DIVISION DE EDUCACION CONTINUA
CURSOS ABIERTOS

VIII CURSO INTERNACIONAL DE CONTAMINACION DE ACUIFEROS
MODULO III: MODELOS MATEMATICOS EN GEOHIDROLOGIA
Y CONTAMINACION DE ACUIFEROS
DEL 2 AL 6 DE OCTUBRE DE 1995

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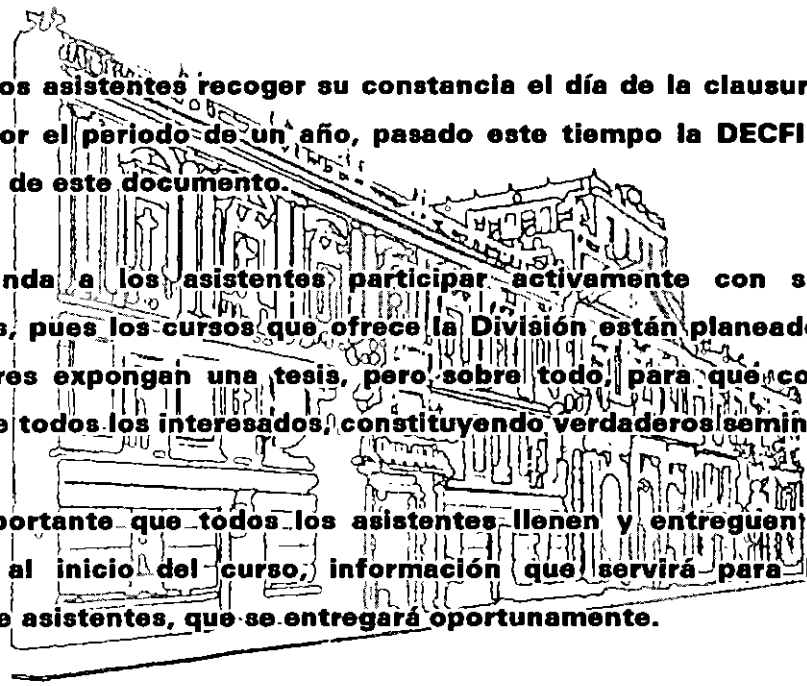
DIVISION DE EDUCACION CONTINUA

A LOS ASISTENTES A LOS CURSOS

Las autoridades de la Facultad de Ingeniería, por conducto del jefe de la División de Educación Continua, otorgan una constancia de asistencia a quienes cumplan con los requisitos establecidos para cada curso.

El control de asistencia se llevará a cabo a través de la persona que le entregó las notas. Las inasistencias serán computadas por las autoridades de la División, con el fin de entregarle constancia solamente a los alumnos que tengan un mínimo de 80% de asistencias.



Pedimos a los asistentes recoger su constancia el día de la clausura. Estas se retendrán por el periodo de un año, pasado este tiempo la DECFI no se hará responsable de este documento.

Se recomienda a los asistentes participar activamente con sus ideas y experiencias, pues los cursos que ofrece la División están planeados para que los profesores expongan una tesis, pero sobre todo, para que coordinen las opiniones de todos los interesados, constituyendo verdaderos seminarios.

Es muy importante que todos los asistentes llenen y entreguen su hoja de inscripción al inicio del curso, información que servirá para integrar un directorio de asistentes, que se entregará oportunamente.

Con el objeto de mejorar los servicios que la División de Educación Continua ofrece, al final del curso deberán entregar la evaluación a través de un cuestionario diseñado para emitir juicios anónimos.

Se recomienda llenar dicha evaluación conforme los profesores impartan sus clases, a efecto de no llenar en la última sesión las evaluaciones y con esto sean más fehacientes sus apreciaciones.

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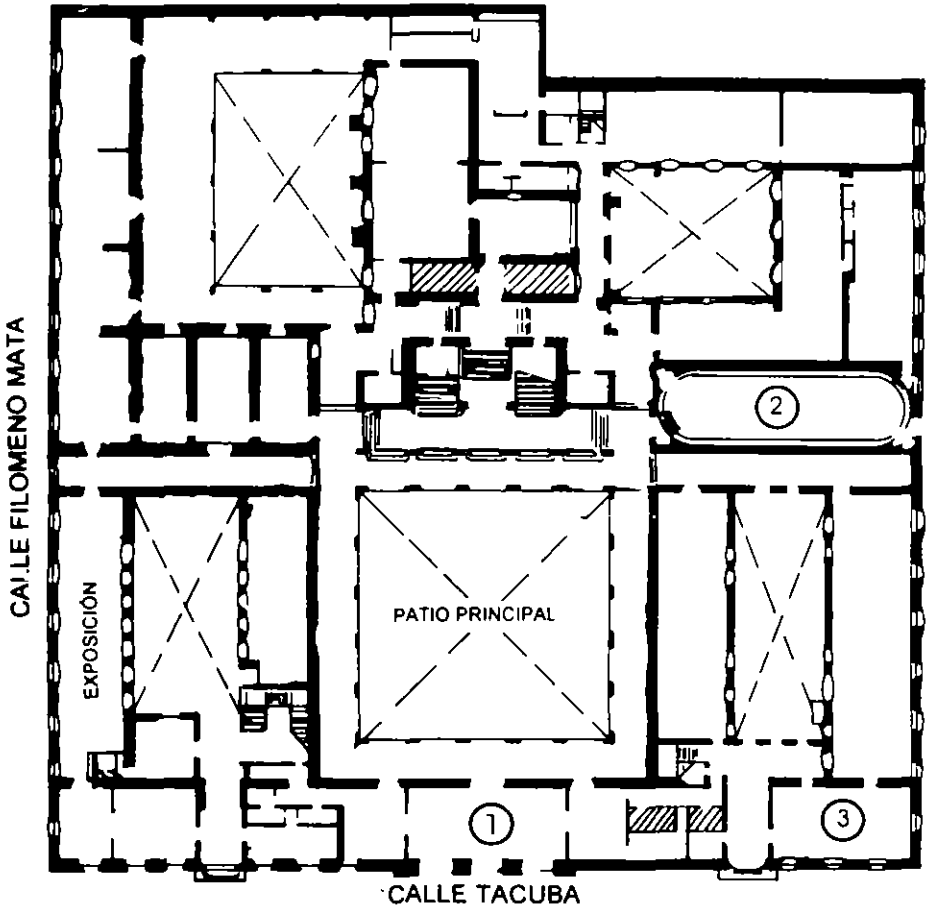

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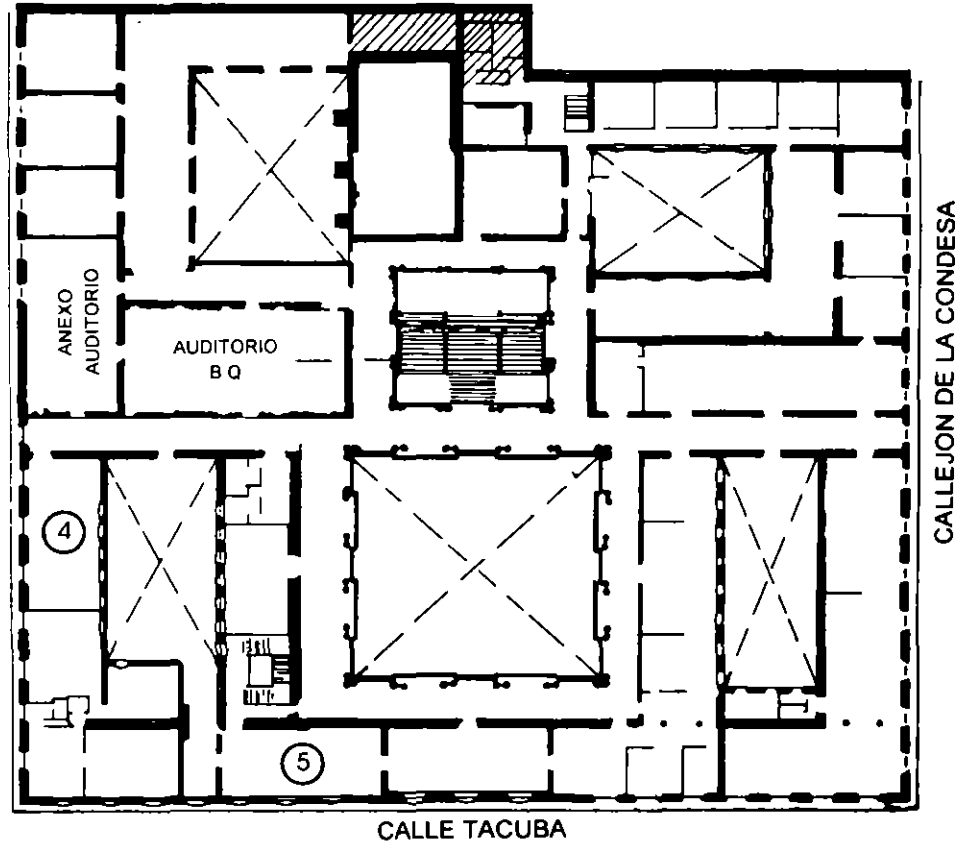

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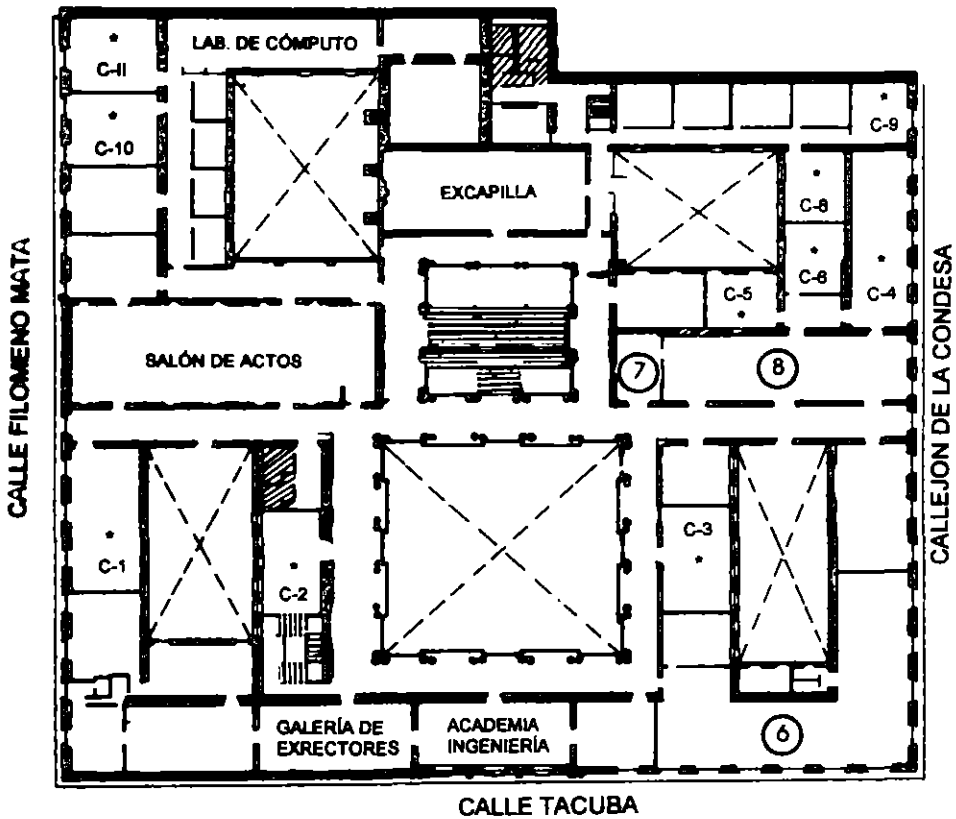

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DIVISIÓN DE EDUCACIÓN CONTINUA
FACULTAD DE INGENIERÍA U.N.A.M.
CURSOS ABIERTOS

VII CURSO INTERNACIONAL DE CONTAMINACION DE ACUIFEROS

MODULO 3.- MODELOS MATEMATICOS EN GEOHIDROLOGIA
Y CONTAMINACION DE ACUIFEROS

2 AL 6 DE OCTUBRE DE 1995

DIA	HORA	T E M A	PROFESOR
LUNES 2	9:00 A 11:00	GENERALIDADES SOBRE MODELOS MATEMATICOS	ING. RUBEN CHAVEZ GUILLEN
	11:00 A 14:00	INTRODUCCION A LAS MICROCOMPUTADORAS	ING. FEDERICO MEIXUEIRO
	16:00 A 17:30	CONTINUACION	ING. FEDERICO MEIXUEIRO
	17:30 A 19:00	MODELO DEL FLUJO "PLASM"	ING. DAVID GLEZ. POSADAS
MARTES 3	9:00 A 14:00	MODELO DEL FLUJO "PLASM" (CONTINUACION)	ING. DAVID GLEZ. POSADAS
	16:00 A 19:00	MODELOS GEOFISICOS EN CONTAMINACION	ING. ALFONSO ALVAREZ MANILLA
MIERCOLES 4	9:00 A 14:00 16:00 A 19:00	MODELOS DE TRANSPORTE	M. EN C. FERNANDO LARA
JUEVES 5	9:00 A 14:00	MODELO DE FLUJO	ING. GUILLERMO HERNANDEZ
	16:00 A 19:00	"MODFLOW"	ING. RODRIGO MEDINA
VIERNES 6	9:00 A 14:00	MODELOS EN GEOHIDROLOGIA	ING. JUAN M. LESSER ILLADES
	16:00 A 19:00	MESA REDONDA	

1. ¿Le agradó su estancia en la División de Educación Continua?

SI ☐ NO ☐

Si indica que "NO" diga porqué: _____

_____

2. Medio a través del cual se enteró del curso:

Periódico *Excélsior*	
Periódico *La Jornada*	
Folleto anual	
Folleto del curso	
Gaceta UNAM	
Revistas técnicas	
Otro medio (Indique cuál)	

3. ¿Qué cambios sugeriría al curso para mejorarlo?

_____

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4. ¿Recomendaría el curso a otra(s) persona(s) ?

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5.¿Qué cursos sugiere que imparta la División de Educación Continua?

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6. Otras sugerencias:

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DIVISION DE EDUCACION CONTINUA
FACULTAD DE INGENIERIA, UNAM
CURSOS ABIERTOS

CURSO: Mód. III: Modelos Matemáticos en Geohidrología y Contaminación de Acuiferos
FECHA: del 2 al 6 de octubre de 1995.

EVALUACIÓN DEL PERSONAL DOCENTE

(ESCALA DE EVALUACIÓN: 1 A 10)

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Ing. Rubén Chávez Guillén				
Ing. Federico Meixueiro				
Ing. David González Posadas				
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M.C. Fernando Lara				
Ing. Guillermo Hernández				
Ing. Rodrigo Medina				
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Promedio _____

EVALUACIÓN DE LA ENSEÑANZA

CONCEPTO	CALIF.
ORGANIZACIÓN Y DESARROLLO DEL CURSO	
GRADO DE PROFUNDIDAD DEL CURSO	
ACTUALIZACIÓN DEL CURSO	
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Promedio _____

EVALUACIÓN DEL CURSO

CONCEPTO	CALIF.
CUMPLIMIENTO DE LOS OBJETIVOS DEL CURSO	
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CALIDAD DEL MATERIAL DIDÁCTICO UTILIZADO	

Promedio _____

Evaluación total del curso _____

Continúa...2

FACULTAD DE INGENIERIA U.N.A.M.
DIVISION DE EDUCACION CONTINUA

CURSOS ABIERTOS

VII CURSO INTERNACIONAL DE CONTAMINACION
DE ACUIFEROS.

MODULO III: MODELOS MATEMATICOS E HIDROLOGIA
Y CONTAMINACION DE ACUIFEROS.

TEMA: DEL METODO DE DIFERENCIAS FINITAS METODO
DE ELEMENTOS FINITOS Y METODO DE CARACTERISTICAS

PROF. GUILLERMO HERNANDEZ GARCIA

1. El Método de Diferencias Finitas

El Método consiste en una aproximación de derivadas parciales por expresiones algebraicas envolviendo los valores de la variable dependiente en un limitado número de puntos seleccionados.

Como resultado de la aproximación, la ecuación diferencial parcial que describe el problema es reemplazada por un número finito de ecuaciones algebraicas, escritas en términos de los valores de la variable dependiente en puntos seleccionados. Las ecuaciones son lineales si las ecuaciones diferenciales parciales son también lineales.

El valor de los puntos seleccionados se convierten en las incógnitas, en vez de la distribución espacial continua de la variable dependiente. El sistema de ecuaciones algebraicas debe ser resuelto y puede envolver un número largo de operaciones aritméticas.

Antiguamente todos estos cálculos eran realizados manualmente, o por el uso de dispositivos mecánicos. En la actualidad, con el advenimiento de las computadoras electrónicas las operaciones son ejecutadas por medio de un programa de cómputo.

1.1. Flujo Estable

Para mostrar este método vamos a considerar el caso de flujo bi-dimensional de un fluido en un acuífero homogéneo, isotrópico confinado, sin fuentes o sumideros. Para este caso, el flujo es descrito por la ecuación de Laplace:

$$\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}=0. \qquad (1.1.1)$$

Esta ecuación debe ser satisfecha en todos los puntos dentro del dominio R del acuífero considerado. En la frontera de R el nivel del agua, h, debe satisfacer ciertas condiciones de frontera. Vamos a asumir que las condiciones de frontera son:

$$\text{en } S_1: \quad h = f, \qquad (1.1.2)$$

$$\text{en } S_2: \quad Q_n = -T\frac{\partial h}{\partial n} = 0 \qquad (1.1.3)$$

donde S_1 y S_2 son partes complementarias de la frontera, las cuales juntas forman la frontera total de la región R. En la primera la altura del nivel es prescrito y en la segunda la frontera es impermeable.

Una retícula de cuadrados es trazada sobre la región R (figura 1.1). El valor de la variable h en un punto nodal de la retícula, o nodo, es expresada como $h_{i,j}$, donde i indica la posición de una linea vertical de la retícula (la *columna*), y j la línea horizontal de la retícula (el *renglón*).

En general, la aproximación de la primera derivada con respecto a x de una función $F(x,y)$, es dada por:

$$\frac{\partial F}{\partial x} \approx \frac{F(x+\Delta x, y) - F(x,y)}{\Delta x} \tag{1.1.4}$$

esta se dice que es la aproximación de *diferencia finita hacia adelante* de la derivada parcial.

La *diferencia finita hacia atrás* es obtenida de la forma siguiente:

$$\frac{\partial F}{\partial x} \approx \frac{F(x,y) - F(x-\Delta x, y)}{\Delta x} \tag{1.1.5}$$

Existen pequeñas diferencias entre las dos aproximaciones. La *diferencia finita central* es a menudo más exacta:

$$\frac{\partial F}{\partial x} \approx \frac{F(x+\frac{1}{2}\Delta x, y) - F(x-\frac{1}{2}\Delta x, y)}{\Delta x} \tag{1.2.6}$$

La segunda derivada es la derivada de la primera derivada; y si utilizamos una aproximación de diferencia finita central, obtendremos:

$$\begin{aligned} \frac{\partial^2 F}{\partial x^2} &\approx \frac{F(x+\Delta x, y) - 2F(x,y) + F(x-\Delta x, y)}{(\Delta x)^2} \\ &= \frac{F_{i+1,j} - 2F_{i,j} + F_{i-1,j}}{(\Delta x)^2} \end{aligned} \tag{1.1.7}$$

La fórmula se ilustra en la figura 1.2, donde la función mostrada tiene segunda derivada positiva, por el incremento de la pendiente en la dirección x.

La aplicación de (1.1.7) a las derivadas parciales el (1.1.1) nos da la aproximación del operador de Laplace. Si por razones de simplicidad se asumen intervalos iguales en las direcciones de x e y:

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} \approx \frac{h_{i,j-1} + h_{i,j+1} + h_{i-1,j} + h_{i+1,j} - 4h_{i,j}}{\Delta^2} \tag{1.1.8}$$

como la parte izquierda de la ecuación se reduce a cero según lo indica la ecuación diferencial básica (1.1.1), se puede hacer la aproximación requiriendo que:

$$h_{i,j} = \tfrac{1}{4}\left(h_{i,j-1} + h_{i,j+1} + h_{i-1,j} + h_{i+1,j}\right) \tag{1.1.9}$$

Los nodos en la frontera requieren atención especial para acomodar las condiciones de frontera. Una posible condición de frontera es la *condición de Dirichlet* (1.1.2), la cual establece que el nivel del agua subterránea sea el especificado a lo largo de parte de la frontera. En este caso ésta se prescribe *a priori* y ya no es una incógnita.

En un nodo de una frontera impermeable, a lo largo de la cual una condición de *frontera de Neumann* (1.1.3) es aplicada, el nivel es una incógnita y la ecuación para ese nodo debe reflejar la condición de no flujo en la frontera.

Para un nodo en una frontera vertical esto puede ser expresado por la condición de que $h_{i-1,j}=h_{i+1,j}$. La sustitución en el algoritmo general nos da:

$$h_{i,j} = \tfrac{1}{4}\left(2h_{i,j+1} + h_{i-1,j} + h_{i+1,j}\right) \qquad (1.1.10)$$

Un ejemplo simple de una región rectangular es mostrada en la figura 1.3. A lo largo del límite superior el nivel se especifica como 100. En la esquina inferior izquierda es especificado el nivel cero. La estimación inicial para los nodos con valor desconocido se considera con el valor promedio de 50.

En la primera parte de la figura se muestran las condiciones iniciales. Estas no satisfacen la ecuación (1.1.9). Son corregidas aplicando la aproximación en una siguiente *iteración* del programa, y el resultado se muestra en la parte central de la figura. Tampoco se satisface la ecuación (1.1.9).

Después de un número dado de iteraciones, en cada una de las cuales todos los valores son actualizados, la solución correcta es obtenida y representada en la parte derecha de la figura.

El método descrito es denominado de *relajación*, porque en cada paso los errores son relajados. En terminología matemática el método de relajación es también conocido como el *método de Gauss-Seidel.*

Como un ejemplo, el programa BV9-1 puede ser utilizado para resolver el problema ilustrado en la figura 1.4. En esa figura las condiciones de frontera son un nivel prescrito de $h = 1$, a lo largo de las fronteras superior y derecha y un nivel dado de $h = 0$, en la esquina inferior izquierda.

El programa inicia preguntando el número de lineas en las direcciones x *e* y; aquí el número 6 debe ser dado. A continuación el programa pregunta las coordenadas x de las líneas verticales; ese debe responder 0, 1, 2, 4, 8, 16, sucesivamente. Para las coordenadas en y, la respuesta debe ser la misma secuencia. A continuación las condiciones de frontera deben ser dadas. Para el caso de la figura 1.4 existen 12 nodos que especificar; por ejemplo, para $i=1, j=1$: $h=0$, para $i=6, j=6$: $h=1$, etc.

Los datos de salida para 36 iteraciones para los nodos en la frontera impermeable son:
h = 0.000, 0.363, 0.530, 0.686, 0.839, 1.000.

1.2. Flujo no estable.

La ecuación diferencial parcial básica para flujo no estable en un acuífero homogéneo e isotrópico, con la posibilidad de suministro de agua por infiltración, puede ser escrita como:

$$S\frac{\partial h}{\partial t} = T\left(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2}\right) + I \qquad (1.2.1)$$

donde I es una función fuente, representando la infiltración (negativa para evapotranspiración). T es la transmisividad y S es el almacenamiento. La formulación completa requiere especificar condiciones de frontera e iniciales como en el caso de flujo estable. En parte de la frontera el nivel es dado y en el resto es impermeable, esto es,

$$\text{en } S_1: \quad h = f, \qquad (1.2.2)$$

$$\text{en } S_2: \quad Q_n = -T\frac{\partial h}{\partial n} = 0 \qquad (1.2.3)$$

Las condiciones iniciales son:

$$t = 0: h = h^0 \qquad (1.2.4)$$

donde, h^0 es una función conocida, especificada a través de todo el dominio R.

La derivada en el tiempo es aproximada por una diferencia finita hacia adelante, porque el problema es predecir los valores futuros de los niveles a partir de los valores iniciales. Por lo tanto, se introduce la aproximación:

$$\frac{\partial h}{\partial t} = \frac{h'_{i,j} - h^0_{i,j}}{\Delta t} \qquad (1.2.5)$$

donde delta t es la magnitud del paso de tiempo y h' es el valor del nivel al final del paso de tiempo.

1.2.1. Método explícito.

La opción de aproximación más simple de las derivadas espaciales es asumir que en (1.1.8) todos los valores de niveles se consideran en el inicio del tiempo. Después de la sustitución de varias aproximaciones en (1.2.1) se obtiene

$$h'_{i,j} = h^0_{i,j} + I\Delta t / S + \alpha\left(h^0_{i-1,j} + h^0_{i+1,j} - 2h^0_{i,j}\right) + \beta\left(h^0_{i,j-1} + h^0_{i,j+1} - 2h^0_{i,j}\right) \qquad (1.2.6)$$

donde las constantes se definen por:

$$\alpha = T\Delta t / \left[S(\Delta x)^2\right] \qquad (1.2.7)$$

$$\beta = T\Delta t / \left[S(\Delta y)^2\right] \qquad (1.2.8)$$

La ecuación (1.2.6) expresa el nuevo valor del nivel en términos de valores iniciales en ese nodo y en sus vecinos inmediatos. Como todos estos valores son conocidos el proceso es llamado *explícito*.

El programa BV9-2 se puede usar considerando el ejemplo de una región cuadrada de dimensiones 100 m. por 100 m., teniendo una transmisividad T = 10 m/d, un almacenamiento S = 0.4 y una infiltración de 0.001 m/d. Para este caso el programa propone un paso de tiempo de un día.

Una posible malla para el problema se muestra en la parte izquierda de la figura 1.5. El orden en el cual los datos deben ser introducidos es: 100, 10, 100, 10, 0, 0.001, 10, 0.4, 1, 100. El resultado para el nivel en el centro como función del tiempo se muestra en la parte derecha de la figura.

1.2.2. Método implícito.

Como una aproximación alternativa, podemos tomar la derivada espacial al final del paso de tiempo, a la mitad del paso de tiempo, o en general, en algún punto intermedio:

$$h_{i,j} = \varepsilon h^0_{i,j} + (1-\varepsilon)h'_{i,j} \qquad (1.2.9)$$

donde ε es un parámetro de interpolación de valor entre 0 y 1. Cuando ε = 0 el valor de $h_{i,j}$ equivale al valor al final del paso del tiempo, $h'_{i,j}$. En ese caso la aproximación de la ecuación básica (1.2.1) es:

$$h'_{i,j} = h^0_{i,j} + I\Delta t / S + \alpha\left(h'_{i-1,j} + h'_{i+1,j} - 2h'_{i,j}\right) + \beta\left(h'_{i,j-1} + h'_{i,j+1} - 2h'_{i,j}\right) \qquad (1.2.10)$$

Esta es la ecuación para el método completamente implícito. El uso del método iterativo de Gauss-Seidel, sugiere que se puede utilizar para formular la ecuación en la forma:

$$h'_{i,j} = \left[h^0_{i,j} + I\Delta t / S + \alpha\left(h'_{i-1,j} + h'_{i+1,j}\right) + \beta\left(h'_{i,j-1} + h'_{i,j+1}\right)\right] / (1 + 2\alpha + 2\beta) \qquad (1.2.11)$$

El proceso iterativo definido por el algoritmo (1.2.11) produce un número de cálculos por paso de tiempo mayores comparados con el método explícito. Sin embargo, esto es balanceado por el hecho de que el proceso es estable para todos los tamaños del paso de tiempo. Así, éstos pueden ser más largos cuando el proceso se hace más lento.

El programa BV9-3 realiza los cálculos para el método completamente implícito. Para resolver el problema ilustrado en la figura 9.5, los datos de entrada deben ser: 100, 10, 100, 10, 0, 0.001, 10, 0.4, 1, 10, 20, 1.5, si el número de iteraciones en cada paso de tiempo es 20 y el factor de relajación es 1.5.

Si en lugar de tomar ε = 0, se toma ε = 1/2, resultará una formulación más exacta conocida como el *Esquema Crank-Nicholson*, ésta es muy exacta e incondicionalmente estable. El método completamente implícito tiene la importante ventaja de que también puede ser usado para estudiar problemas de flujo estable.

1.3 Convergencia y Estabilidad

1.3.1 Convergencia

La condición de convergencia es difícil de verificar, ya que esta condición establece que la solución de la ecuación numérica se aproxima a la solución con ecuación diferencial parcial original si todos los intervalos finitos tienden a cero. Esto puede ser demostrado en forma general en algunos casos simples, como los problemas en una dimensión, para los cuales la solución numérica puede ser expresada en forma cerrada. En muchas aplicaciones en la práctica de ingeniería, es imposible probar la convergencia en forma rigurosa. De allí que es usualmente considerado suficiente si el procedimiento numérico ha sido verificado con respecto a una variedad de soluciones analíticas.

1.3.2 Estabilidad

Una condición necesaria para la convergencia es que los errores, por ejemplo los debidos al redondeo, no se incrementen con en tiempo. Esta es la llamada la *condición de estabilidad.* Es una condición tan importante que implica ciertas restricciones al tamaño del paso de tiempo en un proceso explícito.

El primer caso a considerar es el método explícito para problemas de flujo inestable descrito en (1.2.6),

$$h'_{i,j} = h^0_{i,j} + I\Delta t / S + \alpha\left(h^0_{i-1,j} + h^0_{i+1,j} - 2h^0_{i,j}\right) + \beta\left(h^0_{i,j-1} + h^0_{i,j+1} - 2h^0_{i,j}\right) \qquad (1.3.1)$$

donde las α y β se definen por:

$$\alpha = T\Delta t / \left[S(\Delta x)^2\right] \qquad (1.3.2)$$

$$\beta = T\Delta t / \left[S(\Delta y)^2\right] \qquad (1.3.3)$$

Como el sistema de ecuaciones es lineal, es suficiente investigar la propagación de la distribución del error, considerado como la desviación de la solución particular $h = 0$ de la ecuación homogénea (con $I = 0$). Para acentuar el efecto se asume que en cierto tiempo los errores son:

$$h^0_{i-1,j} = h^0_{i+1,j} = h^0_{i,j-1} = h^0_{i,j+1} = -\varepsilon,\ h^0_{i,j} = \varepsilon$$

de (1.3.1), $h'_{i,j} = (1 - 4\alpha - 4\beta)\varepsilon.$ (1.3.4)

Para que los errores no crezcan, este resultado debe ser menor que ε, y mayor que $-\varepsilon$. De otra manera cada error será mayor que el previo y crecerá sin límite en el tiempo. Con (1.3.2) y (1.3.3) esto conduce a la siguiente condición para el valor del paso de tiempo Δt

$$0 < \Delta t < \frac{1}{2}\frac{S}{T}\frac{(\Delta x)^2(\Delta y)^2}{(\Delta x)^2 + (\Delta y)^2}. \qquad (1.3.5)$$

El proceso implícito presentado en la sección 1.2 es incondicionalmente estable, lo cual significa que para todos los valores (positivos) del paso de tiempo, los errores se disiparán con el tiempo. Esto puede ser demostrado probando que la amplitud de cualquier componente de una serie de Fourier decrecerá con el tiempo. El caso Más simple es el del equivalente en una dimensión de la ecuación (1.2.10), en ausencia de infiltración,

$$h'_{i,j} = h^0_{i,j} + \alpha\left(h'_{i-1,j} + h'_{i+1,j} - 2h'_{i,j}\right) \tag{1.3.6}$$

Ahora considérese un componente del error, el cual puede ser descrito por

$$h^0 = A\exp(i\omega x), \qquad h' = B\exp(i\omega x) \tag{1.3.7}$$

donde ω es la frecuencia de esta componente de la representación en series de Fourier del error, A es su amplitud inicial, y B es su amplitud después del paso de tiempo. Substituyendo (1.3.7) en (1.3.6) nos da

$$\frac{A}{B} = 1 + 2\alpha\left[1 - \cos(\omega\Delta x)\right]. \tag{1.3.8}$$

Este cociente es siempre mayor que 1, para todos los valores de la frecuencia ω o de la dimensión de tiempo α, sin dimensiones. De aquí podemos concluir que el proceso es siempre estable.

El criterio de estabilidad (1.3.5) ha sido incorporado en el programa BV9-2, donde es usado para sugerir al usuario un valor para el paso de tiempo. En el programa BV9-3, es usado para sugerir un valor para el primer paso de tiempo.

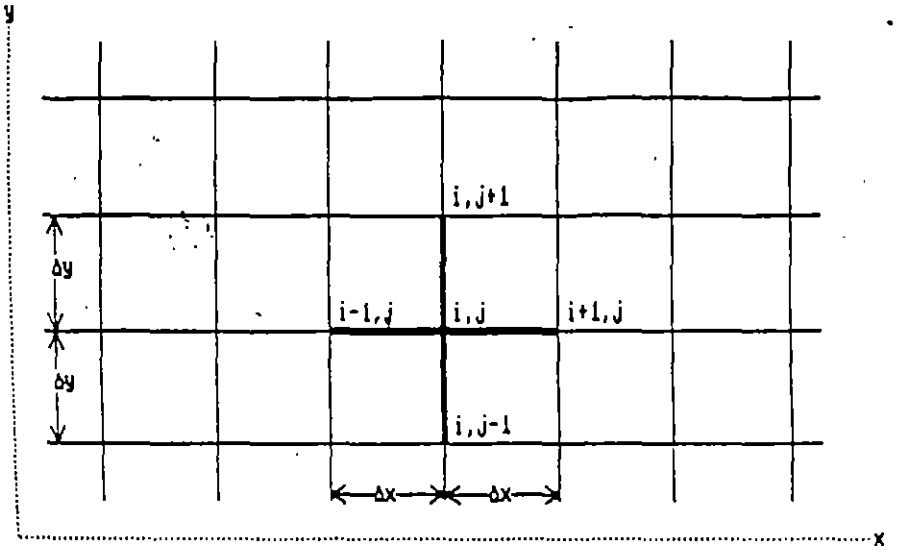


Figura 1.1. Malla rectangular

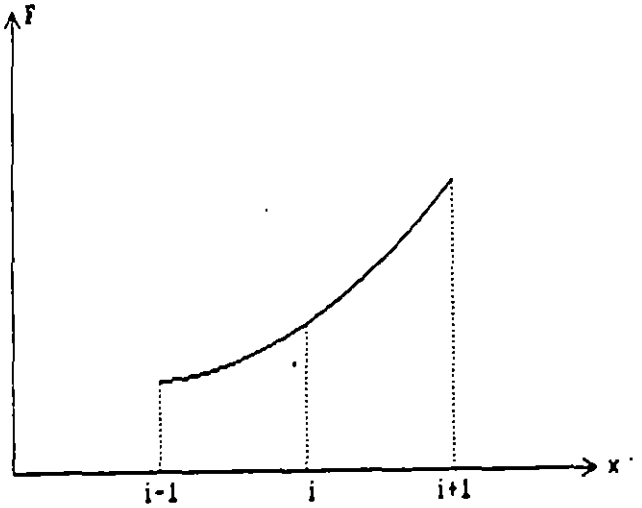


Figura 1.2. Aproximación de segunda derivada

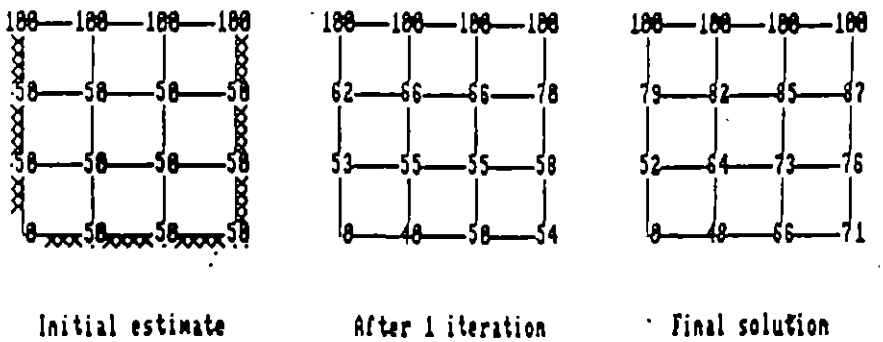


Figura 1.3. Ejemplo del método de diferencias finitas

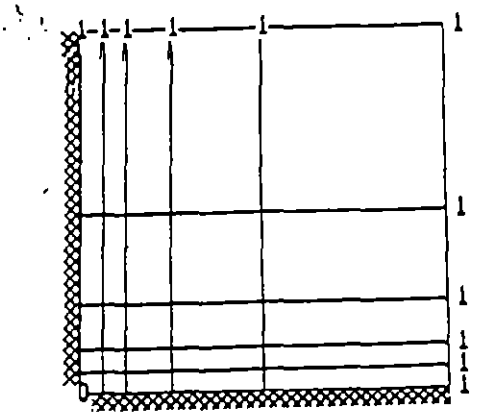


Figura 1.4. Ejemplo resuelto por el método de diferencias finitas

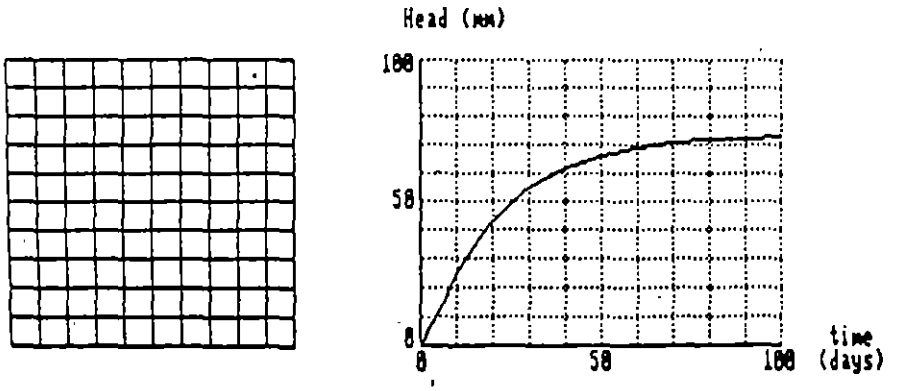


Figura 1.5. Ejemplo de resultados obtenidos pro el programa BV9-2

2. El Método de Elemento Finito

2.1. Flujo estable.

Considérese flujo estable de agua subterránea en el acuífero de transmisividad T, mostrado en la figura 2.1. El acuífero es freático, con flujo desde el acuífero inferior, éste con un nivel conocido. La ecuación diferencial básica puede ser escrita como:

$$\frac{\partial}{\partial x}\left(T\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(T\frac{\partial h}{\partial y}\right)+I-\frac{h-h'}{c}=0 \qquad (2.1.1)$$

donde I es la infiltración, h es el nivel en el acuífero, h' es el nivel del acuífero inferior conocido, c es la resistencia del material separando los dos acuíferos. El último término representa el flujo de infiltración hacia el acuífero. La transmisividad del acuífero superior es $T=kb$, donde k es conductividad y b es el espesor de la capa de agua.

La ecuación debe satisfacerse en una región R en el plano x-y. Las condiciones de frontera especificadas son

$$\text{en } S_1: \quad h=f, \qquad (2.1.2)$$

$$\text{en } S_2: \quad T\frac{\partial h}{\partial n}=qb \qquad (2.1.3)$$

En el método de elemento finito la R, en la cual se da el flujo, es subdividida en un gran número de pequeños elementos, en los que el nivel de agua subterránea es aproximado por alguna función simple. La forma más simple de subdividir la región es mediante el uso de elementos triangulares (Figura 2.2).

Las formas más simples de aproximar las variaciones de nivel dentro de un elemento triangular es asumiendo que el nivel varía linealmente en cada elemento (Figura 2.3). La superficie generada definida por los valores nodales, es una superficie continua; las pendientes son discontinuas a través de las fronteras de los elementos. El nivel del agua subterránea en un punto dentro de un elemento es definido por una interpolación lineal entre los valores en los puntos de la malla o nodos.

Formalmente, el nivel piezométrico h a través de la región puede ser expresado por

$$h=\sum_{i=1}^{n} N_i(x,y)h_i \qquad (2.1.4)$$

donde h_i es el nivel del nodo i y N_i es una función base definida por

$$N_j = 1, \text{ si } j = i, \qquad N_j = 0, \text{ si } j \neq i \tag{2.1.5}$$

con interpolación lineal dentro de cada elemento. Una función base típica es mostrada en la figura (2.4).

La función de interpolación también puede ser usada para el nivel conocido en el acuífero inferior y se puede escribir como:

$$h' = \sum_{i=1}^{n} N_i(x,y) h_i' \tag{2.1.6}$$

En general, la aproximación (2.1.4) no satisfará exactamente la ecuación diferencial parcial (2.1.1). Esta condición es relajada requiriendo que la ecuación diferencial se satisfaga sólo en el promedio, usando un número de funciones de peso, igual al número de incógnitas. Este es llamado el *método de residuos pesados*.

Lo más conveniente es usar las funciones base también como funciones de peso, éste es el *Métodos de Galerkin*. Lo anterior conduce a las siguientes condiciones:

$$\int_R \left\{ \left[\frac{\partial}{\partial x}\left(T\frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y}\left(T\frac{\partial h}{\partial y} \right) + I - \frac{h-h'}{c} \right] N_i \right\} dx\,dy = 0 \qquad (i \in C) \tag{2.1.7}$$

que deben ser satisfechas para cada valor de i, para el cual h_i es desconocida. La integral en (2.1.7) puede ser separada en dos partes:

$$\left[\frac{\partial}{\partial x}\left(T\frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y}\left(T\frac{\partial h}{\partial y} \right) \right] N_i = \frac{\partial}{\partial x}\left(N_i T\frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y}\left(N_i T\frac{\partial h}{\partial y} \right) (\\ -T\frac{\partial N_i}{\partial x}\frac{\partial h}{\partial x} - T\frac{\partial N_i}{\partial y}\frac{\partial h}{\partial y} \tag{2.1.8}$$

sustituyendo (2.1.8) en (2.1.7), junto con (2.1.4) y (2.1.6), nos da:

$$J_1 + J_2 + J_3 = 0 \quad (i \in C) \tag{2.1.9}$$

donde, J_1, J_2 y J_3 son tres integrales definidas por:

$$J_1 = \int_r \left\{ \frac{\partial}{\partial x}\left(N_i T \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y}\left(N_i T \frac{\partial h}{\partial y} \right) \right\} dx\,dy \qquad (2.1.10)$$

$$J_2 = -\int_R \left\{ T \sum_j h_j \left[\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y} \right] \right\} dx\,dy \qquad (2.1.11)$$

$$J_3 = \int_R \left\{ I N_i - \frac{1}{c} \sum_j N_i N_j \left(h_j - h'_j \right) \right\} dx\,dy \qquad (2.1.12)$$

La sumatoria en la segunda y tercera integrales, debe ser ejecutada sobre todos los valores de j desde 1 hasta n, donde n es el número de nodos. La ecuación (2.1.9) es la ecuación básica del método de elementos finitos. Cada una de las integrales va a ser evaluada separadamente.

2.1.1. La primera integral.

La primera integral, expresada por (2.1.10), puede ser transformada en una integral de línea a lo largo de la frontera S de la región R por el *Teorema de la Divergencia* (o *Teorema de Gauss*). Esto nos da

$$J_1 = \int_r \left\{ \frac{\partial}{\partial x}\left(N_i T \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y}\left(N_i T \frac{\partial h}{\partial y} \right) \right\} dx\,dy = \int_S \left\{ N_i T \frac{\partial h}{\partial n} \right\} dS \quad (i \in C) \qquad (2.1.3)$$

Los valores de i son restringidos a los números de nodo donde el nivel es desconocido, los valores de i para los puntos en los segmentos de frontera S_1 son excluidos. Así, la integral en la parte derecha de la ecuación se restringe a valores localizados en la frontera S_2.

El valor de la función de suministro a lo largo de un elemento de frontera es $q_k b$ y la longitud de tal parte de la frontera es L_k. A lo largo de dos segmentos de línea el valor promedio de N_i es 1/2 y la integral será la suma de dos valores, uno en la izquierda y otro en la derecha del nodo i. Esta suma será denotada por Q_i. Físicamente esto significa que el agua total suministrada a lo largo de un elemento de frontera es atribuida a los dos nodos en sus extremos. Por lo tanto:

$$J_1 = \int_r \left\{ \frac{\partial}{\partial x}\left(N_i T \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y}\left(N_i T \frac{\partial h}{\partial y} \right) \right\} dx\,dy = Q_i \quad (i \in C) \qquad (2.1.14)$$

$$Q_i = \tfrac{1}{2} q_k b L_k \tag{2.1.15}$$

2.1.2. La segunda integral.

La segunda integral puede ser definida formalmente como:

$$J_2 = -\int_R \left\{ T \sum_j h_j \left[\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y} \right] \right\} dx\, dy = -\sum_j P_{ij}\, h_j \tag{2.1.16}$$

donde la sumatoria del lado derecho es sobre los elementos R_p incluidos en el dominio R, donde

$$P_{ij} = \int_{R_p} \left\{ T \left[\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y} \right] \right\} dx\, dy \quad (i \in C) \tag{2.1.17}$$

para evaluar esta integral, se toma en cuenta que las contribuciones a esta integral solo existen si el elemento R_p contiene ambos nodos i y j. Si uno u otro nodo no pertenece e este elemento la función base se hace cero y de esta manera no hay contribución a la integral. Así nos podemos restringir a elementos que contengan a ambos nodos.

Como las funciones base son lineales podemos escribir:

$$N_i(x,y) = p_i x + q_i y + r_i, \quad N_j(x,y) = p_j x + q_j y + r_j \tag{2.1.18}$$

donde los coeficientes p_i, p_j, etc., son constantes. Si los tres nodos R_p son denominados por j, k y l (donde i puede ser cualquiera de ellos), entonces N_j debe ser 1 en el nodo j, y 0 en los nodos k y l, por lo tanto:

$$p_j x_j + q_j y_j + r_j = 1, \quad p_j x_k + q_j y_k + r_j = 0, \quad p_j x_l + q_j y_l + r_j = 0$$

este es un sistema de ecuaciones simultáneas con tres incógnitas. la solución a este sistema es:

$$p_j = b_j / D, \quad q_j = c_j / D, \quad r_j = d_j / D(\tag{2.1.19}$$

donde

$$b_j = y_k - y_l, \quad b_k = y_l - y_j, \quad b_l = y_j - y_k$$
$$c_j = x_l - x_k, \quad c_k = x_j - x_l, \quad c_l = x_k - x_j$$

$$d_j = x_k y_l - x_l y_k, \; d_k = x_l y_j - x_j y_l, \; d_l = x_j y_k - x_k y_j$$
$$D = x_j b_j + x_k b_k + x_l b_l \tag{2.1.20}$$

La cantidad D es el determinante del sistema de ecuaciones. Para la evaluación de la integral (2.1.17) las cantidades necesarias son:

$$\frac{\partial N_i}{\partial x} = p_i, \quad \frac{\partial N_j}{\partial x} = p_j, \quad \frac{\partial N_i}{\partial y} = q_i, \quad \frac{\partial N_j}{\partial y} = q_j$$

Si asumimos que la transmisividad T es constante, T_p a través del elemento R_p, entonces obtenemos:

$$P_{ij} = T_p A_p \left\{ b_i b_j + c_i c_j \right\} / D^2$$

donde A_p es el área del elemento R_p, cuya fórmula alternativa es $A_p = \frac{1}{2}|D|$
La expresión formal para los coeficientes P_{ij} es:

$$P_{ij} = \frac{T_p}{2|D|} \left\{ b_i b_j + c_i c_j \right\} \tag{2.1.21}$$

sustituyendo (2.1.21) en (2.1.16) da, para la segunda integral:

$$J_2 = -\sum_j P_{ij} h_j \quad (i \in C) \tag{2.1.22}$$

donde los coeficientes P_{ij} son definidos por (2.1.21).

2.1.3. La Tercera Integral.

La tercera integral definida por (2.1.12), puede ser considerada en dos partes. La primera es la integral de la infiltración I,

$$J_{3-1} = \int_R \{ IN_i \} dx\, dy \quad (i \in C) \tag{2.1.23}$$

La integral sobre un elemento R_p, expresa el promedio del producto $I_p N_i$ en ese elemento, multiplicada por el área del elemento. Como I_p es constante, el promedio de N_i es 1/3, y el área del elemento triangular es $\frac{1}{2}|D|$ la primera parte de la tercera integral es:

$$J_{3-1} = I_p |D| / 6 \quad (i \in R_p) \tag{2.1.24}$$

Físicamente significa que la infiltración del elemento $\frac{1}{2} I_p |D|$, es distribuida en los tres nodos del elemento triangular. Se puede también escribir:

$$J_{3-1} = Q_i \quad (i \in C) \tag{2.1.25}$$

donde Q_i ahora representa la parte de la infiltración atribuible al nodo i. Para los elementos para los cuales el elemento i pertenece tenemos:

$$Q_i = I_p |D| / 6 \quad (i \in R_p) \tag{2.1.26}$$

La segunda parte de la tercera integral es:

$$J_{3-2} = -\int_R \left\{ \frac{1}{c} \sum_j N_i N_j \left(h_j - h'_j \right) \right\} dx\, dy \quad (i \in C) \tag{2.1.27}$$

para el elemento R_p, separando los factores constantes tenemos:

$$J_{3-2} = -\sum_j \frac{1}{c_p}(h_j - h'_j)\int_{R_p}\{N_i N_j\}dx\,dy \quad (i \in C) \tag{2.1.28}$$

$$N_i(x,y) = p_i x + q_i y + r_i, \quad N_j(x,y) = p_j x + q_j y + r_j$$

Estas integrales toman la forma más simple si el origen de las coordenadas coincide con el centroide del elemento, y si esto se asume no se pierde generalidad. En este caso el momento de área de primer orden se elimina:

$$\int_{R_p} x\,dx\,dy = 0, \qquad \int_{R_p} y\,dx\,dy = 0 \tag{2.1.29}$$

El momento de segundo orden puede ser expresado como:

$$\begin{aligned}
&\int_{R_p} x^2\,dx\,dy = \{x_j^2 + x_k^2 + x_l^2\}|D|/24 = \tfrac{1}{2}|D|Z_{xx},\\
&\int_{R_p} y^2\,dx\,dy = \{y_j^2 + y_k^2 + y_l^2\}|D|/24 = \tfrac{1}{2}|D|Z_{yy},\\
&\int_{R_p} xy\,dx\,dy = \{x_j y_j + x_k y_k + x_l y_l\}|D|/24 = \tfrac{1}{2}|D|Z_{xy}
\end{aligned} \tag{2.1.30}$$

Usando (2.1.19), (2.1.29) y (2.1.30), la integral (2.1.28) puede ser escrita como:

$$J_{3-2} = -\sum_j R_{ij}(h_j - h'_j) \tag{2.1.31}$$

donde

$$R_{ij} = \{b_i b_j Z_{xx} + c_i c_j Z_{yy} + (b_i c_j + b_j c_i)Z_{xy} + d_i d_j\}/\{2|D|c_p\} \tag{2.1.32}$$

esto completa la tercera integral.

Con (2.1.14), (2.1.22), (2.1.24) y (2.1.31), la formula (2.1.9) se convierte en:

$$\sum_j \{P_{ij}h_j + R_{ij}(h_j - h'_j)\} = Q_i \quad (i \in C) \tag{2.1.33}$$

2.2 Flujo estable en un Acuífero Confinado.

2.2.1. Un Programa Simple.

Para mostrar el método de solución y un programa simple considerando el caso de flujo estable en un acuífero completamente confinado. Para tal caso, la ecuación diferencial básica (2.1.1) se puede simplificar tomando $I = 0$ y $c = \infty$. La ecuación resultante es:

$$\frac{\partial}{\partial x}\left(T\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(T\frac{\partial h}{\partial y}\right)=0 \qquad (2.2.1)$$

Para este caso el sistema de ecuaciones (2.1.33) se reduce a:

$$\sum_j \{P_{ij}h_j\} = Q_i \quad (i \in C) \qquad (2.2.2)$$

donde de acuerdo a (2.1.21), los coeficientes P_{ij} son sumatorias sobre todos los elementos, cada uno de los cuales hace contribuciones de la forma:

$$P_{ij} = \frac{T_p}{2|D|}\{b_i b_j + c_i c_j\} \qquad (2.2.3)$$

El programa BV10-1 es posible utilizarlo para resolver primeramente un problema simple, como el ilustrado en la figura 2.5. El problema consiste se flujo uniforme de izquierda a derecha. Las dimensiones horizontal y vertical de los elementos son iguales a 1. El nivel del lado izquierdo es de 10, mientras el del derecho es 0. La transmisividad es 1 en todos los elementos. El número de iteraciones es de 50, y el factor de relajación es de 1.5; el orden en que los datos deben ser introducido es:

6,4,50,1.5,
0,0,Y,10,0,1,Y,10,1,0,N,0,1,1,N,0,2,0,Y,0,2,1,Y,0,
1,2,3,1,2,3,4,1,3,4,5,1,4,5,6,1

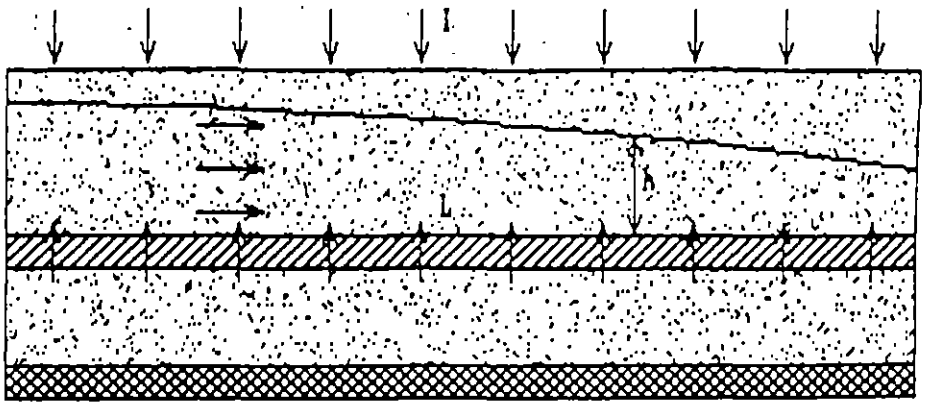


Figura 2.1. Acuífero freático semiconfinado

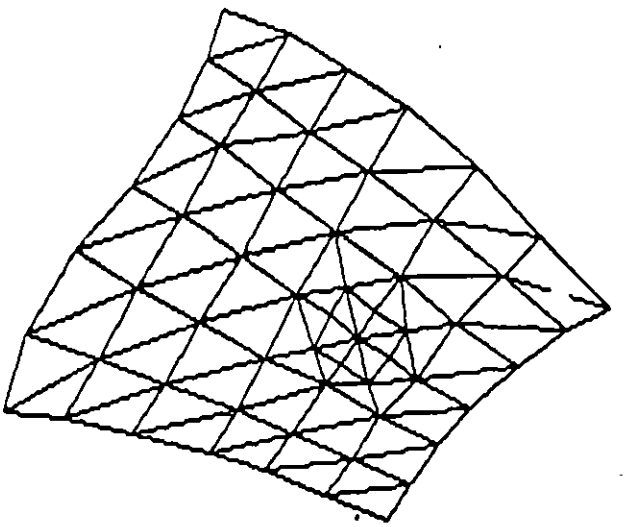


Figura 2.2. Dominio R dividido en elementos triangulares

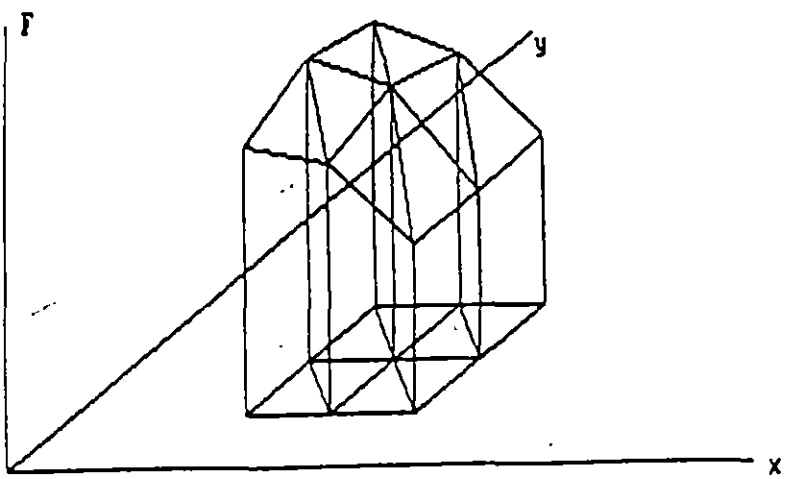


Figura 2.3. interpolación lineal del nivel dentro de los elementos

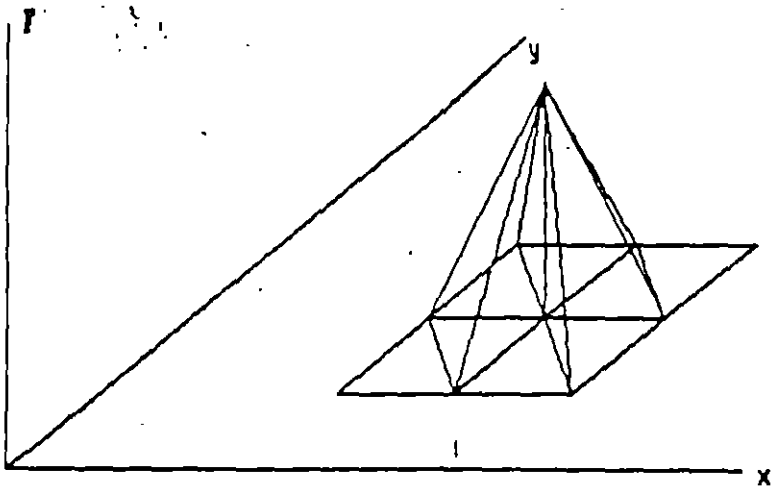


Figura 2.4. Una función típica

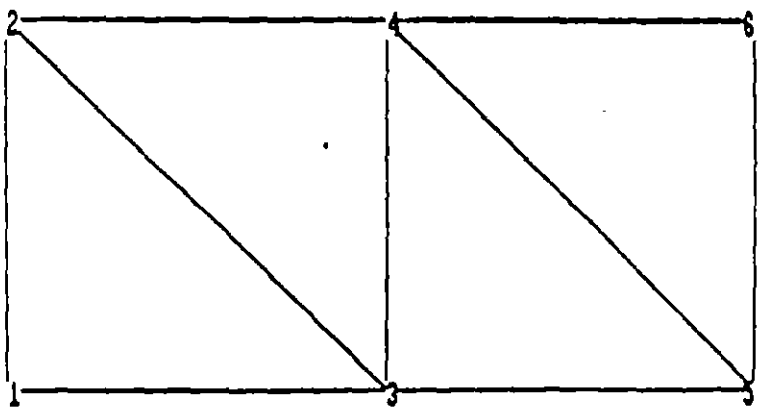


Figura 2.5. Problema elemental

3. EL MODELO COMPUTARIZADO DE TRANSPORTE DE SOLUTOS Y DISPERSIÓN EN DOS DIMENSIONES de L. F. Konikow y J.D.Bredehoeft

Introducción

El modelo calcula los cambios transitorios en la concentración de un soluto no reactivo el agua subterránea fluyendo. El programa de computadora resuelve dos ecuaciones diferenciales parciales de segundo orden. Una ecuación es la de flujo de agua subterráneas que describe la distribución de niveles piezométricos en el acuífero. La segunda ecuación es la de transporte de solutos que describe la concentración química en el sistema. Acoplando la ecuación de flujo con la de transporte de solutos, el modelo puede ser aplicado a problemas tanto de estado estacionario como de flujo transitorio.

Los cambios de concentración que ocurren en un sistema dinámico de agua subterránea se deben principalmente a cuatro procesos distintos:
1) transporte advectivo , en el cual los químicos disueltos se mueven con el flujo de agua subterránea;
2) Dispersión hidrodinámica, en el cual difusión molecular y iónica y variaciones a pequeña escala en la velocidad de flujo a través del medio poroso causa que las trayectorias de moléculas disueltas y iones diverjan o se desprendan de la dirección promedio del flujo de agua subterránea;
3) Fuentes o sumideros, donde el agua de una composición dada se introducida a agua de una composición diferente;
4) Reacciones, en las que una cantidad de una especie química disuelta en particular sea adicionada o substraída del agua subterránea debido a reacciones químicas o físicas en el agua o entre el agua y los materiales sólidos del acuífero.

El modelo asume:
1) Que no ocurren reacciones que afecten las concentraciones que afecten las especies de interés y
2) Que los gradientes de densidad de fluido, viscosidad, y temperatura no afectan la velocidad de distribución
El acuífero puede ser
1) heterogéneo y
2) anisotrópico.

Fundamentos Teóricos

Ecuación de Flujo

La ecuación que describe el flujo transitorio bi dimensional de un fluido compresible y homogéneo a través de un acuífero no homogéneo anisotrópico puede ser escrito en notación cartesiana tensorial como:

$$\frac{\partial}{\partial x_i}\left(T_{ij}\frac{\partial h}{\partial x_j}\right) = S\frac{\partial h}{\partial t} + W \qquad (3.1)$$

donde

$T_{i,j}$ es el tensor de transmisividad, L^2/T;
h es el nivel piezométrico, L;
S es en coeficiente de almacenamiento, adimensional;
t es el tiempo, T;
$W=W(x,y,z,)$ es el caudal volumétrico por unidad de área de signo positivo para salida y negativo para flujo de entrada
x_i, x_j son las coordenadas cartesianas, L;

la expresión para velocidad de filtración del agua subterránea puede ser derivada de la ley de Darcy:

$$V_i = -\frac{K_{ij}}{\varepsilon}\frac{\partial h}{\partial x_j} \qquad (3.2)$$

donde

V_i es la velocidad de filtración en la dirección de x_i, L/T;
K_{ij} es el tensor de la conductividad hidráulica, L/T;
ε es la porosidad efectiva del acuífero, adimensional

Ecuación de Transporte

La ecuación para describir el transporte bi dimensional y la dispersión de una especie química disuelta y no reactiva puede ser escrita como:

$$\frac{\partial(Cb)}{\partial t} = \frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(bCV_i) - \frac{C'W}{\varepsilon}; \quad i,j = 1,2 \tag{3.3}$$

donde

C	es la concentración de la especie química disuelta, M/L^3
D_{ij}	es el coeficiente de dispersión hidrodinámica, L^2/T
b	es el espesor saturado del acuífero, L
C'	es la concentración del soluto en la fuente o sumidero, M/L^3

En la parte derecha de la ecuación:
El primer término represente los cambios de concentración por dispersión hidrodinámica;
El segundo termino describe el efecto del transporte advectivo;
El tercer término represente una fuente o sumidero de fluido.

Coeficiente de Dispersión.

El coeficiente de dispersión puede ser relacionado con la velocidad del flujo del agua la naturaleza del acuífero usando la ecuación de Scheidegger:

$$D_{ij} = \alpha_{ijmn}\frac{V_m V_n}{|V|} \tag{3.4}$$

Para un acuífero isotrópico el tensor de dispersividad puede ser definido en términos de dos constantes; la dispersividad longitudinal α_L y la dispersividad transversal α_T. estas se relacionan con los coeficientes de dispersión por:

$$\begin{aligned} D_L &= \alpha_L|V| \\ D_T &= \alpha_T|V| \end{aligned} \tag{3.5}$$

Expandiendo la ecuación de Scheidegger sustituyendo las identidades y eliminando términos de coeficiente cero, los componentes del coeficiente de dispersión para flujo bi dimensional en un acuífero isotrópico se pueden establecer explícitamente como:

$$D_{xx} = D_L \frac{(V_x)^2}{|V|^2} + D_T \frac{(V_y)^2}{|V|^2}$$

$$D_{yy} = D_T \frac{(V_x)^2}{|V|^2} + D_L \frac{(V_y)^2}{|V|^2} \qquad (3.6)$$

$$D_{xy} = D_{yx} = (D_L - D_T) \frac{V_x V_y}{|V|^2}$$

Métodos Numéricos

Ecuación de Flujo.

La ecuación de flujo puede ser aproximada con la salvedad de que los ejes de coordenadas se alineen con las direcciones del tensor de transmisividad por la siguiente ecuación de diferencias finitas:

$$T_{xx[i-\frac{1}{2},j]}\left[\frac{h_{i-1,j,k} - h_{i,j,k}}{(\Delta x)^2}\right] + T_{xx[i+\frac{1}{2},j]}\left[\frac{h_{i+1,j,k} - h_{i,j,k}}{(\Delta x)^2}\right] + T_{yy[i,j-\frac{1}{2}]}\left[\frac{h_{i-1,j,k} - h_{i,j,k}}{(\Delta y)^2}\right] + T_{yy[i,j+\frac{1}{2}]}\left[\frac{h_{i,j+1,k} - h_{i,j,k}}{(\Delta y)^2}\right]$$

$$= S\left[\frac{h_{i,j,k} - h_{i,j,k-1}}{(\Delta t)}\right] + \frac{q_{w(i,j)}}{\Delta x \Delta y}\frac{K_z}{m}\left[H_{s(i,j)} - h_{i,j,k}\right] \qquad (3.7)$$

donde i,j,k son los índices de las dimensiones en x,y, y el tiempo, y q_W es recarga.

Después de que la distribución de niveles ha sido calculada, para un paso de tiempo, la velocidad para el flujo de agua subterránea puede ser calculada en cada nodo usando un esquema de diferencias finitas explícitas. por ejemplo para la velocidad en la dirección x:

$$V_{x(i+\frac{1}{2},j)} = \frac{K_{xx(i+1,j)}}{\varepsilon}\left[\frac{h_{i,j,k} - h_{i+1,j,k}}{(\Delta x)}\right] \qquad (3.8)$$

Ecuación de Transporte

Método de Características

La ecuación de transporte puede ser escrita, considerando espesor saturado como variable y expandiendo el término de transporte advectivo, como sigue:

$$\frac{\partial C}{\partial t} = \frac{1}{b}\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right) - V_i\frac{\partial C}{\partial x_i} + \frac{C\left(S\frac{\partial h}{\partial t} + W - \varepsilon\frac{\partial b}{\partial t}\right) - C'W}{\varepsilon b} \qquad (3.9)$$

Esta ecuación es la resuelta en el programa de computadora. por conveniencia es escrito como:

$$\frac{\partial C}{\partial t} = \frac{1}{b}\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right) - V_x\frac{\partial C}{\partial x} - -V_y\frac{\partial C}{\partial x} + F \qquad (3.10)$$

La derivada material de la concentración, que asume la razón de cambio observada moviéndose con las partículas es:

$$\frac{dC}{dt} = \frac{\partial C}{\partial t} + \frac{\partial C}{\partial x}\frac{dx}{dt} + \frac{\partial C}{\partial y}\frac{dy}{dt} \qquad (3.11)$$

Para las componentes x y y tenemos las velocidades como:

$$\frac{dx}{dt} = V_x \qquad (3.12)$$

$$\frac{dy}{dt} = V_y \qquad (3.13)$$

si sustituimos en la ecuación (3.11) las (3.10), (3.12) y (3.13):

$$\frac{dC}{dt} = \frac{1}{b}\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right) + F \qquad (3.14)$$

la solución del sistema de ecuaciones (3.11-13) puede ser dada como:

$$x = x(t); \qquad y = y(t); \qquad C = C(t) \qquad (3.15)$$

y son llamadas las curvas características de la ecuación de transporte.

Seguimiento de partículas.

El método de características consiste en poner partículas o puntos en cada celda de la malla de elementos finitos formándolos en una distribución uniforme en el área de interés. La concentración inicial asignada a cada punto es la concentración asociada con el nodo de la celda conteniendo los puntos.

cada paso de tiempo cada punto es movido una distancia proporcional a la longitud del incremento de tiempo y la velocidad el la localidad del punto (fig. 3.1). La nueva posición el calculada siguiendo las formas de las ecuaciones (3.12) y (3.13):

$$x_{p,k} = x_{p,k-1} + \delta x_p = x_{p,k-1} + \Delta t V_{x\left[x_{(p,k)}, y_{(p,k)}\right]} \tag{3.16}$$

$$y_{p,k} = y_{p,k-1} + \delta y_p = y_{p,k-1} + \Delta t V_{y\left[x_{(p,k)}, y_{(p,k)}\right]} \tag{3.17}$$

donde

p es el número índice para identificación del punto; y
δx y δy son las distancias que se movió en las direcciones x y y.

Después que todos los puntos se han movido la concentración en cada nodo es tomada como el promedio de las concentraciones de todos los puntos localizados dentro del área de esa celda; esta concentración promedio es denotada como $C_{i,j,k*}$. Los puntos en movimiento simulan el transporte por advección porque la concentración en cada nodo cambia con cada paso de tiempo conforme diferentes puntos, teniendo diferentes concentraciones, entran y salen del área de esa celda.

La aproximación por diferencias finitas de la ecuación de transporte es expresada como:

$$\Delta C_{i,j,k} = \frac{0.5\Delta t}{b}\left[\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C_{(k-1)}}{\partial x_j}\right) + \frac{C_{(k-1)}\left(S\frac{\partial h}{\partial t} + W - \varepsilon\frac{\partial b}{\partial t}\right) - C'W}{\varepsilon}\right]$$
$$+\frac{0.5\Delta t}{b}\left[\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C_{k*}}{\partial x_j}\right) + \frac{C_{k*}\left(S\frac{\partial h}{\partial t} + W - \varepsilon\frac{\partial b}{\partial t}\right) - C'W}{\varepsilon}\right] \tag{3.18}$$

La nueva concentración al final del incremento de tiempo k es calculada como:

$$C_{i,j,k} = C_{i,j,k*} + \Delta C_{i,j,k} \tag{3.19}$$

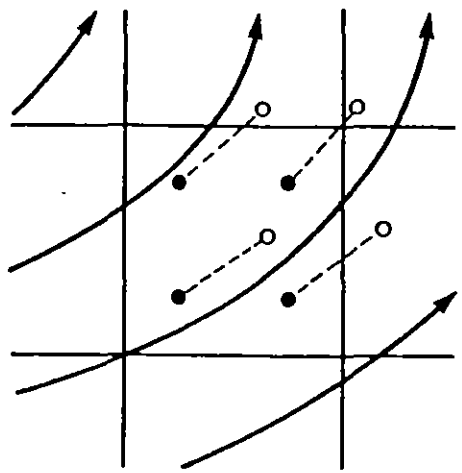
$$\frac{\partial}{\partial x}\left(bD_{xx}\frac{\partial C}{\partial x}+bD_{xy}\frac{\partial C}{\partial y}\right)$$

$$=\frac{bD_{xx[i+\frac{1}{2},j]}(C_{i+1,j}-C_{i,j})}{(\Delta x)^2}-\frac{bD_{xx[i-\frac{1}{2},j]}(C_{i,j}-C_{i-1,j})}{(\Delta x)^2}$$
$$+\frac{bD_{xy[i+\frac{1}{2},j]}(C_{i,j+1}+C_{i+1,j+1}-C_{i,j-1}-C_{i+1,j-1})}{4\Delta x\Delta y}$$
$$-\frac{bD_{xy[i-\frac{1}{2},j]}(C_{i-1,j+1}+C_{i,j+1}-C_{i-1,j-1}-C_{i,j-1})}{4\Delta x\Delta y}.$$

$$\frac{\partial}{\partial y}\left(bD_{yy}\frac{\partial C}{\partial y}+bD_{yx}\frac{\partial C}{\partial x}\right)$$

$$=\frac{\left(bD_{yy}\frac{\partial C}{\partial y}\right)_{i,j+\frac{1}{2}}-\left(bD_{yy}\frac{\partial C}{\partial y}\right)_{i,j-\frac{1}{2}}}{\Delta y}+\frac{\left(bD_{yx}\frac{\partial C}{\partial x}\right)_{i,j+\frac{1}{2}}-\left(bD_{yx}\frac{\partial C}{\partial x}\right)_{i,j-\frac{1}{2}}}{\Delta y}$$
$$=\frac{bD_{yy[i,j+\frac{1}{2}]}(C_{i,j+1}-C_{i,j})}{(\Delta y)^2}-\frac{bD_{yy[i,j-\frac{1}{2}]}(C_{i,j}-C_{i,j-1})}{(\Delta y)^2}$$
$$+\frac{bD_{yx[i,j+\frac{1}{2}]}(C_{i+1,j}+C_{i+1,j+1}-C_{i-1,j}-C_{i-1,j+1})}{4\Delta x\Delta y}$$
$$-\frac{bD_{yx[i,j-\frac{1}{2}]}(C_{i+1,j-1}+C_{i+1,j}-C_{i-1,j-1}-C_{i-1,j})}{4\Delta x\Delta y}.$$

$$(\Delta C_{i,j,k})_{II}=\frac{\Delta t}{\epsilon b_{i,j,k}}\left[C_{i,j,k-1}\left(S\left[\frac{h_{i,j,k}-h_{i,j,k-1}}{\Delta t}\right]\right.\right.$$
$$\left.+W_{i,j,k}-\epsilon\left[\frac{b_{i,j,k}-b_{i,j,k-1}}{\Delta t}\right]\right)$$
$$\left.-C'_{i,j,k}W_{i,j,k}\right].$$



EXPLICACIÓN

- ● Posición inicial de la partícula
- O Nueva posición de la partícula
- → línea y dirección de flujo
- --- trayectoria calculada de la partícula

Figura 3.1. Vista parcial de una hipotética malla de diferencias finitas mostrando la relación entre el campo de flujo y el movimiento de puntos

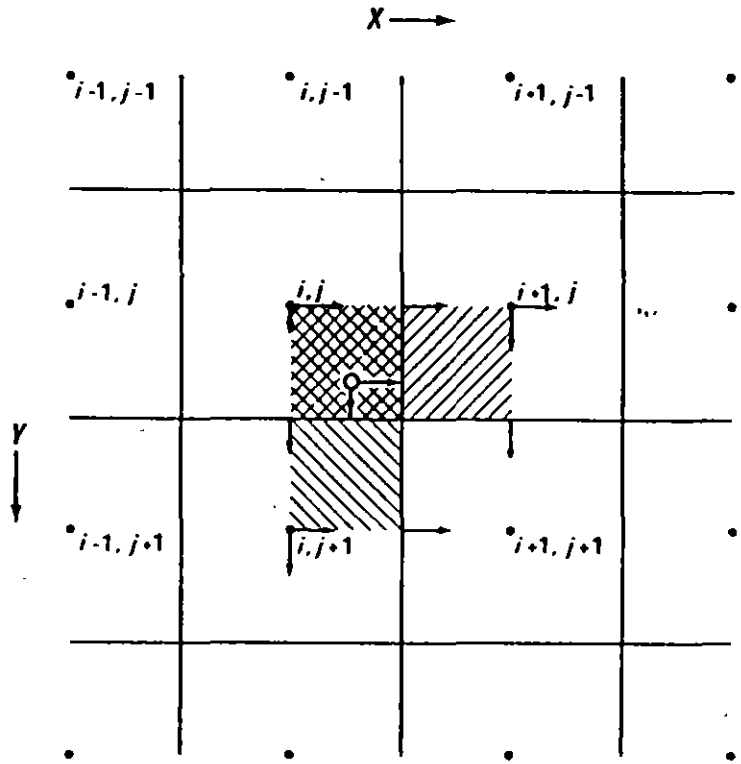


Figura 3.2. Vista parcial de una hipotética malla de diferencias finitas mostrando áreas sobre las cuales la interpolación bilineal es usada para calcular la velocidad en un punto. Nótese que cada área de influencia e igual a 1/2 del área de una celda

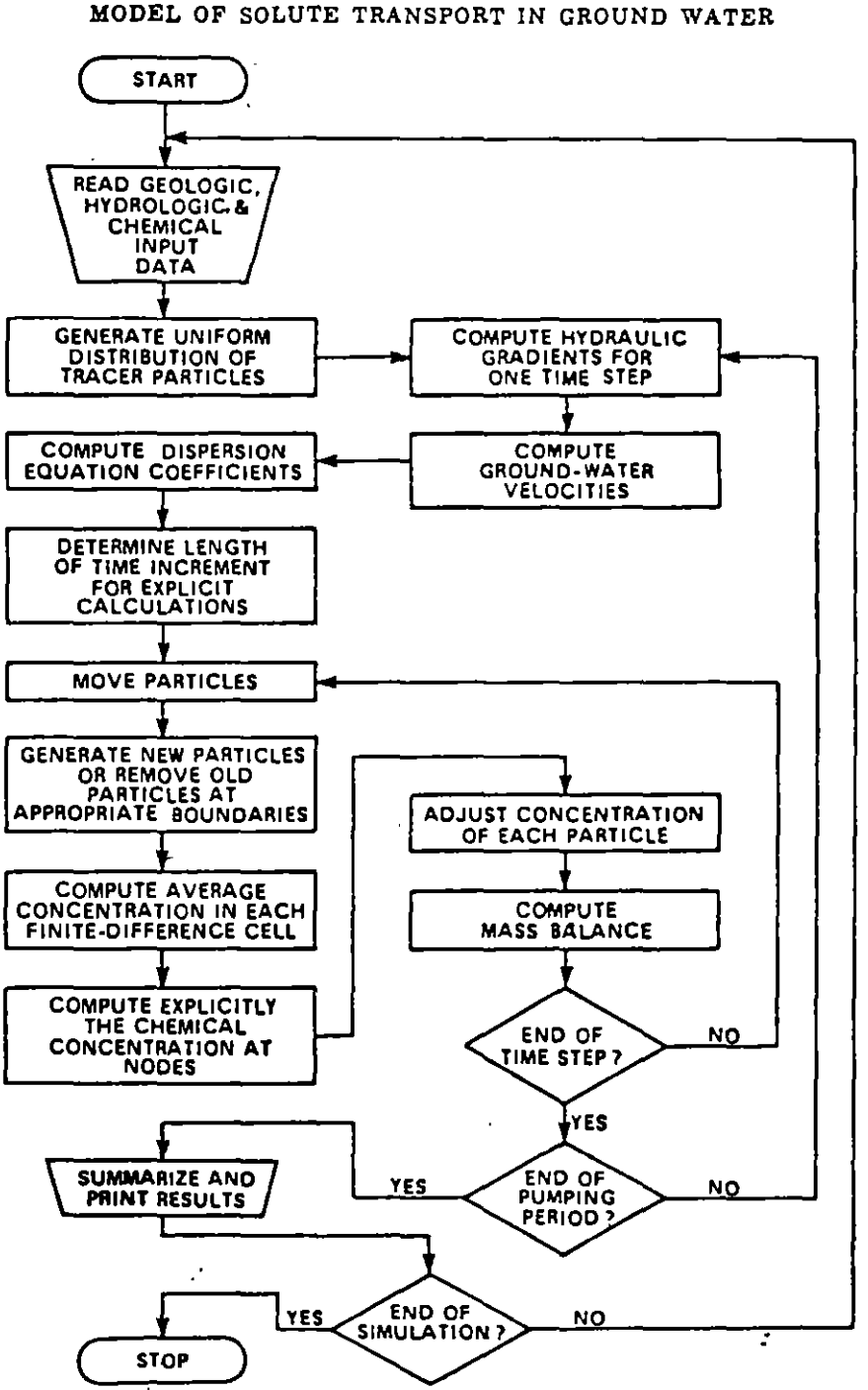


Figura 3.3 Diagrama de flujo simplificado ilustrando las principales etapas en el procedimiento de cálculo

4. MÉTODOS DE SOLUCIÓN DE ECUACIONES LINEALES

4.1 Métodos Directos de Resolución de Sistemas de Ecuaciones Lineales

Un muy bien conocido método directo para solución de sistemas de ecuaciones lineales de la forma

$$\sum\{P(I,J)\times F(J)\} = G(I) \qquad (I = 1...N)$$

es el *método de eliminación Gaussiana*. En este método la primera ecuación es usada para expresar la primera variable en términos de todas las otras variables, entonces la primera variable es eliminada de todas las ecuaciones subsecuentes. Queda un sistema de N-1 ecuaciones con N-1 variables; el proceso puede ser repetido hasta que solo una ecuación con una variable quede. Esta ecuación puede ser fácilmente resuelta y entonces las ecuaciones previas pueden ser resueltas en una serie de sustituciones hacia atrás.

4.2 Métodos Iterativos de Resolución de Sistemas de Ecuaciones Lineales

En esta sección se presenta el *método iterativo de Gauss-Seidel*, con el énfasis puesto en la ejecución en una computadora pequeña. La teoría del Método puede ser encontrada en libros de texto de análisis numérico. El sistema de ecuaciones lineales será escrito como:

$$\sum\{P(I,J)\times F(J)\} = G(I) \qquad (I = 1...N) \qquad (4.2.1)$$

donde la sumatoria debe ser ejecutada desde J=1 a J=N.

En el método de Gauss-Seidel una solución inicial estimada es continuamente actualizada corrigiendo la I-ésima ecuación modificando la variable I. La estimación inicial puede ser arbitraria, por ejemplo, $F(I)$ = 0 para todos los valores desconocidos de $F(I)$. En forma alternativa, se puede hacer alguna estimación razonable para las incógnitas. En general la ecuación (4.2.1) no será satisfecha por la solución estimada. La variable $F(I)$ será corregida por una cantidad $DF(I)$, de mido que la ecuación I sea satisfecha. Si la solución estimada es representada por $FA(I)$, esto significa que

$$\sum\{P(I,J)\times FA(J)\} + P(I,I)\times DF(I) = G(I)$$

La corrección de la incógnita $DF(I)$ puede ser despejada de la ecuación

$$DF(I) = \left[G(I) - \sum\{P(I,J)\times FA(J)\}\right] / P(I,I) \qquad (4.2.2)$$

El algoritmo Gauss-Seidel consiste en la ejecución repetida de la ecuación (4.2.2) para todos los valores de I. Puede ser demostrado que el proceso converge si la matriz es positiva

definida. La convergencia es razonablemente rápida si la diagonal principal de la matriz es dominante.

El algoritmo de Gauss-Seidel puede ser ejecutado por la siguientes proposiciones en lenguaje de programación BASIC:

```
1000 FOR K=1 TO NI
1010 FOR I=1 TO N
1020 A=G(I):FOR J=1 TO N: A=A-P(I,J)*F(J):NEXT J
1030 F(I)=F(I)+A/P(I,I):NEXT I:NEXT K
```

El número de iteraciones es *NI*, el cual a menudo es asignado con la magnitud del número de ecuaciones *N*. Algunas veces el número de iteraciones necesario puede ser mayor, especialmente si la diagonal principal no es dominante. Entonces un método diferente puede ser más eficiente.

Una variante del algoritmo de Gauss-Seidel es el *método de Jacobi*, en el cual todas las correcciones son calculadas primero, y entonces todos los valores de *F(I)* son actualizados en un paso. Esto puede ser ejecutado por las siguientes líneas:

```
1000 FOR K=1 TO N
1010 FOR I=1 TO N
1020 A(I)=G(I):FOR J=1 TO N:A(I)=A(I)-P(I,J)*F(J):NEXT J,I
1030 FOR I=1 TO N:F(I)=F(I)+A(I)/P(I,I):NEXT I:NEXT K
```

Este procedimiento requiere un mayor tiempo de cálculo y usa más memoria a causa de que el vector de incrementos tiene que ser almacenado. La convergencia es más lenta. Es por esto que el método de Gauss-Seidel sea usualmente preferido excepto por propósitos especiales.

La experiencia práctica con el método de Gauss-Seidel ha demostrado que la convergencia puede ser mejorada multiplicando la corrección en cada paso por un factor algo mayor que 1. Esto significa que en cada paso el error no se hace igual a cero, sino que por un impulso extra se hace que cambie de signo. en anticipación a futuras correcciones. El factor, llamado *factor de sobre-relajación* debe ser menor que 2 y, al menos, igual a 1. El algoritmo ahora es el siguiente:

```
1000 FOR K=1 TO NI
1010 FOR I=1 TO N
1020 A=G(I):FOR J=1 TO N: A=A-P(I,J)*F(J):NEXT J
1030 F(I)=F(I)+R*A/P(I,I):NEXT I:NEXT K
```

4.3 Método Implícito de dirección Alternante (ADI).

Consideremos la ecuación en dos dimensiones transitoria para un acuífero confinado:

$$\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}=\frac{S}{T}\frac{\partial h}{\partial t} \tag{4.3.1}$$

Para el caso especial $\Delta x = \Delta y = a$, la aproximación de diferencias finitas completamente implícita es:

$$h'_{i-1,j}+h'_{i+1,j}+h'_{i,j-1}+h'_{i,j+1}-4h'_{i,j}=\frac{Sa^2}{T}\frac{h'_{i,j}-h^0_{i,j}}{\Delta t} \tag{4.3.2}$$

Poniendo la incógnitas del lado izquierdo de la ecuación y los valores conocidos a la derecha:

$$h'_{i-1,j}+h'_{i+1,j}+h'_{i,j-1}+h'_{i,j+1}+\left(-4-\frac{Sa^2}{T\Delta t}\right)h'_{i,j}=-\frac{Sa^2}{T}\frac{h^0_{i,j}}{\Delta t} \tag{4.3.3}$$

La base del método Implícito de dirección Alternante (ADI) es obtener una matriz de coeficientes tridiagonal escribiendo alternativamente las ecuaciones de diferencias finitas primero implícitamente a lo largo de las columnas y explícitamente a lo largo de los renglones y entonces viceversa. Las ecuaciones que resultan son:

$$h'_{i,j-1}+\left(-4-\frac{Sa^2}{T\Delta t}\right)h'_{i,j}+h'_{i,j+1}=-\frac{Sa^2}{T}\frac{h^0_{i,j}}{\Delta t}-h^0_{i-1,j}-h^0_{i+1,j} \tag{4.3.4}$$

$$h'_{i-1,j}+\left(-4-\frac{Sa^2}{T\Delta t}\right)h'_{i,j}+h'_{i+1,j}=-\frac{Sa^2}{T}\frac{h^0_{i,j}}{\Delta t}-h^0_{i,j+1}-h^0_{i,j-1} \tag{4.3.4}$$

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TEMA: MODFLOW SIMULACION COMPUTACIONAL DE FLUJO EN MEDIOS POROSOS SATURADOS

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Introducción:

El análisis del comportamiento observado de un acuífero, y la predicción de su evolución futura, son objetivos importantes que se pretende alcanzar mediante una serie de estudios multidisciplinarios que permiten simular el movimiento del agua en medios porosos.

La implementación de un modelo numérico de simulación requiere de información proveniente de diversas disciplinas. Los resultados proporcionados por estudios geológicos, geofísicos, hidrogeoquímicos, hidráulicos, climatológicos, etc. constituyen los archivos de datos que caracterizan al acuífero estudiado.

La metodología que se emplea en el proceso de modelación numérica, consiste en obtener una solución aproximada de la ecuación diferencial que gobierna el movimiento del agua en un medio poroso saturado. La región de simulación se define de acuerdo a la geometría del sistema acuífero estudiado, y se le imponen condiciones de frontera justificables por la geología y la hidráulica subterránea. Adicionalmente, para la solución transitoria se requiere de condiciones iniciales (observadas o deducidas) para el tiempo de inicio de la simulación.

Una vez que se dispone de los archivos de datos, el algoritmo numérico de solución de la ecuación de flujo, condiciones iniciales y de frontera especificados, se procede a ejecutar las simulaciones de calibración del sistema, enfocadas a reproducir el comportamiento observado. La incertidumbre en los valores asignados a los parámetros hidráulicos y a la recarga del sistema, entre otros factores, pueden conducir a una discrepancia entre los niveles piezométricos observados y los simulados. La calibración del modelo consiste en modificar los archivos de datos propuestos originalmente, hasta obtener un funcionamiento del sistema que sea similar al observado históricamente.

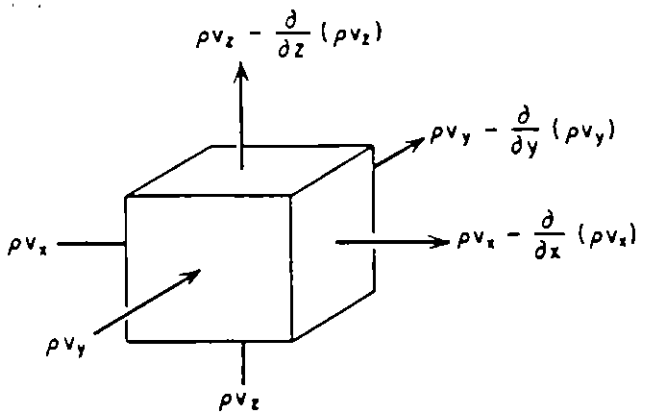
Las simulaciones predictivas se realizan utilizando los archivos de datos calibrados y permiten prever el comportamiento que el sistema acuífero adoptará en el futuro al ser sometido a diversas políticas de explotación.

Las configuraciones de niveles piezométricos obtenidas mediante simulaciones predictivas, son determinantes en la toma de decisiones para el manejo racional de los recursos hidráulicos y para el diseño de las estructuras requeridas.

En los subcapítulos siguientes se presentan algunos aspectos importantes del proceso de simulación numérica, entre estos la deducción de la ecuación diferencial que describe el movimiento del agua en medios porosos, algunos comentarios acerca de los problemas con valores a la frontera, un ejemplo del procedimiento de solución analítica de un problema con valores a la frontera, y finalmente un artículo referente a la simulación numérica del acuífero de San Luis Potosí que ilustra concretamente la metodología expuesta.

DEDUCCION DE LA ECUACION DIFERENCIAL DE FLUJO EN MEDIOS POROSOS

La deducción de la ecuación de flujo para un medio poroso saturado se puede realizar mediante un balance de materia en un volumen de control:



Según la ecuación de continuidad (Ley de Conservación de la Materia), las entradas (E) menos las salidas (S) en un sistema, son iguales al cambio de volumen almacenado dentro del mismo (ΔV).

$$E-S=\Delta V$$

La masa que pasa por unidad de tiempo a través de una cara del volumen de control $\left(\frac{M}{L^2T} \right)$ se puede expresar como ρvA

donde:

ρ = Densidad del fluído $\left(\frac{M}{L^3} \right)$

v = Descarga específica $\left(\frac{L}{T} \right)$

Las entradas menos las salidas en la dirección x serán:

$$\rho vx\ \Delta y\ \Delta z - \left[\rho vx + \frac{\partial(\rho vx)}{\partial x} \Delta x \right] \Delta y\ \Delta z$$

Análogamente:

en la dirección y:

$$\rho vy\ \Delta x\ \Delta z - \left[\rho vy + \frac{\partial(\rho vy)}{\partial y}\Delta y \right] \Delta x\ \Delta z$$

en la dirección z:

$$\rho vz\ \Delta x\ \Delta y - \left[\rho vz + \frac{\partial(\rho vz)}{\partial z}\Delta z \right] \Delta x\ \Delta y$$

Las entradas menos las salidas en el volumen de control serán:

$$E - S = - \left[\frac{\partial(\rho vx)}{\partial x} + \frac{\partial(\rho vy)}{\partial y} + \frac{\partial(\rho vz)}{\partial z} \right] \Delta x\ \Delta y\ \Delta z$$

Dividiendo entre el volumen $\Delta x\ \Delta y\ \Delta z$, se obtiene el cambio en el almacenamiento por unidad de volumen del sistema:

$$\Delta V = - \left[\frac{\partial(\rho vx)}{\partial x} + \frac{\partial(\rho vy)}{\partial y} + \frac{\partial(\rho vz)}{\partial z} \right] \qquad (1)$$

Para un sistema en estado estacionario la variación del volumen almacenado con respecto al tiempo (Δv) es igual a cero:

$$\Delta V = 0$$

Suponiendo densidad del fluído constante:

$$- \left[\frac{\partial vx}{\partial x} + \frac{\partial vy}{\partial y} + \frac{\partial vz}{\partial z} \right] = 0 \qquad (2)$$

Sustituyendo la ecuación de Darcy:

$$v = - K \frac{\partial h}{\partial L} \quad \text{en cada componente}$$

$$\frac{\partial}{\partial x}\left(Kx\,\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(Ky\,\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(Kz\,\frac{\partial h}{\partial z}\right) = 0 \qquad (3)$$

Suponiendo que el material es isotrópico (Kx = Ky = Kz) y homogéneo (K = cte).

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial z^2} = 0 \qquad (4)$$

Esta ecuación es conocida como la Ecuación de Laplace y es de gran utilidad en hidrogeología. La solución de esta ecuación describe el valor de la carga hidráulica en estado estacionario en cualquier punto en una región tridimensional.

Flujo transitorio en medio saturado.

La ley de conservación de masa requiere que la masa que se almacena por unidad de tiempo por unidad de volumen dentro del volumen de control, sea igual a la variación con respecto al tiempo de la densidad ρ del fluido que se encuentra dentro de los poros del material limitado por el volumen de control

$$-\left[\frac{\partial(\rho vx)}{\partial x} + \frac{\partial(\rho vy)}{\partial y} + \frac{\partial(\rho vz)}{\partial z}\right] = \frac{\partial(\rho n)}{\partial t} \qquad (5)$$

donde n es la porosidad del material.

Desarrollando el lado derecho de la ecuación.

$$-\left[\frac{\partial(\rho vx)}{\partial x} + \frac{\partial(\rho vy)}{\partial y} + \frac{\partial(\rho vz)}{\partial z}\right] = n\,\frac{\partial \rho}{\partial t} + \rho\,\frac{\partial n}{\partial t} \qquad (6)$$

$n\,\frac{\partial \rho}{\partial t}$ es la masa producida por la expansión del agua por unidad de tiempo cuando cambia su densidad.

$\rho\,\frac{\partial n}{\partial t}$ es la masa producida por la compactación del medio poroso

por unidad de tiempo cuando cambia su porosidad.

Se puede demostrar que el cambio en ρ y el cambio en n se producen al variar la carga hidráulica h, y que el volumen de agua producido por los 2 mecanismos cuando la carga hidráulica h disminuye una unidad, es Ss (coeficiente de almacenamiento específico $[L^{-1}]$)

$$Ss = \rho g(\alpha + n\beta) \tag{7}$$

α = compresibilidad de la matriz sólida

β = compresibilidad del fluído

El cambio de masa de fluído almacenado por unidad de tiempo es:

$$\Delta V = \rho \, Ss \, \frac{\partial h}{\partial t} \tag{8}$$

La ecuación (6) se puede expresar como:

$$-\frac{\partial(\rho v\dot{x})}{\partial x} - \frac{\partial(\rho vy)}{\partial y} - \frac{\partial(\rho vz)}{\partial z} = \rho \, Ss \, \frac{\partial h}{\partial t} \tag{9}$$

Desarrollando los términos del lado izquierdo por medio de la regla de la cadena, y considerando que los términos $\rho \frac{\partial vx}{\partial x}$ son mucho mayores que los $vx \frac{\partial \rho}{\partial x}$, y sustituyendo la Ley de Darcy, se obtiene:

$$\frac{\partial}{\partial x}\left(Kx \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(Ky \frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(Kz \frac{\partial h}{\partial z}\right) = Ss \frac{\partial h}{\partial t} \tag{10}$$

Considerando medio isótropo: $Kx = Ky = Kz$

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial z^2} = \frac{Ss}{K} \frac{\partial h}{\partial t} \tag{11}$$

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial z^2} = \frac{S}{T} \frac{\partial h}{\partial t} \tag{12}$$

Esta ecuación se conoce como la ecuación de difusión. La solución $h(x,y,z,t)$ describe el valor de la carga hidráulica en cualquier punto (x,y,z) de la región para cualquier tiempo t.

Problemas con valores a la frontera

Un problema de valores a la frontera es un modelo matemático

La técnica de análisis de un problema de valores a la frontera es un proceso de 4 pasos:

1) Examen del problema físico
2) Planteamiento del problema físico en términos de un problema matemático equivalente
3) Solución del problema matemático con técnicas matemáticas
4) Interpretación de los resultados matemáticos en términos del problema físico.

Los problemas de flujo en medios porosos dan lugar a un problema matemático de la forma de problema con valores a la frontera.

Para definir completamente un problema transitorio de valores a la frontera en flujo subterráneo se necesita conocer:

1) El tamaño y forma de la región de flujo (geometria del sistema)
2) La ecuación de flujo dentro de la región
3) Las condiciones de frontera alrededor de la región
4) Las condiciones iniciales en la región
5) La distribución espacial de los parámetros hidrogeológicos que controlan el flujo
6) Un método matemático de solución

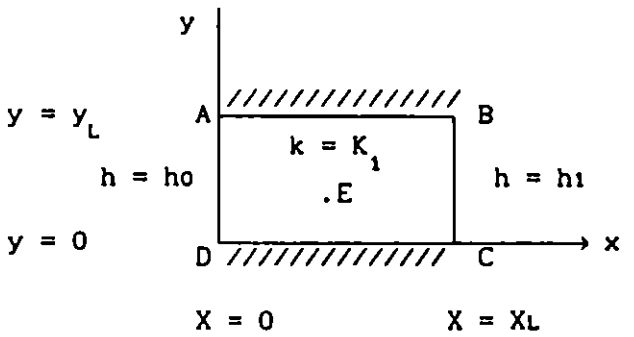
Si el problema con valores a la frontera es para estado estacionario, no se requiere conocer las condiciones iniciales del sistema.

Los métodos de solución para un problema con valores a la frontera pueden ser clasificados en 5 enfoques:

1) Solución por inspección
2) Solución por técnicas gráficas (redes de flujo)
3) Solución por modelos analógicos (circuitos eléctricos)
4) Solución por técnicas matemáticas analíticas
5) Solución por técnicas matemáticas numéricas (modelos computacionales)

Ejemplo de una solución analítica a un problema de valores a la frontera

Considere el problema de flujo subterráneo mostrado en las figuras:



La ecuación de flujo en dos dimensiones para flujo en zona saturada y estado estacionario es:

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = 0 \qquad \text{- - - (1)}$$

La expresión matemática de las condiciones de frontera es:

$$\frac{\partial h}{\partial y} = 0 \quad \text{en} \quad y = 0 \quad y \quad y = y_L \qquad \text{- - - (2)}$$

$$h = h0 \quad \text{en} \quad X = 0 \qquad \text{- - - (3)}$$

$$h = h_1 \quad \text{en} \quad X = X_L \qquad \text{- - - (4)}$$

Se obtendrá h (x,y) usando la técnica de separación de variables:
Se supone en el método de separación de variables que la solución es un producto de la forma:

$$h(x,y) = X(x)\ Y(y) \qquad \text{- - - (5)}$$

La ecuación (1) se expresa ahora como:

$$Y \frac{\partial^2 X}{\partial x^2} + X \frac{\partial^2 Y}{\partial y^2} = 0 \qquad \text{- - - (6)}$$

Dividiendo entre X Y se obtiene:

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = -\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} \qquad - - - (7)$$

El lado izquierdo es independiente de y. El lado derecho, a pesar de su apariencia, debe ser independiente de y, debido a que es igual al lado izquierdo. Análogamente, el lado derecho es independiente de x, y también el lado izquierdo. Si los dos términos de la ecuación son independientes de x y y, cada término debe ser igual a una constante.

entonces:

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = G \quad y \quad \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} = G \qquad - - - (8)$$

La constante G puede ser positiva, negativa o cero. Los 3 casos conducen a una solución tipo producto. Pero sólo el caso G = 0 dá lugar a una solución que tiene significado físico para este problema. Por lo tanto:

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = 0 \quad y \quad \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} = 0 \qquad - - - (9)$$

Estas son ecuaciones diferenciales ordinarias cuyas soluciones son bien conocidas:

$$X = Ax + B \quad y \quad Y = Cy + D \qquad - - - (10)$$

La solución producto (5) es:

$$h(x,y) = (Ax + B)(Cy + D) \qquad - - - (11)$$

Los coeficientes A, B, C y D se evaluan mediante las condiciones de frontera. Diferenciando (11) con respecto a y se obtiene:

$$\frac{\partial h}{\partial y} = (Ax + B)C \qquad - - - (12)$$

La condición de frontera (2) implica que C = 0. La ecuación (11) queda como:

$$h(x,y) = (Ax + B)D = Ex + F \qquad - - - (13)$$

De acuerdo a las condiciones de frontera (3) y (4);
F = ho y E = -(ho - h1)/xL. La solución es entonces:

$$h(x,y) = ho - (ho - h1)\frac{x}{xL} \qquad - - - (14)$$

Se aprecia claramente que la ecuación (14) satisface las condiciones de frontera (3) y (4). La derivada con respecto a y es igual a cero satisfaciendo la condición (2). La segunda derivada de h(x,y) con respecto a x también es igual a cero. Por lo tanto la solución (14) satisface la ecuación de flujo (1).

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EVALUATION OF HYDROTHERMAL SOURCES THAT SUSTAIN AN OVEREXPLOITED AQUIFER AT SAN LUIS POTOSI, MEXICO.

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ABSTRACT. A numerical model is implemented for the aquifer of the City of San Luis Potosi, which takes into account the contribution of an underlying thermal source. Previously, it was thought to be overexploited. By means of the numerical model, it is shown that this is not the case, because there is a contribution from the underlying thermal source. Since the properties of the thermal source are not known, the procedure used to incorporate them is to adjust the values of the vertical hydraulic conductivity between the thermal source and the aquifer until the actual piezometric levels in the aquifer were reproduced. For this case study, such a procedure has produced useful results.

INTRODUCTION

The Valley of San Luis Potosi, is located in the high plateau of the Republic of Mexico (Fig.1) and it lies in the semi-arid region. The water demand of the City of San Luis Potosi, capital of the state of the same name, for agricultural, urban and industrial uses, has been steadily increasing. Most of the water supplied to the city is from underground sources, because due to the reduced rainfall, the surface water contribution is small (only 8 %).

There is concern with respect to the future evolution of the aquifer, because in the last few years the observed speed of drawdown has reached the rate of 1.3 m $year^{-1}$. However, if the hydraulic balance of the aquifer is carried out taking into account only what is known about the aquifer, the predicted rate of drawdown is even larger. On the basis of thermal, chemical and hydraulic evidences, in a previous study: Instituto de Geofisica, UNAM (1988), it was established that the differences between the observed and the predicted rate of drawdown is due, to water supplied by deeper geological formations with thermal activity.

Taking into account these facts, it was decided to implement a numerical model of the aquifer to improve the understanding of its behavior, specially with respect to the deep thermal sources, and to predict the system behavior under different exploitation policies for the next twenty years.

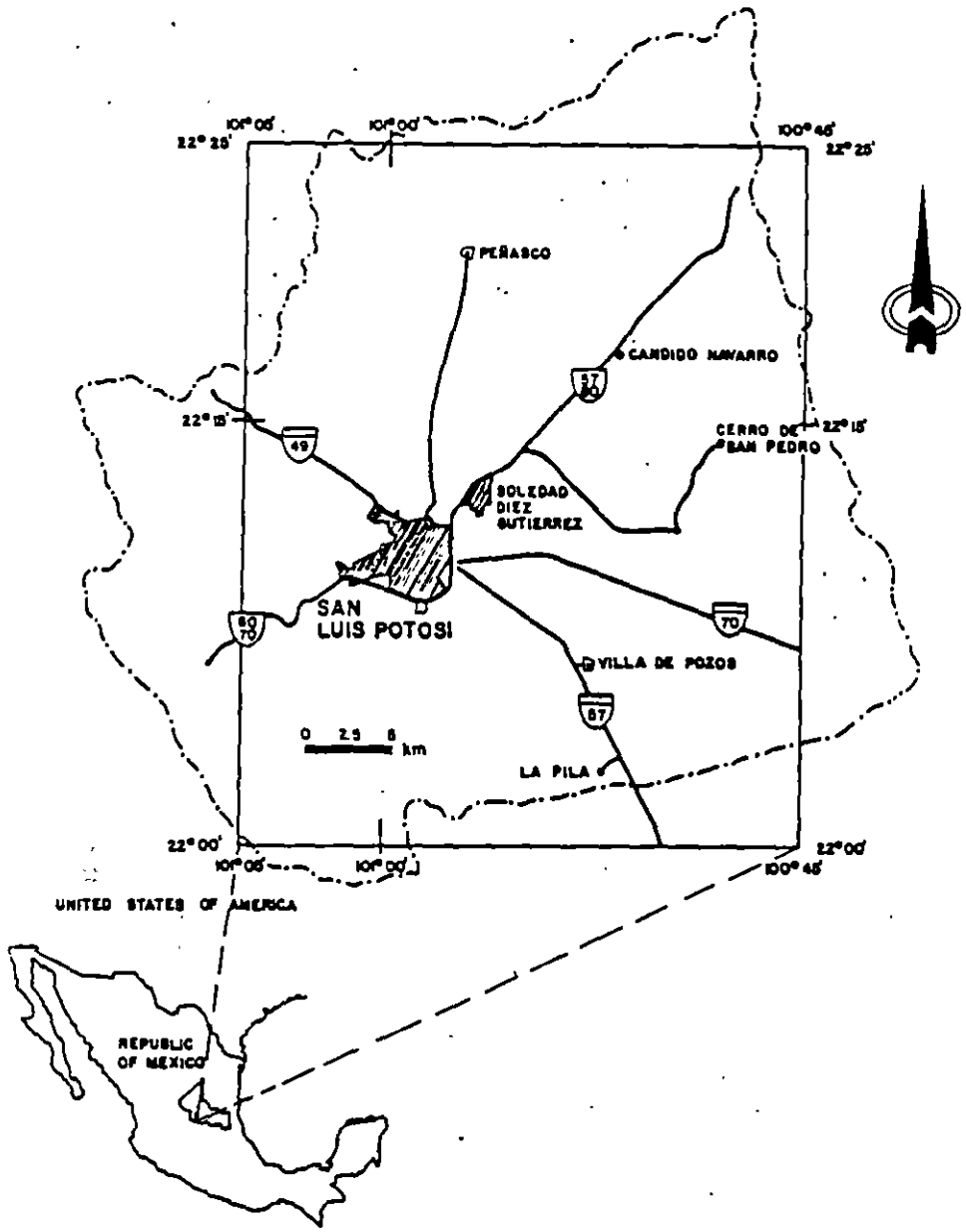


Figure 1: Location map of San Luis Potosi Basin

HYDROGEOLOGIC MODEL

On the basis of the available geological, geophysical, piezometric an hydrochemical information, the proposed hydrogeological model of the syste includes a "shallow aquifer" of reduced yield and poor quality water. Thi aquifer overlies a "clay formation" which in turn confines a deeper aquifer Most of the water is produced at this "deep aquifer", which has therma activity (Fig.2). Below it, lay the "thermal sources".

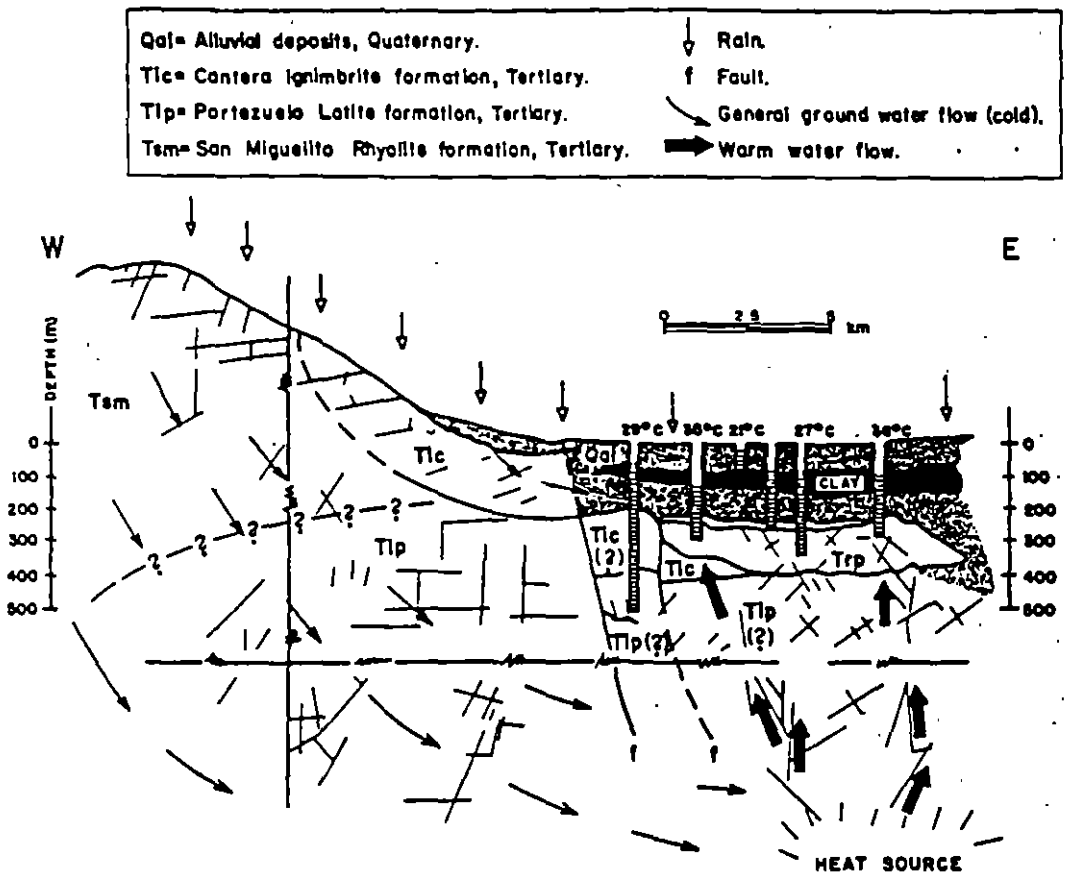


Figure 2: The hydrogeological model

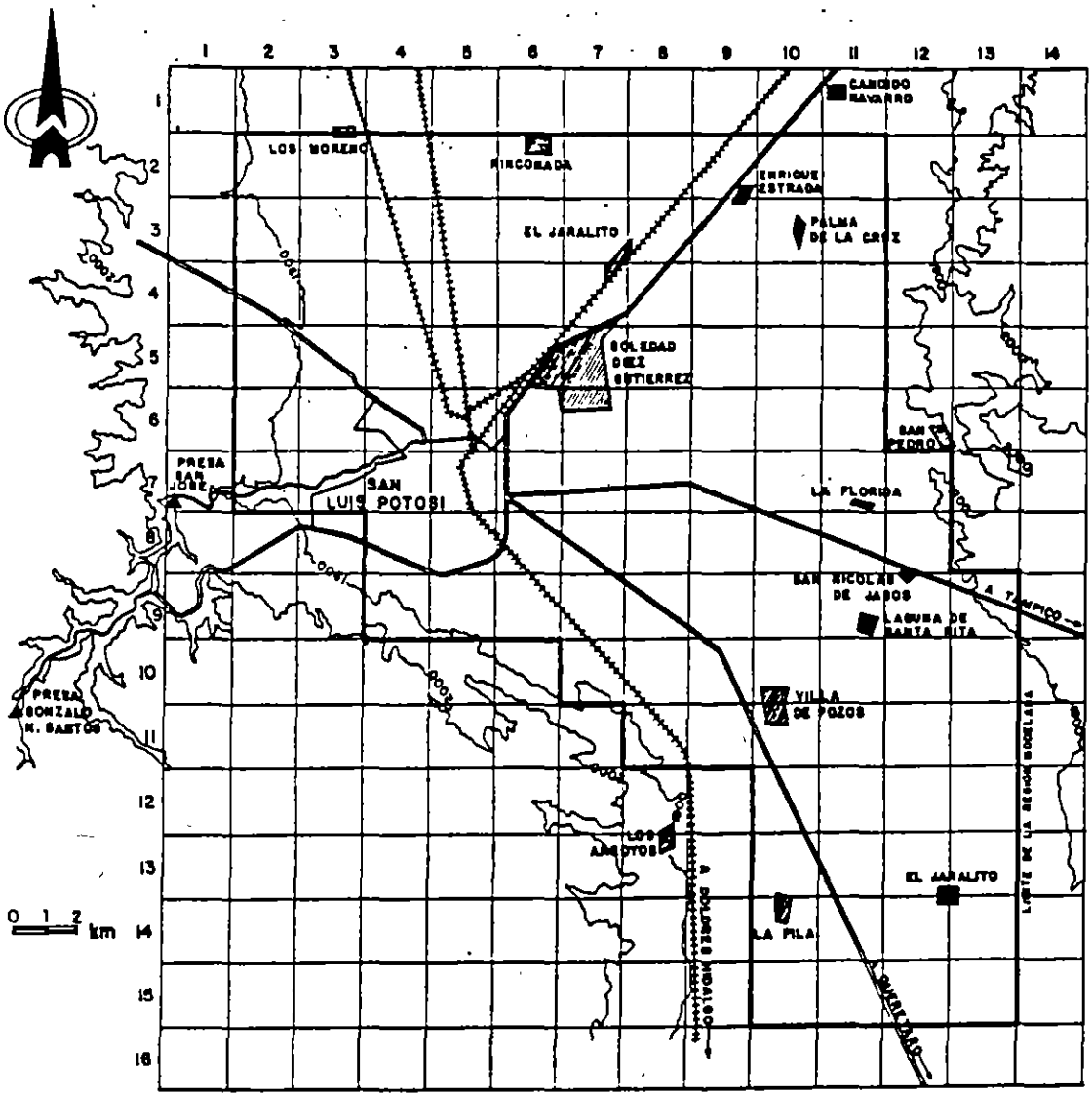
In this figure, it can be observed, that the system of regional flow is important for aquifer performance, producing a vertical component of hot water. For a detailed geological description of the system, the reader is referred to the previous study: Instituto de Geofisica, UNAM (1988).

MODELLING OF THE SYSTEM

For the implementation of the numerical model, a conceptual model of its behavior was defined, suitable differential equations were adopted, a computer program was selected and its calibration was carried out using the available information. The piezometric levels produced by the program, were interpolated using the package *SURFER*: Golden Software, Inc., (1989) to obtain a more convenient graphical representation.

The conceptual model

The limits of the area included in the model, are shown in Fig. 3 and were based on geological considerations.



Limit of the modeled region.

Figure 3: Grid used in the numerical simulation

The San Miguelito range at the west and the San Pedro range at the east, constitute natural boundaries because they present conditions of no flow, and at some places constant head (Fig. 4).

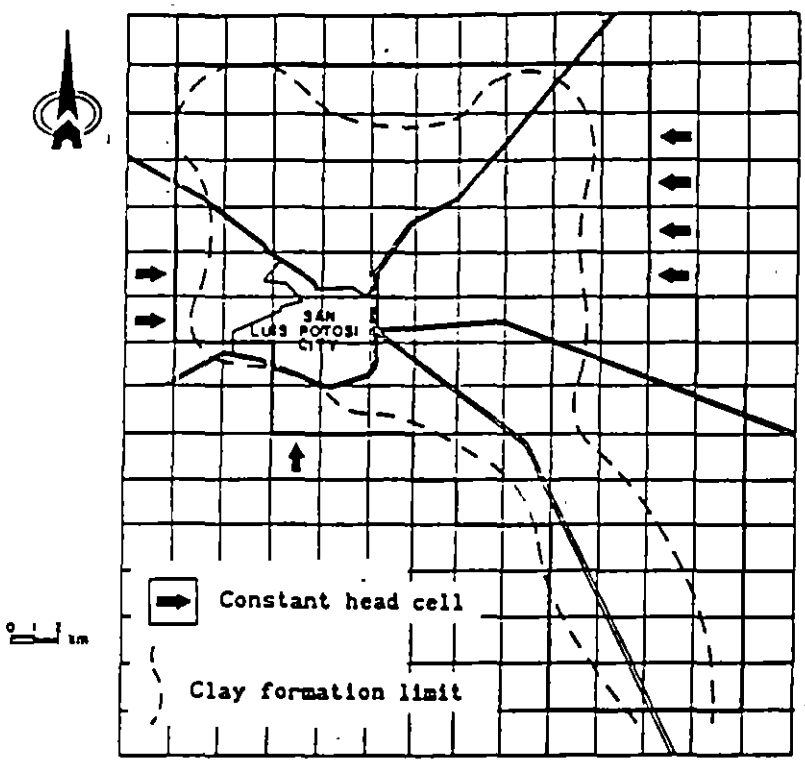


Figure 4: Area covered by the clay formation

The northern and southern limits were selected on the basis of the piezometric information that was available and they were taken as impermeable, because there is evidence that the flow there, is negligible. The shallow aquifer, located on the upper part of the system, functions as a unit independent of the deep aquifer, because the clay layer that separates them is sensibly impervious. Taking into account that most of the water is produced at the deep aquifer, the purpose of the model is the prediction of its behavior exclusively, leaving aside the shallow aquifer.

The Basic Equation

The governing equation used was:

$$\frac{\partial}{\partial x}\left(Kx\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(Ky\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(Kz\frac{\partial h}{\partial z}\right) = S_s \frac{\partial h}{\partial t} \qquad (1)$$

where Ss = specific coefficient of storage $[L^{-1}]$

K = Hydraulic conductivity $[LT^{-1}]$

h = Hydraulic head [L]

t = Time [T]

However, the analysis of the flow was mainly two-dimensional, because only two horizontal layers were incorporated in the model.

The computer code MODFLOW: McDonald & Harbaugh, (1984), was used in all calculations. This model applies the cells method which yields finite differences approximations.

The deep aquifer can be satisfactorily modelled using a 2x2 Km grid and applying finite difference schemes on them, as illustrated in Fig. 4. Layer I includes the best known part of the system, where the value of the hydraulic properties are known or at least can be estimated. Layer II was introduced to model the deeper, less known geological formations which supply the thermal water. The flow and interaction between layers I and II, is due to the differences of hydraulic head between them. In layer II, it was assumed a constant hydraulic head that remained greater than the head of layer I, throughout the runs. This induces a vertical component of flow whose magnitude can be adjusted varying the ratio of the hydraulic conductivity (Kz) to the thickness of the layer where the flow takes place.

An upper boundary condition of no flow was considered in layer I, which corresponds to the clay layer whose hydraulic conductivity is neglected. In the horizontal limits of the aquifer, either constant head or no flow boundary conditions were considered, as indicated in Fig. 4.

CALIBRATION

In the period January 1987- July 1989, heads were measured monthly in observation wells distributed throughout the region that was modelled. At the same time, the pumping rate was measured in some cases and estimated by indirect means in others.

In addition, the piezometric head distribution corresponding to 1960, is available and there are estimates of the historical evolution of the pumping rates.

The hydraulic properties of the known part of the aquifer were obtained by means of pumping tests and also some pumping tests available from previous studies were interpreted. Transmissivity varies between $1x10^{-5}$ and $8x10^{-4} m^2 s^{-1}$. The calibration for layer I, started with these values and then were modified on the basis of the results of the calibration. The properties of layer II were adjusted until the behavior of the system was reproduced in a satisfactory manner.

In spite of the additional piezometric information that was available, the calibration was based on the period 1987 - 1989, which covers 30 months only. This was due to the better quality of the data for that period. Once the results of the calibration were obtained, the data of less quality that were available for the period 1960 - 1988, were used to verify it.

In the evaluation of the storage coefficients of the region modelled, 10 values that were determined by pumping tests were incorporated. The extension

of the confining clay layer was determined by means of the analysis of the prevailing geological conditions (inferred from well logs) and geophysical surveys. The values of the storage coefficients that were used for the cells that behave as confined, are between 2×10^{-4} and 7×10^{-3}. In the case of cells that perform as unconfined, values between 0.02 and 0.15, were used.

The initial runs, using the estimated values of S and T, led to the distribution of the piezometric heads shown in Fig. 5.

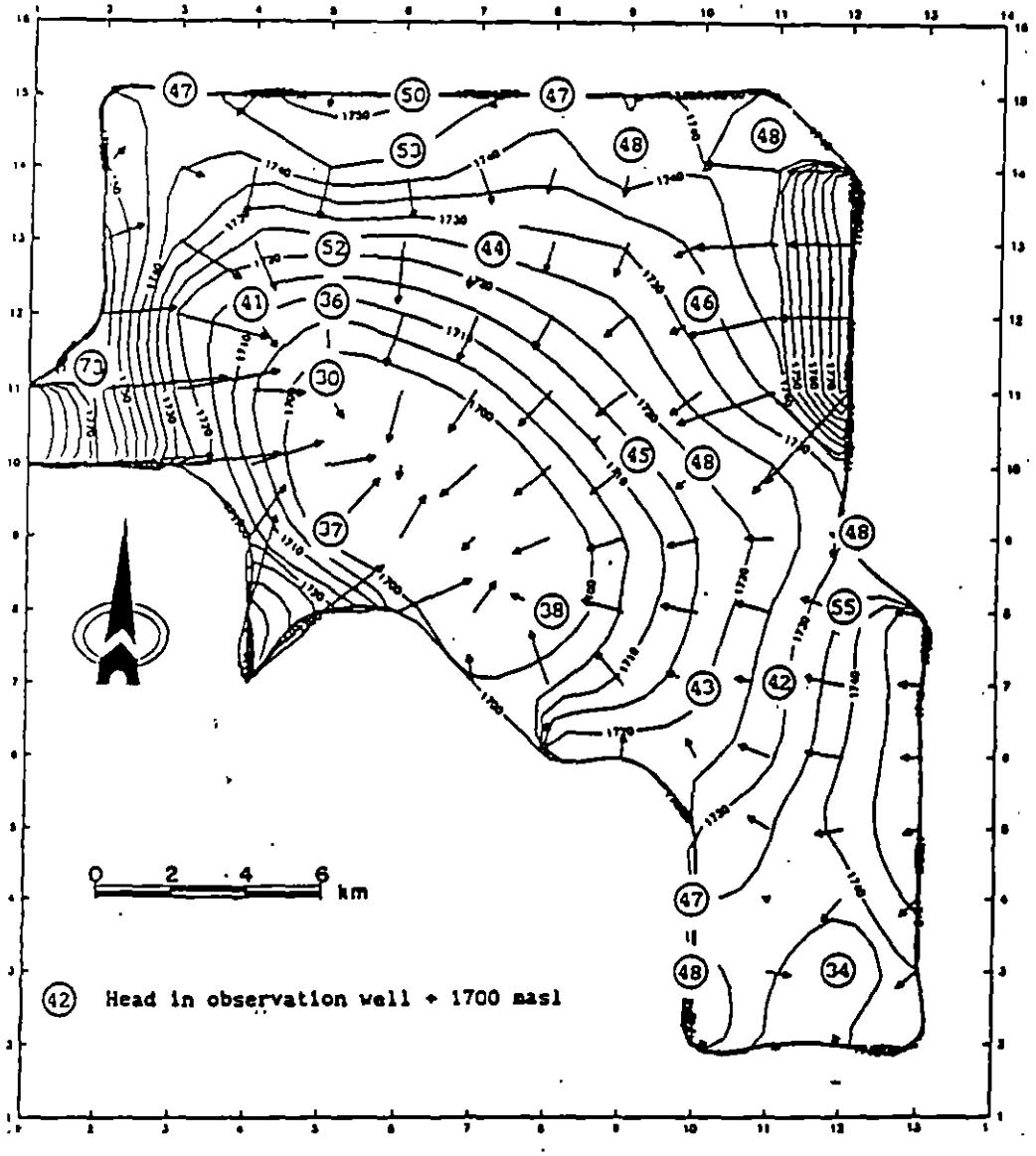


Figure 5: Contour map of predicted piezometric heads, without thermal sources

In this figure the predicted drawdowns deviate drastically from those observed, the greatest deviations occurring in the area where the thermal manifestations have been observed (Fig. 6).

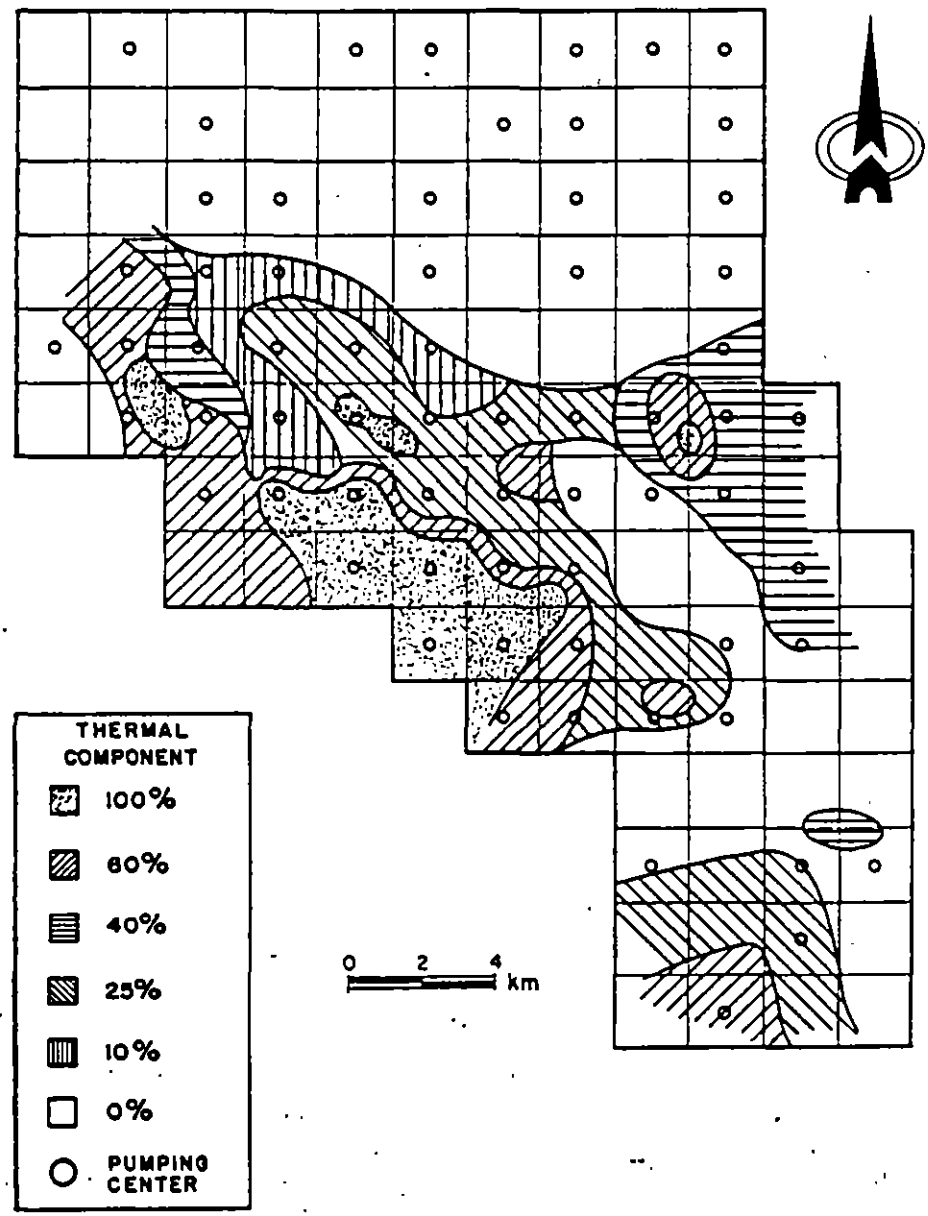


Figure 6: Location of thermal sources

The general conclusion drawn from these results, was that the observed behavior cannot be predicted satisfactorily using the observed values of S and T, when only horizontal flow is modelled. The yield of the actual system is much larger than the one obtained in such model.

The discrepancy between the observed and predicted heads, can be reduced in one of the following manners:

a.- Increasing the storage coefficient of the aquifer, considering it as unconfined in all the region modelled.
b.- Incorporating additional sources of water in the cells, where required.

The first option is unrealistic, since it contradicts geologic evidence directly supplied by well logs and must be discarded, in spite of the fact that it was used in a previous study: Niedzielsky, (1990).

On the other hand, the inclusion of additional sources in the model is fully justified by the hydrochemical and thermal evidences: Cardona (1990), Carrillo-Rivera (1992). They represent the vertical component of the regional system of flow that has been observed in the thermal area of the Valley of San Luis Potosi (Fig. 6). Therefore, this was the option that was adopted in the model. It was incorporated by means of an additional layer (layer II) whose properties were adjusted in the calibration of the model, assuming the piezometric head of that layer is constant.

Since the hydraulic properties of the main aquifer (layer I) are the best known, in the calibration, emphasis was placed in determining the properties of the thermal sources. A first guess of the values of the hydraulic conductivity in the vertical direction (Kz) between layers I and II, based on the temperatures and well discharges measured in the field, was used in the initial simulations, and then they were adjusted until the actual piezometric distributions in the thermal area were reproduced. The stopping criterion for the calibration process was that the actual heads should be predicted with an error of less than one meter in the thermal zone, as shown in Fig. 7.

Using the calibrated model, a global mass balance of the region was carried out. The results obtained are listed in Table 1.

Table 1: Mass Balance of the Aquifer

Concept	$Q(m^3s^{-1})$	%
Aquifer storage	0.34	13
Lateral recharge (cold water)	0.36	14
Upward supply (hot water)	1.90	73
Total well extraction	2.60	100

The distribution of the supply, shows clearly that the most important contribution comes from the vertical flow which originates in the regional system and exhibits thermal anomalies.

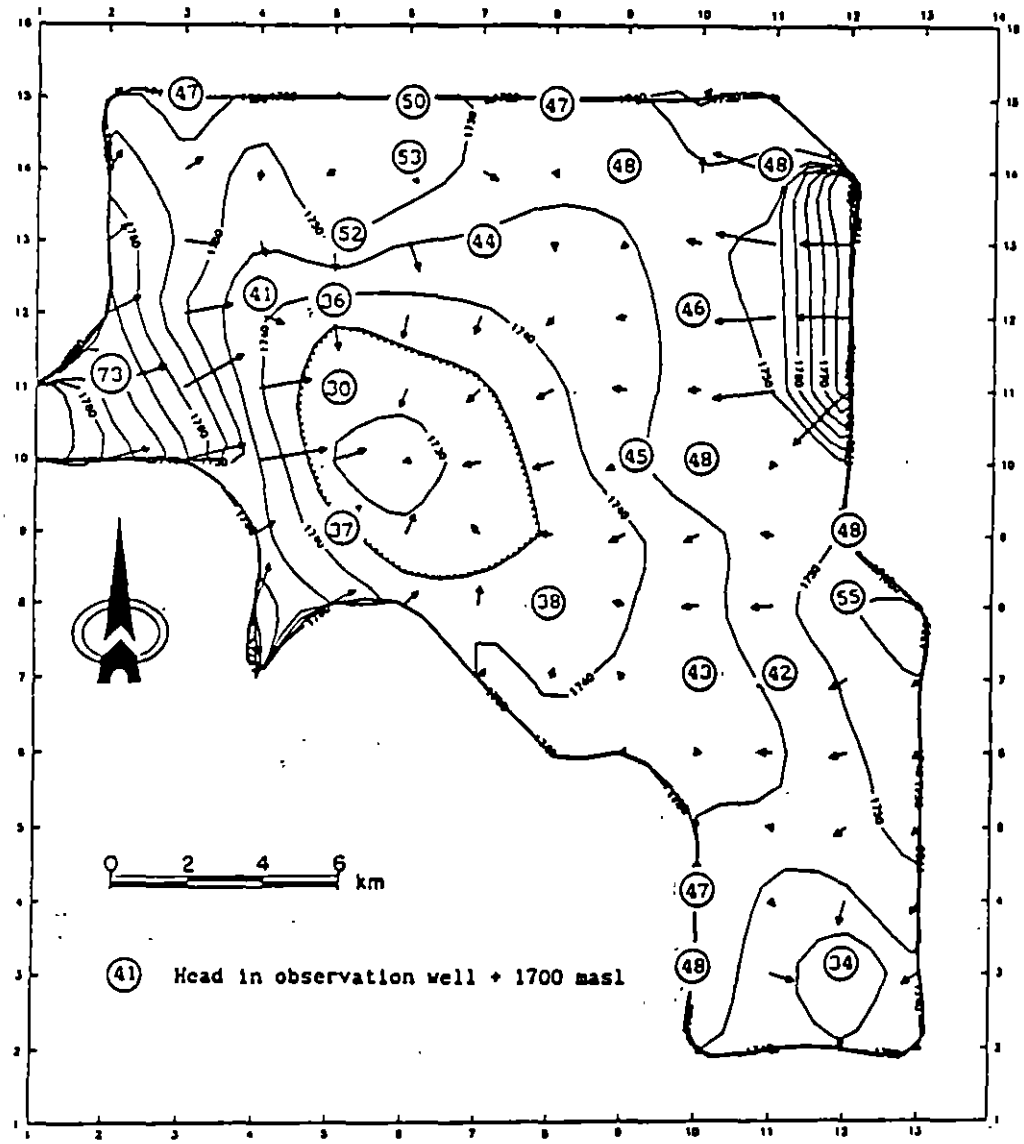


Figure 7: Contour map of predicted piezometric heads, after calibration

Long period verification

As was already mentioned, the information available for the period 1960 - 1988, was used to test the results of the calibration. Thus, after the calibration was completed, a run covering that period was carried out.

Taking the known initial conditions for 1960 and estimating the evolution of the rate of pumping in the period, the piezometric heads were predicted, using the calibrated model. The results of the simulation after 29 years, had differences of less than 3 meters between the observed and computed heads, in the thermal area. This indicates, specially taking into account the low quality of the information available for the period, that the parameters that were obtained in the calibration, are acceptable to make predictions of the behavior of the system, within a moderate range of accuracy.

TESTING DIFFERENT PUMPING POLICIES

The analysis of a wide range of exploitation policies of the system is necessary, to quantify the potential of the thermal sources, as a water supply for the city of San Luis Potosi.

Predictions of the behavior of the system for a period of 21 years (1989 - 2010), under different exploitation policies were carried out. The options considered were:

I.0- Keeping the present extraction rate fixed during the whole period.
I.1- Increasing the rate of extraction 5 % every 5 years.
I.2- Increasing the rate of extraction 10 % every 5 years.
I.3- Increasing the rate of extraction 20 % every 5 years.

II.1- Increasing the rate of extraction in the thermal area exclusively (13 cells) 5% every 5 years.
II.2- Increasing the rate of extraction in the thermal area exclusively (13 cells) 10% every 5 years.
II.3- Increasing the rate of extraction in the thermal area exclusively (13 cells) 20% every 5 years.
II.4- Increasing the rate of extraction in the thermal area exclusively (13 cells) 40% every 5 years.

In Table 2 the results obtained for the different policies that were tested are shown. For each policy the total volume extracted during the period of 21 years is given and then the percentages which originate in the thermal sources, the storage of the aquifer and the neighboring regions is indicated. Finally, in the last column the total volume of drawdown produced during the whole period in the modelled region, is given in millions of cubic meters. These results are also illustrated in graphical form, in Fig. 8. Clearly, to ensure a drawdown as low as possible, locating the additional demand in the thermal region is the best option.

Table 2: Predictions for the period 1989 - 2010 under different policies

Policy	Total Pumped Volume ($m^3 \times 10^6$)	Of Thermal Origin (%)	From Aquifer Storage (%)	From the Boundary (%)	Drawdown Volume ($m^3 \times 10^6$)
I.0	1698	81	3	16	3440
	When increments in pumping are uniformly distributed				
I.1	1915	81	5	14	6000
I.2	2153	76	7	17	8800
I.3	2702	77	11	12	16000
	When all increments of pumping are taken from thermal area				
II.1	1866	83	4	13	4800
II.2	2069	81	5	14	6400
II.3	2184	82	6	12	7600
II.4	2946	82	8	10	13600

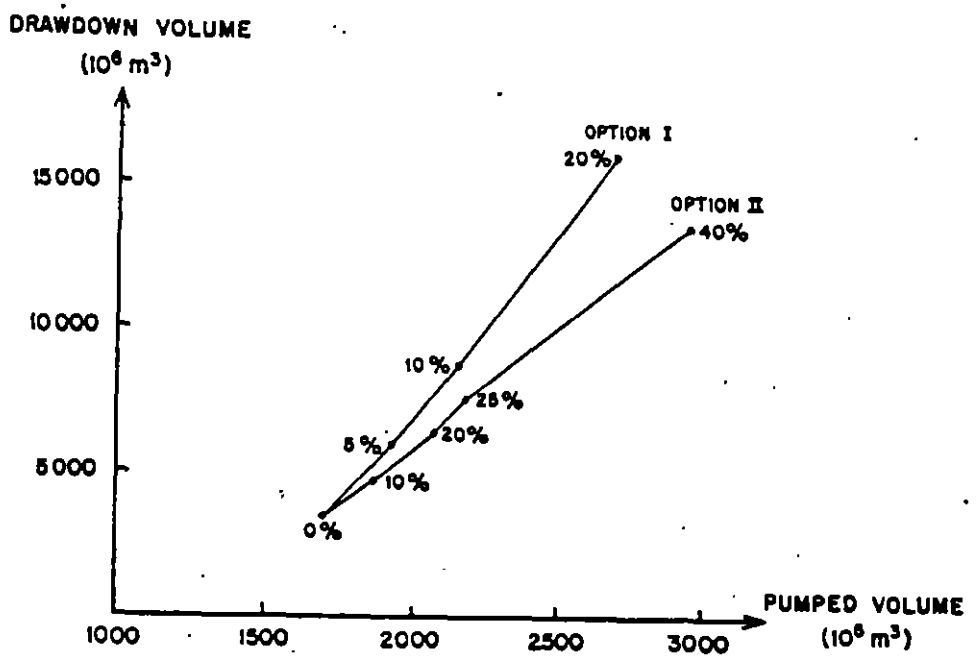


Figure 8: Comparison of simulated policies

CONCLUSIONS

A numerical model that takes into account the contribution of thermal sources was developed, and using it, different operation policies have been tested, for the aquifer of the City of San Luis Potosi.

Initially, it was intended to implement a model without thermal sources. However, it turned out to be impossible to achieve a model capable of predicting the observed behavior, when only horizontal flow was modelled. This pointed out the need of incorporating thermal sources in the model, in order to explain the vertical flux coming from deeper geological formations, whose hydraulic properties are unknown. This vertical supply was incorporated in the model, introducing a layer of constant hydraulic head in the lower aquifer.

Since the properties of such layer were unknown, it was necessary to derive them during the calibration process. The main parameter that was adjusted was the vertical hydraulic conductivity that exists between layers I and II. At the same time, the hydraulic properties, T and S, of the aquifer and the boundary conditions were also adjusted. The fact that an additional parameter was introduced in the calibration, made this process more complicated than is usual for this kind of applications. However, this form of proceeding is similar to what is usually done when applying modelling techniques in the horizontal plane, for which it is standard to eliminate neighboring regions with insufficient hydrological information by imposing suitable boundary conditions. In many cases, the supply coming from such regions is quite significant for the behavior of the part of the aquifer which is modelled.

The results of the calibration were satisfactorily verified by reproducing the observed behavior in a longer period (1960-1988) of exploitation of the aquifer, for which incomplete hydrometric information was available. The results of this study indicate that the procedure used here, to study a deep geological formation for which no information is available, may be useful more generally. In particular, in the case study here reported, in spite of the insufficient knowledge of the deep formation, it was possible to make recommendations for the policies to be followed in the production of the aquifer. These recommendations are better founded than if the lack of information about the thermal sources, had inhibited the development of such model.

The distribution of piezometric heads predicted on the assumption that the present rate of pumping is continued through the whole period, 1989 - 2010 (Fig. 9 option I.0) indicates that the present extraction can be continued without producing exceedingly large drawdowns.

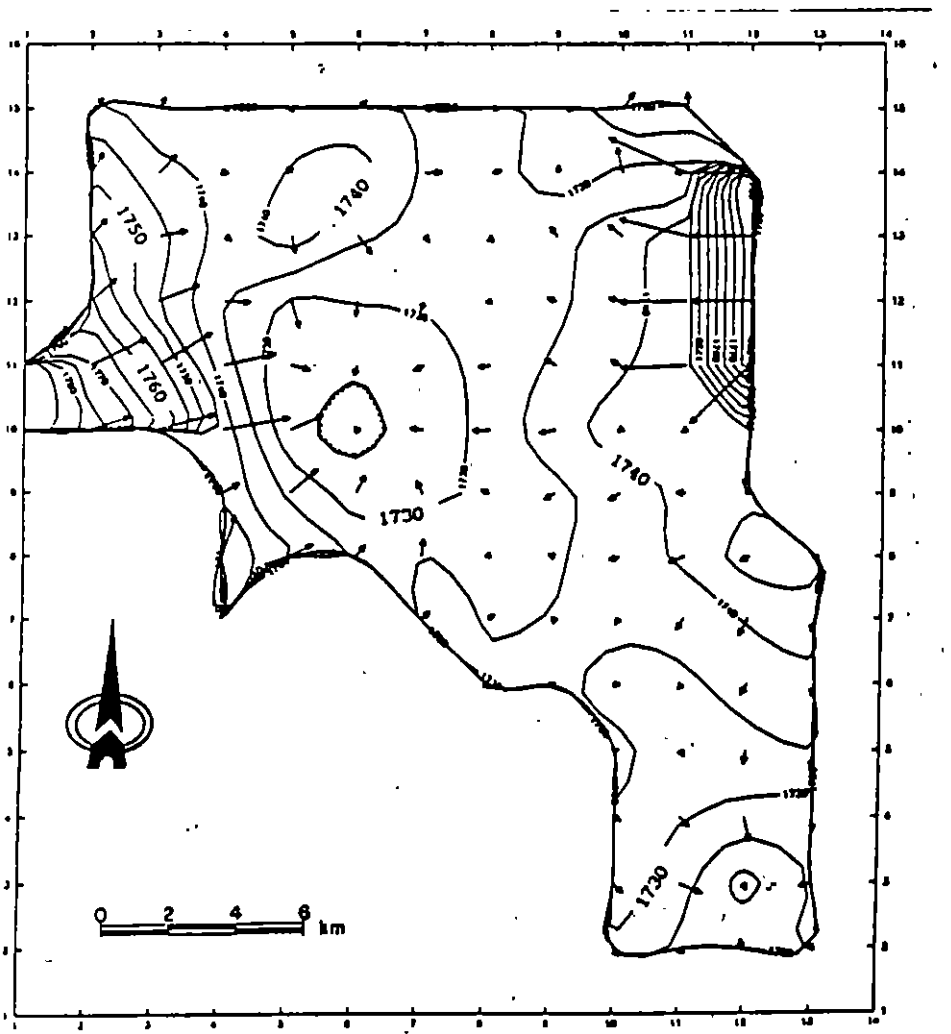


Figure 9: Contour map of predicted piezometric heads (1989 pumping rate)

Figure 8, clearly illustrates the fact that if the pumping rate is to be increased, the most convenient option from the point of view of keeping the drawdowns as small as possible, is to concentrate the demand in the thermal area. However, if such policy is adopted, the supply would contain a greater volume of thermal water, which would deteriorate its quality. Thus, in such case, it would be important to monitor the dissolved ions and the water temperature. If this is done, it should be recommended that the information gathered in this manner, be used to improve the numerical model and to test the assumptions on which it is based.

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FACULTAD DE INGENIERIA U.N.A.M.
DIVISION DE EDUCACION CONTINUA

CURSOS ABIERTOS

VI CURSO INTERNACIONAL DE CONTAMINACION DE ACUIFEROS

MODULO III: MODELOS EN GEOHIDROLOGIA Y CONTAMINACION DE ACUIFEROS

MODELOS MATEMATICOS Y COMPUTACION APLICADA A LA GEOHIDROLOGIA

ING. JUAN MANUEL LESSER ILLADES

GROUND WATER SOFTWARE

PART ONE

DATA BASES AND UTILITIES

USER'S MANUAL

United Nations
Department of Technical Co-operation for Development
Division of Natural Resources and Energy
Water Resources Branch

Version 1.0, December 1989

Software written by: Dr.J.Karanjac and Dr. D.Braticevic

Manual written by: Dr. J.Karanjac

Typesetting and Graphical Layout: Zorana Stanojkovic

November 1991

Updating notes

Since December 1990, many of the programmes have been corrected, and improved. The latest corrections were made in June 1991. The following are notes on features that have been added or changed in the programs after the manual was printed.

1. DOS Versions

The GW programs now work under DOS.3, DOS.4 and the new DOS.5. In the revised DEFCNF utility that can also be called by SETUP, you have to tell the program what DOS version you are using. If you were working with DOS3.X and upgraded your system to DOS.50 do not forget to run SETUP to tell the GW program that the DOS has been changed.

2. Set Up and Super VGA Drivers

You can set up the GW program in your computer by typing SETUP or as mentioned in the manual by typing DEFCNF. Two high resolution VGA drivers were added. You can use the 800 x 600 resolution only if your computer is equipped with a VGA card that is based on Tseng Laboratories chips, and if you have a super VGA color monitor. The higher resolution of 1024 x 756 may or may not work even if you have the right super VGA card and monitor. More details on these two new drivers appear on the screen during the setup procedure.

3. Text Editor

A text editor DAVE is included in the GW Software. It was written by Dr. Robert B.K. Dewar, a professor of Computer Science at New York University, who kindly allowed the UN to use the Text Editor in the GW software.

The DAVE Text Editor is very easy to use. Once you have correctly installed the GW Software in your computer, type DAVE [file name], and the first screen appears. To learn the Editor function, type ALT-H, and the help menu appears.

GW6 (well logs) program is set up to call the DAVE Editor automatically for preparing a new well log file or to edit an existing one. To save a file press ALT-F1. There is, however, one deficiency in this Text Editor. It does not allow lines longer than 80 characters. This may not be enough for all the comments that one may have in a well log. To overcome it, replace the DAVE editor by another editor which can work within the GW6 program such as Norton editor, QEDIT etc... Modify the file GW6.GEN in the GW directory and in the data directory accordingly. Another way to solve this problem is to use DAVE editor as it is and later edit

the file created by the GW6 program with another text editor/word processor, and add the additional comments. With DAVE Editor you can increase the comments line to 150 characters by typing DAVE/L [file name].

4. Sample Files

Sample data files are included with the GW Software. Data files for GW2, GW3, GW5, GW6 and GW11 are found in a subdirectory GWD. It is on diskette No.4 of the 5 1/4" 1.2MB diskettes, on diskette No.8 of the 5 1/4" 360MB diskettes and on diskette No.6 of the 3 1/2" 720MB diskettes.

The data files for GW2 - hydrochemistry is Vietnam and Nepal; the data file for GW3 - pumping test is named India, that for GW5 - hydrographs is Sample. You call the data files for GW6 - hydrographs by *.1th. The data files for GW11 - mapping appear on the screen automatically.

The data files for the modeling programs GW7, GW8, GW9 and GW10 are always in separated subdirectories GW7D, GW8D, GW9D and GW10D.

5. Monographic (Hercules) Users

In GW6 on the graphic screen for digitizing the cross section line with the mouse, the text message on how to use the mouse is garbled. Instead of the text you will see horizontal dotted lines in the upper part of the monitor. The garbled text is as follows:

TO DIGITIZE CROSS SECTION:
1. Move cursor to the first point,
2. Press left button,
3. Move cursor to the last point,
4. Press left button.

Esc=Exit

You can digitize the line on the screen. The dots will not appear in the printed cross section.

6. If your computer uses diskettes of another format than you received, and you do not have the means to copy the GW software to your format, please return the diskettes and indicate what format you need, and we will send it to you.

GROUND WATER SOFTWARE, PART ONE: DATA BASES AND GROUND WATER UTILITIES

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CHAPTER 7. GRAPHICS

INTRODUCTION

1. Acknowledgment

This series of ground water programs has been developed by the United Nations Department of Technical Co-operation for Development, Natural Resources and Energy Division, Water Resources Branch, New York. The programming is an outcome of a sub-contract within the UN/DTCD project in Bermuda, BER/86/001, "Advanced Modelling and Ground Water Software Development". The co-operation of the Bermuda Government is highly appreciated. Likewise, acknowledgment is extended to the UNDP office in Kingston, Jamaica, notably to former Resident Representative **Dr. Brenda McSwinney**, and to Mr. **Norman Thomas**, former Director of Public Works Department of the Government of Bermuda, for their interest and support of the project. A portion of the programming work was also supported by the UN/DTCD project in Nepal, NEP/86/025, "Shallow Ground Water Investigations in Terai". The authors of programs in this series are **Dr. Jasminko Karanjac**, UN/DTCD Consultant Hydrogeologist and Modelling Specialist in BER/86/001 and NEP/86/025, and **Dr. Dusan Braticevic**, who designed the system of windows and the user interface. **Dr. Braticevic** also programmed all graphical routines and displays.

The authors wish to acknowledge the role of **Mr. Uri Golani**, Special Technical Adviser in the Water Resources Branch, for masterminding the whole project, supporting and advising the authors, and providing useful hints for improving the whole package. Without his active involvement this Ground Water Series would not have been produced.

All inquiries concerning this Manual and/or software, including recommendations for corrections and improvements, may be directed to:

The Chief, Water Resources Branch
Natural Resources and Energy Division
Department of Technical Co-operation for Development
United Nations, New York, N.Y.10017
Cable: UNATIONS NEWYORK
Fax: 212-9638542

All inquiries with respect to technical matters, program deficiencies, suggestions for program improvements, and the like, should be addressed to **Dr. J.Karanjac**, J.Gagarina 185, 11070 Belgrade, Yugoslavia. Inquiries related to the distribution of program diskettes and user manuals should be directed to **Mr. Uri Golani**, One UN Plaza, room 764, New York, NY 10017, U.S.A.

2. Disclaimer

The United Nations Department of Technical Co-operation for Development assumes no responsibility and shall have no liability, consequential or otherwise, of any kind arising from the use of this program material.

The programmers have used their best knowledge and judgment in making the programs. Any suggestions for program improvement and/or correction shall be gratefully appreciated.

3. List of Programs

The Ground Water Software package (Part One: Data Base and Utilities) consists of the following programs:

GW1. Hydraulic Conductivity
GW2. Ground Water Chemistry
GW3. Pumping Tests
GW4. Well Hydraulics and Well Construction
GW5. Water Level Data Base and Hydrographs
GW6. Well Logs and Lithological Cross-sections
GW11. Graphics

The major features of each program are briefly described below.

GW1. Permeability Calculations and Conversions

This is a utility program consisting of the following components:

- Conversions
- Calculations from grain sizes using empirical formulas (Hazen, USBR, Slichter, Kozeny, Zamarin, Terzaghi)
- Average values in layered media (horizontal and vertical flow)
- Permeameter tests (constant head, falling head, no discharge)
- Pumping tests (steady state)
- Tables

GW2. Ground Water Chemistry

This is a data base program, with several retrieval (applications) options and a report printing capability. The following options are available:

- Select input for data base
- Input data
- Edit data
- Browse
- Delete
- Stiff diagram (screen display and printout)
- Piper diagram (screen display, printout, plot)
- Wilcox diagram (screen display, printout, plot)
- Reporting
- ASCII file for reporting

GW3. Pumping Tests

This is a data base program, with data analysis and presentation capabilities (screen graphics, printout). It is made up of the following components:

- Define units
- Data input and editing, etc.
- Test analysis (Jacob, Theis, Hantush, recovery, dug wells; screen graphics, printing, plotting)

GW4. Well Hydraulics and Well Construction

This is a utility program with the following major components:

- Define units
- Well functions (standard "Theis" well function, leaky well function, Bessel functions, error function)
- Pump tests (step drawdown test with second and nth power well loss, orifice weir, flowing well discharge, etc.)
- Well construction (recommended well diameter, optimum screen length, etc.)

GW5. Water Level Data Base and Hydrographs

This is a data base program which creates a water level data base, displays results on the screen, print or plots a hydrograph.. The user controls what is to be edited, input, displayed, or printed (depth to water versus absolute water level elevation, whole hydrograph or only a selected time interval, individual data connected by a line or left as scattered points, etc.).

The program has the following components:

- Define units
- Data input, editing, deleting, etc.
- Data analysis (display, print, plot)
- Working time interval
- Change depth for altitude and vice versa
- Select connecting interval in days, hours, minutes

GW6. Well Logs and Lithological Cross-sections

This is a data base program which is used to create a drilling data base; update and edit it; create, display, print or plot well construction and lithological log; display, print or plot lithological cross sections in any direction and length as selected by the user. The user inputs and edits data using his/her favorite word processor from inside the program. The program has about 30 built-in lithological symbols, but the user can create almost any additional symbol. This manual offers guidelines for creating additional symbols.

This program has the following components:

- Edit data
- Well log
- Select files
- New file
- Delete a file
- Cross sections (calculation, display, print, plot)
- Edit general data
- Produce a table with data summary
- Percentage of permeable versus impermeable layers

GW11. Graphics

This is a utility program which is used by GW6 (Lithology) to create maps with wells, boundaries, river roads, etc. It is made of the following components:

- Create or edit a coordinate system
- Display, print or plot a graphics content
- Add lines, points, text, and contours to the coordinate system
- Create contour lines

In this package, the contouring portion of the program cannot be used.

4. Program Files

To run this software package you must create a directory GW branching from the root directory (that is \GW). Each of the program modules is comprised of at least four files: one, with extension EXE, is executable file; three files are with extensions MST, CMN and WND.

The following files must be copied from distribution diskettes to the \GW directory on the hard disk.

GW.EXE
GWA1.EXE
GWB1.EXE
UN.MST
UN.CMN
UN.WND
DEFCNF.EXE
DVIRX120.EXE (driver for 9-pin printer),
DVILQ180.EXE (driver for 24-pin printer).
DVISCR.EXE
DVIHPGLF.EXE (driver for Hewlett-Packard compatible plotter)
CGA.DRV, EGA.DRV, VGA.DRV, ATT.DRV, WYSE.DRV, HGC.DRV
GW1.EXE, UN1.WND, UN1.CMN, UN1.MST
GW2.EXE, UN2.WND, UN2.CMN, UN2.MST
GW3.EXE, UN3.WND, UN3.CMN, UN3.MST
GW4.EXE, UN4.WND, UN4.CMN, UN4.MST
GW5.EXE, UN5.WND, UN5.CMN, UN5.MST
GW6.EXE, UN6.WND, UN6.CMN, UN6.MST, GW6.DLT, GW6CF.EXE, GW6.STM, DIGXSC.EXE
GW11.EXE, UN11.WND, UN11.CMN, UN11.MST
PLTCSY.EXE, PLTLIN.EXE, PLTPTS.EXE, PLTTXT.EXE, PLTCNT.EXE

The main program, GW.EXE, which ties all of the others together, requires the files GW.EXE, GWA1.EXE, and GWB1.EXE to run, plus the files UN.MST, UN.CMN, UN.WND to establish communications with the user. "MST" stands for "menu structure", "CMN" stands for "communication", "WND" stands for "windows".

In order to display graphics on the screen one of the screen graphics drivers (one of the files with a .DRV extension, such as CGA.DRV) must be present in the \GW directory. The screen driver executable file, DVISCR.EXE, program must also be present. If you wish to save space on your hard disk, you can remove all of the .DRV files from the GW directory except the one that you need for your computer.

Also, to print any of printouts one of the two printer drivers must be copied to the \GW directory: DVIRX120.EXE (for 9-pin EPSON-compatible printer), DVILQ180.EXE (for 24-pin EPSON-compatible printer). To plot graphics on a Hewlett-Packard compatible plotter, the executable file DVIHPGLF.EXE is

used. It plots directly to the plotter or creates an ASCII file. Such an ASCII file can be edited and/or used later on when a plotter becomes available.

Prior to running the program you must create a configuration file, CONFIG.CFG. You can create this file in either of two ways:

(1) Execute the file DEFCNF.EXE by typing DEFCNF, and provide answers to three prompts: (a) Screen driver, (b) Printer driver, (c) Color monitor [Y/N].

(2) Use a text processor or the DOS "COPY CON CONFIG.CFG" command, and create the file CONFIG.CFG. The first line of this file contains the name of the screen graphics driver you will use; the second line contains the name of the printer driver you will use; and the third line contains a Y or N, depending on whether your computer has a color monitor. The CONFIG.CFG file may look as follows:

```
EGA.DRV
DVILQ180.EXE
Y
```

CAUTION: If you attempt to run the program GW without first creating a CONFIG.CFG file in the GW directory, you will be prompted by the program to answer three questions and as a result a CONFIG.CFG file will be created, but the program will terminate abnormally and the computer will hang. You will have to reboot the system.

All files in the GW software package occupy about 3 MB of hard disk space. However, each of the six programs plus the seventh, graphics, can run independently. For that you need only four program-dependent files (GWx.EXE, UNx.MST, UNx.CMN, UNx.WND), plus DVISCR.EXE and one of screen drivers, one of printer drivers, and a plotter driver. Only the GW6 program (Well Logs and Lithology) needs also the files GW6.DLT and GW6.STM for the program to run correctly.

For more instructions on individual program modules check chapters 1 through 7 of this manual.

5. Hardware Requirements

The GW programs are written for personal computers running under the PC-DOS or MS-DOS operating system. This section describes the hardware requirements for running the programs.

Mathematical Co-processor. Although you can run any of the programs without a math co-processor, some of programs will run very slowly if the system is not equipped with a co-processor. For example, the pumping tests program (GW3) may take about one hour to process a pumping test with 99 test points (time-drawdown pairs) using the Hantush leaky method if a co-processor is not used. By comparison, the same test completes in several minutes with a co-processor. Likewise, the GW6 (Lithology) program involves extensive calculation in rasterizing drawings for screen display or printout. Writing the textual part of a graphics screen can also be very slow unless a co-processor is installed.

Mathematical co-processor is strongly recommended.

Memory Requirement. Some of programs require all available memory accessed by DOS Version 3 or 4. The executable files (those with extension of .EXE, such as GW1.EXE) are distributed in compressed form; the minimum memory required for running each program is normally equal to the actual size of its executable file. However, the screen driver demands an additional 140 KB of memory, and the printer driver about the same. Both drivers share the same memory space, and are never engaged at the same time. If you run this program through the GW shell, an additional 16 KB of memory is used in keeping the track of all modules.

With the exception of the GW1 and GW4 modules, which do not have presently graphics routines, the programs are very memory-intensive. It is almost mandatory that these programs run from a computer equipped with 640 KB of RAM (random access memory).

The following instructions should normally be observed:

(a) Run the program GW in a computer with at least 640 KB memory.

(b) Remove all memory-resident programs.

(c) Modify your CONFIG.SYS file and reduce Buffers and Files to a small number. The maximum number of open files (by DOS and the program) is 10 (for the GW6 program). Buffers could be 5. Remember that each file and buffer uses about 500 bytes. The "shortage" of several kilobytes of memory may be critical in running the GW6 program.

WARNING. Memory problems may appear in GW6 program. If printout fails or appears incomplete, you have a memory problem! GW6 will not run on a computer equipped with less than 640 KB RAM.

Hard disk. Although all programs except GW6 can be run from a floppy disk, it is highly recommended that all programs be installed on a hard disk. Some of programs write some scratch files to disk, and erase them later. The capacity of a floppy (except high density 3.5-in 1.4 MB drive, or 5.25-in 1.2 MB drive) may not be sufficient to hold this additional information. One megabyte free space on hard disk is normally sufficient to hold scratch and output files.

Mouse. The programs GW2, GW3, GW5, GW6, and GW11 have graphics routines which may be enhanced by using the mouse. The programs have been tested with a Microsoft Mouse, a Logitech Mouse, and a Genius Mouse. The mouse is very useful in zooming the Piper trilinear diagram (GW2), and in zooming the lithological log and/or cross section in GW6. Its primary importance is in selecting a lithological cross section line directly from the map of wells in GW6. However, all program can run without the mouse, so its use is optional, although strongly recommended.

Video Display Adapter. The following video adapters are supported by the programs: color graphics adapter (CGA), color enhanced graphics adapter (EGA), Hercules, a special SGA for AT&T 6300 or Olivetti computers, VGA, the high-resolution WYSE adapter. To run the programs with a Hercules graphics adapter you must have the command "HGC full" in your AUTOEXEC.BAT file, or you should execute that command prior to running the GW software. Note: the WYSE driver is not completely correct in the mixed alpha-numeric and graphics mode. Also, the CGA display card on a color monitor will produce black and white graphs. This is explained by the fact that to have the resolution of 620x200 CGA mode 1 is used which is two-color mode, that is black and white.

The programs will run without video display adapters, but you will not be able to see any graphics display on the screen. Nevertheless, you will be able to process most of the information and print it (pumping tests, hydrographs, etc.). Each program first looks for a file CONFIG.CFG in the \GW directory. This is the file which contains the information on the type of video adapter you have selected to work with.

Printer. Programs GW2, GW3, GW5, GW6, GW11 can direct their output to a printer. 9-pin and 24-pin EPSON-compatible printers are supported. With some other printers it was noted that there was double line spacing due to the printer and program both issuing a carriage return and line feed. If you have a printer which is not EPSON-compatible, try to eliminate printer-generated line feed if possible by setting a switch on your printer.

Plotter. Each graph can be either displayed, printed or plotted. Only the Hewlett-Packard plotters using the HPGL (Hewlett-Packard Graphical Language) or emulating it, are supported. The output is directed to COM1 serial port, which should be configured with DOS command MODE as follows:

```
MODE COM1:9600,N,8,1
```

If you sometime experience dropouts in data, you might reduce the baud rate (instead of 9600 try 2400) and try sending the data again. You may also try the mode command as

```
MODE COM1:9600,N,7,1
```

6. Software Requirements

DOS 2.11 or higher is required. In your CONFIG.SYS file there must be a line "DEVICE=ANSI.SYS". The device (file) affects cursor movement, erases specific areas of the screen and sets the graphics mode.

If there is a CONFIG.SYS file on your disk or diskette, which is read during booting the system, you must modify it by adding the above line "DEVICE=ANSI.SYS", provided your ANSI.SYS file is in root directory. If it is in a subdirectory, for example the DOS subdirectory, modify the line by establishing the path, such as:

DEVICE=\DOS\ANSI.SYS

If CONFIG.SYS does not exist on your disk, create a new one. The modification and/or creation can be done using the COPY CON routine in the following way (COPY CON is a standard DOS routine which is used to create small files by typing lines directly from the keyboard):

a) First check whether you have the file CONFIG.SYS on your DOS disk directory by typing DIR. If CONFIG.SYS does exist, view its contents by typing TYPE CONFIG.SYS (and RETURN). Write down the contents of the CONFIG.SYS file or memorize its contents. Use the DOS routine COPY CON to rewrite the CONFIG.SYS file by typing:

COPY CON CONFIG.SYS (RETURN)

Retype all existing lines in your CONFIG.SYS file and add the following:

DEVICE=ANSI.SYS

followed by RETURN. You will terminate this file by typing either Ctrl Z (which means End-of-File) or by pressing F6 (which means the same), followed by RETURN.

b) If the CONFIG.SYS file does not exist, create one by typing:
COPY CON CONFIG.SYS (RETURN)

and enter only one line of text: **DEVICE=ANSI.SYS**, followed by RETURN, F6 and RETURN. At the end, your CONFIG.SYS file will most probably look like this:

FILES=10
BUFFERS=10
DEVICE=ANSI.SYS
DEVICE=MOUSE.SYS

or simply **DEVICE=ANSI.SYS**

You can view the contents of the file by typing **TYPE CONFIG.SYS**.

As mentioned earlier, the GW software needs the "configuration" file, CONFIG.CFG, to identify the video adapter, type of printer, and whether you are using a color or monochrome monitor.

Add the subdirectory \GW to the DOS PATH command in your AUTOEXEC.BAT file. This line may read as follows:

PATH=C:\;C:\DOS;C:\UTIL;C:\GW;C:\NORTON

7. Units

Most of the programs offer you a choice of units for distance, time, pumping rates, and transmissivity. When you select a unit, you are expected to use the same unit throughout the program, unless directly instructed by the program to differently. Each of categories of units has a provision for user-defined units. This makes the program more flexible. However, you will be prompted for two additional parameters, should you decide to use your own units: (1) unit notation, (2) scaling factor, which is the conversion from your unit to the program's built-in default units, which are metric.

The program has several built-in units for each category. For example, the distance can be input as meters and/or feet. Any other choice requires a conversion. If you select inches as the basic input unit, you must provide the scaling factor of 0.0254, which is the number of meters per inch. The conversions from some other popular units are given here below.

Transmissivity:	1 feet^2/day	= 0.0931098 m^2/day
	1 m^2/sec	= 86400 m^2/day
Pumping rate:	1 l/sec	= 86.4 m^3/day
	1 m^3/hr	= 24 m^3/day
	1 f^3/sec	= 2446.78 m^3/day
	1 cm^3/sec	= 0.0864 m^3/day

The program built-in units are the following:

distance:	m, feet
time:	day, hr, min
pumping capacity:	m^3/day, gpm
transmissivity:	m^2/day, gpd/ft

8. General Hints

(a) First of all back up programs. This is to say that before you install the programs, make back-up copies of all the programs on the distribution diskettes.

(b) Back up data files. It is highly recommended that you keep a back-up copy of your data files. Data bases for programs such as GW2, GW3, GW5, and GW6 especially need to be backed up.

(c) All programs have a full-screen user interface. Normally, the bottom two lines are reserved for messages and instructions to you. All programs are designed to be user-friendly; that is there is enough instruction on the screen to guide you without too much need for a manual. Likewise, most of the programs are transparent to you; that is, you are informed what the program is doing at any given moment. In all but the GW1 program, there is a list of options on the right side of the screen. Each option is activated by pressing a single key. The program branches to a subroutine depending on the key you press.

(d) Restore control with ALT -F10 key sequence. If, while you are running any of the programs, the screen appears corrupted, or some messages are printed at the very bottom of the screen below the message line, simultaneously press the ALT and F10 keys. In most cases the screen will return to the correct form. This works only when the program is waiting for your input. If the program is running and computation is in progress, you will have to wait until it stops.

(e) Use the ESC key to back up. The ESC key is normally used to back one step, or to clear the current window and return to the previous window. The CTRL-F3 key sequence normally deletes all characters after the cursor (to the end of field). The Page Up and Page Down keys are used in the normal way, the same as Home and End. In some programs Ctrl Home moves the cursor to the first line in the data file, and Ctrl End moves the cursor to the bottom line.

(f) You may delete any files in your subdirectories which have the form FORTx, where x is any number. You may view the contents of these files, since they are ASCII files, but the contents will be meaningless to you. (These files are generated by a routine which programmers used to follow the performance of programs, but which has not yet been removed from the code.) The same applies to files GRAF.AGR, which is a graphics scratch file, and some other scratch files.

(g) If, after starting a program, you see some characters at the screen bottom, such as [2J or any combination of letters and numbers with [, you must have forgotten to add the line DEVICE=ANSI.SYS into your CONFIG.SYS file. Or, the file ANSI.SYS was not properly located. If it resides in the DOS subdirectory, the command should be DEVICE=\DOS\ANSI.SYS.

(h) All ASCII (or DOS) files can be viewed with the routine SHOW, the use of which was made possible by kind permission of Summit Information System Inc.

(i) It is advisable to have a memory mapping utility (file) installed on your computer to tell you how much memory is available for user programs. This is especially important when running the GW6 program, which requires almost 590 KB of memory when used with a screen and/or a printer driver. One such utility is MAPMEM ("map memory") by TurboPower Software.

(j) You must create the directory GW directly from the root directory. If this is done on the hard disk partition which is in the same time the boot drive, there is already COMMAND.COM file in the root directory. However, if you decide to install the software in D:\GW directory, and D drive is not the boot drive, you must copy COMMAND.COM into the root directory of the D drive.

(k) It is recommended that you keep your data files and/or examples separate from the \GW directory. For example, if you are working with a lithological data base for a district called "DISTRICT", you are advised to create a subdirectory DISTRICT, create your data files in or copy them into that directory. Before running the GW6 program, log in to the directory DISTRICT (you must also have the GW6.GEN file in that directory; see Chapter 6), and type GW or GW6.

(l) Check for Non-ASCII characters in data files. The final hint is probably the most important. In some programs you may use your favorite text editor to create ASCII files, which are than input into the program. For example, this is an option in GW3 (pumping tests), GW5 (hydrographs), and GW6 (lithology). However, some text editors, such as WordStar, do not automatically produce an ASCII file, whether you use a Nondocument or Document option. You may notice some strange characters (above ASCII code 128), which you must remove by editing the file or by converting the file to an ASCII file. To check whether such characters are present, use the utility SHOW supplied with this package. The command is "SHOW filename". In the case of WordStar, you must print the file, selecting for the printer ASCII, and renaming the WordStar-created ASCII.WS file to something that is meaningful to you. For further explanation see Chapter 6, Section 6.5.1.

Report Problems to Authors

The programmers attempted to provide you with the full control over program termination. Ideally the program should always warn or inform you that something went wrong. Much less ideal is when the computer hangs and you have to reset it. This may happen in some instances which the programmers were not aware of. Any such case should be brought to our attention either directly, or via UN/DTCD, Water Resources Branch, New York.

The most problems were experienced in the pumping test program, GW3. The Hantush, and sometimes the Theis method will cause the program to abort. This will happen in rare occasions when there is either underflow or overflow (too large or too small exponent, negative logarithm, etc.). You are advised to check pumping test raw data and eliminate suspicious data, such as fluctuations of level, or zero decline of level near the end of test. Chances are that even such a test will provide useful results using the Theis and/or Hantush method.

9. Graphics Routines

The following graphics routines are available in this version of the Ground Water Software package:

GW2. Chemistry	Piper and Wilcox diagrams
GW3. Pumping Tests	Screen display of raw data; data fitting with Jacob, Theis, Hantush, recovery methods, Rushton & Singh dug well matching method
GW5. Hydrographs	Water level graphs
GW6. Lithology	Well log, map of wells, lithological cross sections
GW11.Graphics	Coordinate system, superimposed boundaries, rivers, roads and other lines; points such as wells; text; contours (not used in this package).

Each of the graphics screens allows the zooming a detail using a mouse. Zooming can be repeated sever times.

10. Summary

To use this Ground Water Software package to its greatest potential you need an MS-DOS compatible computer with 640 KBytes of memory, a fixed disk with at least 10 megabytes of storage capacity, a high-resolution monitor (monochrome or color), a video display adapter card, and a mouse.

The following table shows the memory requirements for individual program modules. In order to conserve disk space, each EXE file is distributed in a compressed form. However the minimum memory requirement is controlled by its normal or uncompressed size.

	Memory in KB Actual	Compres.	Co-processor	Disk	Video
GW1	235	152	Not required	Floppy/hard	Not required
GW2	292	208	Recommended	Floppy/hard	Recommended
GW3	427	314	Recommended	Hard rec'd	Highly rec'd
GW4	298	222	Not required	Floppy/hard	Not required
GW5	400	281	Highly rec'd	Hard rec'd	Highly rec'd
GW6	447	227	Highly rec'd	Hard mand.	Highly rec'd
GW11	230	156	Highly rec'd	Hard rec'd	Highly rec'd

Abbreviations: "Compres" – compressed, "rec'd" – recommended
"req'd" – required, "mand." – mandatory

11. Future Improvements

The improvements will be in two directions: (a) hardware/software, (b) program universality and additional routines.

In the first group come various additional screen drivers (notably super VGA); printer drivers (notably a laser driver); plus various fonts to make printout more attractive and usable. More plotter drivers could be included.

The chemical program, GW2, may have more retrieval routines, such as bar diagrams plotted directly onto the map; the data base may include coordinates, land surface elevations, and some other well construction parameters, which will make contouring of random data possible; and a contouring routine (gridding from random data) may be added.

The pumping test may include corrections for partial penetration, improved handling of Hantush and/or Theis method in the case of unexpected input. Programs could also detect the presence of a recharge or impermeable boundary during pumping test, etc. Especially in pumping test program, GW3, improvements are needed.

The well hydraulics and construction program, GW4, may add the design of gravel pack on the basis of aquifer grain-size analysis. Cost of pumping and energy requirements could make the program more versatile. The step-drawdown test should be visible on the screen.

The hydrographs program, GW5, needs a better control over printout, such as title of drawing in different fonts and sizes, format larger than A4, etc.

Well logs could be made user-defined as far as their content is concerned. Likewise, lithological symbols could be edited on the screen.

Plotter output, which was added at the last moment, is not yet fully tested. You are advised to read additional comments on the plotter use. These will be found at the end of this Introduction.

12. Running the GW Program

To start this software, you should log to a directory in which you keep your data files (GW2, GW3, GW5, GW6). For GW1 and GW4, which are the utility programs, it is not important in which directory you may be. You may log to the \GW directory as well.

Type GW. After few seconds the screen as shown in Fig. A will be displayed. This is the program's Main Logo, with the software package title, United Nations, and authors.

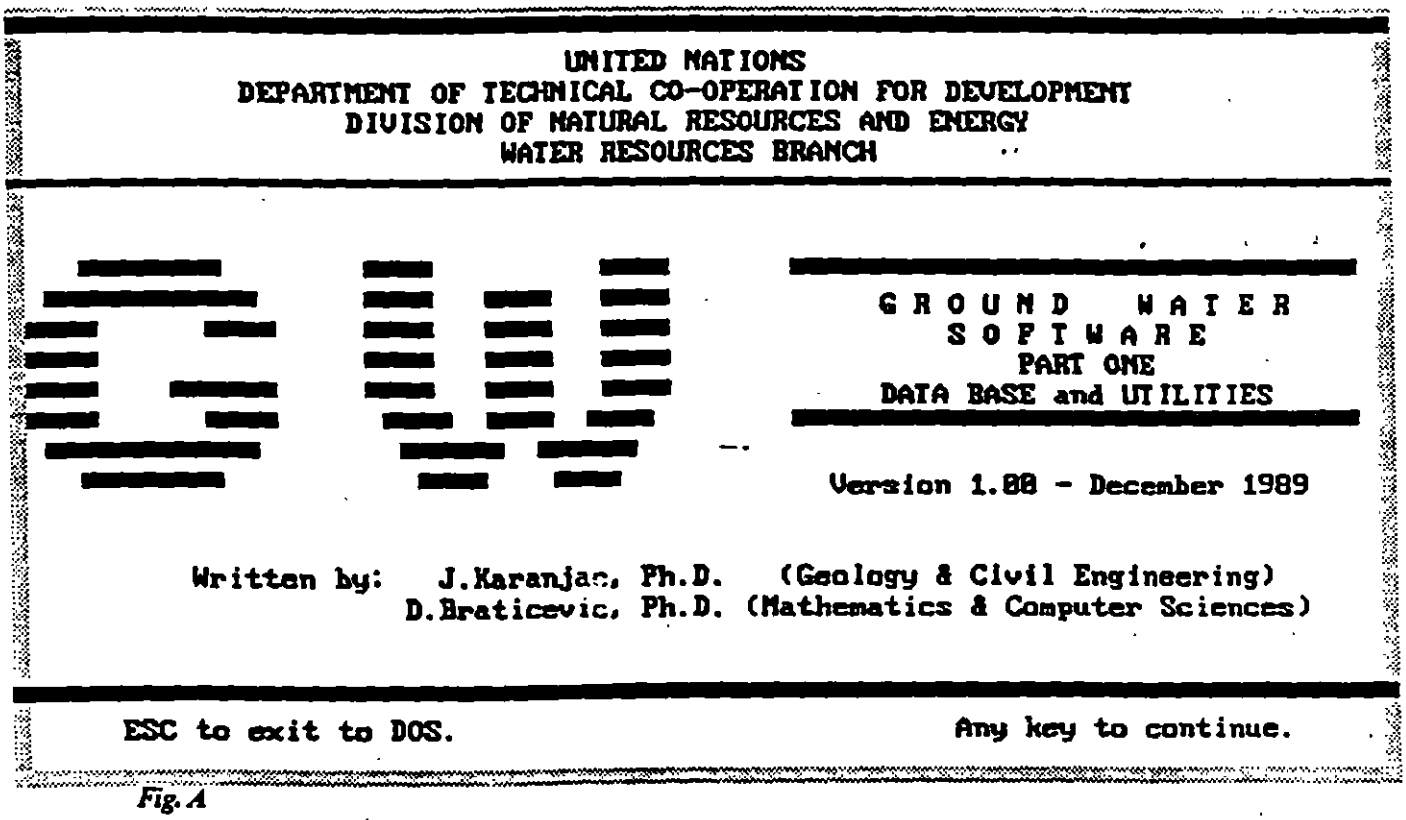

Fig. A

Press any key to see the second screen, Fig. B, which is the copyright notice and instructions on whom to contact if you have problems or need assistance with the software.

Press any key. The program comes to the Main Program Selection Menu, Fig. C. From here the program branches to one of 6 working modules or the graphics utility.

```
                    COPYRIGHT NOTICE

  These ground water programs were prepared by the Water Resources Branch,
Division of Natural Resources and Energy, Department of Technical Co-opera-
tion for Development, United Nations, New York. The programs were developed
under the UNDP's and Government of Bermuda project "Advanced Mathematical
Modelling and Software Development" (BER/86/001), and were tested and
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assumes no responsibility and shall have no liability, consequential or
otherwise, of any kind arising from the use of this program material.

NOTES. (1) All correspondence related to technical program matters should be
           addressed to J.Karanjac,J.Cagarina 185,11070 Belgrade,Yugoslavia.
       (2) Correspondence related to program diskettes and User's Manual
           distribution should be addressed to Uri Goiani, Special Technical
           Advisor, UN, DTCD, One UN Plaza, room 764, New York, NY 10017.

Press any key to continue.                                  ESC to quit.
```

Fig. B

```
UN/DTCD -- GROUND WATER SOFTWARE                          Version 1.00
PROGRAM SELECTION                                      December 1989

  1. Hydraulic Conductivity                  FUNCTIONS :
  2. Ground Water Chemistry
  3. Pumping Tests                           X=Exit to DOS
  4. Well Hydraulics & Construction
  5. Hydrographs
  6. Lithology
 11. Graphics

Use cursor keys and [Enter] to select program module.
```

Fig. C

13. Additional Comments

The plotter output is not yet fully tested. Almost every graphics screen can be either directly plotted to the COM1 (serial) port, or an ASCII plot file can be created for later editing. The following should be observed:

. Use A3 (ISO) or B (ANSI) format of paper. (Some programs may be plotted to A4 or A format) but you must edit the ASCILplt file by adding the HPGL command RO90 after the initial two HPGL commands, IN;DF;.)

. Modify, if you wish, the pen selection numbers. When viewing the ASCILplt file you will notice the HPGL command SP 1, SP 2, or like. This is interpreted by the plotter as Select Pen.

. Well logs can be plotted only in the default size, that is the A4 format (21 cm horizontal by 29 cm vertical; or 8.5 by 11 inch).

. Only graphical characters will be plotted. Thus, some lettering that may appear on the screen, will not be plotted if the characters are from the ASCII alphanumeric set.

. You will have to press the key R every time the plotter changes the pen. There will be a message displayed:

Write fault error writing device COM1
Abort, Retry, Ignore, Fail?

Answer with R and wait until another halt. This will be fixed in the second release.

For your reference, the HPGL standard commands most often used in this program package are:
IN .. a command to initialize plotter
DF .. a command to return the plotter to a predefined (default) state
PA .. sets absolute plotting
PU .. raises the pen
PD .. lowers the pen
RO90 .. rotates the coordinate system 90 degrees.

Permeability Calculations and Conversions

1.1. General

This is primarily a utility program for calculating permeability values (hydraulic conductivity) from grain-size analysis (grain-size distribution curves) and for converting permeability values from one system of units to another, etc.

Since there are no graphics routines in this program, a video adapter is not required. A mathematical co-processor is not required. To run this program, you must have copied the following files to the \GW directory: GW1.EXE, UN1.CMN, UN1.MST, UN1.WND. You may log to any subdirectory, provided you have a path to the GW directory in your AUTOEXEC.BAT file (see the Introduction). Alternatively, you may run this program by typing GW1 and RETURN. The total disk space occupied by the four required files is 247,884 bytes. The memory requirement for the GW1.EXE program is 235 KB; the program comes in a compressed version occupying 155,476 bytes.

1.2. Program Overview

The GW1 program consists of 6 parts (see Fig. 1.1):

- Conversions
- Calculation from grain sizes
- Average values in layered media
- Permeameter tests
- Permeability from pumping tests
- Tables

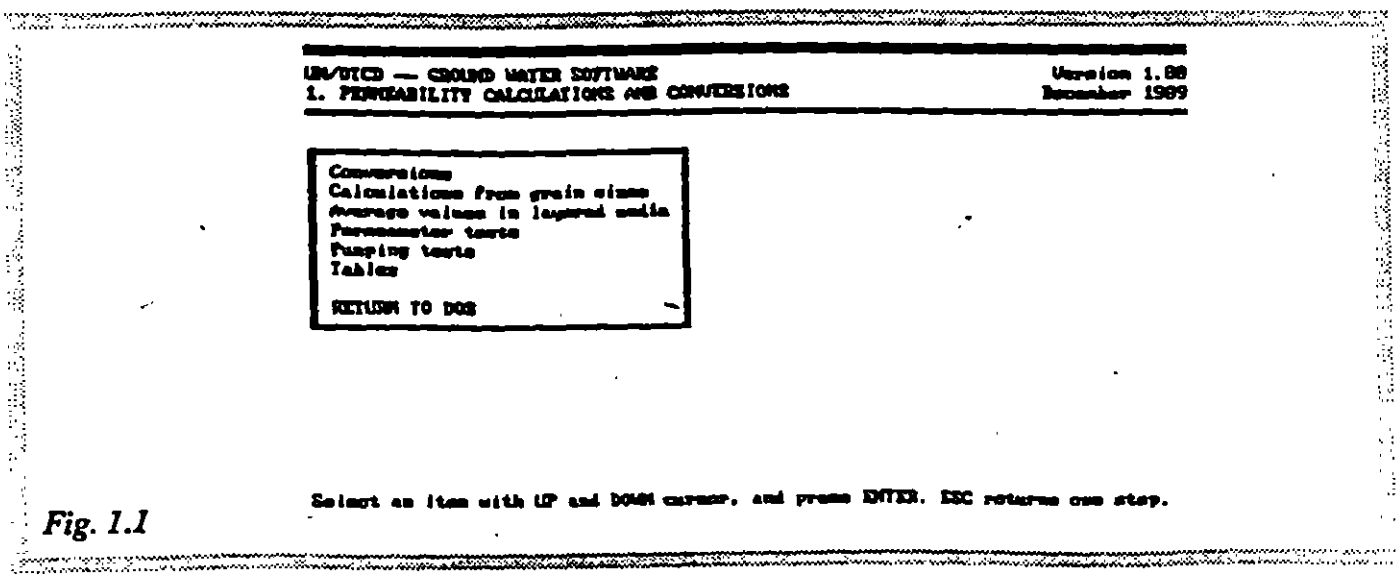


Fig. 1.1

1.3. Conversions

The first part converts permeability values (hydraulic conductivity) from one system of units to another system. The options are: US gpd/ft^2, Imp gpd/ft^2, m/day, cm/s. Press ESC to terminate this part of the program. Place the cursor on the top line (Conversions) and press RETURN (ENTER). The window titled FROM appears offering the choice of units to convert from. Select a unit using cursor up and down keys. Press RETURN. The right part of the window titled TO, as shown in Fig.1.2, is displayed offering you the choice of units to convert to. Select a unit and press RETURN. The cursor shall come to Input data. Type a value and you will see the converted result. In this example, 1000 US gpd/ft^2 is equal to 40.74140 m/day.

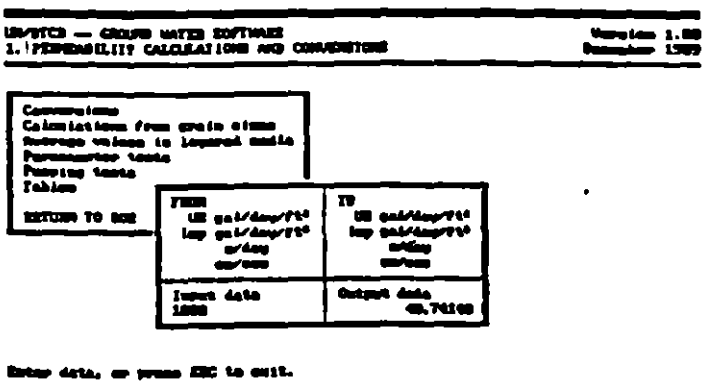


Fig. 1.2

1.4. Calculation From Grain Size

The second part calculates the permeability coefficient (hydraulic conductivity) using one of six available empiric formulas:

HAZEN	ZAMARIN
CREAGER, JUSTIN, HINDS (U.S.B.R. formula)	KOZENY
SLICHTER	TERZAGHI

Each calculation requires some or all of the following input parameters: (a) effective grain diameter (d_{10} or d_{20}), or the total grain-size distribution; (b) temperature of water in aquifer formation (due to viscosity dependence on temperature); (c) empirical coefficient which distinguishes between smooth and clean sand on one side and angular and clayey sand on the other side; (d) total porosity of sand. When in doubt as to what to accept for formation water temperature, type 10. (The corrections are probably not important; the empirical formulas produce only a correct order of magnitude considering the way in which formation samples are usually collected.)

You run this portion of the program by moving the cursor one line down to Calculations from grain size and pressing RETURN. You will be given 6 options. Select one with cursor keys (up/down) and press RETURN.

The HAZEN formula applies to sands and gravels with effective grain diameter between 0.1 and 3.0 mm and uniformity coefficient d_{60}/d_{10} less than 5. To select the empirical coefficient which takes care of grain uniformity, sorting, and cleanness, have in mind that typical values are as follows:

0.4 – 0.8 for clayey and nonuniform sand

0.8 – 1.2 for clean and uniform sand

The more uniform sand, the higher the coefficient. An example is shown in Fig. 1.3.

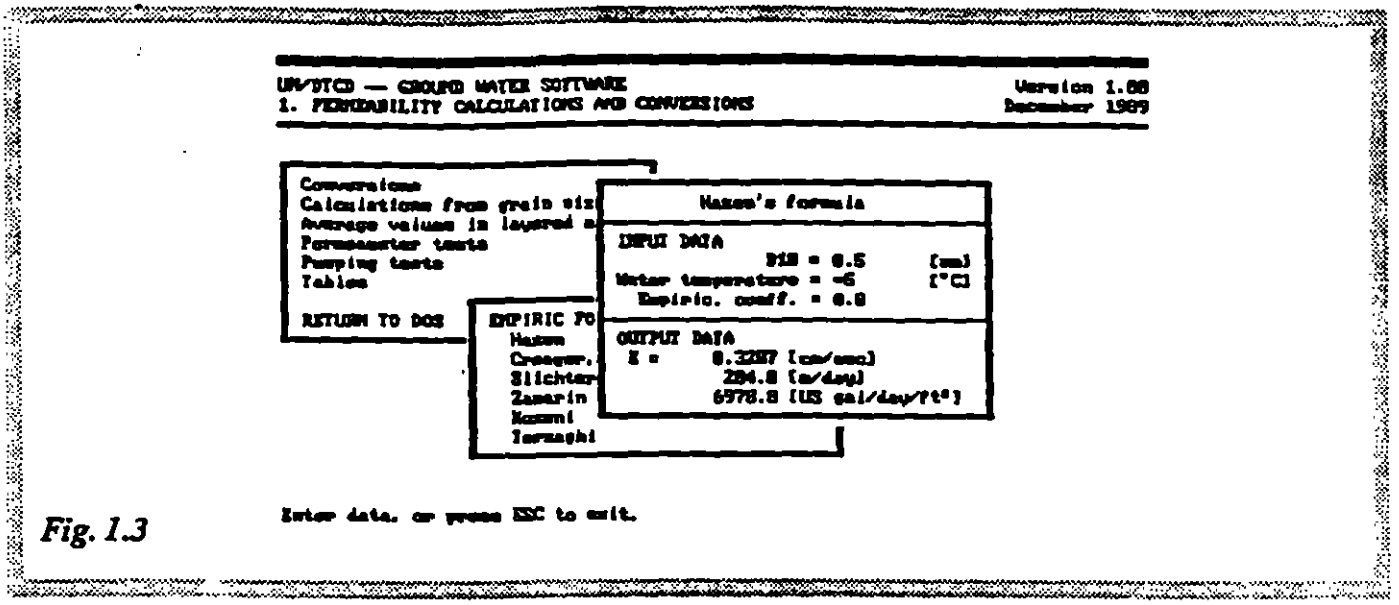


Fig. 1.3

The **U.S.B.R. formula** (due to Creager, Justin and Hinds) requires the d_{20} as the effective grain diameter (in mm), without any corrections (temperature, empiric. coefficient).

The **Slichter formula** applies to sands and gravels with effective grain diameter between 0.1 and 3.0 mm and uniformity coefficient d_{60}/d_{10} less than 5. The formula requires the knowledge of total sand porosity, and there is also a correction for formation water temperature. With the Slichter formula, the porosity (total) must be typed as a fraction of 1.0, temperature in °C, and d_{10} in mm (screen diameter of 10% of the total sample retained on the screen).

The **Zamarin formula** requires the input of the whole grain-size curve in the following ranges:

less than 0.01 mm	(288.60)	0.50–1.00 mm	(1.38)
0.01–0.05 mm	(40.25)	1.00–2.00 mm	(0.69)
0.05–0.10 mm	(13.80)	2.00–3.00 mm	(0.27)
0.10–0.15 mm	(8.05)	3.00–5.00 mm	(0.25)
0.15–0.25 mm	(6.07)	5.00–7.00 mm	(0.17)
0.25–0.50 mm	(2.76)	7.00–10.0 mm	(0.11)

Each fraction of sample analysis (typed as, e.g., 0.12 if 12% of the whole sample falls within the interval) is multiplied by a corresponding weighting factor which assigns a greater importance to finer than to coarser fractions. These factors are shown in the above table in brackets. The effective diameter is obtained as one over the sum of the products of weighting factors and fractions of each interval. The temperature correction is also introduced in the same way as in the Slichter formula.

The **Kozeny formula** requires the following input: total porosity as a fraction of one, effective diameter (d_{10}) in mm, and the formation water temperature.

The **Terzaghi formula**, which applies mostly to coarse-grained sand and gravel, needs the input values of d_{10}, porosity as a fraction of one, and temperature. There is also a correction coefficient which takes into account two categories of sand grains: smooth and angular.

1.5. Average Values In Layered Media

This section of the program calculates an average permeability coefficient for horizontally stratified terrain. The flow may be either parallel or perpendicular to the layers of different permeabilities.

(1) Flow parallel to layers

layer 1	K_1, H_1	K_i and H_i are hydraulic conductivitie and thicknesses of individual layers, respectively
layer 2	K_2, H_2	
layer 3	K_3, H_3	

From the continuity-of-flow consideration, the specific flow through each layer is equal to:

$q_1 = K_1 H_1 i \quad q_2 = K_2 H_2 i \quad q_3 = K_3 H_3 i$

where i is the gradient of flow. The total flow through all layers is equal to

$q = q_1 + q_2 + q_3 + \ldots + q_n$ or $q = (K_1H_1 + K_2H_2 + K_2H_3 + \ldots K_nH_n)$

The same total flow can be expressed in terms of an average hydraulic conductivity, K_{av}, as

$q = K_{av}Hi$

where H is the sum of all individual thicknesses ($H_1+H_2+H_3+\ldots+H_n$). Equating the two expressions the following is obtained:

$K_{av} = (K_1H_1+K_2H_2+K_3H_3+\ldots+K_nH_n)/(H_1+H_2+H_3+\ldots+H_n)$

The GW1 program prompts for (a) the number of layers, (b) hydraulic conductivity of each layer, (c) thickness of each individual layer.

(2) Flow perpendicular to layers

layer 1		K_1, H_1
layer 2		K_2, H_2
layer 3		K_3, H_3

In a similar way one obtains the following expression for the average hydraulic conductivity when the flow is perpendicular to the stratification:

$K_{av} = (H_1+H_2+H_3+\ldots+H_n)/(H_1/K_1 + H_2/K_2 + H_3/K_3 + \ldots + H_n/K_n)$

The input is prompted for from the screen in the same way as in the flow parallel to stratification. An example is shown in Fig. 1.4.

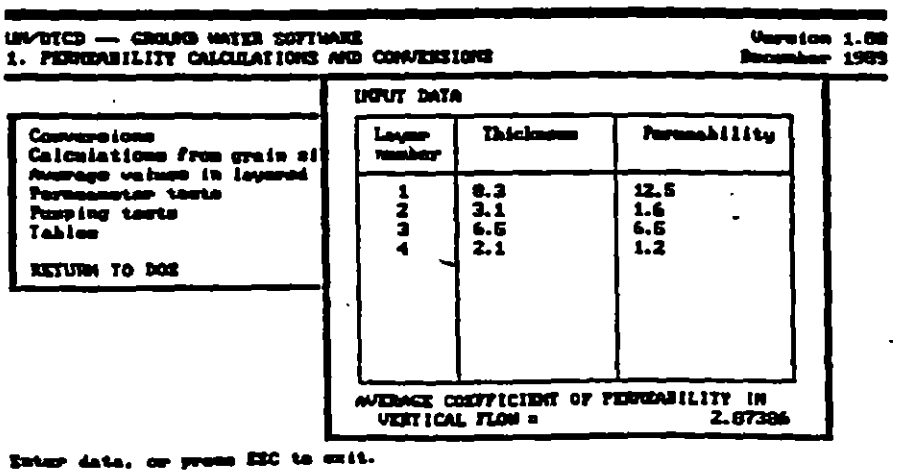


Fig. 1.4

1.6. Permeameter Tests

Permeameters are used for laboratory determinations of permeability from small samples of permeable materials. Several types have been developed, such as constant-head, falling-head, and nondischarging permeameters. The first submenu that appears when you select "Permeameter tests" from the main menu prompts for the system of units; the options are American units (US gallon, foot, second) and metric units (cm^3,cm^2,sec). The next window prompts for the type of permeameter. Three types can be handled by the program: (a) constant head, (b) falling head, (c) nondischarging permeameter.

The *constant-head permeameter* is used to measure permeabilities of consolidated or unconsolidated formations under low heads. The parameters needed for calculation are the following: V is the flow volume in time t, L is the length of sample, A is the horizontal area of sample, h is the water level difference between two cylinders. You are prompted to input all these values in units you have selected two windows before.

In the *falling-head permeameter*, water is added to the tall column, flows upward through the medium cylinder and is collected as overflow. Both consolidated and unconsolidated samples can be tested in this manner. The permeability coefficient is calculated from the following parameters: d_c, the sample cylinder diameter; d_t, the water tube diameter; L, the vertical length of sample; t, the time in which water level drops in the tall water tube from initial h_o to end value h. One example is shown below and in Fig. 1.5.

Sample cylinder diameter = 4.8 [cm]
Water tube diameter = 1.3 [cm]
Vertical length of sample = 7.9 [cm]
Initial water head = 11.3 [cm]
Water head at end of test = 7.3 [cm]
Test duration = 12.7 [cm]

PERMEABILITY = 0.01994 [cm/sec]
= 17.2 [m/day]

The third type of permeameter, the *nondischarging permeameter*, is used for measuring permeability of unconsolidated formations under very low head. The parameters to define the permeability coefficient are the following: A, the area of supply and discharge reservoirs; L, the total length of the "U" tube; a, the area of the sample in the "U" tube; t, the time at which the difference of levels between supply and discharging reservoirs becomes equal to h, starting from some initial head difference h_o at t=0.

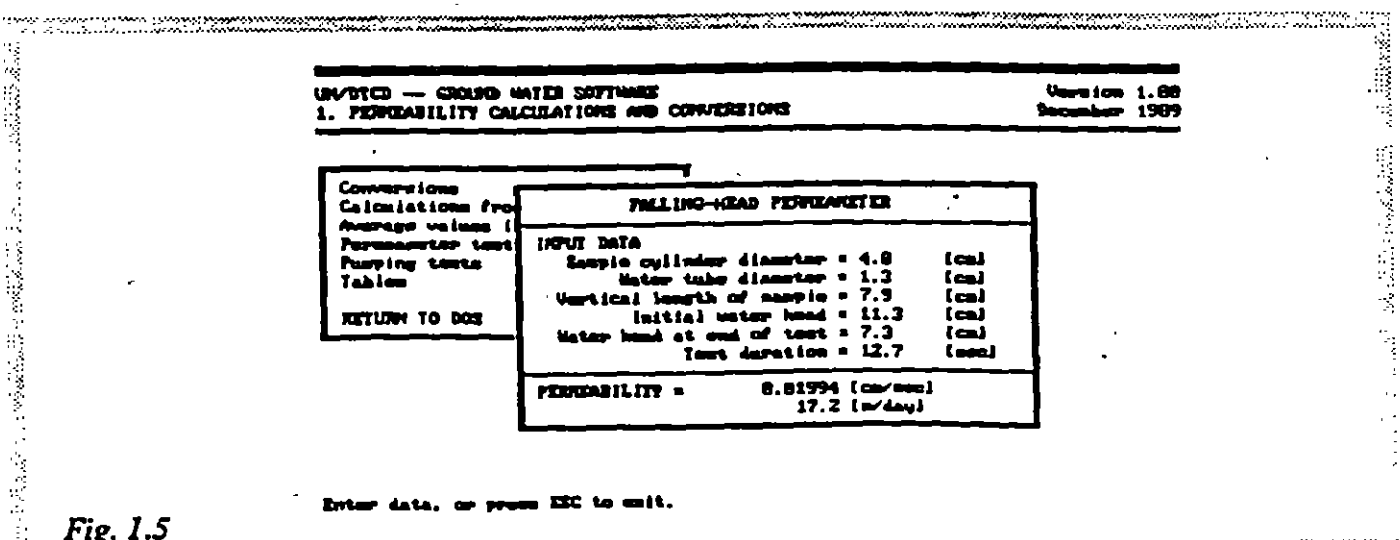


Fig. 1.5

1.7. Permeability from Pumping Tests

In this section the permeability coefficient is calculated from pumping tests in steady radial flow to a well, under both confined and water table conditions. The first window that appears when you select "Pumping tests" is selected from the main menu, prompts you to select pumping rate units. Five options are built into the program: (a) gpm, (b) gpd, (c) l/sec, (d) m^3/day, (e) m^3/hr. The second window prompts you to select the type of aquifer, confined or unconfined (water table).

If you select "confined aquifer" , you are expected to supply the following data:

(a) pumping rate, (b) aquifer thickness, (c) distance to first observation well, (d) distance to second observation well, (e) head in first observation well, (f) head in second observation well. If only one observation well is used during the pumping test, the distance to the first observation well becomes the pumped well diameter.

The coefficient of permeability K is calculated from the "equilibrium" or Thiem formula.

In the case of "unconfined" or water-table aquifer, the information supplied is the same except there is no prompt for aquifer thickness, which does not appear in the equation for pumping rate or permeability. An example is shown in Fig. 1.6.

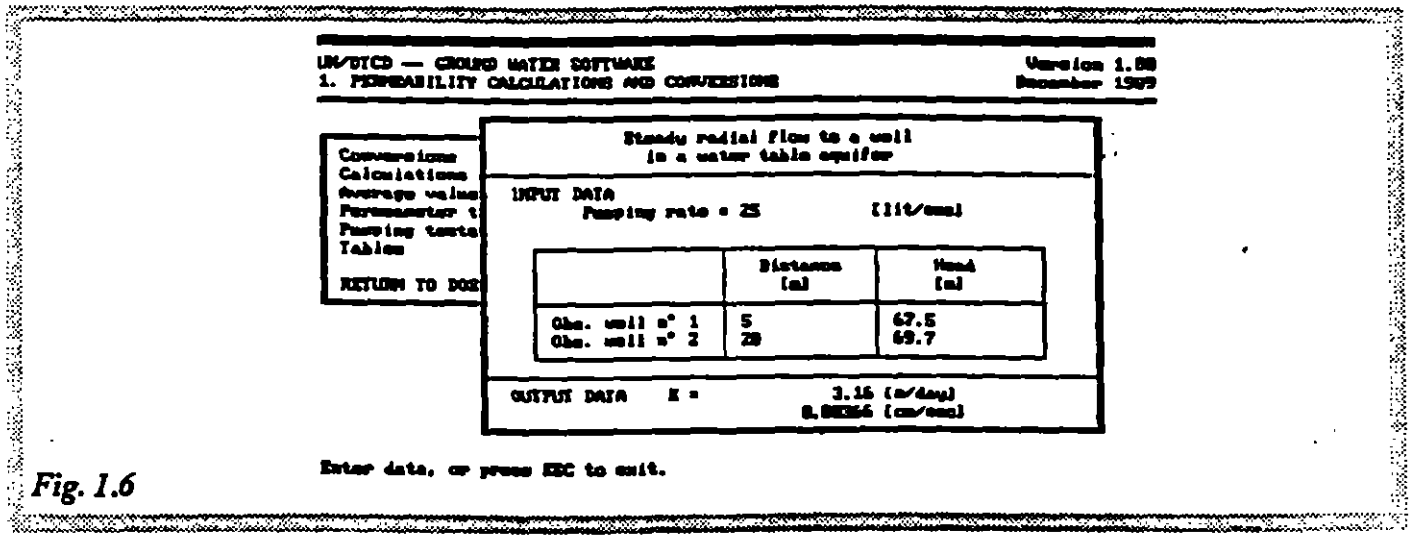


Fig. 1.6

1.8. Tables

Several tables are included in the GW1 program for your reference. The selection window for the tables looks as follows:

SELECT TABLE

Average values of permeability
Average values of k and K
Representative values of k and K
Units for length, area and flow rate
Conversion factors

Ground Water Chemistry

2.1. General

This is a utility program that allows you to create, manage, and display or print reports for a ground water quality data base.

The program requires about 300,000 bytes of memory. A video display adapter is required (see Introduction) for viewing the Piper and Wilcox diagrams. The Stiff diagram printing program uses only ASCII characters and can be used with any dot matrix or daisy-wheel printer. The Piper and Wilcox graphics programs require a dot matrix printer with graphics capabilities. Plotter is optional for plotting Piper and Wilcox diagrams. A mathematical co-processor is not absolutely necessary, but it speeds up the writing of textual part on graphics screens. A mouse is not required, but is useful for zooming in on details in the Piper diagram.

In order to run the GW2 program you must copy the following files to the \GW directory: GW2.EXE, UN2.CMN, UN2.MST, UN2.WND. The executable program, GW2.EXE, comes in a compressed form, occupying about 213,000 bytes. As an option you may copy TABLE.EXE plus six TABLEx files (*x* is 1,2,3,4,5,6) to any subdirectory in which you wish to keep your chemical data base. (TABLE.EXE is independent from the GW2 program.)

You can start the GW2 program either by typing GW2 at the DOS prompt, or by selecting GW2 from the main menu of the GW program.

The following keys have special functions:

The **F2** function key erases the data field completely

The **F3** function key erases the data field from current cursor position to the end of the field

The **ALT-F10** key, pressed simultaneously, "fix" the screen if it appears corrupt

PgDn ("Page down") and **PgUp** ("Page up"), display on the screen one page down or up, respectively, provided the data base has more than 14 samples

The **HOME** key positions the cursor to the top of the screen

The **END** key positions the cursor to the bottom of the current screen

The **CTRL+HOME** key sequence brings up sample number one

The **CTRL+END** key sequence brings up the last sample in the data base

2.2. Creating Ground Water Quality Data Base

The creation of a ground water quality data base is the most important portion of this program. The program starts with an Opening Screen (Fig. 2.1) prompting you to type the name of a Chemistry Data File. Here, you are given two alternatives.

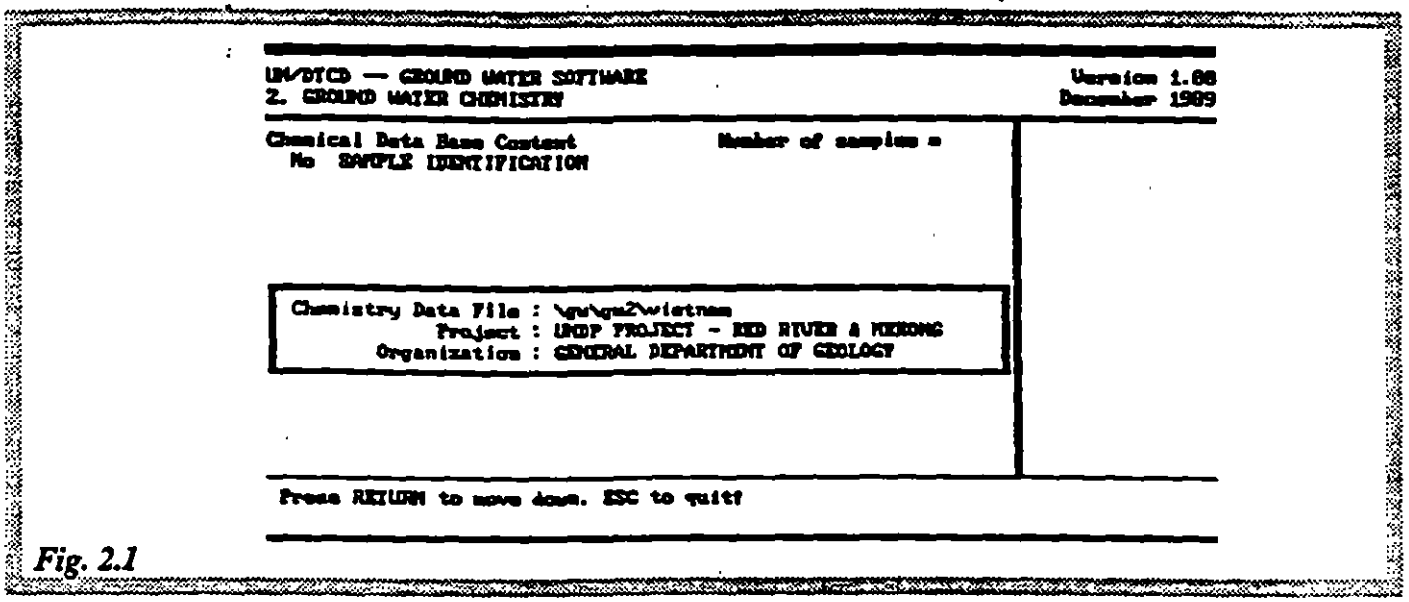


Fig. 2.1

(1) If this is the first time a Chemistry Data File is being created, i.e. if such a file had not been created before and does not exist on the disk, there will be a message displayed at the bottom of the screen, after the name of the file is typed:

This file does not exist.

Press C to create new file or Esc to exit.

(2) If the file exists on the disk, the program displays two lines identifying the file (Project and Organization), and the cursor moves to the second line (Project:). You may modify the title of the project and then press RETURN. The cursor then moves to the third line (Organization:) which can also be edited. When you press RETURN, the screen displays another window with the total number of samples in the data base shown at the top of the screen (Number of samples =), and lists the first 14 samples (sequential number and identification), as shown in Fig. 2.2.

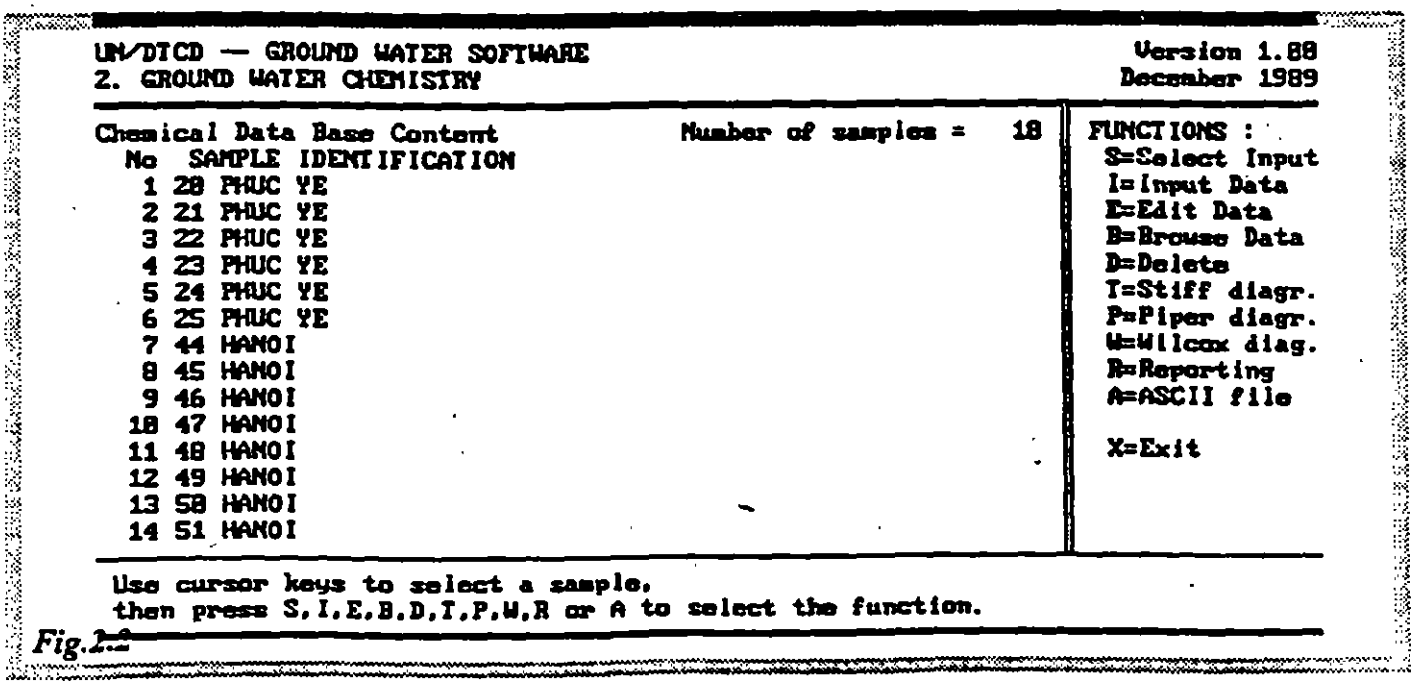


Fig. 2.2

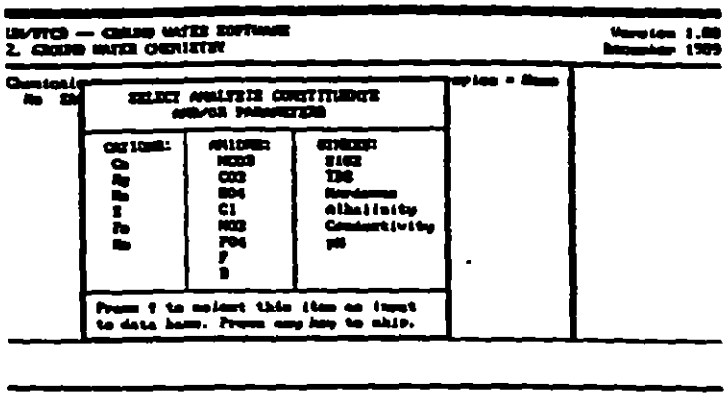


Fig. 2.3

2.3. Procedure to Create a New Data File (Data Base)

After you enter the name of the new file and press the C key to create the file, you are prompted to fill in the "Project" and "Organization" fields.

The screen then displays the choice of constituents (parameters) that may be entered into the ground water chemistry data base (Fig. 2.3). The table is divided into three columns. The first column, cations, contains Ca, Mg, Na, K, Fe, and Mn. The second column, anions, contains HCO_3, CO_3, SO_4, Cl, NO_3, PO_4, F, and B. The third column, others, contains SiO_2, TDS, Hardness, Alkalinity, Conductivity, pH. A total of 20 parameters can be entered into the data base.

Since not all of these constituents and/or parameters are analyzed and/or collected in all projects, the program enables you to select the parameters you wish to enter into the data file. You may select parameters by moving the cursor and pressing Y whenever you wish to add a parameter to the data base list. Pressing any other key will skip the current line. The data base will contain internally all 20 fields, regardless of the selection you make. This means that the data base can be updated with new samples by changing the contents, i.e. by adding new parameters to the data base. This selection is programmed to make input of data easier, that is, to allow you to input only the data which have some positive value.

After you select the data parameters you are given two options: (1) you can reselect the parameters by typing "S". (2) you can begin to input data input by typing "I". The first option returns you to the beginning of the parameter selection procedure described above. The second option allows you to enter your actual data from field notes or laboratory forms into the computerized data base. After you type "I", the screen displays the following (Fig. 2.4): Sample No appears in the upper right corner, the Identification field in the second line,

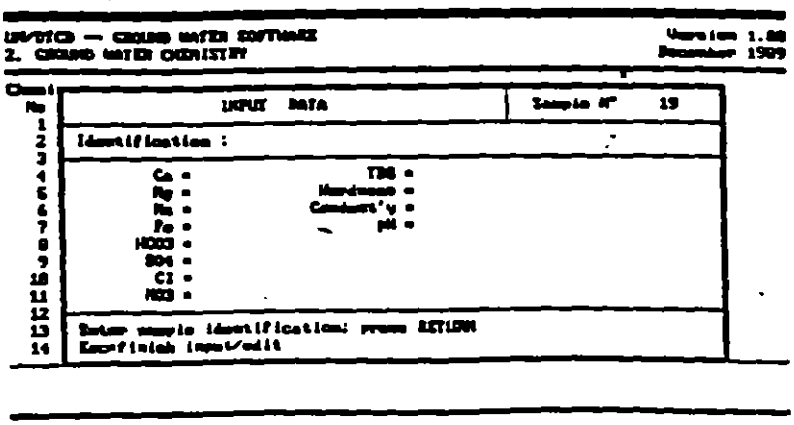


Fig. 2.4

followed by the list of parameters that you have selected. The program enters the sample number for you, starting with the number 1 for a new data base. The cursor moves to the second line – Identification, and the following message appears at the bottom of the screen: "Enter sample identification". The sample identification can be up to 46 characters long. It is used by the program only to identify a sample. You may type the number, laboratory sample number, locality, name, depth of a well, date of sampling, etc. Any combination of ASCII characters is permitted. After the identification is entered, the cursor moves to the first of the selected parameters (normally it will be Ca). Type the values, one by one, using the back arrow key to erase errors. After the last parameter is input (normally pH value), the screen displays Sample N° 2, and the cursor moves to the new identification field. (Any error can be corrected later in EDIT mode.)

Once you have entered the initial data for your data base, the remaining procedures are identical to those for already created data bases; these are described below.

2.4. Available Program Functions

As mentioned above, if the data file had been created before and exists on the disk (directory), the Project and Organization which are associated with the file will be shown automatically. After you press the RETURN twice, the total number of samples contained in the data file will be shown in the right corner of the first line, and the identification of the first 14 samples is displayed sequentially.

The right portion of the screen displays the list of available functions. The following functions can be selected (see Fig.2.2):

- S – select input
- I – input data
- E – edit
- B – browse
- D – delete
- T – Stiff diagram
- P – Piper diagram
- W – Wilcox diagram
- R – Reporting
- A – ASCII file

The role of the "S" – select input function was explained before. Likewise the "I" – input data function was used to start creating a new data file. The "I" function can be used in an existing file to continue with the input of new samples. For example, if an existing data file contains already 20 samples, by pressing "I" the Sample N° 21 will be displayed in the first line and the cursor will be at the Identification field. The parameter fields shall be blank waiting for you to input data.

The "E" – edit function allows you to make corrections and modifications to be made in data files. Before pressing the E key , first move the cursor to the sample number that you want to edit. The screen looks as shown in Fig. 2.5. The sample number is displayed, its identification shown and data values reproduced as

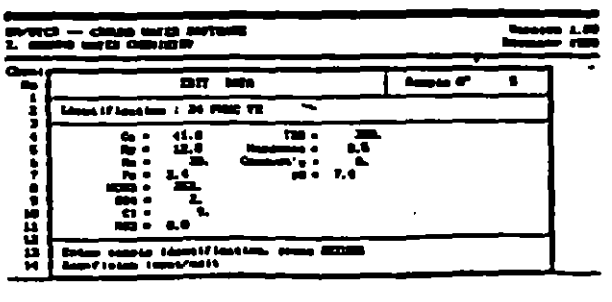


Fig. 2.5

input into the data base. Any parameter can be changed by pressing RETURN and moving down the data analysis form. The previous value can be erased either by using DEL key or the F2 and F3 function keys.

The "B" – browse function permits you to view the contents of the data base. Pressing the up/down arrow keys displays one sample at a time either toward the beginning or end of the data base. Likewise, HOME and END keys display the first or last sample in the data base, respectively. Browsing is shown in Fig. 2.6.

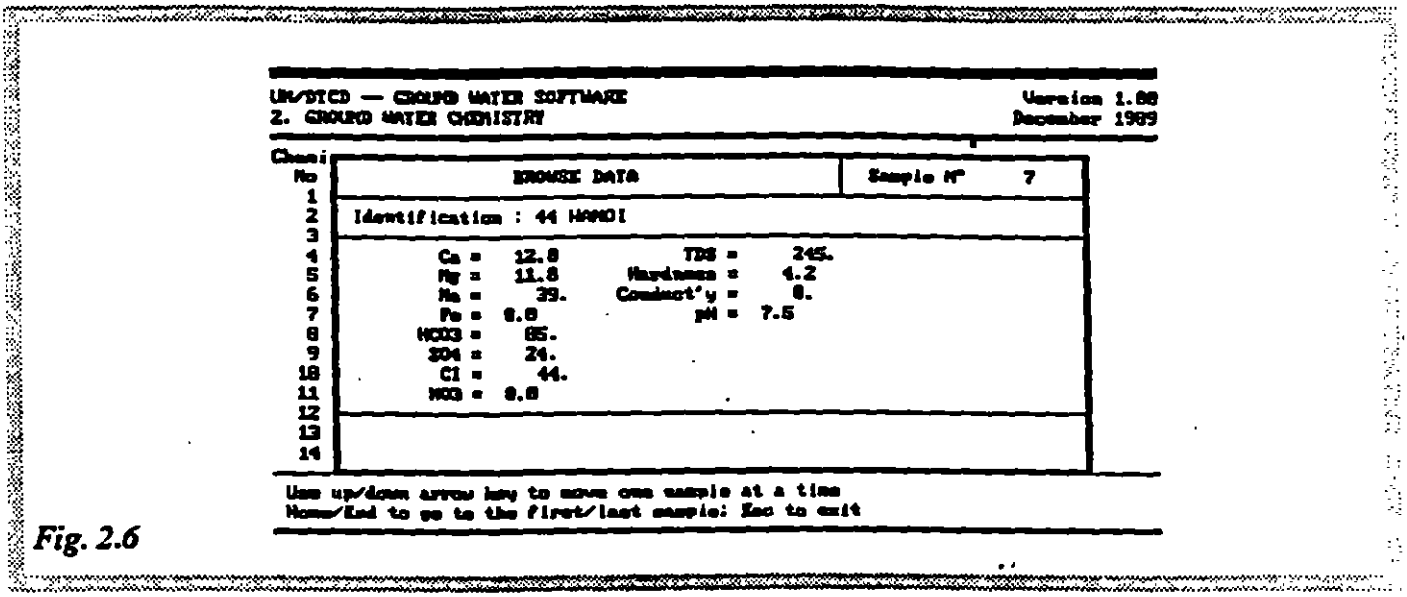


Fig. 2.6

The "T" – STIFF diagram key starts one of retrieval programs, that of displaying/printing the STIFF diagram. The STIFF diagram is shown in Fig. 2.7. Before you press the key "T" you must place the cursor on the line with the sample for which the STIFF diagram is required. The STIFF diagram processing will be explained later.

The "P" – PIPER diagram key is used to view on the screen, or to plot on the printer/plotter, the PIPER diagram. The PIPER diagram processing will be explained later.

The "W" – WILCOX diagram key is used to view or to print/plot the WILCOX diagram. The WILCOX diagram processing will be explained later.

The "R" key is used to activate the reporting subroutine.

The "A" key is used to make a copy of the data base in ASCII format. Such a file may then be used as input file to other retrieval programs, or it may be edited by a text processor.

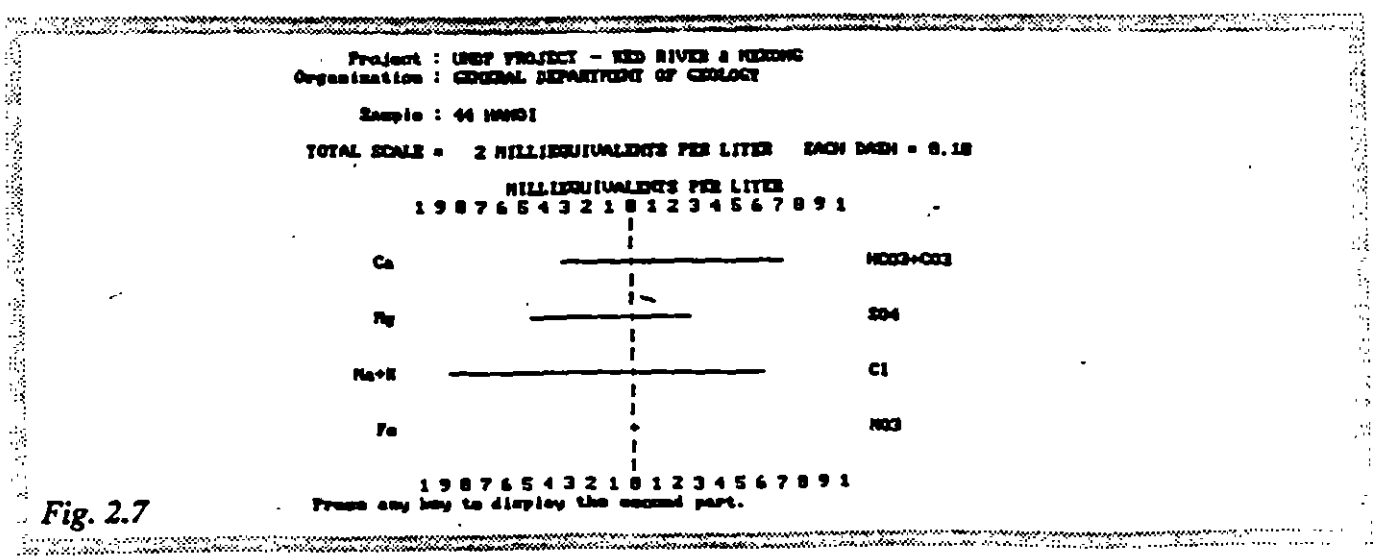


Fig. 2.7

5. Application Programs

STIFF Diagram. Named after H.A.Stiff, Jr. (*STIFF, H.A., Jr., 1951. The Interpretation of Chemical Water Analysis by means of Patterns, J.Petrol., Tech.pt. 15.*) the STIFF graphical method plots four major cations (Ca, Mg, Na+K, Fe) on the left side, and four major anions (HCO_3+CO_3, SO_4, Cl, NO_3) on the right side. The original STIFF plot connects the points on the diagram and produces a pattern which, when compared to another analysis, can be useful in making comparisons of waters. This program presents a modified STIFF diagram in which the length of each line defines the concentration of a particular cation and anion. Concentrations on the diagram are expressed in equivalents per million (milliequivalents per liter). One example is shown in Fig. 2.7. Since iron and nitrates are normally present in insignificant concentrations, most natural waters can be represented as solutions of three major cations (calcium, magnesium, sodium with or without potassium) and three major anions (bicarbonate plus carbonate, sulfate, chloride). If any of these is missing, the program declares such analysis as incomplete.

After a sample is highlighted (selected) from the list of all samples in a data base, and the key "T" pressed, you will have several options where to direct the output – to screen ("D" for display), to printer ("P" for printer), and to an output disk file ("W" for write) for later editing and/or printing.

Provided that the analysis is complete (at least Ca, Mg, Na or K, HCO_3 or CO_3, SO_4, Cl present with nonzero positive values) and the analysis is balanced (the sum of anions matches the sum of cations within 5%, or within any other tollerance specified by you), the output, composed of two parts, will be generated. The first part is a graphical presentation of the analysis in the form of the modified STIFF diagram. The second part contains all important parameters and/or constituents, such as total dissolved solids (TDS), type of water (defined by the dominant cation and dominant anion), all major cations and anions (expressed in ppm and epm), and other parameters if available (hardness, electrical conductivity, pH, alkalinity, etc.). The program also calculates and prints the SAR value (sodium adsorption ratio).

If an analysis is incomplete, the program displays the message "Analysis incomplete" and shows the constituents which are missing or zero. Nothing else will be displayed in the case of an incomplete analysis.

If an analysis is not balanced, which in the context of this program means that the sums of anions and cations expressed in epm differ by more than 5% (or anything specified by you), the message "CATIONS AND ANIONS DO NOT BALANCE" is displayed, followed by the sums of cations and anions and percentage error. The error is expressed as twice the absolute difference of cations and anions divided by the sum of cations and anions, all in equivalents per million, multiplied by 100. The diagram will not be shown, but the rest of information (constituents, type of water, SAR, etc.) will be printed and/or displayed.

PIPER Diagram. Named after A.M.Piper (*PIPER, A.M., 1953. "A Graphic Procedure in the Geochemical Interpretation of Water Analysis," U.S.Geol.Surv. Ground Water Note 12.*), the trilinear diagram (see Fig. 2.8) presents graphically a group of analyses on the same plot. The text that explains the structure of the PIPER diagram is taken from Walton (*"Groundwater Resource Evaluation", McGraw-Hill, 1970*).

"Piper (1953) developed a form of the trilinear diagram which is an effective tool in segregating analysis data for critical study with respect to sources of the dissolved constituents in groundwaters, modifications in the character of a water as it passes through an area, and related geochemical problems. For the PIPER trilinear diagram, groundwater is treated substantially as though it contained three cation constituents (Mg, Na, and Ca) and three anion constituents (Cl, SO4, and HCO3)...

The PIPER trilinear diagram combines three distinct fields of plotting, two triangular fields at the lower left and lower right, respectively, and an intervening diamond-shaped field. All three fields have scales reading in 100 parts. In the triangular field at the lower left, the percentage reacting values of the three cation groups (Ca,Mg,Na) are plotted as a single point according to conventional trilinear coordinates. The three anion groups (HCO3, SO4, Cl) are plotted likewise in the triangular field at the lower right. Thus, two points on the diagram, one in each of the two triangular fields, indicate the relative concentrations of the several dissolved constituents of a groundwater... The central diamond-shaped field is used to show the overall chemical character of the groundwater by a third single-point plotting, which is at the intersection of rays projected from the plottings of cations and anions. The position of this plotting indicates the relative composition of a groundwater in terms of the cation-anion pairs that correspond to the four vertices of the field. The three trilinear plottings will show the essential chemical character of a groundwater according to the relative concentration of its constituents, but not according to the absolute concentrations".

When you press the "P" key, the message Enter drawing identification appears on the screen. Type an identifying title for the Piper plot. The identification will be centered on the 80-column wide paper (standard A4 format, width 210 mm). One may type e.g. PIPER TRILINEAR PLOT, or the name of the project, district,

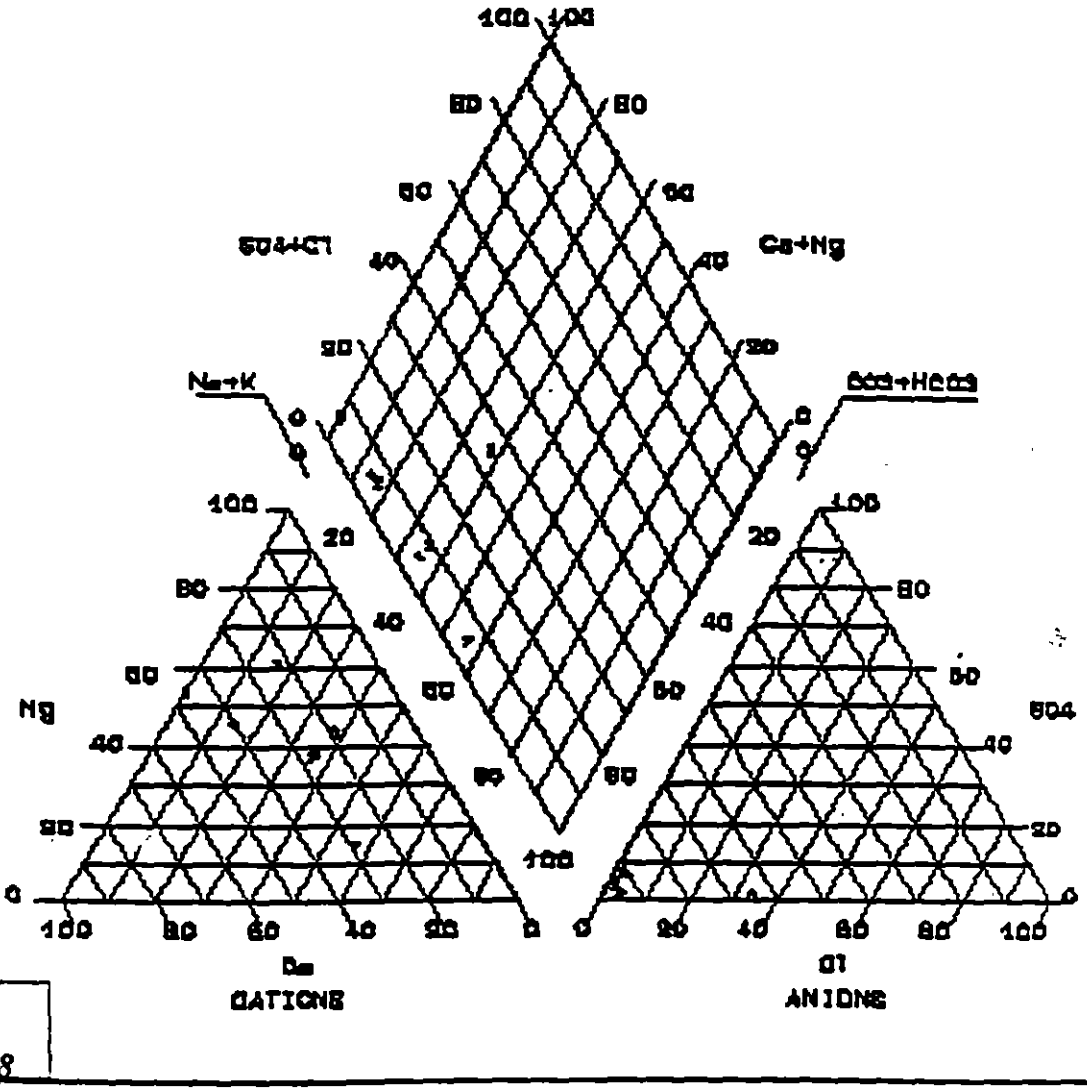


Fig. 2.8

etc. After the plot is identified, you are prompted to select water sample analyses to be plotted on the PIPER diagram. This is one of major advantages of the program – you are able to select analyses to be shown on a PIPER plot. Thus, you may create a rather large data base, and retrieve on one PIPER plot only samples that belong to the same project, or the same area, or that were taken at a certain date. You may use the cursor keys, or CTRL+HOME (to move the pointer to the beginning of the file), or CTRL+END (to move the pointer to the end of the file), or PgDn (PgUp) keys. When you have selected a sample to be plotted press "P", move the cursor to another sample, and repeat the operation of sample selection. When the last sample is selected, press "X" to start the plot.

After pressing the "X" key, you will have four options: (1) to print the graph (press P), (2) to view the graph on the screen (press D), (3) to send the graph directly to the plotter through COM1 serial port (press H), (4) to create an ASCII plot file to be used on another plotter or in another application (press A). Normally you will want to see the graph first. Press D. After the graph is shown you may enlarge some detail by zooming a rectangle. For this you will need a mouse. Read the message on the right side of the screen. If you select P to print the graph, provided that there is paper in printer and printer is switched on, a table identifying all samples

to be plotted will be printed first. The programmers decided to convert all small numbers and identifications to one character only. This is for the sake of readability of the plot in the case of many samples with similar chemical content. However, this limits the number of samples that can be shown on one PIPER diagram to 59 (numbers 1 through 9, capital letters A through Z, small letters a through z). Yet, it is believed that one PIPER diagram should not contain more than, say, 20 to 30 samples for the diagram to be conclusive. Before and after the first table identifying samples is printed, the program pauses giving you the chance to replace or realign the paper. Samples are located on the Piper diagram in the center of the respective character (letter, number).

You may plot the graph on a plotter using or emulating the Hewlett-Packard Graphical Language (HPGL). You must have configured your COM1 serial port according to instructions in your plotters' manual, or following the instructions in Introduction. The plot shall not display the table. Only the graphical screen shall be reproduced in the plot.

Wilcox Diagram. A diagram for use in studying the suitability of ground water for irrigation purposes, named after Wilcox (*Wilcox, L.V, 1955. "Classification and Use of Irrigation Water," U.S. Dept. of Agr. Circular 969*), is based on the sodium adsorption ratio (SAR) and conductivity of water expressed in micromhos/cm at 25 degrees Centigrade. The SAR value is defined by

$$SAR = \{Na/[0.5x(Ca+Mg)]\}^{0.5}$$

High content of exchangeable sodium is highly undesirable for agriculture, and likewise is the high total dissolved solids content, expressed as conductivity of water. An example of the Wilcox diagram is shown in Fig. 2.9.

The processing of the Wilcox diagram is very similar to the routine used in creating the Piper diagram. After selecting the function W (for Wilcox), you have to choose which samples to include in the diagram. This is

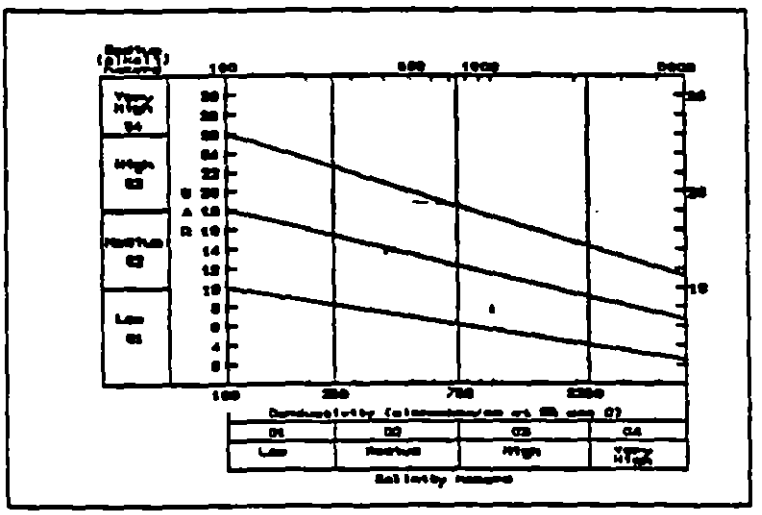


Fig. 2.9

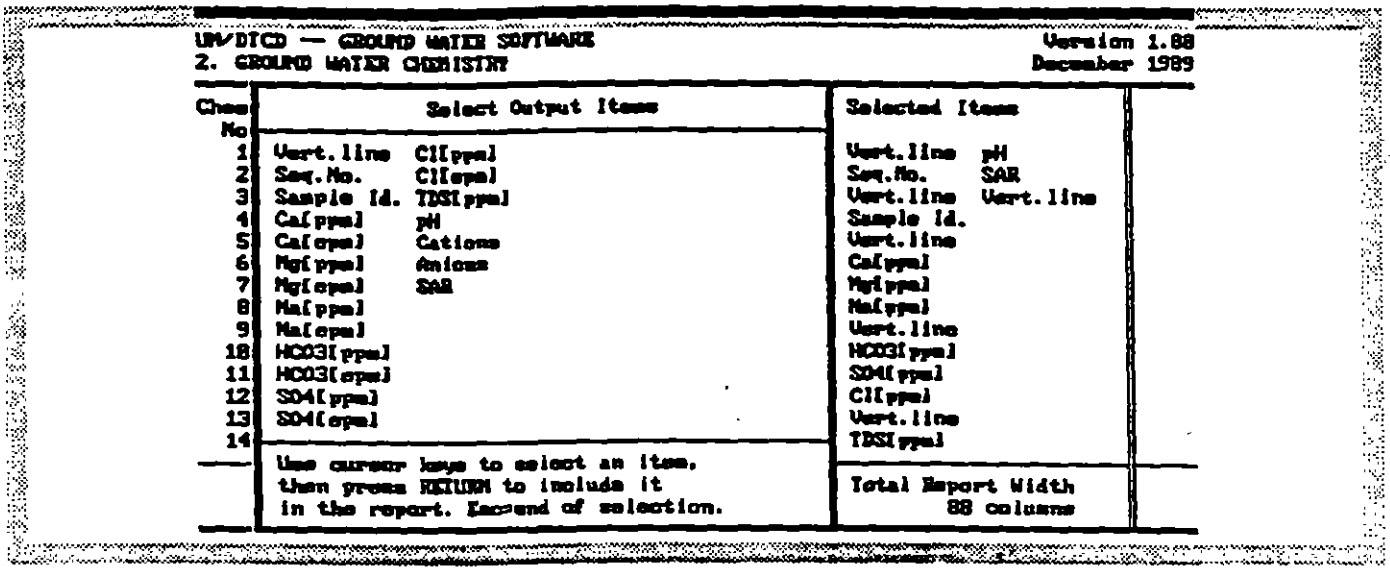
done, as instructed on the bottom line of the screen, by moving the cursor up and down and pressing the key P for each sample to be included. The program checks instantly whether both SAR and conductivity are nonzero positive values. If either of the two is missing and/or zero, there will be a message

Not enough data for Wilcox diagram
Press any key to continue

In either case, continue with the selection of other samples. After selecting the last sample press X to process the Wilcox diagram. The rest of the processing is very similar to the Piper diagram subroutine.

2.6. Reporting

With the "R" key you can print a report on your chemical data base. When you type R, a window entitled "Select Output Items" pops down, showing all output items that are currently included into the data base. As shown in the example from Nepal, Fig. 2.10, there is a total of 20 items currently in the data base. In addition



to major cations and anions, which were manually input in ppm, the program calculated epm values of cations and anions, the SAR value, and sums of cations and anions in epm. In some other cases, there may be more input parameters, e.g. conductivity, alkalinity, boron, manganese, etc.

Table 2.1. Example of Reporting

Seq. No.	Identification	Ca	Mg	Na	HCO3	SO4	Cl	C.	A.	TDS	pH	SAR
1	267–SEMARI	26	22	39	276	6	5	4.80	4.79	206	8.30	1.36
2	268–SARAHAWA	20	33	17	258	9	3	4.45	4.50	226	8.20	0.54
3	269–ASNIYA	35	31	56	374	23	5	6.73	6.75	398	8.30	1.66
4	270–GULARIA	30	21	12	216	6	3	3.75	3.75	280	8.10	0.41
5	271–CHIVPURWA	38	27		212	4	5	4.12	3.70	242	8.10	
6	272–BAIDULI	26	37	61	278	5	84	6.99	7.03	200	8.40	1.80
7	273–CHAVNAR TO	26	8	59	265	5	5	4.52	4.59	360	8.20	2.60
8	274–S.P.OFFICE	80	6	7	270	13	4	4.79	4.81	340	8.20	0.20
9	275–DHARMANAGA	20	27	34	278	2	4	4.70	4.71	248	8.30	1.17
10	276–BELAHIYA	30	23	25	264	2	4	4.48	4.48	260	8.10	0.84
11	277–DUMRAHA	26	23	32	270	4	2	4.58	4.56	240	8.00	1.10
12	278–AMUWA	23	30		188	2	4	3.61	3.24	280	8.00	
13	279–PACHHEDAWA	16	28	22	234	6	4	4.06	4.07	210	7.90	0.77
14	280–SONBRASA	24	33		180	5	5	3.91	3.20	210	8.00	

C – Cations
A – Anions

Each of the parameters to be reported, excluding the Sample identification, has a default column width. All cations and anions in ppm are 6 characters wide (including blanks between two parameters) and all cations and anions in epm are 7 characters wide. The TDS is also 6 characters wide (with separating blanks), the SAR and pH values are each 7 characters wide. You may decide on (1) content of report, (2) width of report, (3) number and place of vertical lines to separate parameters.

Each vertical line occupies 2 characters (one for line, one for blank), the Sequential number (1,2,3...) occupies 5 characters, and Sample identification 14 characters by default. This may be altered as prompted by the program. Table 2.1 is an example of a report form for the data base from Nepal. Included are the following: Sequential number, sample identification, major cations and anions in ppm, sums of cations and anions in epm, TDS, pH, SAR. Several vertical lines separate groups of items. The total width of the report is 112 columns. After you select all the items to be included in the report, the program prompts first for Report title, then for Number of lines per page, and finally for Left margin. If the width of the report is limited to 80 or less characters, the whole data base may have to be printed in more than one page. Thus, identifications can remain the same on two-page report, with constituents reported in ppm on one page, and epm on another page. TDS, SAR, pH, alkalinity, conductivity, hardness, etc. can be reported on either of the two pages. Alternatively, the whole report can be condensed on a standard A4 format by instructing the printer to print in condensed mode (15 or 17 characters per inch – cpi). For this you can use any of available routines (printer's Escape codes, PC-PRINT or similar utility, SIDEWAYS, and so forth).

2.7. ASCII File

You can copy your data base file to an ASCII disk file by pressing the "A" key. You have the option to select items from the data base to transfer to an ASCII file. The procedure is similar to selecting items for reporting, except that the output goes to a disk file from which you can retrieve it by any of available DOS routines (TYPE, for example), third-party utilities (e.g., SHOW), or text processors. You can use the ASCII file as input file for other ground-water quality retrieving programs that are not contained on this diskette.

2.8. TABLES

The program TABLE.EXE can be used to display several water-quality related tables:

1. *Conversion factors (PPM to EPM)*
2. *Maximum permissible concentrations of radio-nuclides in ground water*
3. *Standards – U.S. Public Health Service 1962*
4. *Boron in irrigation water*
5. *List of inorganic constituents*
6. *List of organic constituents*

You execute the program by typing the following command at the DOS prompt: **TABLE**.

The menu with options for 6 tables appears on the screen and you may select any one of these. Since all 6 tables are written in ASCII format in disk files TABLE1, TABLE2, ..., etc., they can be viewed with the utility SHOW, or typed with DOS utility TYPE TABLE& > LPT1, where & is any number from 1 through 6. You can edit these tables just like any ASCII file. (WORDSTAR was used to create the tables.)

Pumping Test Data Base and Analysis

3.1. General

This is a data base program, with data analysis and presentation capabilities (screen graphics, print, plot). Although this program will run on computers without a mathematical co-processor, absence of a co-processor seriously impairs processing speed. This is especially noticeable in the Hantush leaky theory analysis, which works in iterative cycles and requires a large number of floating-point calculations. Because there are several screen-display graphics routines a video display adapter is highly desirable, although not mandatory.

The program's output to printer was tested on EPSON LQ800/1000 printers. Although not tested, any matrix printer with graphics capability emulating the EPSON Escape Sequence code should be sufficient. The data base editor is independent of the printer, and so are all procedures excluding printing out results. In other words, the program can be used and results obtained without a printer. All data contained in the data base can be shown on the screen in either alphanumeric mode (time, drawdowns, levels, pumping rates, calculated parameters, etc.), or in graphics mode (time-drawdown diagrams). Pumping test graphs can also be plotted on a Hewlett-Packard (HPGL) compatible plotter.

The distribution program comes with several examples. These are contained in files INDIA.PT1, INDIA.PT2. The examples are from a current UN/DTCD project in India. The pumping test data base is prepared by this program in such a way that two files are created, with extensions PT1 and PT2, respectively. One contains general information about wells (location, aquifer, static water level, pumping rate, type of aquifer, type of well, etc.), while the other contains pumping test data (pairs of water levels or drawdowns versus time).

At certain places during program execution the program may appear slow. Either edited data are being written to the disk file, a scratch file is being created, or calculations are being performed. Depending on the main processor clock rate, and the availability of a mathematical co-processor, this time lag may be from several seconds to a minute or two. Please be patient. If the program is not running correctly a message will be displayed on the screen. In some cases, though rarely, the program will terminate without producing results. Moreover, the termination might be abnormal, and you might need to reset the computer. This will be corrected in the second release.

In order to run the GW3 program you must copy the following files to the \GW directory: GW3.EXE, UN3.CMN, UN3.MST, UN3.WND. With the GW3.EXE file in a compressed version occupying itself 317,216 bytes, these four files occupy about 369,000 bytes. The memory required for running this program is 437,000 bytes for the program without graphics screen and/or printer support. For the maximum memory see Introduction. While running the program it is advisable that you prepare your example or actual data base files in a directory other than the \GW directory. You may log into that directory and type GW to start the ground water software. Then select "3. Pumping Tests" with cursor and press ENTER.

3.2. Program Overview

The program creates a pumping test data base. Once data are transferred into the computer, several methods of analysis should be attempted, and standard deviation of the fit recorded. The method which produces the least standard deviation should be accepted as being most representative, provided this agrees with the local hydrogeological situation.

The test data file is limited to 100 time-drawdown or time-level pairs.

The methods selected for analysis are the classical THEIS, JACOB and HANTUSH type-curve matching or semilogarithmic approximations, plus the recovery method and large-diameter dug well pumping test method. Only corrections for water-table aquifer are incorporated in the program. There is no correction for partial penetration, neither for boundary effects nor for variable pumping rates. The dug-well test routine differs from the others. While in the classical theory the program fits the data with assumed values of transmissivity and storage coefficient, in dug-well test you should supply "guess values" of transmissivity and storage coefficient. The program fits test values (levels) with guessed values and generates a drawdown curve which is plotted along with test drawdown curve. You select the pair of coefficients with the best fit.

3.3. Running Program

The program starts by displaying the screen as shown in Fig. 3.1; you are prompted to type the name of a pumping tests file. The cursor is at "Pumping Tests File". Such file, whether existing or about to be created, may contain one or many pumping test data. This file may contain up to 200 pumping tests from any number of different wells. The idea is to group all pumping tests from a project or an area into one data base.

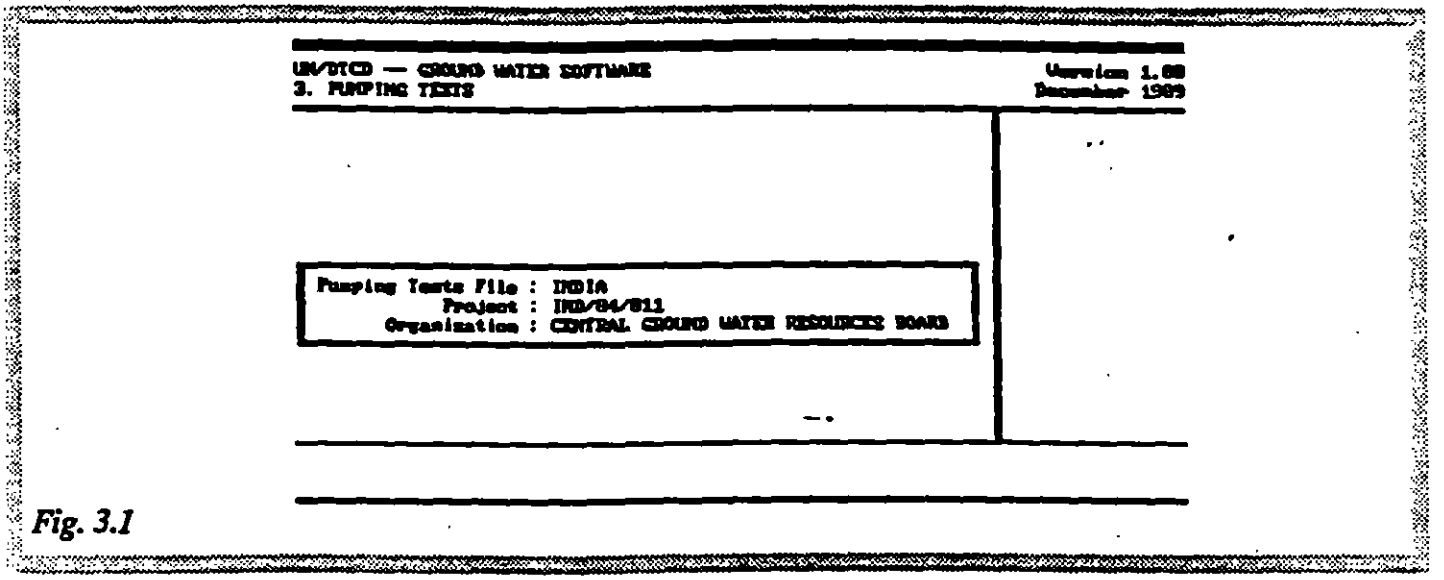


Fig. 3.1

Type in the name of a pumping test file without extension. After you type the data file name the program checks whether such a file exists in the directory that you have specified. If it exists the cursor moves to the second field: Project, and then to the third: Organization. You may type anything that will identify your project and/or organization, or you may press RETURN on both prompts. However, if the program discovers that your data file name is incorrect or nonexisting, there will be a message at the bottom of the screen (message window):

This file does not exist.
Press C to create new file or ESC to exit.

This message is quite clear. Typing C brings the cursor to the second line: Project, to which you may type anything identifying your project or you may press RETURN to move further. If you typed the data base file name incorrectly, you may correct this by pressing RETURN on the first prompt. The cursor is again on the first line and the program waits for another file name.

In the case you are working with an existing data base, you may edit (change, modify) your project identification and organization title. This screen may have a final look as shown in Fig.3.1.

The next screen is the main menu (Fig. 3.2). From here the program branches into three directions: (1) defining units, (2) input and editing data, and (3) analyzing test data. The main menu screen has several "working" sections. The program identification remains on top. The main portion is filled with only two items:

(a) Data base name, and (b) Number of tests in the current data base. The bottom (message) section contains the instruction 'Press U,D or A to select a function group'. The function groups are defined on the right side of the screen. Unless the default units are selected as shown on the right side lower corner, which are in essence the standard metric units, you should select the letter U to define another set of units. The selection

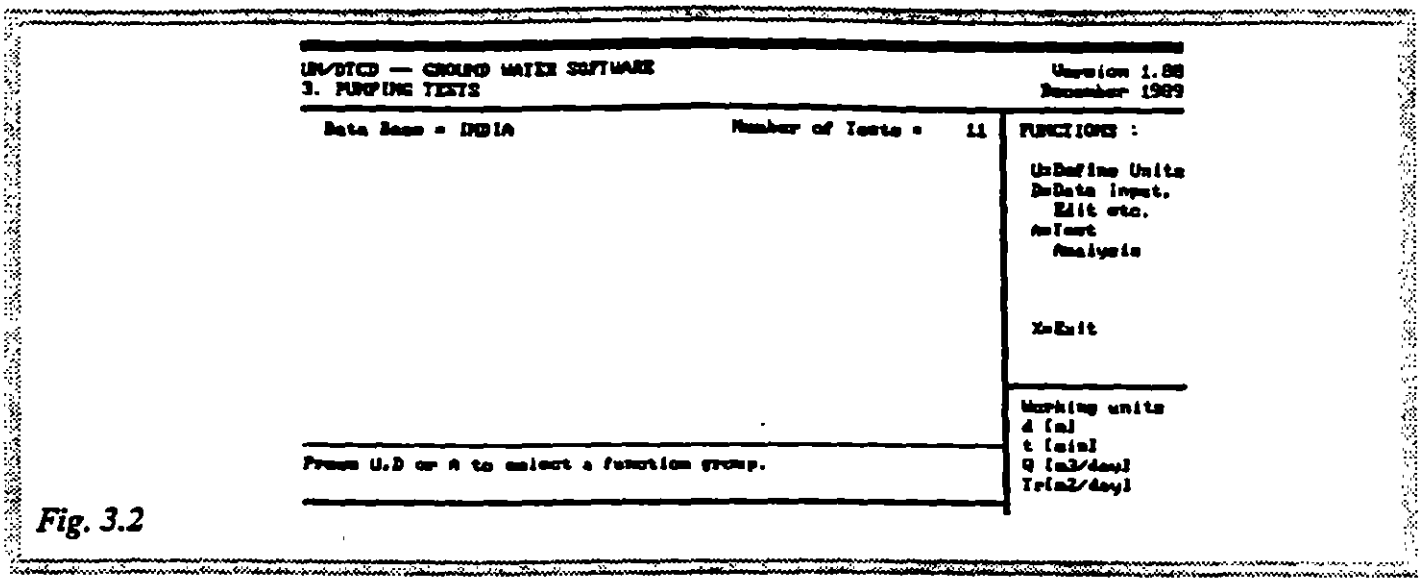


Fig. 3.2

of units is explained in Introduction. The corner with currently selected units will remain visible throughout most of the program. Only from this main menu you may return to the main menu of the Ground Water Software program and/or exit to DOS by pressing X.

3.4 Data Input, Editing, Screen Display, Deleting Analysis, etc.

The second group of operations is activated by pressing the letter D from main menu. In the case that the data base exists with one or more pumping test data in it, the next screen shall display the list of tests (wells) in the current data base. The example shown in Fig. 3.3 is from India, from a Central Ground Water Board – UNDP project in the Kasai-Subarnarekha area. If you are creating a new data base, only the list of functions will appear on the right side, while the message on the top shall display 'Number of Tests: None'.

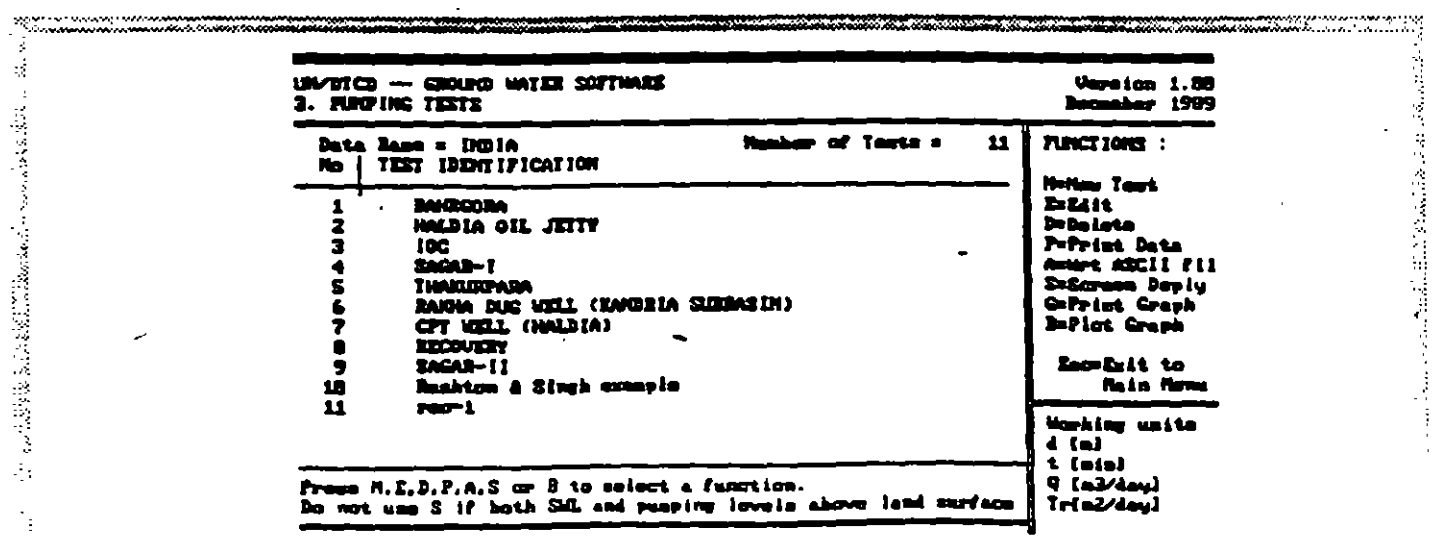


Fig. 3.3

UNDP project in the Kasai-Subarnarekha area. If you are creating a new data base, only the list of functions will appear on the right side, while the message on the top shall display "Number of Tests: None".

New Test. If you are creating a new data base, type the letter N. The cursor appears on the message li prompting for test identification. You can type anything that identifies the test, but the identification cannc. go beyond the light line. In the example shown in Fig. 3.4, the identification "New Test, date 1/2/87" was entered. After pressing RETURN, you will be prompted for pumping rate and distance from the observation well. All programs are prepared for constant pumping rate during a test. When the prompt for "Distance

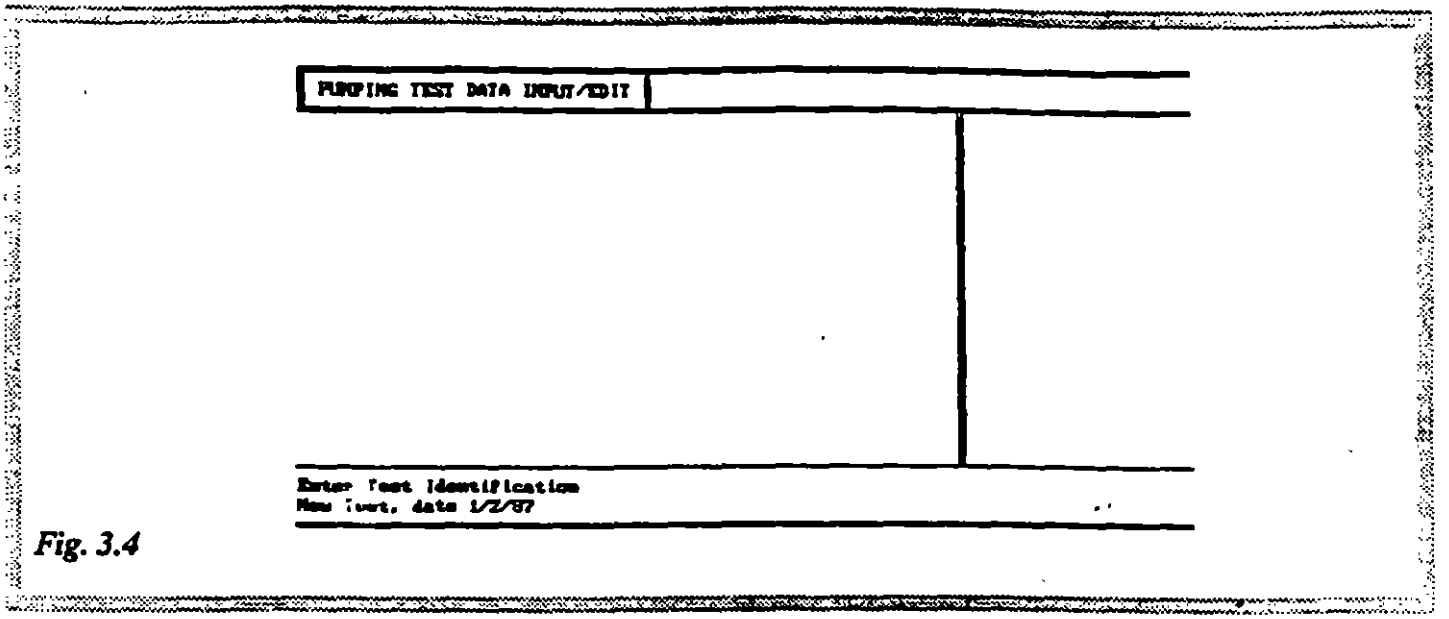


Fig. 3.4

from Pumping Well" appears, you should type either actual distance or well radius in the case that no observation wells are available. (In the latter case, the distance is hypothetical, since the storage coefficient cannot be obtained from the pumped well alone, but the program demands that a distance be input.)

The next prompt is for the type of aquifer, confined or unconfined. The program adjusts drawdown data for decrease in the transmissivity using the formula derived by Jacob:

$$s' = s - (s^2/2m)$$

where: s' = drawdown that would occur in an equivalent nonleaky artesian aquifer;
s = observed drawdown under water-table conditions;
m = initial saturated thickness of aquifer.

If you type the letter U, indicating an unconfined aquifer, the next prompt will be for initial saturated thickness of aquifer. If a confined aquifer is indicated, the next question asks if you will input drawdowns or water levels. Possible answers are the letters D (drawdowns) and L (levels). If you select L (water levels), the next question asks for Static Water Level and a message is displayed at the bottom of the screen telling that when the SWL is above land surface (flowing wells) it should be typed as positive value; when the SWL is below the land surface a negative sign should precede the value.

The next prompt asks whether that well is a standard or dug well. "Standard" here implies any well except a dug well for which assumptions on which the classical Theis, Jacob and Hantush theories are based apply. The main difference between these two categories of wells is that in a "standard" well water is instantaneously released from the aquifer and no storage in the well is allowed. In the case of a dug well, most of water during the abstraction phase is taken from storage in the well, but when the pump is switched off, water continues to flow from the aquifer to refill the well. If standard well is the response, the general data input phase is finished, and the screen may display something similar to Fig. 3.5. If dug well is the answer, four additional parameters should be input:

Well Radius to Face of Aquifer
Well Radius of Storage Portion
Pumping Duration
Test Duration

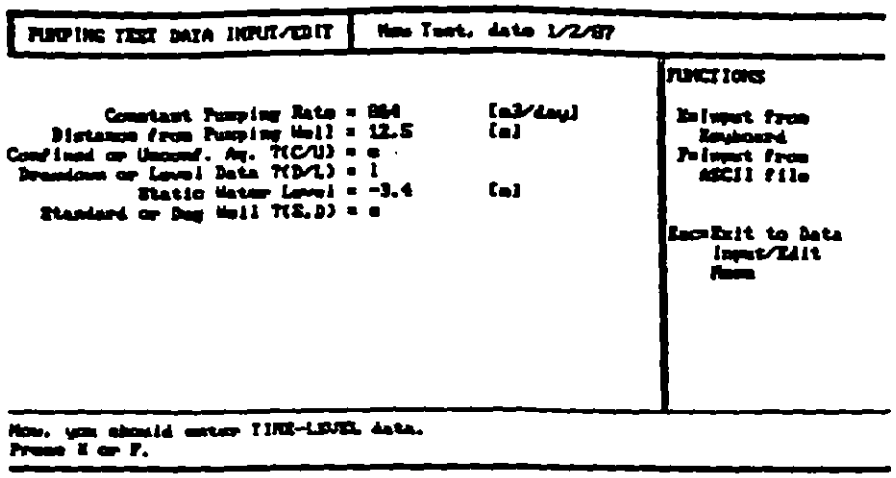


Fig. 3.5

"Pumping duration" is the duration of abstraction (pumping) phase, while "Test duration" is the total duration of the test, including abstraction phase and level recovery phase.

You have two options for inputting test data: (1) from keyboard, one by one; (2) from ASCII file created either by a word processor or text editor, or from another program. The options are invoked by letters K or F as shown in Fig. 3.5 in the function section.

After you type the letter K to select keyboard input, the screen looks as shown in Fig. 3.6. You should type time and drawdown values. You may speed up the input by first typing all the time values, using the down arrow key to move the cursor, and then return to the drawdown/level column and repeat the input for levels/drawdowns. Or, you may type one pair of values after another. To switch from time to drawdown or vice versa, you should press RETURN. Several function keys are also available for input/editing (F1, F2, F3,

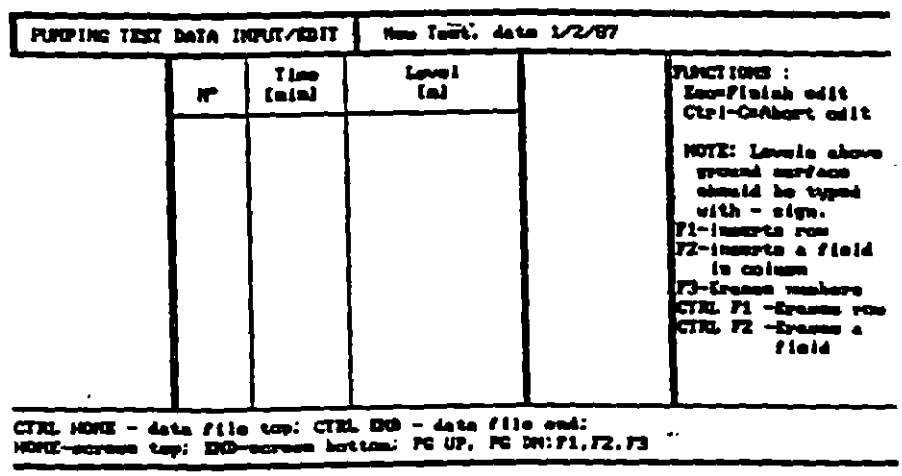


Fig. 3.6

Ctrl F2, etc.). Their functions are shown on the right side of the screen. Since the same screen is used for editing an existing data file, the bottom message line describes the function of some other keys. E.g., simultaneous pressing Ctrl HOME brings the data file to the top of the file (data pair number 1), Ctrl END brings the cursor to the last data pair, HOME and END move the cursor to the top or bottom of the current screen, and Page Up or Down have usual meaning.

You can terminate input either by pressing the ESC key for normal termination, or Ctrl C to abort the input process. In either case the program returns to the Edit/Input menu. The program will notice if you have made a mistake by typing zero or negative time, or if you have not completed an input line with both time and drawdown/level values.

The second possibility is to transfer an existing data file created by a text processor. In that case at the submenu with two functions K and F, type F. The data file must be prepared in ASCII format, with time and level/drawdown data separated by either a comma or a blank. There will be a prompt displayed at message line: Enter input file name. After you type the file name, you will be prompted to specify in which way the data file is prepared: with time data as the first entry or with level/drawdown data in the first place. The answer can be Y (time data first) or N (level or drawdown data first). The program reads the data file and writes in the message line:

Number of input pairs = .
Press any key to continue.

After a key is pressed, the data file is transferred into the data base and the screen displays the list of all tests in the data base, including the new entry at the last line. In the same time the count "Number of Tests" in the upper right corner is updated.

An example of an ASCII data file is given below:

1	7.350
2	8.300
3	8.910
4	9.120
5	9.330
..	.....
18	10.450
19	10.500
20	10.520
..	.....
1200	14.210
1740	14.430
1800	14.440

In this example the order of data is time followed by level; time is in minutes.

Editing Existing Data. You select the edit function placing the cursor on the test sample you wish to edit, and pressing the letter E. The screen shown in Fig. 3.7 appears. The data are divided into two categories: (G) general data, (M) measured data. If you type the letter G to edit general data and supplying the answer BAHRGORA for the test name, the screen may look as shown in Fig. 3.8. If you type the letter M to edit measured data the screen may appear as shown in Fig. 3.9.

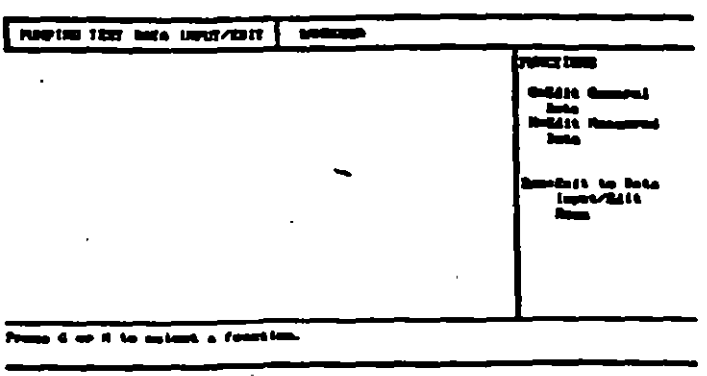


Fig. 3.7

Editing data is straightforward. Several function keys may assist. Their functions are shown on the screen. As a reminder the following keys can be used:

F1 – Inserts a row. Repeated pressing of F1 key makes space for several rows (time-level or time-drawdown data pair).

F2 – Inserts a field in a column. It is normally used when all time data are typed first, followed by the column

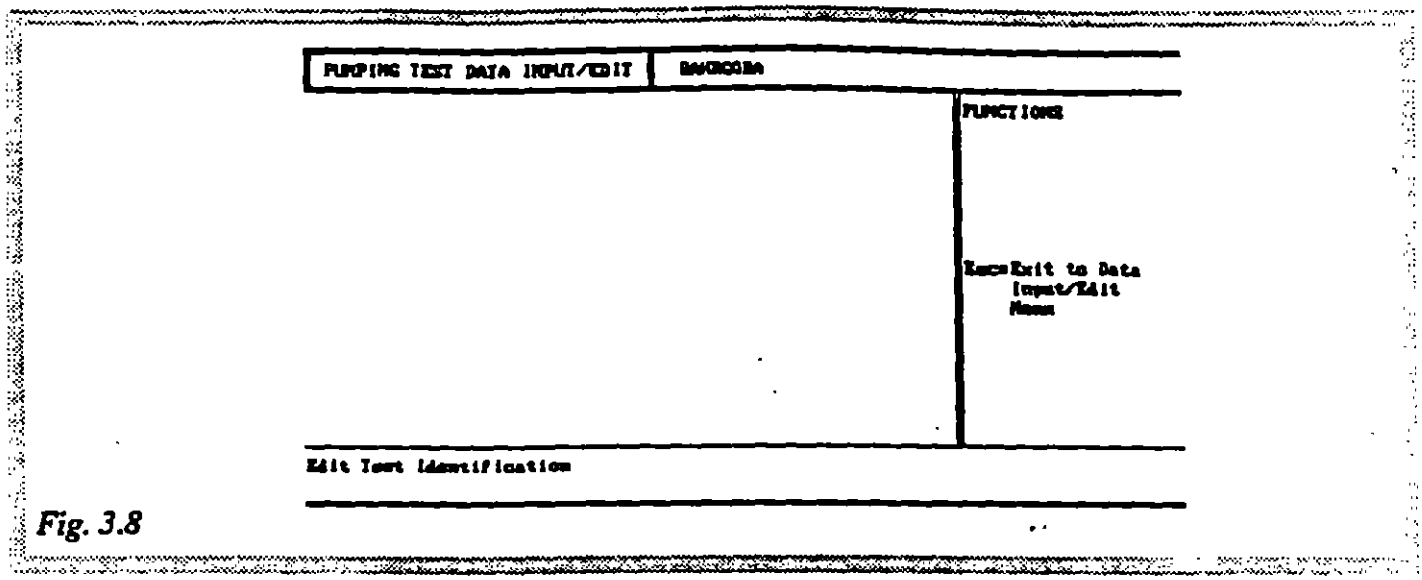


Fig. 3.8

of drawdown data. If you accidentally omit a value, you can create an extra space for the missing value by pressing F2.

F3 – Erases all numbers in a field to the right of the cursor position.

Ctrl F1 – Erases a row.

Ctrl F2 – Erases a field.

Editing is terminated by pressing the ESC key (normal termination after which the new version of the test overwrites the old one) or by simultaneous pressing of CONTROL and C keys (edit abort). In the case of normal termination of editing, the program returns first to the screen which offers editing (functions G and M), and then, after another ESC is pressed, to the Data Input/Edit Menu. In the case of aborting the editing operation, a message

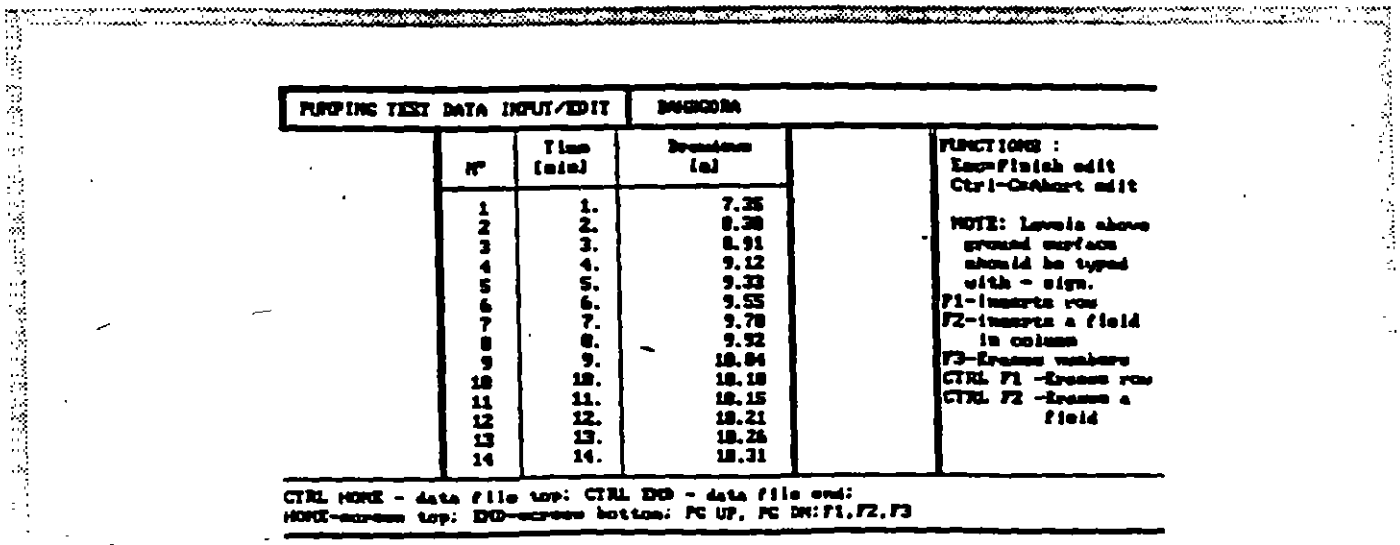


Fig. 3.9

All entered/edited data will be lost!
Is this what you want? (Y/N)

will be displayed. Pressing any key except "Y" will bring back the data file for repeated editing. Pressing the "Y" key returns the program to the Data Input/Edit Menu.

Delete Test. An entire test can be deleted by placing the cursor to that particular test and by pressing the letter D. Once deleted a test cannot be restored. It is advisable to have a floppy disk copy of the data base prior to editing and/or deleting test data.

Print Data. In order to print your test data, place the cursor on a test and type the letter "P"; the selected data file will be printed in the following form: (a) data base and project identification, (b) general data about that particular test, (c) time-drawdown (level) data.

Write to ASCII File. From the Data Input/Edit Menu a test file from the data base can be written in an ASCII format. First place the cursor on the test to be saved in an ASCII file. Then type the letter "A". The message line shall display: "Enter Output File Name". After you enter a file name press RETURN, an ASCII file shall be created.

Screen Display. One of main objections to using the computer to analyze a pumping test stems from the fact that a hydrogeologist cannot see the data, how they fit on an arithmetic or logarithmic scale, whether there may be boundary effects, etc. In other words, if the computer is left alone to make interpretation, the results may be erroneous without the user knowing or appreciating it. For this reason in this program there are several checking possibilities. One is to view the raw input data in a semilogarithmic scale, another is to eliminate some time-drawdown pairs from interpretation, and the final check is to compare the standard deviation (root-mean-square) and accept only the best fit.

You may view input data from this Data Input/Edit Menu by pressing the letter "S" (screen display).

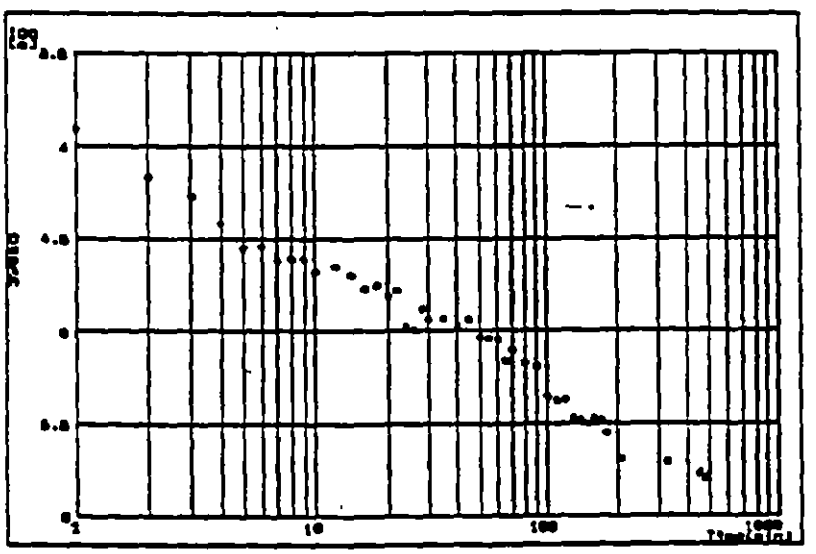


Fig. 3.10

Print Graph. The displayed screen can be printed, along with the project and data base identification, by returning to the Data Input/Edit Menu (any key pressed in the Screen Display mode) and pressing the letter "G". An example is shown in Fig. 3.10.

Plot Graph. The displayed screen can be plotted to a Hewlett-Packard (HPGL) compatible plotter. Only the displayed graph shall be reproduced, without project identification and results. (To obtain a complete hard copy of a test, use printer.) Press letter B. Have your plotter connected to COM1 serial port, which must be properly configured (see Introduction).

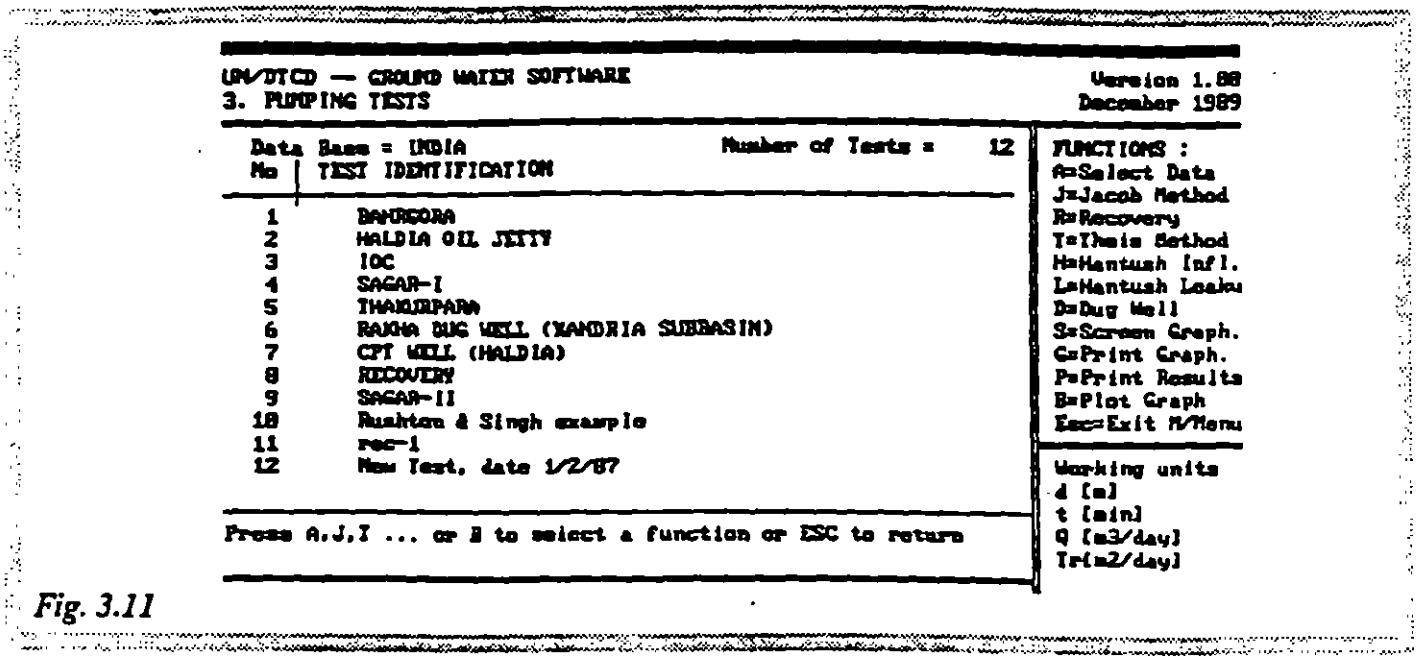


Fig. 3.11

3.5. Test Analysis

The third group of procedures is the analysis of pumping test data from the existing data base. After you type the letter "A" on the main menu, the screen shall look something like the one shown in Fig. 3.11. The cursor is always on the first line (test No.1). The following functions are available:

Select Data. This offers you a possibility to eliminate some unwanted data pairs, either because of an evident error in measuring or because such data do not fit into the method selected for analysis (e.g., early data in Jacob's approximation).

Jacob Method. Semilogarithmic approximation of the THEIS nonequilibrium method. In some cases it may offer a better fit than the THEIS method due to some restrictions involved in the THEIS method.

Recovery Method. This is the Theis method used to determine the aquifer constants from the analysis of the recovery of a shutdown well. The test data prepared for the recovery method cannot be analyzed with another alternative method.

Theis Method. Theis nonequilibrium type curve matching method, one of principal methods of pump test data analysis.

Hantush Inflection Point Method. One of methods of testing a leaky aquifer using the inflection point on a semilogarithmic time-drawdown scale. The method is less accurate than the next one, but sometimes it works when the type curve method fails. It is much faster than the next one.

Hantush Leaky Method. This is the classical Hantush type curve matching method for nonsteady-state time-drawdown.

Dug Well. A recent method of analyzing pumping and recovery phases of large-diameter dug wells, with the consideration given to the seepage face. The method is due to Rushton and Singh.

Screen Graphics. Viewing of test data and the best fit line produced by the method selected.

Print Graphics. Printing the time-drawdown test data along with the best-fit line and test results.

Print Results. Printing project and test identification and a table with field data, calculated data by the computer and differences. Printing results of analysis and standard deviation.

Plot Graph. Plots the displayed screen, without project and test identification, and results. Use only plotters emulating HPGL (see **Introduction**).

3.6. Method of Analysis

Selection of Data. When you type the letter A you will be given a possibility to eliminate some of erroneous data pairs. The cursor is in the column labeled S. Move the cursor using up and down cursor keys to the row you wish to eliminate. Type the sign "*". This eliminates the pair of data from computation. (The message to that effect is displayed in the message line.) An example is shown in Fig. 3.12.

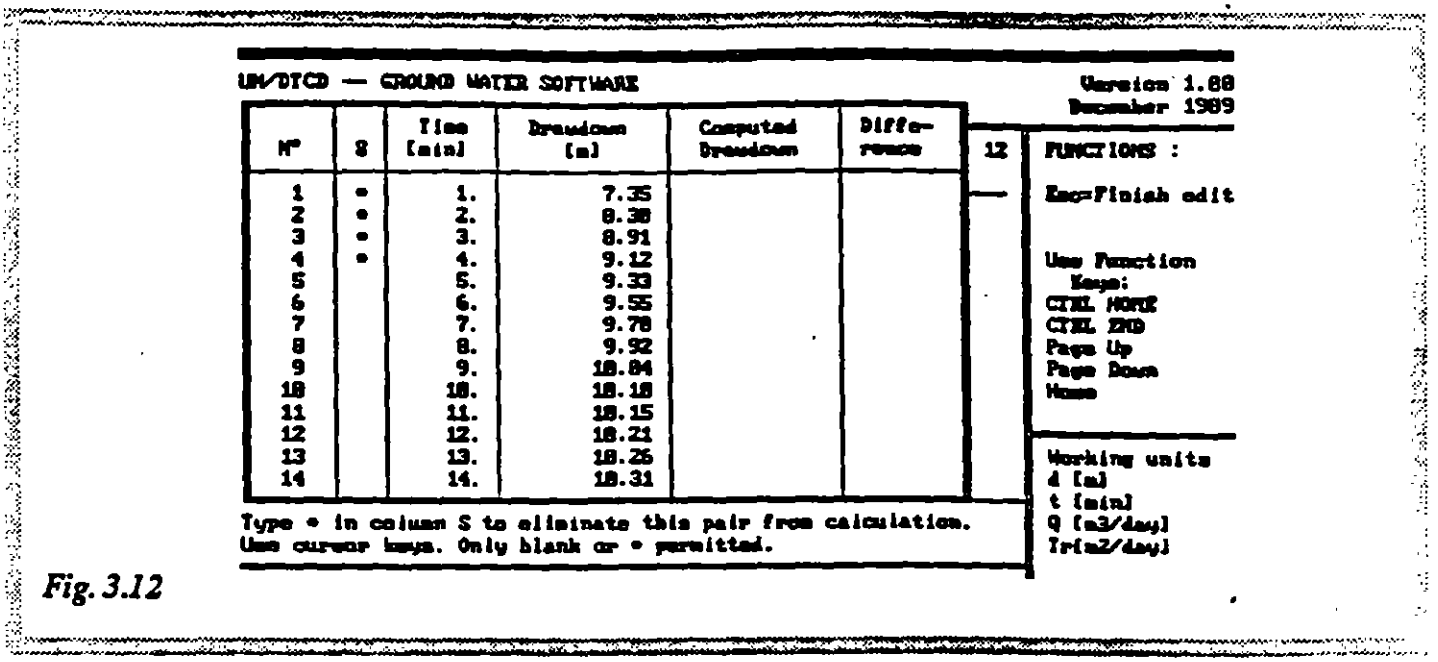


Fig. 3.12

Theis Method. The Theis method is activated by typing the letter T. The method of analysis is well explained in any text book on ground water. The method of computer interpretation is based on the Kansas Geological Survey Groundwater Series 3 publication "*The Theis Equation: Evaluation, Sensitivity to Storage and Transmissivity, and Automated Fit of Pumptest Data*", authored by C.D.McElwee. The automated fit is an iterative process in the course of which the transmissivity and storativity coefficients are changed until a "best" fit is obtained. As a measure of the error in fitting, the root-mean-square in drawdown is calculated for the "best" transmissivity and storage coefficient. The root-mean-square is actually the standard deviation defined as the square root of the arithmetic mean of the squared differences between field and calculated drawdowns.

The results are reported on the screen in the way as shown in Fig.3.13 for American units and in Fig. 3.14 for metric units.

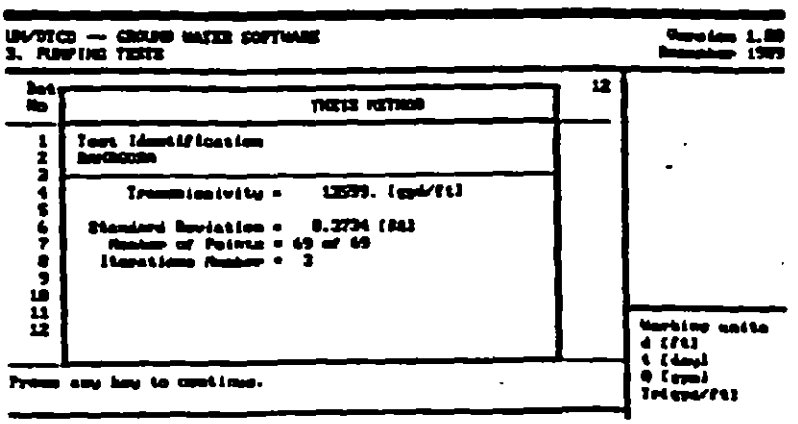


Fig. 3.13

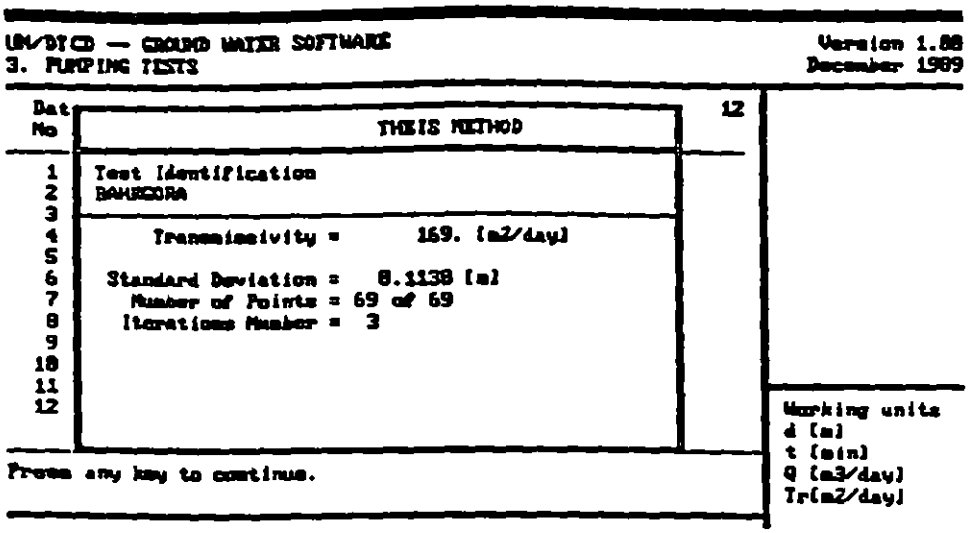


Fig. 3.14

The screen displays the following results:

Transmissivity	Number of points	Storage Coefficient
Number of iterations	Standard Deviation	

The standard deviation is the criterion of the goodness of the fit. The fit in the case of Bahrgora well (India) is very good, 0.113 m, considering that 69 points were involved in the calculation (see Fig. 3.14). However, the goodness of the fit is best demonstrated in Fig. 3.15, which is obtained by selecting the G option from the Test Analysis Menu.

The number of iterations is an indicator of convergence of the solution to an acceptable level of error. In the case of the THEIS program, the criterion is that between two successive iterations the "improvement" of relative transmissivity and storage coefficient is less than 0.0001.

You should expect a relatively small number of iterations, since the initial guess for transmissivity and storage coefficient is already a good guess, i.e. the values obtained from Jacob's semilogarithmic approximation.

JACOB's Method. This is a semilogarithmic approximation which is good for small values of well function's argument u (i.e., for small r and/or large t). The method is also well documented in any text book on hydrogeology. The method of solution is the least square regression analysis and the fit of a straight line through the test data in a semilogarithmic diagram. The computer method provides very quick result. However, one should check whether initial test data satisfy the condition that

$$(r^2 * S)/4Tt < 0.01$$

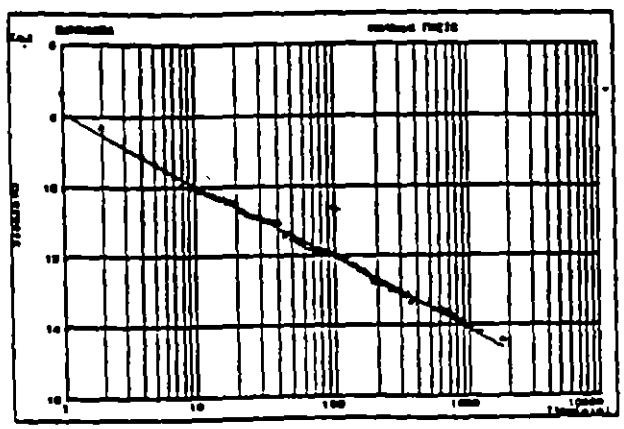


Fig. 3.15

where: r = distance from pumped well to the observation well; S = coefficient of storage; T = transmissivity; t = time since pumping started.

The early data which do not satisfy this condition should be eliminated from computation using the opti A (Select) and typing * in the appropriate rows. A typical test result is shown in Fig. 3.16. The parameters A_0 and A_1 are the coefficients in the linear regression equation, from which transmissivity and storage coefficients are calculated.

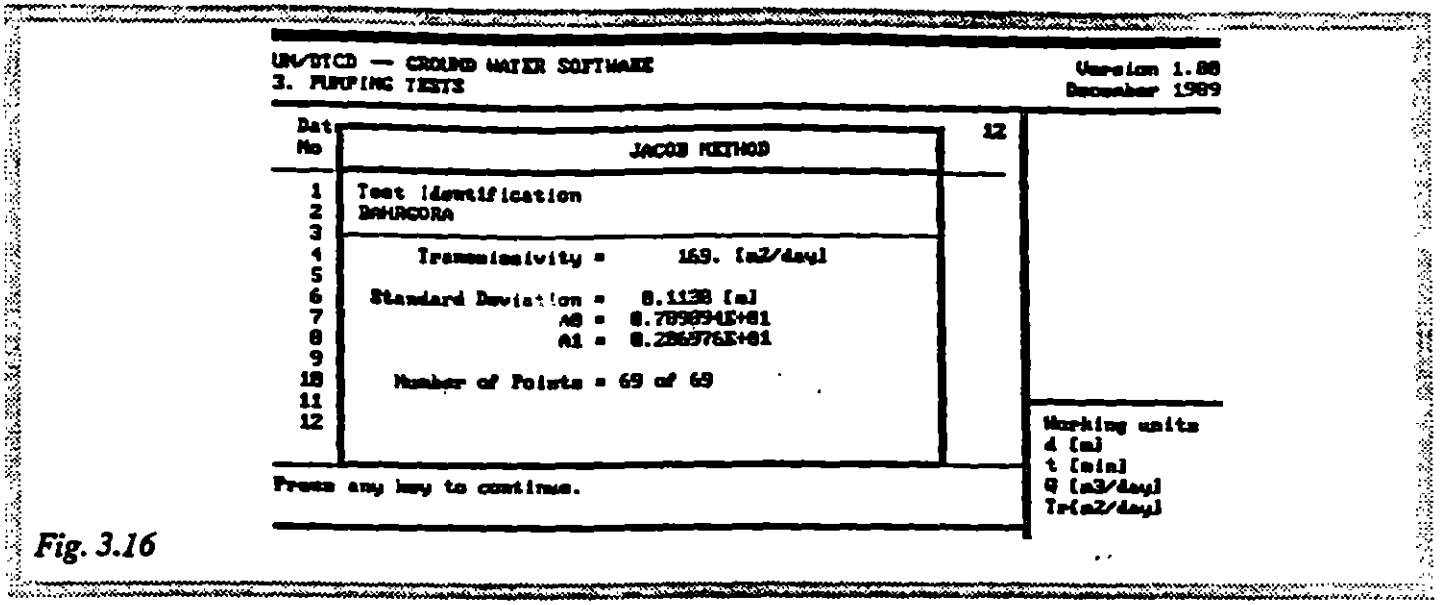


Fig. 3.16

HANTUSH Inflection Point Method. This method will not work in all cases. Most probably it will not work in the case of the pumped well without observation wells, in which the drawdown in the first two or three measurements is greater than 50% of the final drawdown. The method assumes that the steady-state drawdown has been reached at the end of the test, or that steady-state drawdown can be extrapolated at the end of the test data. The method is fast, although not that accurate as the classical HANTUSH type-curve matching method, which is explained next.

Both this method and the next method (HANTUSH leaky type-curve method) produce the values of transmissivity, storage coefficient and leakance (alternatively defined as leakage coefficient). The latter is the ratio of vertical permeability of semiconfining layer to its thickness. If the thickness of the semiconfining layer (through which the leakage occurs) is known, the vertical permeability (hydraulic conductivity) of that layer

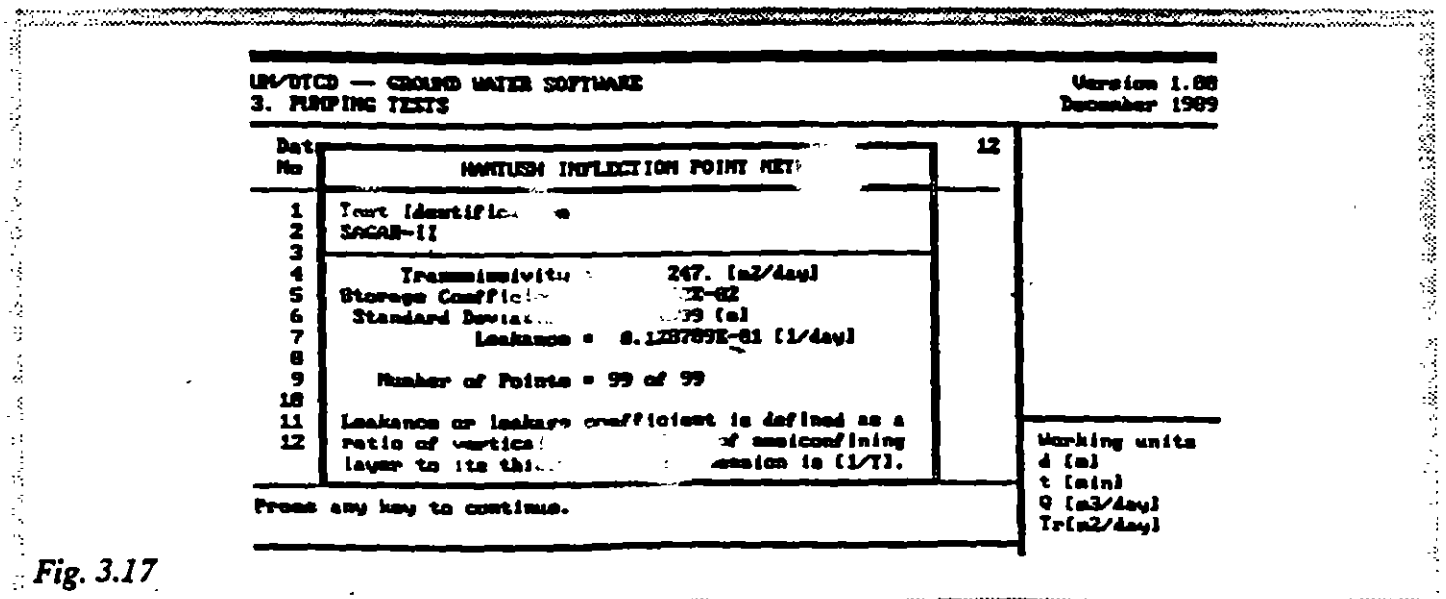


Fig. 3.17

is calculated by multiplying the leakance with thickness. An example is shown in Fig. 3.17. The fit is relatively acceptable, considering that 99 points were involved, although the standard deviation amounts to 0.30 m. The leakance of 0.01287 day^{-1} is interpreted in the following way. If the thickness of the semiconfining layer is about 20 m, its vertical permeability will be about 0.26 m/day, which is characteristic for a mixture of silt, clay and sand.

HANTUSH Leaky-Aquifer Type-Curve Method. The method of solution is an improved version of the method reported by P.M.Cobb et al., in the 1982 publication of Kansas Geological Survey titled "*An Automated Numerical Evaluation of Leaky Aquifer Pumping Test Data: An Application of Sensitivity Analysis.*" The procedure for solution is an iterative algorithm in which the values of transmissivity, storage coefficient and leakance are modified between iterations until an acceptable convergence is obtained. The criterion of convergence is the relative standard deviation. In all tested cases the solution converged in less than 70 iterations. The maximum allowed number of iterations is 100. The processing may take considerable time if a test includes many test points (over 50) and if the number of iterations is large (over 50). However, in a system equipped with a numerical co-processor and in which the main processor works at, say, 12 MHz clock rate, the processing is remarkably fast. To speed up the processing, the initial guess of transmissivity and storage coefficient is taken from the Theis method which is called first. The solution will not be achieved only if the test data do not follow one of leaky-aquifer formulas even approximately. When testing the program, this happened in one out of 30 tests.

The example in Fig. 3.18 is the same as the one shown in Fig. 3.17. The Hantush Leaky-Aquifer Type-Curve method (Fig. 3.18) is superior to the Hantush Inflection Point method (Fig. 3.17). This is reflected in the value of standard deviation which is 0.16 m in the former compared to 0.30 m in the latter. Otherwise, all

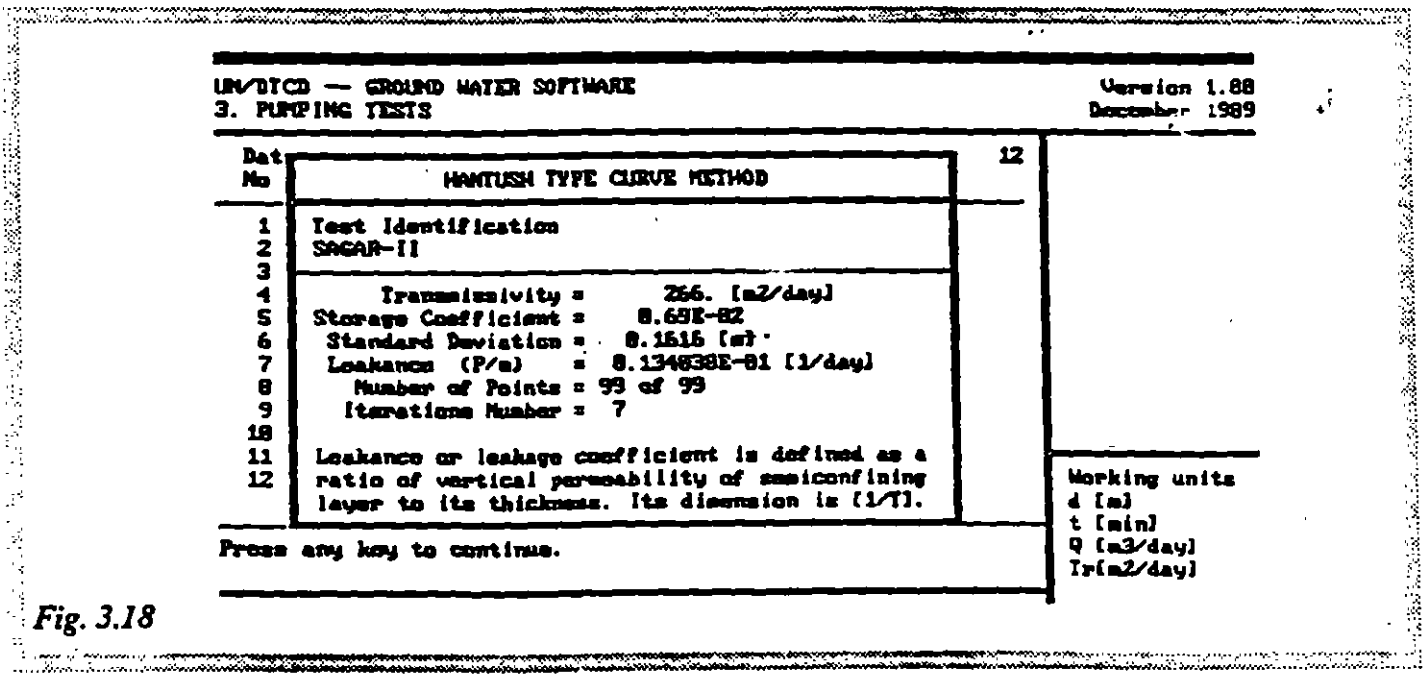


Fig. 3.18

other parameters are very close and the differences are quite acceptable.

Well SAGAR-II (Kasai-Subarnarekha project, India)

	Leaky Type-Curve	*Inflection Point*
Transmissivity	266 m^2/day	247 m^2/day
Storage Coef.	0.00686	0.00618
Leakance	0.0134 1/day	0.0129 1/day

The fit in the case of the HANTUSH Leaky-Aquifer Type-Curve method is demonstrated in Fig. 3.19.

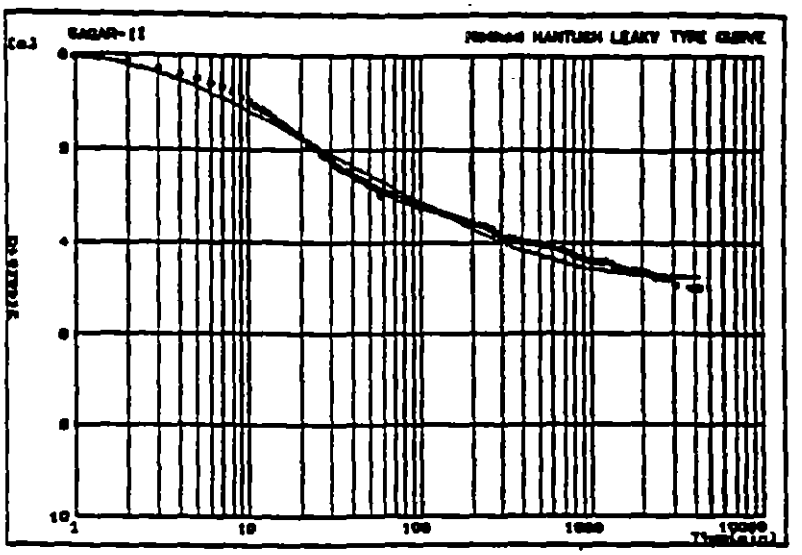


Fig. 3.19

Recovery Method. After you select the recovery method by typing the letter R, you must answer two additional questions (Fig. 3.20):

Pumping Phase Time
Final Drawdown

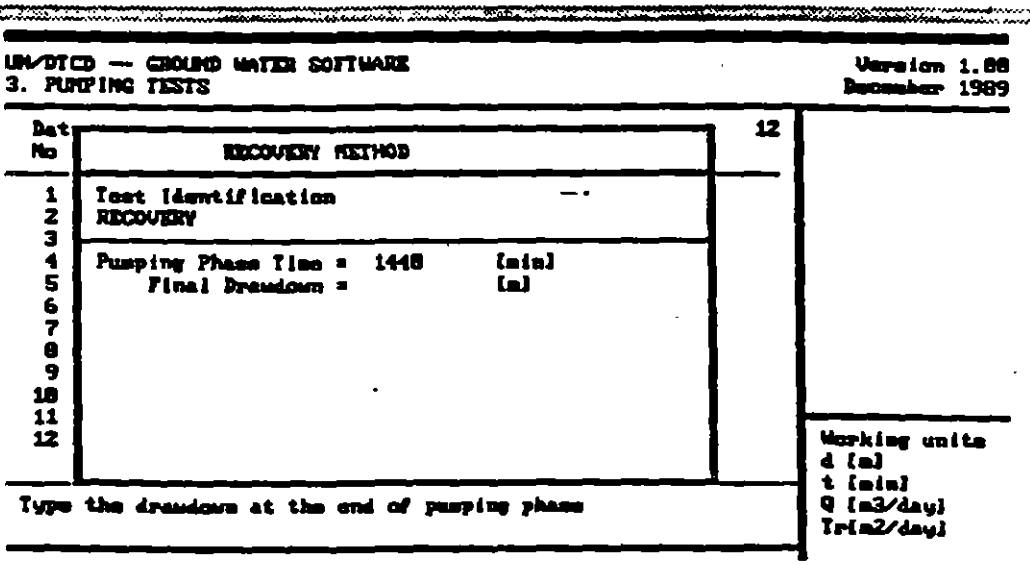


Fig. 3.20

The first is the duration of the pumping phase (from the moment a pump is started until it is switched off), and the second is the total duration of the test, both pumping and recovery phases included. The method of solution is a regression analysis of the system "residual drawdown" on the ordinate axis versus the logarithm to the base 10 of the "modified time". The modified time is defined in the following way:

$$t_{mod} = (t + t')/t'$$

where:

t = time since the test started
t' = time since the pump was shut down and levels started to recover.

The equation for residual drawdown has the following form:

$$S_r = A \log(t_{mod})$$

which is a straight line in the semilogarithmic diagram passing through the origin set at infinite time or at logarithm of 1. The slope of the line allows for the determination of transmissivity. Storage coefficient is determined from the value of the drawdown at the time of shutdown. The method may provide an acceptable value for the value of transmissivity, but the storage coefficient determination, based on only one value, inevitably may or may not be correct.

One example is given in figures 3.21, which is a test from the E.E.Johnson,Inc. book "Ground Water and Wells", 1966, page 138. The computer fit is shown in Fig.3.21a. The values of transmissivity reported in the book are 10,200 and 10,400 gpd/ft, while the computer program reported 11,089 gpd/ft (Fig.3.21b). The storage coefficient in the computer program is 0.0027 while the book reports none.

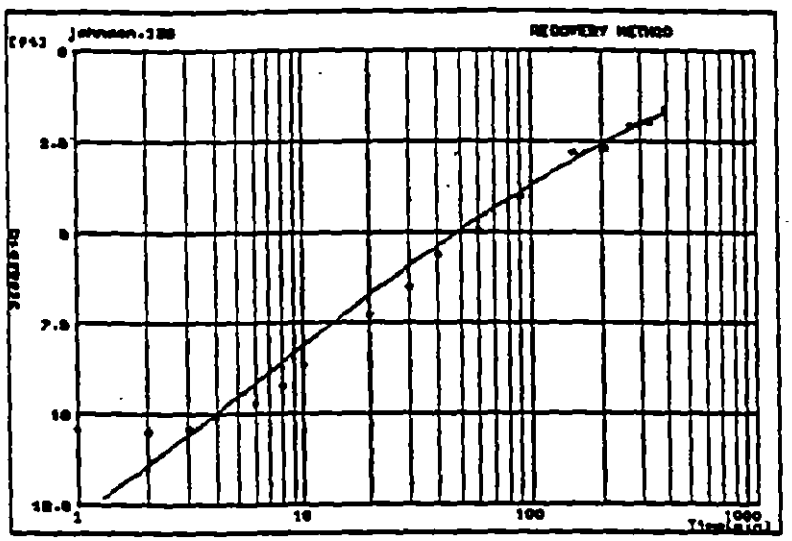


Fig. 3.21A

UN/DTCD — GROUND WATER SOFTWARE Version 1.00
3. PUMPING TESTS December 1989

Dat No	RECOVERY METHOD	1
1	Test Identification Johnson.139	
	Transmissivity = 11889. [gpd/ft] Storage Coefficient = 0.27E-02 Standard Deviation = 0.7164 [ft] A = 0.475248E+01 [ft] Number of Points = 17 of 17	

Working units
d [ft]
t [min]
Q [gpm]
Tr[gpd/ft]

Press any key to continue.

Fig. 3.21B

Dug Well Pump Test Method. A method of analyzing the pumping and recovery phases of large diameter wells based on a Kernel function was recently (January-February 1987) presented by K.R.Rushton and V.S.Singh in the journal of Ground Water. The method was selected by the authors of this software package for the following two reasons:

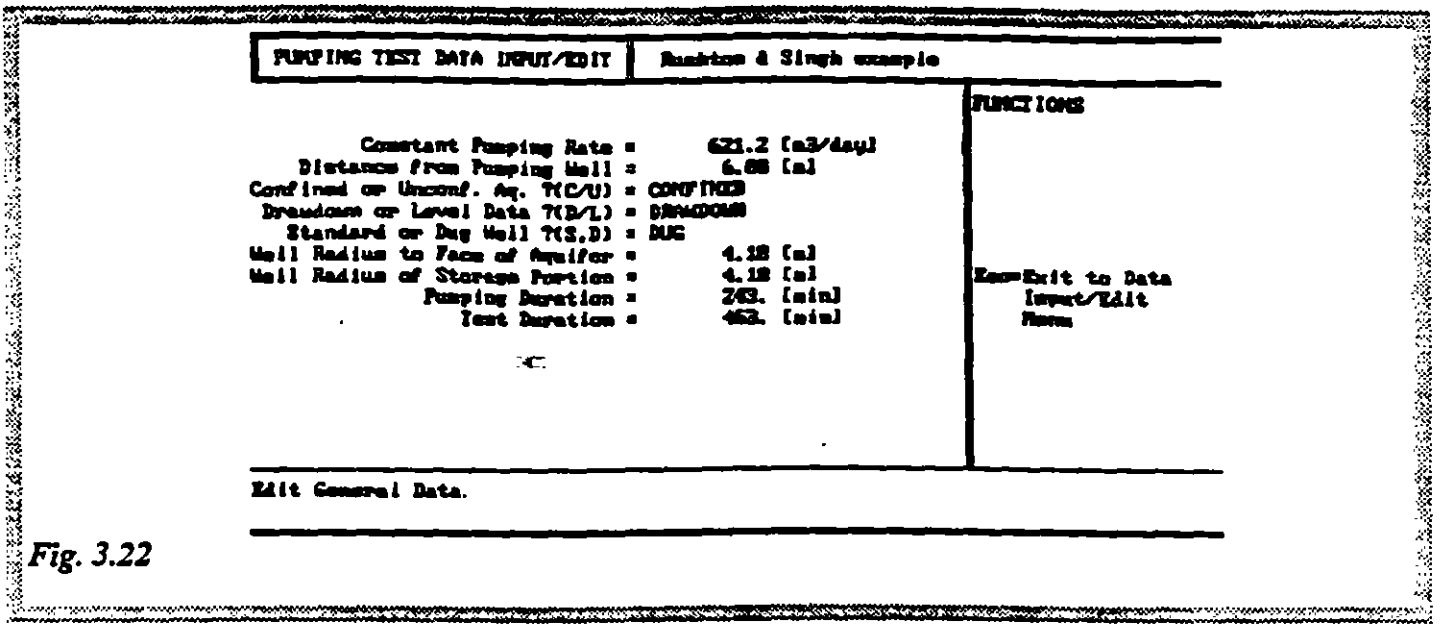


Fig. 3.22

(1) In India alone in early 1985 there were about 8.7 million dug wells. The forecast was that another 1.3 million dug wells shall be constructed over the period of next five years, implying that by the year 1990 there may be about 10 millions dug wells in India alone. It was also reported that in India about 71% of the total ground water draft comes from dug wells.

(2) The method of testing and interpretation needs improvements and a computer program which speeds up the processing may be of great help. As originally programmed by Rushton and Singh, the user was to draw the computer-calculated curve on top of his/her field data every time he/she made a computer run. With this program the whole procedure becomes extremely fast and the interpreter learns in the process about the behavior of test data when either transmissivity or storage coefficient are modified. Yet, as the authors state, the method needs some additional verification.

The use of the test is explained in Figs. 3.22, 3.23, 3.24 and 3.25. Figure 3.22 shows the input data (general) for the well used by Rushton and Singh in their original paper. (As explained before, when you elect to answer

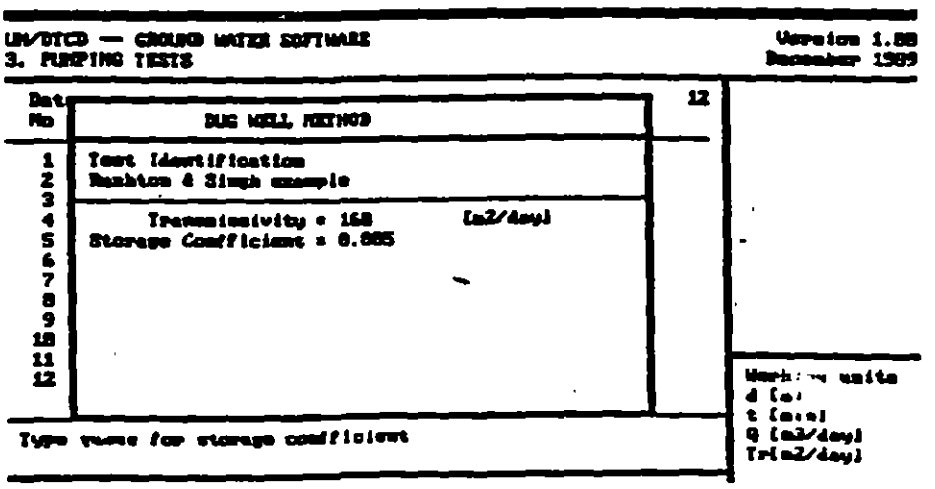


Fig. 3.23

in the Data Input/Edit mode with D the question "Standard or Dug Well?", you must answer several more questions prompted from the screen.) In the Test Analysis mode you are prompted for initial guesses of transmissivity and storage coefficient. The screen looks as shown in Fig. 3.23. The height of the seepage face, which may be correct only in the case of metric units, is still a week point of analysis, as admitted by the authors by saying that "further careful work in a variety of field situations is required to gain a greater understanding of the significance of these coefficients." The coefficients referred to above are G_1 and G_2, which describe the height of the seepage face in the following way:

$$f = G_1 \times Q + G_2 \times Q^2$$

where f is the height of seepage face, Q is the withdrawal rate from the aquifer, and G_1 and G_2 are deduced from field measurements.

The test results are presented in Figs. 3.24 and 3.25. Accepting the transmissivity of 160 m^2/day and storage coefficient of 0.005, with fixed G_1 and G_2 coefficients (0.001 and 0.0001, respectively) the standard deviation for the whole test equals 0.07 m, and the seepage face height at the end of pumping phase equals 0.25 m. The fit is as shown in Fig. 3.25.

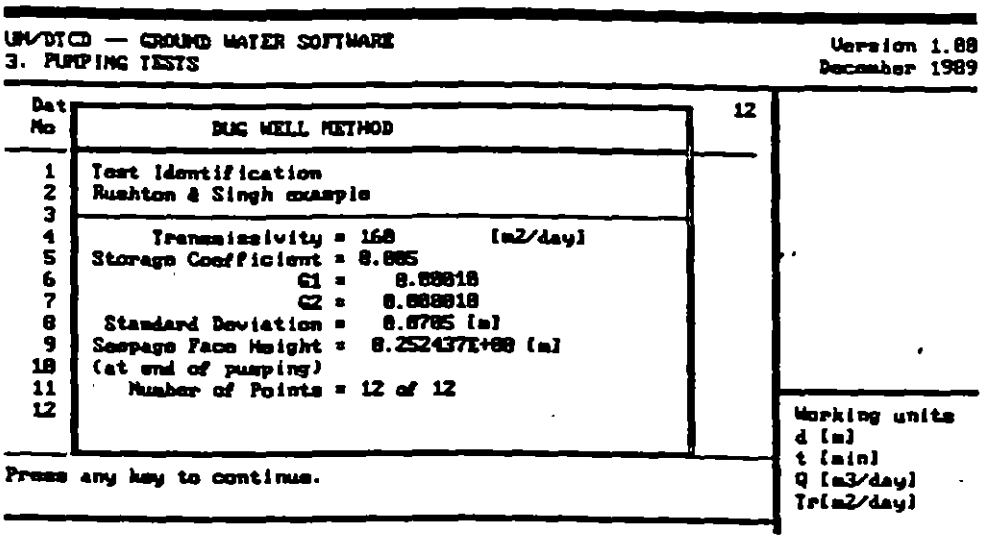


Fig. 3.24

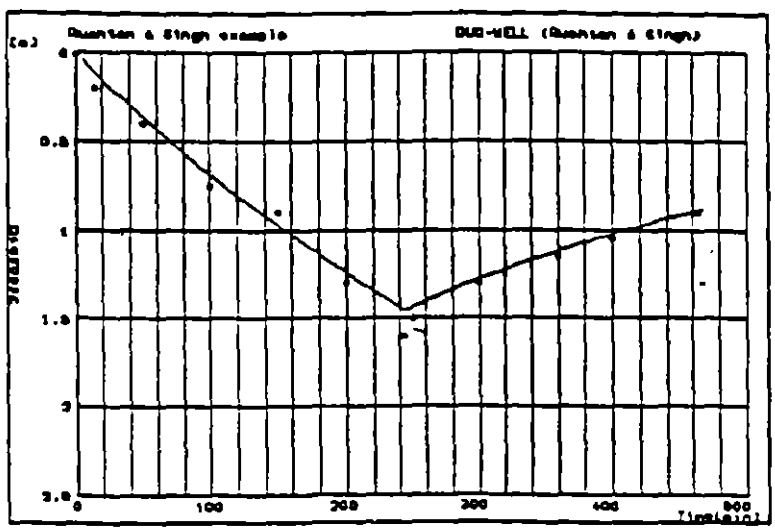


Fig. 3.25

Screen Graphics. The difference between this Screen Graphics and Screen Graphics from the Data Input/Edit Menu is in the following. In the latter, only test data (from data base) were shown on a time-drawdown semilogarithmic graph (arithmetic, in the case of dug wells). In the former, both test data are shown plus the "best fit" with the method selected (calculated with reported values of transmissivity, storage coefficient and, eventually, leakance). It is easy to see whether the parameters calculated by the program satisfy. They will be acceptable if the fit is acceptable.

Print Graphics. The screen discussed above can be printed. The top part of printout is the identification of the project and test, plus some of general data (pumping rate, distance from observation well, aquifer type, etc.). Then the graph is shown, followed by calculated transmissivity, storage coefficient, standard deviation, and, eventually, leakance. The last line is the number of points included in the graph.

Printing Results. The printout of results starts also with project and test identification, plus some general data, followed by calculated values of transmissivity, storage coefficient, standard deviation, etc., and a table with the values of test data in one column, computed drawdown in another column, and difference in still another column.

Plotting Graph. The graph displayed on the screen can be plotted using a HPGL-compatible plotter. The plot size is fixed, that is A4, and only graphical part is drawn.

3.7. Pumping Tests Reported In Literature

The programs presented in this package have been tested against many published pumping tests. The sources of information are the following:

WALTON, W.C., 1969. Selected Analytical Methods for Well and Aquifer Evaluation. Illinois State Water Survey Bulletin 49. Third printing, 1969.
WALTON,W.C. 1970. Groundwater Resource Evaluation. McGraw-Hill.
DeWIEST, R.J.M., 1967. Geohydrology. John Wiley & Sons, Inc.
E.E.JOHNSON, INC. 1966. Ground Water and Wells. UOP Johnson, first edition.
LINSLEY,R.K. and J.B.FRANZINI, 1964. Water Resources Engineering. McGraw-Hill Book Co.

Both published results and computer produced results are presented herein for comparison of methods.
T = Transmissivity P' = Vertical Permeability of Confining Bed
S = Storage Coefficient S.D.= Standard Deviation

1. Well No.19 near Dieterich (Walton, 1969, page 32)

Method: *Leaky Artesian Conditions*

Walton:	Computer:
T=1510 gpd/ft	T = 1791 gpd/ft
S=0.0002	S = 0.00018
P'=0.11 gpd/ft^2	P' = 0.16 gpd/ft^2
	S.D. = 0.127 ft

2. Well No.1 at Gridley (Walton, 1969, page 33)

Method: *Nonleaky Artesian Conditions*

Walton:	Computer:
T=[illegible]0 gpd/ft	T = 9908 gpd/ft
S=0.[illegible]02	S = 0.000021
	S.D. = 0.091 ft

Comment. In the computer program, leaky aquifer method gives slightly better fit. Standard deviation is 0.082 ft, T=9391 gpd/ft, S=0.000022.

3. Well No. 15 near Mossville (Walton, 1969, page 35)

Method: *Water-table conditions with partial penetration*

Walton:	Computer:
T=315,000 gpd/ft	T = 386,712 gpd/ft
S=0.082	S = 0.019
	S.D. = 0.057 ft

4. JOHNSON's book page 111

Method: *Nonleaky confined aquifer*

JOHNSON:	Computer:
T=100,000 gpd/ft	T = 100,630 gpd/ft
S=0.00019	S = 0.0002
	S.D. = 0.007 ft

5. JOHNSON's book page 138

Method: *Recovery*

JOHNSON:	Computer:
T=10,400 gpd/ft	T = 11,089 gpd/ft
	S = 0.00275
	S.D. = 0.71 ft

6. DeWIEST's book, page 265

Method: *Theis nonequilibrium*

DeWIEST:	Computer:
T=20,500 gpd/ft	T = 26,210 gpd/ft
S=0.000315	S = 0.00030
	S.D. = 0.67 ft

Comment: Hantush leaky method provides better fit. The results are the following:

T = 15,991 gpd/ft
S = 0.00043
S.D. = 0.135 ft
P'/m' = 0.02 1/day

7. DeWIEST's book, page 267

Method: *JACOB*

DeWIEST:	Computer:
T=4860 gpd/ft	T = 4933 gpd/ft
S=0.0045	S = 0.00427
	S.D. = 0.146 ft

8. WALTON (1970, page 283)

Method: *Theis nonequilibrium method*

WALTON:	Computer:
T=358,000 gpd/ft	T = 358,889 gpd/ft
S=0.00047	S = 0.000395
	S.D. = 0.043 ft

9. WALTON (1970, page 286)

Method: *Leaky artesian aquifer*

WALTON:	Computer:
T=182,000 gpd/ft	T = 219,227 gpd/ft
S=0.002	S = 0.002
P'=0.87 gpd/ft^2	P '= 0.54 gpd/ft^2
	S.D. = 0.008 ft

10. LINSLEY & FRANZINI (1964, page 88)

Method: *Theis nonequilibrium*

L & F:	Computer:
T=11,800 gpd/ft	T = 10,752 gpd/ft
S=0.0478	S = 0.0495
	S.D. = 0.258 ft

Method: *Jacob's approximation*

T=12,000 gpd/ft	T = 12,283 gpd/ft
S=0.0402	S = 0.0388
	S.D. = 0.145 ft

Comment: First five minutes are excluded in both cases.

Well Hydraulics and Well Construction

4.1. General

This program requires about 305,000 bytes user-available memory. Video adapter is not required. Mathematical co-processor is not required. There is no printer output. Four files are mandatory and each of them must be copied to the \GW directory: GW4.EXE, UN4.CMN, UN4.MST, UN4.WND.

4.2. Program Overview

The program GW4 – Well Hydraulics and Well Construction – has three major parts: (1) Well Functions, (2) Pumping Tests, and (3) Well Construction. Each of the three parts has several subprograms. Primarily, it is a utility program for pumping tests, well hydraulics and well construction.

This program is a collection of many problem-solving routines from everyday well-construction and testing practice. It will not save input data in a form of a data base. The results should be hand written if needed. Same as in other programs in this series, pressing ESC returns the program (screen) one step back, or exits to the main program. Functions are activated by selecting the appropriate single letter command.

When you start the program by typing GW and selecting "4. Well Hydraulics and Construction" from the main menu, the program's main menu appears as shown in Fig. 4.1. From the main menu you may select units, then select either FUNCTIONS, PUMPING TESTS and WELL CONSTRUCTION.

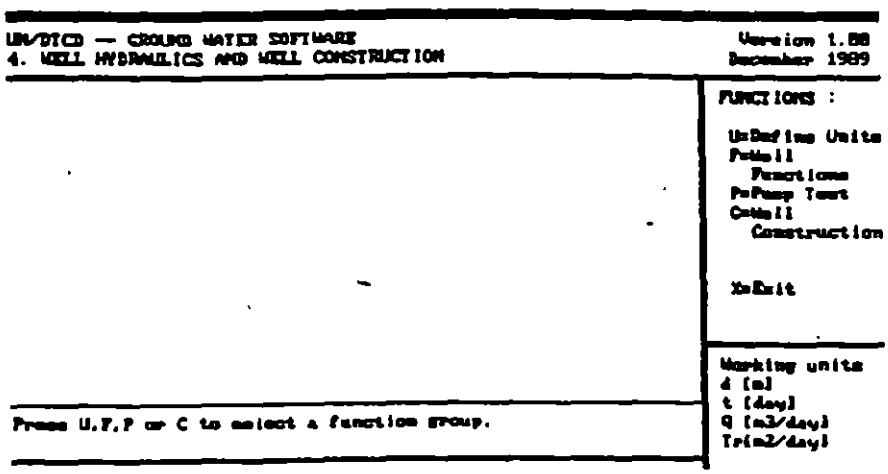


Fig. 4.1

FUNCTIONS, shown in Fig. 4.2, are well functions frequently used in ground water hydraulics. The first one, W(u), is the well function for the infinite artesian aquifer in which a well is pumped at a steady rate. The second well function is the function used in Hantush leaky aquifer theory. The next one is a well function used in partially penetrating wells pumping from anisotropic aquifers. Further, two Bessel functions are also included, same as error and complementary error functions, which are used in many specific cases.

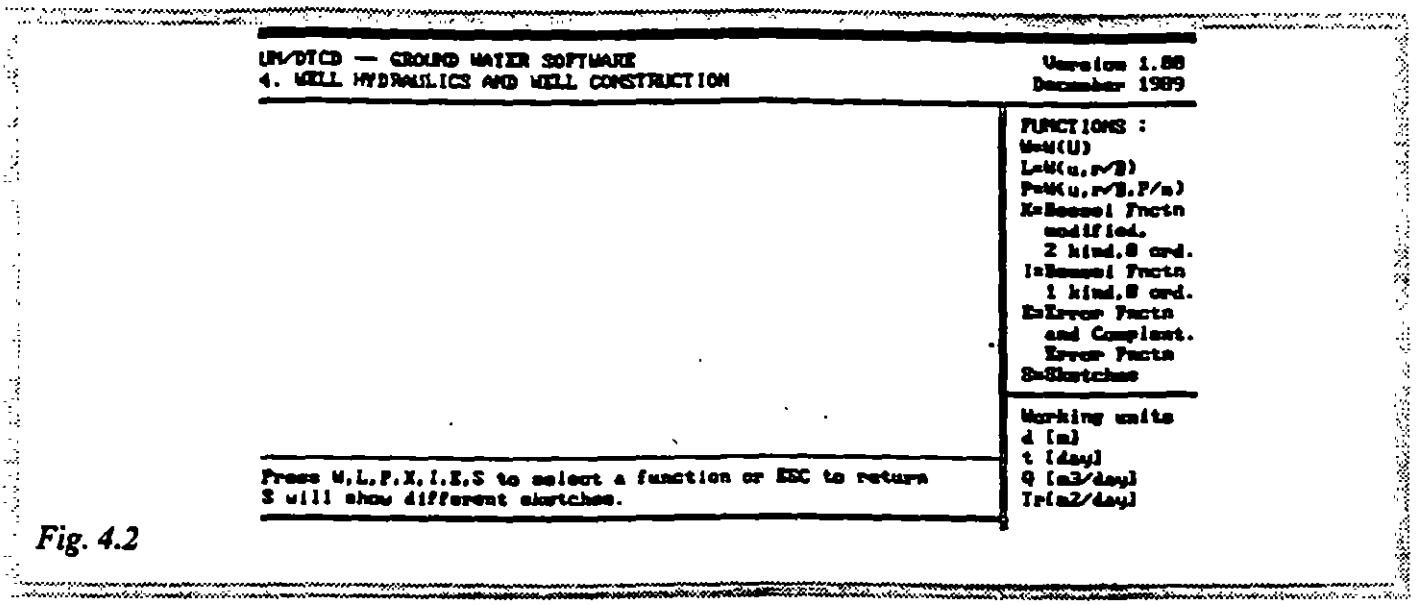


Fig. 4.2

PUMPING TESTS program, shown in Fig. 4.3, contains two subprograms dealing with step-drawdowns tests (also called well-production tests; Q to power 2 and to "n" power), a routine to calculate pumping rate from a circular orifice weir, a routine for estimating discharge from a flowing artesian well, etc.

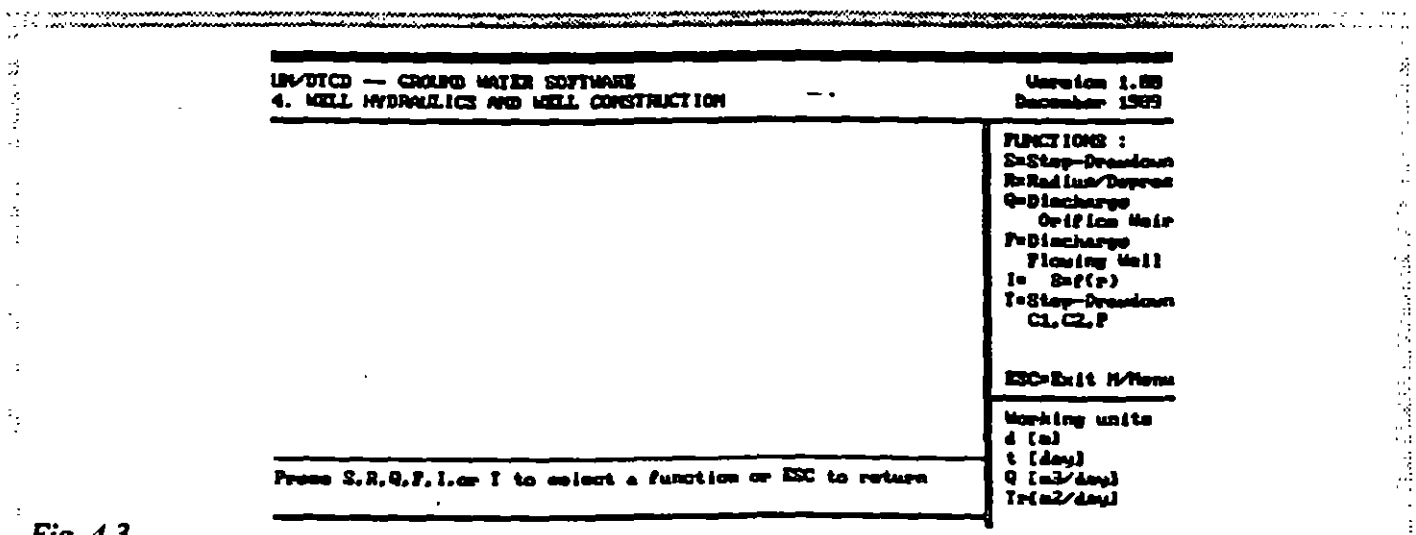


Fig. 4.3

WELL CONSTRUCTION, shown in Fig. 4.4, helps to calculate maximum permissible entrance velocity to screen. Actually it offers a recommendation for selecting optimum screen length as a function of discharge, well diameter, open screen area, and aquifer permeability. There are also some other subprograms that make recommendations as to which drilling diameter to select for a particular pump discharge, etc.

All the time, in every program or subprogram, the right lower corner displays currently selected working units.

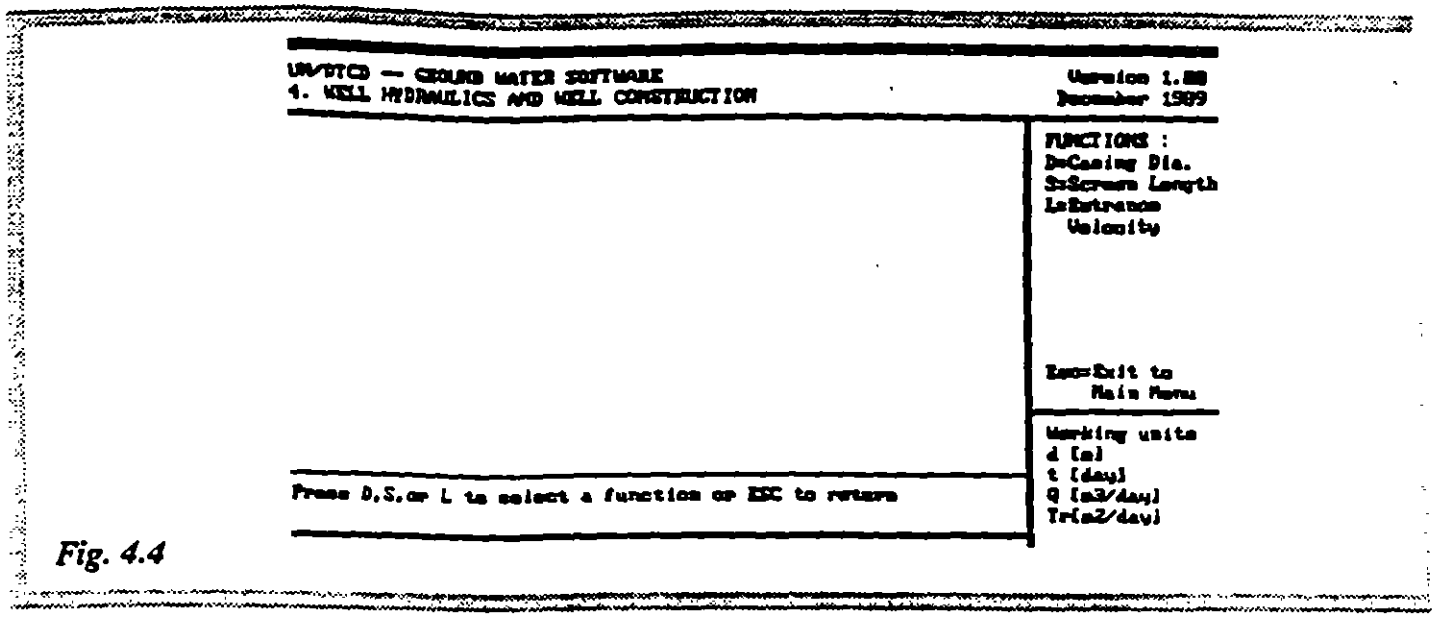


Fig. 4.4

4.3. Well Functions

After you select WELL FUNCTIONS by typing the letter F from the main menu, you can choose among the following functions (Fig. 4.2):

W = W(u)
L = W(u,r/b)
P = W(u,r/b,P/m)
K = Bessel Function, modified, 2 kind,0 order.
I = Bessel Function, 1 kind,0 order.
E = Error Function and Complementary Error Function
S = Sketches
ESC = Exit M/Menu

4.3.1. W(u)

You select this function by typing W from the well functions menu. W(u) is the well function for a nonleaky isotropic artesian aquifer fully penetrated by wells and constant-discharge conditions. In other words, this is the standard well function for the most common case of ideal representation of confined aquifers. When this function is multiplied by Q/(12.5664 T), where Q is the constant pumping rate and T is the transmissivity of the aquifer, the drawdown in the well is obtained.

You can display the sketch of a confined aquifer on the screen by typing the letter S (sketch), followed by letter A (see Figure 4.5).

The theory leading to the nonequilibrium equation, or Theis theory, is well documented in every ground water textbook, and will not be repeated here. The well function is tabulated as a function of the argument u, which lumps together two most important aquifer parameters (transmissivity and storage coefficient), distance from pumping well at which the drawdown in calculated, and time since the start of pumping.

Thus, the argument u is equal to

$$u = r^2S/4Tt$$

where, r is the distance from pumped well to observation point, or to point at which drawdown is being calculated; S is the storage coefficient; T is coefficient of transmissivity; t is time after pumping started.

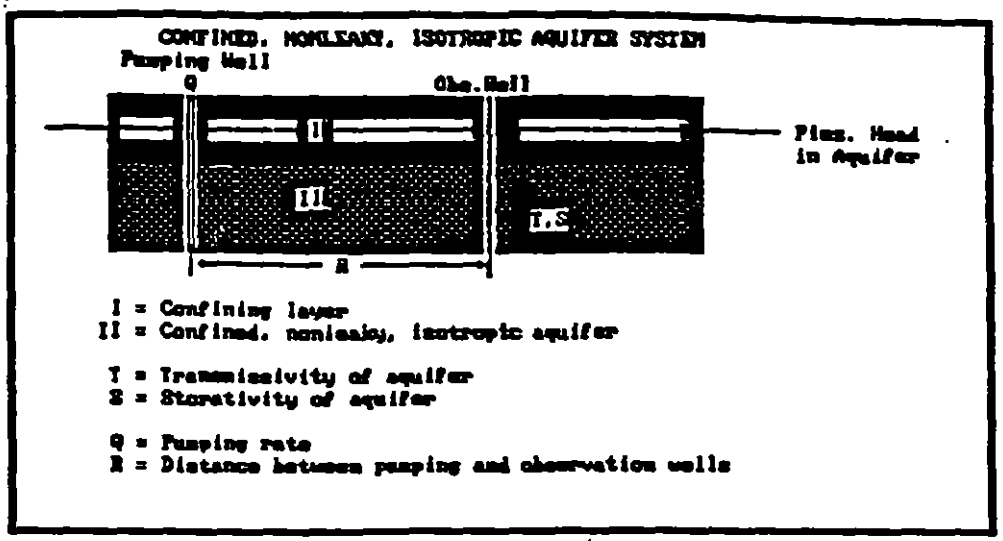


Fig.4.5

Drawdown, as a function of r and t, is expressed as follows:

$$s = (Q/12.56\,T) \times W(u)$$

This part of the program prompts you to input all parameters that define the argument u. First, you have to input the distance from pumped to the observation point, then the storage coefficient, the transmissivity, and the time of pumping. At that point the argument u and well function W(u) are displayed on the screen (Fig. 4.6). You will be finally prompted for well discharge if the drawdown is to be calculated. Alternatively you may press ESC key to terminate this portion of the program.

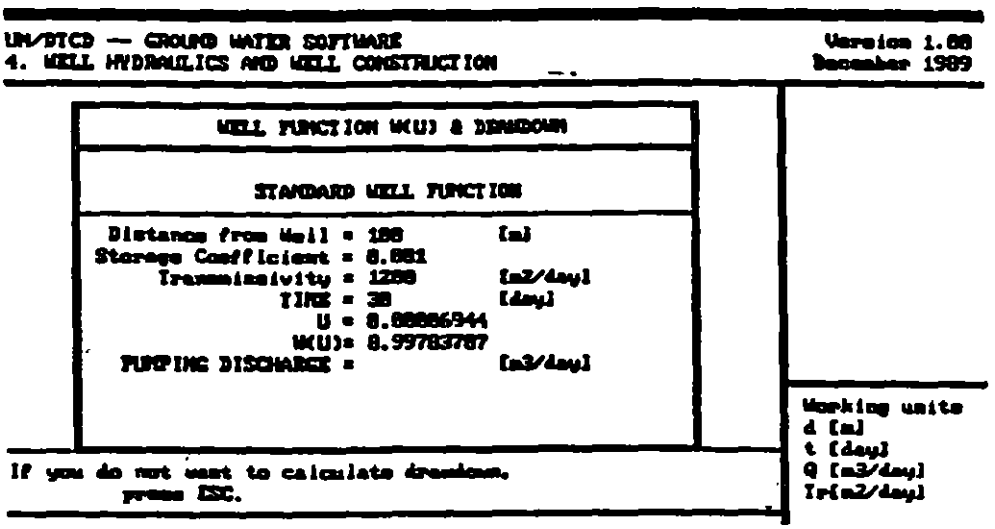


Fig. 4.6

The calculation of the well function W(u) and drawdown at a specific point may be repeated over and over to produce a total drawdown at a point which may be under influence of pumping from several wells. You may add individual drawdowns by writing them down on paper.

The correspondence between computer-produced well functions for particular values of the argument u and tabulated values in textbooks is demonstrated with following examples.

(1)	r = 10 m	(2) r = 100 m
	S = 0.001	S = 0.001
	T = 1000 m^2/day	T = 3000 m^2/day
	t = 10 days	t = 30 days
	u = 2.5×10^{-6}	u = 2.8×10^{-7}
	W(u) = 12.3220062	W(u) = 14.5192289

Tabulated values (Walton, 1970; Wenzel, 1942; De Wiest, 1965; etc.)

W = 12.322 u = 2.5×10^{-7} W(u) = 14.62

u = 3.0×10^{-7} W(u) = 14.44

4.3.2. W(u,r/B)

You select this function by typing the letter L (stands for "leaky") from the WELL FUNCTIONS menu. This routine calculates the well function for a leaky artesian aquifer with fully penetrating wells without water released from storage in aquitard and under constant-discharge conditions. Although the values of W(u,r/B) in terms of practical range of u and r/B are given by Hantush (1956) in tabular form, this portion of the program calculates not only the function W(u,r/B) but also the arguments u and r/B from basic hydrogeological and pumping parameters.

These parameters are, in the following order:

r, S, T, t, P, m

where:

r = distance from pumped well
S = storage coefficient
T = transmissivity
t = time of pumping
P = vertical permeability of semiconfining layer
m = thickness of semiconfining layer.

Of course, all units must be consistent, or as selected at the beginning of the program (see right lower corner: Working Units). Storage coefficient is dimensionless (fraction); time, distance and transmissivity are reported in the units you selected at the beginning. Permeability and thickness of semiconfining layer must be in working units of length over time (permeability) and length (thickness). Thus, if American or British units are used, you may not input for permeability gpd/ft. The correct units would be ft/day if foot was selected for distance and day for time. Some conversion hints are shown on the message line.

The sketch of a leaky system is shown in Fig. 4.7. The same display can be obtained by selecting letter S (for Sketch), followed by letter B. The situation could be reversed: the upper layer may be leaky (semiconfining)

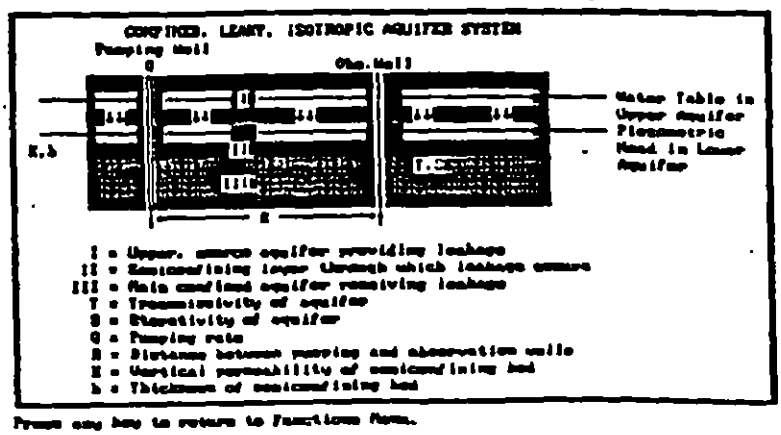


Fig. 4.7

providing water from above, and the lower layer could be absolutely impermeable. The solution is still the same.

The parameter B, which is important in the Hantush leaky aquifer theory, is defined as follows:

$B^2 = (T/P/m)$

The ratio r/B is dimensionless.

After you answer all prompts for input parameters, the program displays the values of the arguments B and u, and the value of the function W(u,r/B). Finally, you will be prompted for pump discharge and the value for drawdown is calculated and displayed (Fig. 4.8).

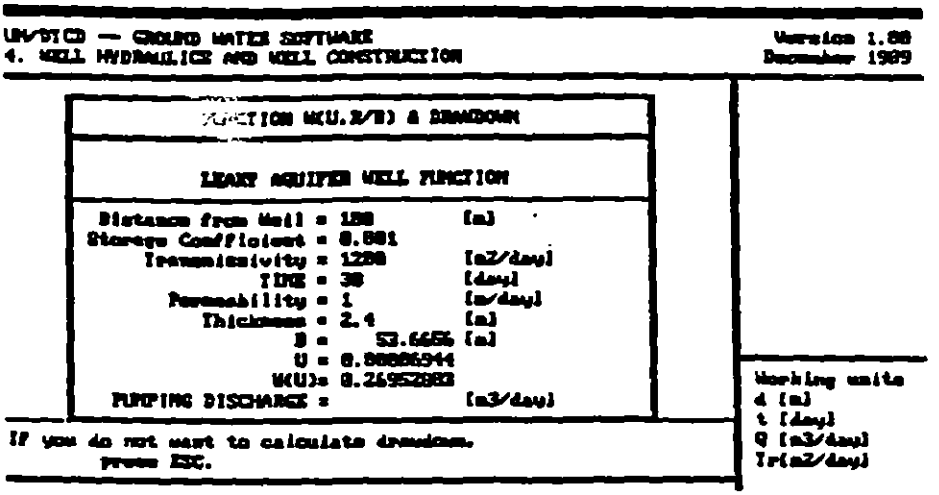


Fig. 4.8

As an example, the following parameters are input:

r = 15 m
S = 0.001
T = 2000 m^2/day
t = 30 days
P = 1 m/day
m = 5 days

The program-calculated values are the following:

B = 100.00 m
u = 0.00000094
W(u)= 4.06005

(The "book" value for W(u,r/B) is 4.0595.)

For pumping discharge Q=2000 m^3/day, the calculated drawdown is 0.323 m.

4.3 P(u,r/B,Pv/Ph)

You select this function by typing the letter P from the WELL FUNCTIONS menu. This is the well function for a nonleaky anisotropic aquifer with partially penetrating pumping and observation wells, and steady-state conditions. The following parameters are required (in this order the program prompts for input):

R = distance from pumped well
m = aquifer thickness
P_v= vertical permeability of aquifer
P_h= horizontal permeability of aquifer

L = penetration length (length of penetration of pumping well from the top of aquifer)
D = distance to screen (vertical distance from the top of aquifer to top of screen)
Y = observation well length

A sketch of definitions for parameters is shown in Fig. 4.9.

The program returns several ratios (R/m, L/m, D/m, Y/m), and a well function which, when multiplied by the value of 0.16*Q/T, returns the value of drawdown under steady-state conditions.

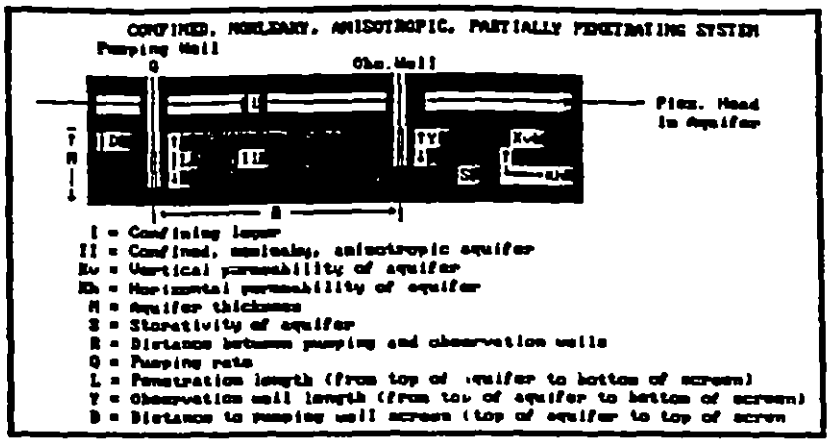


Fig. 4.9

4.3.4. Ko(r/B)

You select this function by typing the letter K from the WELL FUNCTIONS menu. When discharge from a well (aquifer) is balanced by leakage in the case of a leaky aquifer and water levels stabilize at permanent stages, a steady state is reached. The solution for drawdown under such conditions is described by the following equation:

$$s = [Q/6.28\ T]xK_o[r/b]$$

where $K_o(r/B)$ is the modified Bessel function of second kind and zero order. This function is frequently used in leaky aquifer theory. This is also a tabulated function, but in this program the input parameter is not the argument of the function, r/B, but a value calculated from hydrogeological and pumping information.

You will be prompted to provide the values of vertical permeability and thickness of semiconfining layer through which the leakage takes place. The storage coefficient is of no importance under steady-state conditions because the entire yield of the well is derived from leakage only. For example, when

r = 100 m
P = 0.1 m/day
m = 5 m
T = 1000 m^2/day

r/B shall be 0.4472, and $K_o(r/B)$ 1.0182. The "book" value for $K_o(r/B)$, when r/B=0.45, is 1.0129.

In this case, if the well is pumped at 2000 m^3/day, the steady-state drawdown will be equal to 0.32 m.

4.3.5. Io(r/B)

You select this function by typing the letter I from the WELL FUNCTIONS menu. This is the zero-order Bessel function of the first kind. It appears in several equations describing unsteady-state radial flow in isotropic or anisotropic leaky artesian aquifers. The argument r/B is defined in the following way.

$$B^2 = T/P/m$$

where:

T = transmissivity of aquifer
P = coefficient of permeability of aquitard (semiconfining layer)
m = thickness of aquitard
r = effective radius of well, or distance to observation well

4.3.6. Error and Complementary Error Functions

You select these functions by typing the letter E from the WELL FUNCTIONS menu. The error function, erf(x), and its complementary function, erfc(x), frequently appear in ground water hydraulics. They are defined in the following way:

$$erf(x) = 1\text{-}erfc(x) = 1.1283778 \times_0 \{\text{Integral } [\exp(-y^2)\, dy]\}$$

The program prompts for only the value of x and returns the values of error function and complementary error function for x. The error function is used, e.g., in calculating unsteady-state radial flow in isotropic leaky artesian aquifer with fully penetrating wells with water released from storage in aquitard.

4.4. Pumping Tests

The pumping tests program offers several subprograms for testing well performance and/or measuring pumping discharge during a pumping test. In addition, one subprogram makes possible the determination of aquifer parameters (transmissivity and storage coefficient) if three or more observation wells are available.

The following menu appears when you select letter P (pump test) (Fig. 4.3):

S=Step-Drawdown
R=Radius/Depression
Q=Discharge Orifice Weir
F=Discharge Flowing Well
I= S=f(r)
T=Step-Drawdown C_1,C_2,P
ESC=Exit M/Menu

Step-Drawdown Test. Since this is a test of productivity of a well, it is often called well-production test. This is a variable-rate well-production test. Well is pumped at a constant rate for a certain period of time (between one and 24 hours) and drawdown is recorded at the end of the pumping step. Pumping rate is then changed, normally increased, and well is pumped for the same period of time. Water level is measured and drawdown calculated. The same procedure is repeated with different pumping rates one or more times (minimum 3 steps). It is understood that each step must be of the same duration as the others.

According to classical theory, the total drawdown in a production well has two major components: the drawdown s_a (aquifer loss) due to laminar flow of water through the aquifer toward the well and s_w (well loss) due to the turbulent flow of water through the screen or well face and inside the casing to the pump intake. Other components, such as additional drawdown due to the partial penetration of an aquifer, or the drawdown due to barrier boundaries of the aquifer or the build-up due to recharge boundaries of the aquifer, are normally contained within the aquifer loss.

According to Jacob (1946), well loss may be represented approximately by the following equation

$$s_w = C_2Q^2$$

where

s_w = well loss, [L]
C_2 = well-loss constant, [T^2/L^5]
Q = discharge, [L^3/T]

Aquifer loss, s_a, is linearly proportional to pumping rate, i.e.

$$s_a = C_1Q$$

Thus the equation of total loss during pumping may be written as

$$s = C_1Q + C_2Q^2$$

When a well is pumped with three or more steps, the computer subprogram makes it possible to estimate th values of coefficients C_1 and C_2.

You are prompted to input the values of drawdowns and pumping rates for each step. The minimum require number of steps is three and the maximum is five. (In most cases, three is the actual number of pumpin steps.)

After all pairs of values are input (Fig. 4.10), the screen displays the values of coefficients for aquifer loss (C and well loss (C_2). On the second screen, which is shown after any key is pressed, there will be a table showin

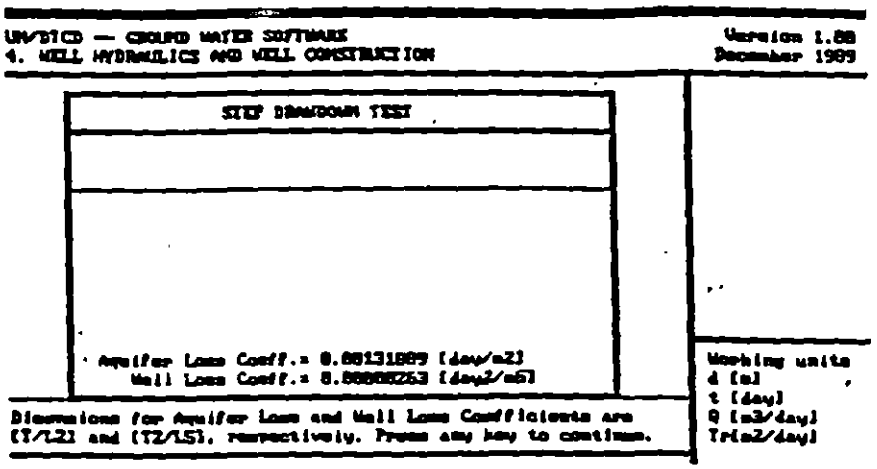


Fig. 4.10

actual drawdowns for each step, plus aquifer loss and well loss for particular step. In addition, well efficiency will be calculated and displayed for each step (Fig. 4.11). Well efficiency, in this case, is defined as the ratio of aquifer loss to measured drawdown. This is equivalent to saying that aquifer loss is unavoidable but all well losses could have been avoided provided that the well had been correctly constructed (large enough casing diameter, below-critical entrance velocity, proper gravel pack, proper development, pumping rate commensurate with well construction and aquifer potential, etc.).

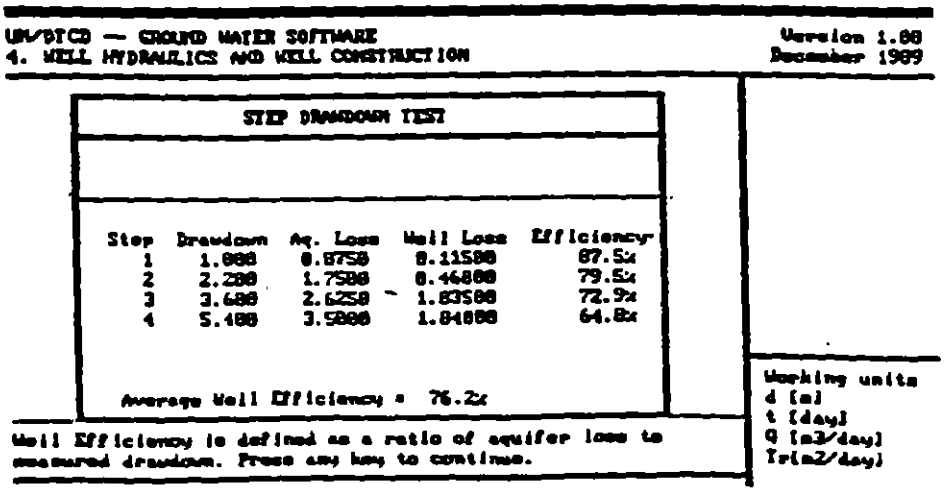


Fig. 4.11

The use of the subprogram is demonstrated with an example from the Walton's book (1970, p.357). A variable pumping-rate well-production test was conducted with the following results:

Step	Pumping rate gpm	Drawdown ft
1	100	3.25
2	151	5.72
3	199	8.53

Before entering the test values, you should select as working units feet for distance and gpm for pumping rate. After you input all three pairs of drawdown-discharge values, the screen displays the values of coefficients C_1 and C_2:

Aquifer loss = 9.959397 sec/ft^2

Well loss = 21.371817 sec^2/ft^5

After you press any key, the second screen displays a table of measured drawdowns and calculated aquifer loss and well loss. Finally, the last column displays well efficiency defined as a ratio of aquifer loss to measured drawdown. The results are as follows:

Step	Measured drawdown ft	Aquifer loss ft	Well loss ft	Well efficiency %
1	3.25	2.2044	1.04698	67.8
2	5.72	3.3286	2.38723	58.2
3	8.53	4.3867	4.14616	51.4

Average efficiency = 59.13%

In Walton (1970), the well loss coefficient equals 21.6 sec^2/ft^5, and well loss for pumping rate of 152 gpm equals 2.46 ft.

Radius of Depression. You select this function by typing the letter R from the PUMPING TESTS menu. The formula for the radius of depression, which is derived from the nonequilibrium equation in the case of an infinite artesian isotropic and homogeneous aquifer without any recharge from the surface, is equal to

R = {Square Root of} (2.25*T*t)/S

where

T is aquifer transmissivity
t is duration of pumping
S is storage coefficient

The expansion of cone of depression during constant-rate pumping to almost infinity is a rather ideal situation. It does not consider any boundary, whether recharging (which might slow down or stop the expansion of depression) or less permeable (which might make the expansion faster). The use of the formula should be restricted to rather limited spread of depression, say of at most several ten kilometers.

The program prompts for the values of transmissivity, storage coefficient and time. The output is the radius of depression for ideal conditions of an artesian, isotropic, homogeneous, infinite aquifer.

Example:

T = 2000 m^2/day	T = 50,000 gpd/ft
S = 0.001	S = 0.0001
t = 10 days	t = 30 days
R = 6708.2 m	R = 67,165.7 ft

Circular Orifice Weir – Pumping Discharge Measurement. The circular orifice weir is one of most commonly used devices to measure the rate of discharge from a pump. The details of construction of an orifice and the measuring setup are explained in several books (*Ground Water and Wells*, Johnson Division, 1972). The program contained in this ground water software helps to calculate the discharge rate when discharge pipe

diameter, orifice plate diameter and the height of water column in the piezometric tube (head) are known. Numerous combinations of pipe and orifice sizes and applicable tables are available. This program closely follows a standard developed at the Engineering School of Purdue University.

The program prompts for pipe diameter, orifice diameter and water column height. This is the only subprogram in this package which overrides the working units. No matter which units you have selected, the input for pipe and orifice diameters, as well as for the head, must be in inches. The output is in gpm, m^3/day and l/sec.

Example (Fig. 4.12): Pipe diameter = 6 in.
Orifice diameter = 4 in.
Head = 5 in.

Discharge rate = 142.8 gpm
= 778.3 m^3/day
= 9.01 l/sec

The values obtained from the program correspond within 2-3% to the values reported in 103-D-1468 (*"Measurement of Water Flow through Pipe Orifice with Free Discharge", Purdue University, Lafayette, Ind., 1949*).

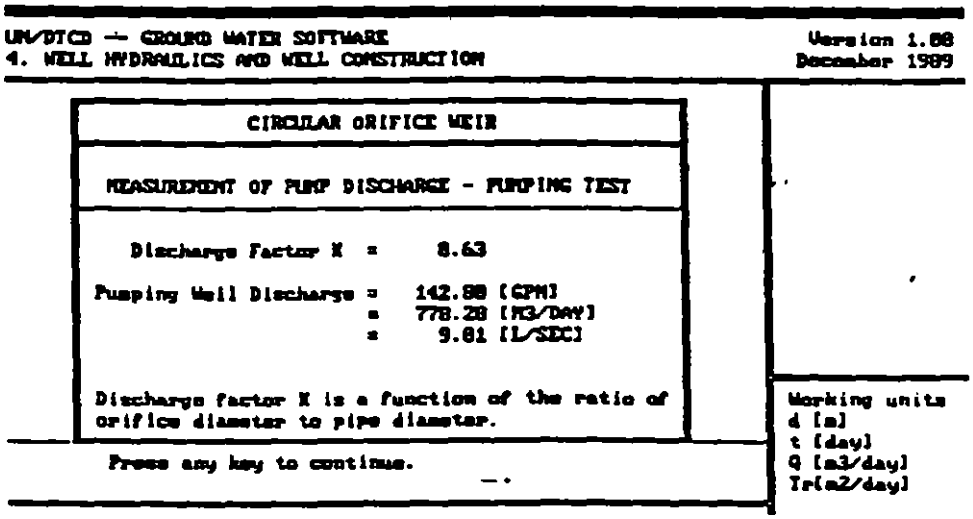


Fig. 4.12

Discharge from Flowing Wells. The dimension of a stream flowing from an open pipe, either vertical or horizontal, can be used to obtain a rough estimate of the flow rate. This subprogram calculates the free flow from a vertical pipe when the diameter of the pipe and the height to which the water rises above the pipe are known. The basis for the estimate is the classical formula for velocity head, $V^2=2gh$, where g is acceleration due to gravity, and h is the head. The final results, with appropriate correction factors, are close to flow rates from Lawrence and Braunworth data (*"Fountain Flow of Water in Vertical Pipe", Transactions, 1906, vol.57,p.264, ASCE*).

The major prerequisite for the application of the program is that all water from the well flows upward through the pipe and that there is no any flow bypassing the pipe and reappearing at the surface from the borehole annulus. The flow must be sufficiently constant so that the height of water does not vary appreciably. The vertical pipe should be a straight length, not less than 0.9 m (3 ft) long, so that the open end is at least this far above from the nearest elbow, bend, or valve. Also, the values are for standard steel pipe with smooth inner surfaces.

The program produces rather correct values for the height of water of at least 10 cm (4 inch), from a pipe diameter 2 to 8 inches.

Example: Nominal diameter of pipe = 6 in.
Height of crest = 10 in.
Q = 576.32 gpm

(Value from a table in "Ground Water and Wells, 1972, is 580 gpm.)

NOTE: In this program you may select any units. The flow will be displayed in selected units for discharge.

Distance-Drawdown Method for Calculating Aquifer Parameters. When Jacob's approximate solution to Theis nonequilibrium formula is solved for drawdown as a function of distance, for a fixed time, the following is obtained:

$$s = [(0.183xQ)/T]x\log(2.25Tt/S) - (0.366Q/T)x\log r$$

where

s = drawdown at a distance r
Q = constant pumping discharge
T = aquifer transmissivity
t = time of pumping
S = storage coefficient
r = distance from pumped well

Since this is an equation of straight line in the "s" – "log r" system, one may calculate aquifer parameters T and S if three or more observation wells are available during the pumping test. It is a standard routine in aquifer evaluation tests to plot drawdowns on a semilog paper, with drawdowns on arithmetic scale and distances on logarithmic scale. The straight line equation becomes equal to

$$s = A_o + A_1 \log r$$

Transmissivity is calculated from the slope (coefficient A_1) of the straight line "delta s" (change of drawdown between any two points one log cycle apart)

$$T = 0.366Q/\text{delta S}$$

and storage coefficient from the coefficient A_o and known T,

$$S = 2.25\ Tt\ x\ \exp(-12.56\ A_oT/Q)$$

Example:

From Walton's book (1972, p.284, problem 4.2)

Distance from production well ft	Drawdown ft
100	8.40
1,000	5.65
10.000	2.84

When these three pairs are input as prompted by the program, the following values are obtained:

T = 94,784.39 gpd/ft
S = 0.000527

and the fit between measured and calculated drawdowns is displayed:

Well	Meas. drawdown (ft)	Calc. drawdown (ft)
1	8.40	8.41
2	5.65	5.63
3	2.84	2.85

The results in Walton's book are: T=93,000 gpd/ft; S=0.0006.

Step-Drawdown Test with Well Loss Proportional to "n" Power of Q. This program differs from Step-Drawdown part of the program (letter S) in the following way. The first program assumes that aquifer loss is linearly proportional to pumping rate, while well loss is proportional to Q raised to second power. This part of the program is in line with Rorabaugh's (1953) finding, according to which n is not fixed to 2, but varies according to aquifer and well situation from less than 2 to 3.5. Values of n less than 2 may occur if Q is relatively low and full turbulence has not yet developed in the entire well-entry flow. For very low values of Q, the flow may even be laminar throughout the system, in which case the well loss coefficient will be zero. To conclude, the basic formula for drawdown is

$$s = A\,Q + B\,Q^n$$

The computer program prompts you for three or more pairs of drawdown – discharge values. After all values are input, the aquifer and well loss coefficients are displayed, together with the power of the Q term. The measured drawdowns are compared with computed drawdowns, and the average well efficiency is displayed. Efficiency is defined as the ratio of aquifer drawdown to total drawdown, "declaring" all well losses as inefficient and unnecessary.

Example.

From Bouwer (1978) book "Groundwater Hydrology" (Fig. 4.13):

Q(m^3/day)	1000	2000	4000
s(m)	4.56	10.74	29.48

graphical calculation produced the following values:

$n = 2.3$ $A = 0.004$ $B = 7 \times 10^{-8}$

The program calculates the following:

$n = 2.3$

$A = 0.004$

$B = 6.76 \times 10^{-8}$

and an average well efficiency of 76.5%. Thus average well loss component is about 23.5% of the drawdown.

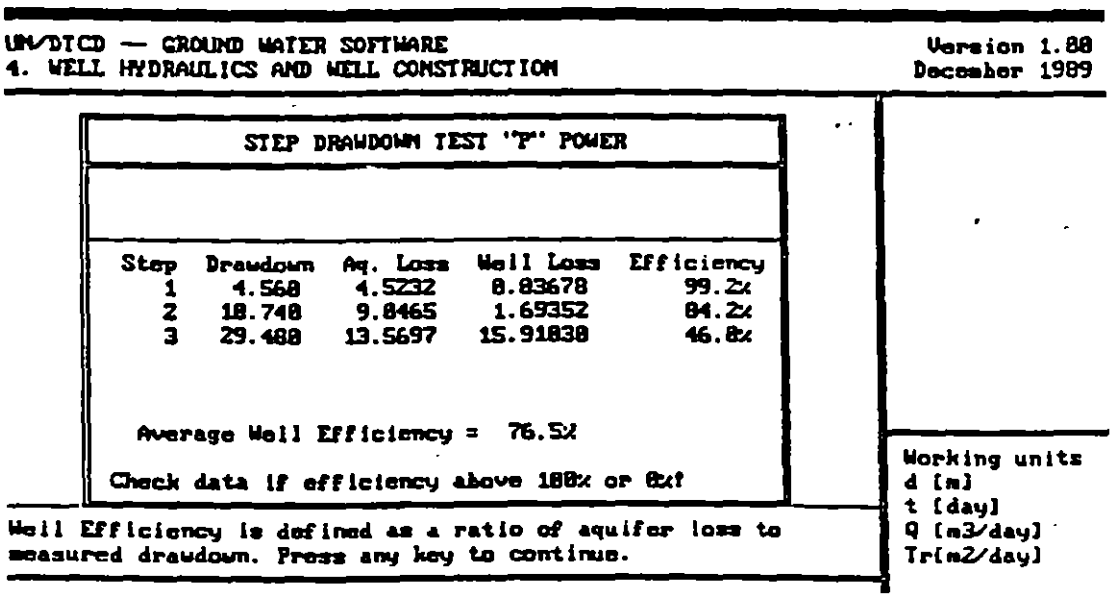


Fig. 4.13

The step-drawdown test gives information regarding the relation between pumping rate and drawdown of a given well. This is important in selecting the optimum pump and depth of pumping. The test also shows how much head loss occurs in the aquifer, and how much in and around the well. Excessive well losses indicate poor design and construction, poor development of the well, or deterioration of the screen.

4.5. Well Construction

General. This portion of the program deals with several subprograms that help to select proper casing diameter, proper screen length, to evaluate whether the screen entrance velocity is eventually above a critical velocity, etc.

The following menu appears after you type the letter C from the main menu (Fig. 4.4):

D=Casing Dia
S=Screen Length
L=Entrance Velocity
ESC=Return to M/Menu

Casing Diameter. The program relates the design pumping rate of the well with optimum casing diameter. The diameter of the production-well casing should be two nominal sizes larger than the bowl size of the pump to prevent the pump shaft from binding, to reduce head losses, and to allow measurement of water levels in the well. The casing diameter may be reduced below the maximum anticipated pump setting depth. Suggested casing diameters for various pumping rates are calculated by this subprogram according to recommendations in Walton (1972, p.299).

The program prompts for only one parameter, the pumping rate of the well (Fig. 4.14). When this is answered, the optimum (recommended) casing diameter is displayed in inches. (This is one of rare routines in this package in which the result is in inches no matter what is the unit for length.)

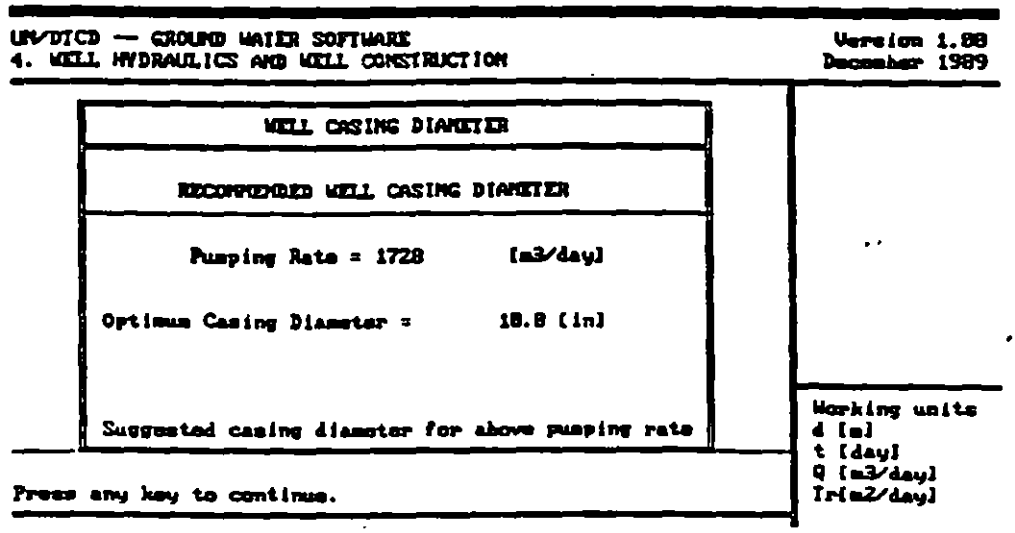


Fig. 4.14

Examples:

Pumping rate	Casing diameter
1728 m^3/day	10 in.
3000 gpm	24 in.
35 l/sec	12 in.

The open area of a screen increases with the diameter of the screen. Thus selection of the production-well diameter may depend upon the desired open area rather than the probable pump required. Yet, the result of this program may be a first step in selecting the correct casing diameter.

Screen Length. The recommended screen length is a function of entrance velocities into the well. The screen length as calculated in this program is based in part on the effective open area of a screen and an optimum (critical) screen entrance velocity. If the length of a screen is less than recommended, implying higher entrance velocities than permitted, there will be a possibility of clogging screen openings by migration of finer particles from aquifer toward the screen. This process, and critical screen entrance velocity, depend largely on the type of aquifer material, which is reflected in aquifer permeability. Thus the input to the program consists of two components: (a) open screen area, (b) selected critical (optimum) entrance velocity. The first may be known for a particular screen, or it may be calculated from another subprogram in this package (section L – entrance velocity) in which the parameters are screen diameter, percentage of open area of the screen, and screen

length. If "1" is selected for the screen length, with known screen diameter and percentage of open area, the screen open shall be calculated and displayed per one unit length of the screen (e.g. m^2/m). This value can then be used in the "S" portion of the program to calculate a recommended optimum screen length.

The second input parameter, optimum (critical) screen entrance velocity, as a function of aquifer permeability, is displayed on the screen suggesting to you which value to choose.

Example: From program "L" - screen diameter = 0.2 m (8 in.)
screen length = 1 m
open area = 11%

Result: Open screen area = 0.069 m^2/m
In program "S" - open screen area = 0.069 m^2/m
entrance velocity = 2600 m/day (this is a value for K=80 m/day - coarse sand)
well discharge = 1728 m^3/day, or 20 l/sec.
Result: Screen Length = 9.63 m

Another example is shown in Figures 4.15 and 4.16.

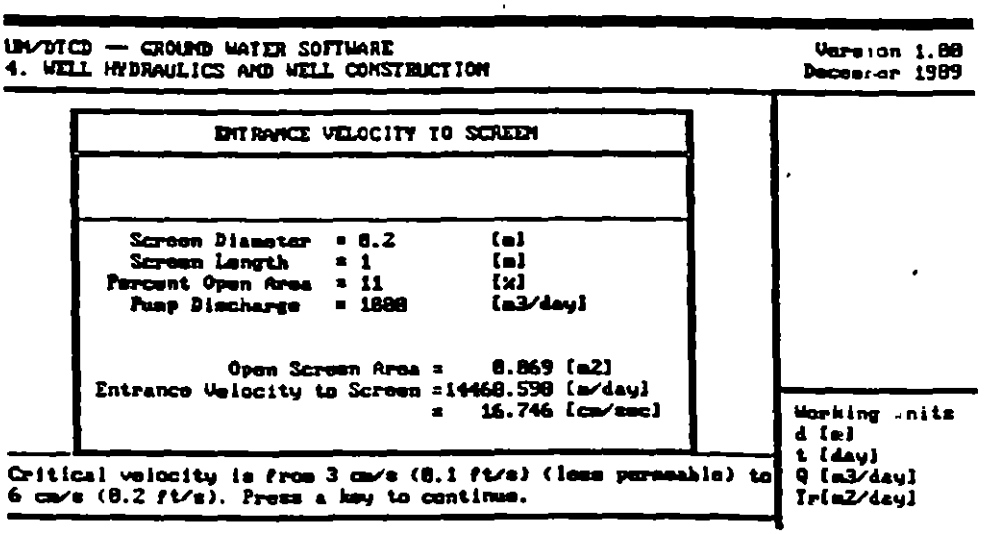


Fig. 4.15

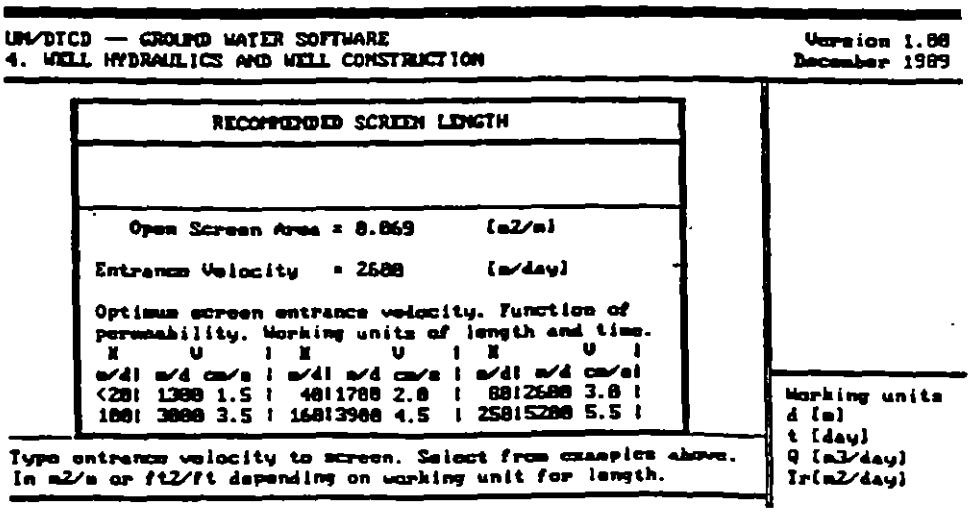


Fig. 4.16

The relationship between optimum screen entrance velocity and the coefficient of permeability of the aquifer which is used in this program, applies mostly to naturally gravel-packed wells. The same procedure is followed in selecting the optimum screen length for an artificially packed production well except that the average of the permeabilities of the aquifer and pack is used to determine the optimum entrance velocity.

Entrance Velocity. This program calculates the actual entrance velocity to the screen as a function of pumping rate, screen diameter, length and percentage of openings. It involves simple arithmetics. Input parameters are:

screen diameter
screen length
percentage of open screen area

The result is the entrance velocity to screen in several units. For comparison, at the message line a comment is displayed suggesting critical permissible entrance velocities as a range from 3 cm/sec to 6 cm/sec depending on aquifer permeability.

Example (Fig. 4.17):

Screen diameter = 0.2 m (8 in.)
Screen length = 6 m
% Open area = 11%
Well discharge = 2000 m^3/day

Results:

Open screen area = 0.415 m^2
Entrance velocity = 4822 m/day
= 5.582 cm/sec

The message at the bottom line suggests that the critical entrance velocity for less permeable medium could be about 3 cm/sec and for more permeable medium up to 6 cm/sec. In this case the decision whether the entrance velocity is above or not the recommended maximum entrance velocity will depend on the permeability of the aquifer.

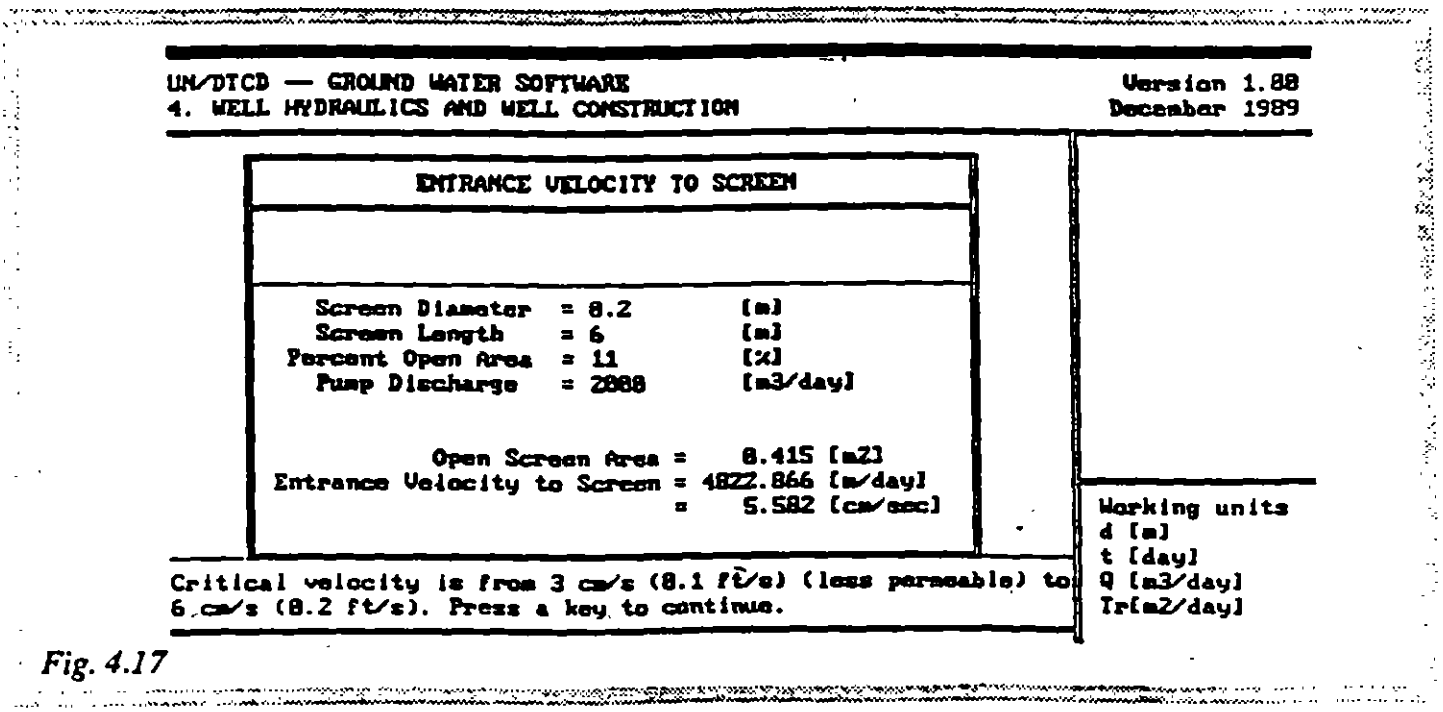


Fig. 4.17

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Hydrographs

5.1. General

This program allows you to create, edit, update a ground water level data base, and to display hydrographs on the screen, print or plot them.

In order to run the GW5 program you must copy the following files to the GW directory: UN5.WND, UN5.CMN, UN5.MST, and GW5.EXE. The minimum memory required for running the program is about 400 KB. In order to view hydrographs on the screen and/or to print them, you will need at least 550 Kbytes of memory. A video display adapter is required for viewing hydrographs on the screen; a dot-matrix printer with graphics capabilities is required for printing and a HPGL-compatible plotter for plotting hydrographs. The four mandatory files take up about 355,000 bytes of the disk.

Program Features

(a) You can input irregularly observed water levels. The program will find the correct time of observations on the time scale. You determine the interval for connecting the points on the hydrograph.

(b) You can input data either as water levels in absolute elevations (above mean sea level) or as depths from a certain measuring point. Hydrographs are always displayed with double scale: depth to water on the left, absolute elevation on the right.

(c) Regardless of the time interval used in a ground water level data base, you can select the time interval to display, print or plot.

(d) One data base can contain a maximum 500 observation wells, and each well may have up to 500 water levels (depths).

(e) The program automatically determines the time and level scales to fill one screen with the graph.

(f) The data input is twofold: (1) from an ASCII file prepared either by a word processor with Nondocument or ASCII option, (2) directly from the program.

(g) When the data are input interactively from the program, the input must be year by year. This means that you should select the time interval for the starting year, type in the data for that year, change the time interval to the next year and type in the data for that year, etc. In a similar way you may edit the data, year after year.

Water levels and/or depths must be input in a time-sorted order. The program will notice and display a message to the effect that some values are not sorted.

5.2. Running the Program

After you select this program module from the main program menu, and press RETURN, the opening screen is displayed and you are prompted for the file name of the ground water level data base, as shown in Fig. 5.1.

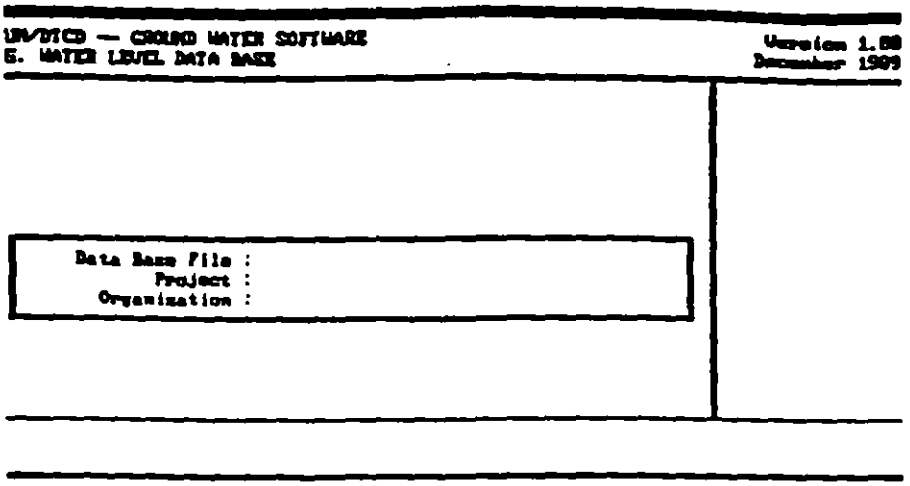


Fig. 5.1

You are prompted to supply the name of the data base (standard DOS file name, without extension). If the file with such a name exists (or, has been created before) the program will fill in the other two fields (Project and Organization). These two fields are used only for labeling the printout. If this is your first attempt to create a data base, such a data base file name shall not exist and the program will display a message:

This file dos not exist.
Press C to create new file or Esc to exit.

Press C. The first line will display the file name (data base name) which you have just typed, and the cursor shall be on the second line: Project. You may type anything you want, or skip by pressing RETURN. Press RETURN anyway whether you typed something or not. The cursor moves to the third line: Organization. Enter a value and press RETURN. After you press RETURN, if this is your first attempt to create a data base, the screen will prompt you for units for distance, followed by the "Working Time Interval" prompt, as in Fig. 5.2.

The preprogrammed default unit for distance (depth, elevation, altitude) is meter, but you may select either meter, foot, or define your own unit. The idea of defining the working time interval is to have the possibility of creating a large data base, with water levels input over a long period of time. However, when it comes to editing, analyzing, displaying, or printing hydrographs, you may reduce the interval by assigning a shorter period of time, the one that you may have interest in.

The program has several logical controls built in. E.g., the program will notice that you have not specified the month or date. In the case of a wrong input the message will warn you that "month must be between 1 and 12". Likewise, you cannot specify the ending date earlier than the starting date. Since both "Units for Distance" and "Working Time Interval" exist as functions on the Main Menu, you may change either at any time. However, care should be exercised in selecting the time interval. Most of errors are due to improper working time interval.

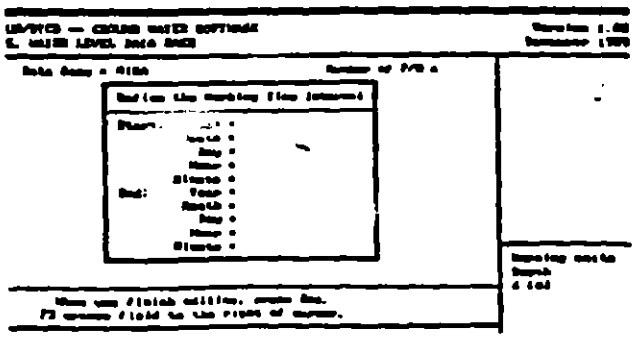


Fig. 5.2

Main Menu. The main menu, shown in Fig. 5.3, contains the following functions:

U = Define Units
D = Data Input, Edit, etc.
A = Data Analysis
T = Working Time Interval
! = Change Depth (–) Altitude
X = Exit to DOS

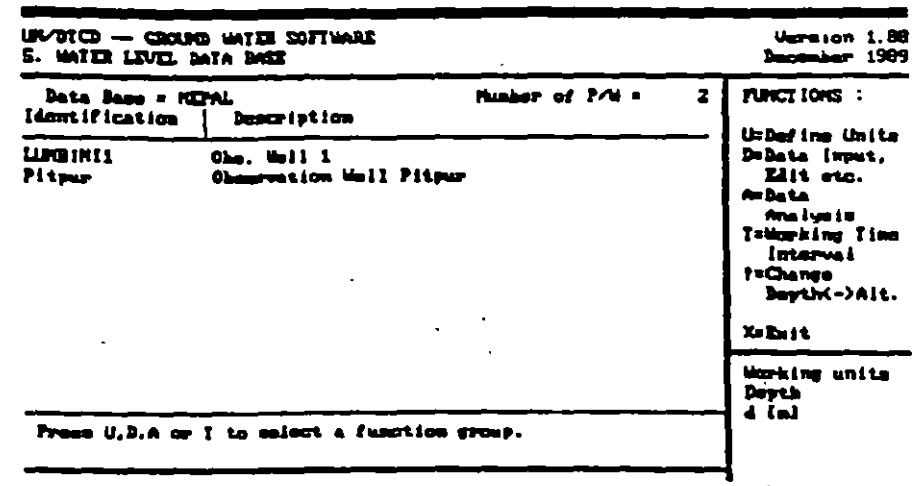


Fig. 5.3

Notice also the message in the lower right corner:

Working Units
Depth
d (m)

indicating that the data base contains levels in the form of depth (from a measuring point), and that the unit for length is meters.

The message line at the bottom contains the instruction: Press U,D,A, or T to select a function group.

In preparing a new data base, you should first type the letter U to define your default units. You should select meters or feet as units for length, select a time interval large enough to accommodate all presently available data, and change "altitude" for "depth" if levels are already expressed in absolute elevations above the mean sea level. Then go to option D to input data.

5.3. Data Input

After you type the letter D, the menu shown in Fig. 5.4 will appear. The following functions are available:

I – for input from an ASCII file
O – for output to an ASCII file
N – for new data input from keyboard
E – for editing data
A – for data analysis (display and printout of hydrographs)
D – for deleting data
Esc – to return to Main Menu

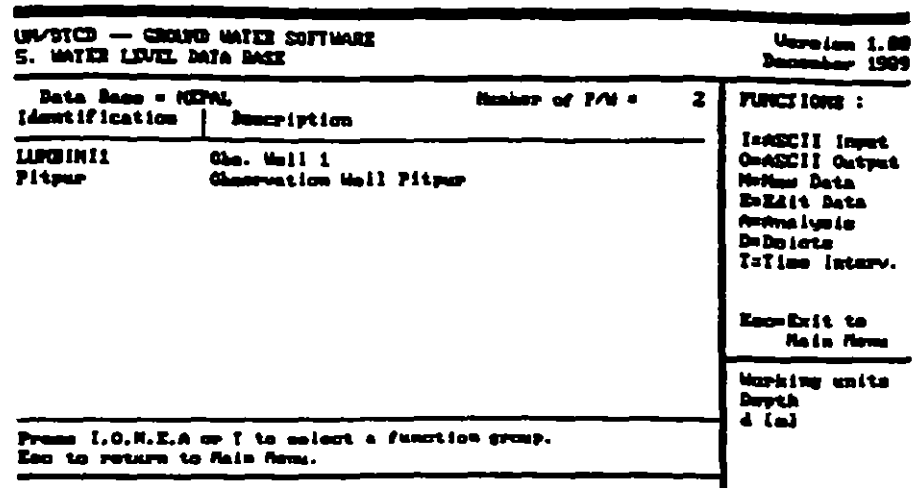


Fig. 5.4

Option I is used when data are to be read from an existing ASCII data file. The file could have been created either with a word processor (WordStar, Word, WordPerfect, Personal Editor, etc.) or from this program using the option N.

Option O is used when the data that have been created from the program (option N) or edited (option E) are to be stored in a separate ASCII file.

Option N is used for interactive input of new data and creation of a data file.

Option E is used for editing existing data, or for extending the period of record.

Option A is used for displaying the graphs, or their printing.

Option D is used for deleting one or more data files (individual wells).

Option T is used to modify the time interval. It is very important because depending on the time interval selected the data will be displayed and available for editing. For example if a wrong time interval is selected the data may not be "visible" and corrections or extension of data will be impossible.

Pressing Esc will return you to one menu backward, i.e. to main menu.

Input from an ASCII Data File. To input data from an ASCII file, type the letter I and answer the program's prompt for a file name. You may have created the file with a word processor in which case the file should have the following format and appearance:

line 1: file name

line 2: description of observation well, any character

line 3: description of aquifer (e.g. Quaternary, dolomite, Ogallala)

line 4: x, y coordinates, land surface and measuring point elevations, format 4F10.0

line 5: the starting year, typed with four digits in columns 1 through 4

line 6: the starting month, typed with one or two digits in columns 1 and 2 (if the month is one from January through September the one-digit value is typed in the column 2)

line 7: day, hour, minute, and the level or depth, in the format I2,2I3,F10.0

line 8: continue input in the same month

line 9: same as above.....

When one month is terminated the next line contains only one "*" character typed in the column 1. The next month follows same as in line 5. The year is terminated with two "*" characters. The entire data file is terminated with three "*" characters. An example is shown on the next page.

```
Pitpur                                  line  1
Observation Well Pitpur                 line  2
Quaternary                              line  3
1000  1000  0.00  0.00                  line  4
1987                                    line  5
5                                       line  6
1 12  0          -1.77                  line  7
*                                       line  8
6                                       line  9
1 12  0          -0.46                  line 10
*                                       line 11
7                                       line 12
1 12  0           1.21                  line 13
*                                       line 14
8                                       line 15
1 12  0           1.28                  line 16
                                        line 17
9                                       line 18
1 12  0           1.36                  line 19
*                                       line 20
10                                      line 21
1 12  0           1.03                  line 22
*                                       line 23
11                                      line 24
1 12  0           1.70                  line 25
*                                       line 26
12                                      line 27
1 12  0           1.54                  line 28
*                                       line 29
**                                      line 30
1988                                    line 31
1                                       line 32
1 12  0           0.04                  line 33
*                                       line 34
2                                       line 35
1 12  0          -1.84                  line 36
*                                       line 37
3                                       line 38
1 12  0          -3.15                  line 39
*                                       line 40
4                                       line 41
1 12  0          -5.00                  line 42
*                                       line 43
5                                       line 44
1 12  0          -2.80                  line 45
*                                       line 46
**                                      line 47
***                                     line 48
```

Immediately after you enter thedata file name and press RETURN, the first line on the screen shows Number of P/W = 1. The letters P and W stand for "piezometer" and "well", respectively. Also on the same line the name of the data base is shown.

Important instructions: (a) Eachmonth must terminate with one star; (b) each year must terminate with two stars; (c) data file must terminate with three stars; (d) press RETURN after the last entry (three stars).

The cursor must be in column 1 of the last line. If it is located anywhere within the line, but not in column 1, there will be an error message "End of file before end of line". If you accidentally leave one blank line at the bottom of the data file (one additional RETURN was pressed), the error message: "Premature end of file." will appear.

However, most errors occur if your word processor does not produce an ASCII file. (With WordStar, unless you "print" the file to ASCII printer, you will not always get a 100% ASCII file. Check this with the utility SHOW.COM that is appended to this software package. If you see some strange character, such as a light rectangle, heart, or the like, you have problem!)

You may prepare several hydrographs in the same data file. After three stars (***), which implies the end of one hydrograph, you may continue with second well name, followed by description, aquifer, coordinates, etc.

Input from keyboard (inside the program). If you want to create a data file interactively from inside the program, the N option (for "new data") should be used. Prior to pressing N be sure that the time interval is the right one. The program will respond by prompting for identification. Type any meaningful name. The program ignores characters beyond the 16th.

Next a table for general data will appear (Fig. 5.5). The message at the screen bottom is as follows:

When you finish editing, press Esc. Table with time-level data will come next.

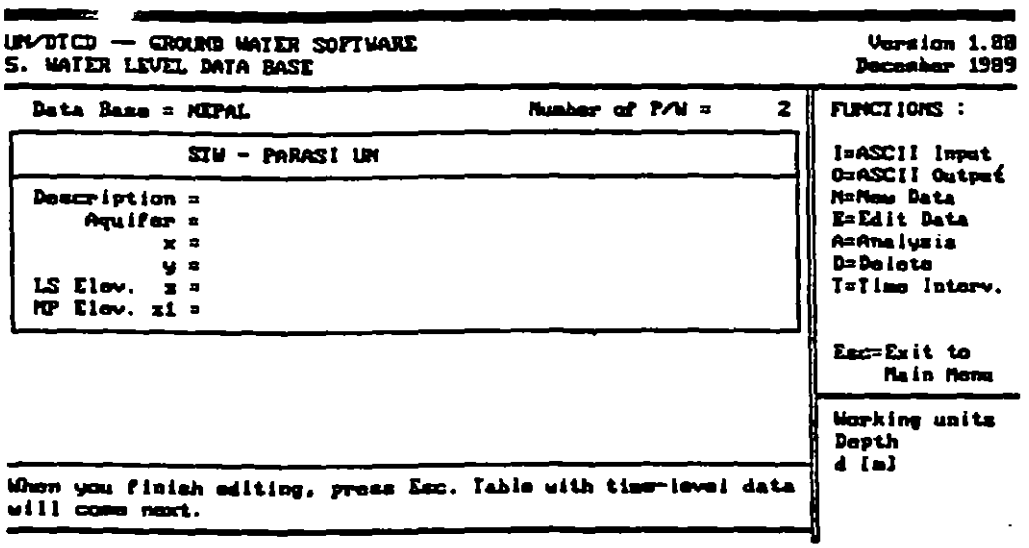


Fig.5.5

Although such a message may not be quite relevant at this moment, this routine is used also for editing existing general data (option E). "Description" and "aquifer" entries are optional. You may press RETURN for either. Their content is used only for labeling the printout, if so selected. Likewise, X and Y coordinates shall be used in future program's revision, for creating a water level contour map from available observation wells. You may type actual coordinates, or press RETURN twice. The last entry, "Measuring point elevation, Z1", is important, if observation well elevation is available. Each graph displays and prints two scales: on the left the depth from measuring point, on the right absolute elevation of the water level. If Z1 elevation is not known or input, both scales shall be the same, starting from 0. (One inconsistency is noted in this version of the program. When the level goes above the land surface, one should type the level with minus sign. Yet, the scale on the left side of the graph is somewhat peculiar: plus sign down from "0" ordinate, minus sign above the "0" ordinate.)

The table that will come next looks as shown in Fig. 5.6. Before typing or editing time-level data, confirm or modify the year on the top left. (The program notices the last year of your "Working Time Interval" and offers the last year to start the input. The logic is the following. In updating a data base, one normally continues

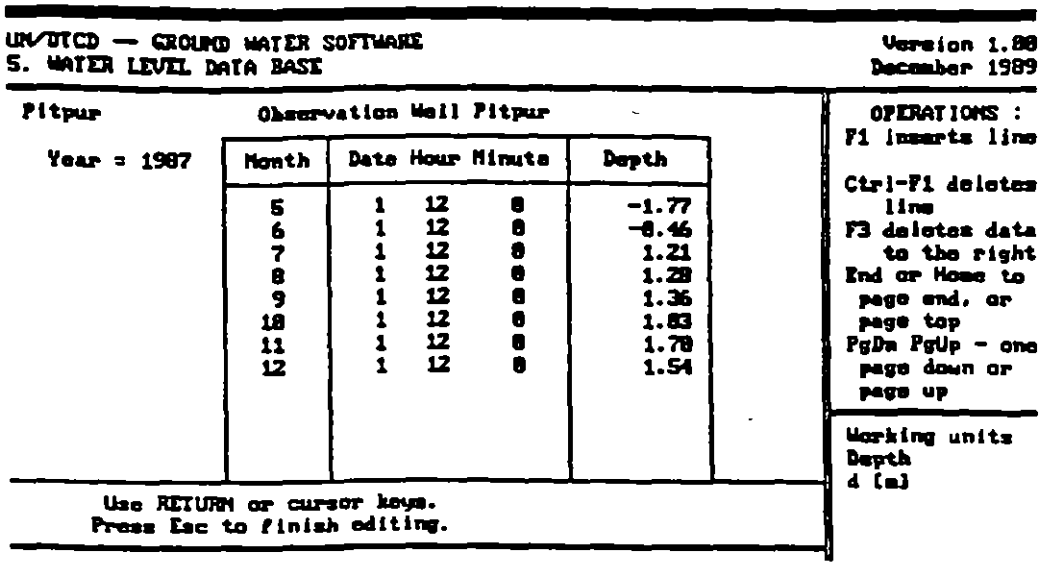


Fig. 5.6

from the last available information. So, if the data base was last time updated in June 1989, when the job is taken up, the next month shall be July of the same year. However, in creating a new data base, if you specify the time interval spanning a two-year period, say 1988-1989, the year that is displayed, that is 1989, should be modified to 1988.

You may move along rows or columns using the cursor control keys, space bar, return, page up and down, home, and end. After you finish your input, press Esc to return to the Data Menu. It is a good practice to write the new data to an ASCII file. Press O and supply the name for the file.

> *Warnings*. **Remember to terminate the last line in the data file with RETURN before exiting (Esc). Do not try to continue after the 12th month. (Program will ignore the input beyond the month 12.) Data must be in time sequence. After one year is finished, the year displayed in the top left corner is updated for one, and you will be prompted to confirm or modify it. You may also escape now by pressing ESC.**

5.4. Editing Data

The procedure for editing data is almost the same as the procedure for entering new data(option N). The difference is that the cursor should be placed on data file which is to be edited. (The program will not ask for the file name or identification.) The table with general data will appear filled with old values. Edit the data or escape. The time-level table will come next. Remember that editing is waiting for your confirmation of the year which is displayed on the top left. The real table with time-level data will not appear until you confirm the year. Nothing prevents you from editing one year after the other.

Writing Data to an ASCII Data File. The option O allows you to write the data, both general and time-level, into an ASCII file. Place the cursor on the line to be copied to an ASCII file and type the letter O. You are then prompted for the name of the file to which you will write the data.

Deleting a File. In order to delete a file, place the cursor on the line with the file to be deleted and press the letter D . Remember, there is no way to "undelete" the file. As a precaution, have all data files transferred to ASCII files one by one prior to deleting any file from a data base. The program warns you that you have pressed D for "Delete", and asks you to confirm this operation.

Changing Time Interval. This is a critical concept in this software package. All "evil" will normally come from an erroneous time interval. No matter how large is the time span in the data base, only the available data will be shown when editing is invoked.

5.5. Analysis

You may display and/or print hydrographs from this menu or from the main menu. In either case the option is invoked by pressing the letter A. The procedure is explained here below.

Typing the letter A will take you to the Data Analysis Menu (Fig. 5.7). The following options are available:

- D – for displaying hydrograph
- P – for printing hydrograph
- Q – for printing a table with data
- T – for selecting the time interval to be displayed and/or printed.
- C – for changing the size of connecting interval
- B – for plotting hydrograph
- A – for creating an ASCII plot file, to be eventually edited and/or used in some commercial plotting program.

First select a file with the cursor. Next check the time interval which will be used. Type T and modify the time interval if necessary. In some cases, when you type A from Main or Data menu, the program automatically asks you to confirm the Time Interval for displaying the data. If you wish details, reduce the time interval. By modifying the time interval you may enlarge or squeeze the graph. Display the hydrograph by typing D. Print hydrograph by typing P. The first prompt will ask you to make printer ready and press RETURN. After that you will be given chance to select between two formats for printing hydrographs. You may print hydrograph with all the information (general data) in data file, such as project name, organization, coordinates, elevations, aquifer description. In this case the graph itself shall be centered on a A4 page with general data preceding the graph. However, you may opt for only graph and its identification. In this case you may have two hydrographs on one A4 page. Answer this prompt by either F for full page with data, or R for "reduced" data. Print data table by pressing "Q". Plot hydrograph by pressing B.

You may decide whether you want to connect some missing intervals or not. If, e.g., data in two months are missing but you still want to have a continuous (connected) graph, press C and type 61 for "Connection interval (days)", followed by two returns. The program scans the time interval between two successive time values and connects them if the time elapsed is less than 61 days.

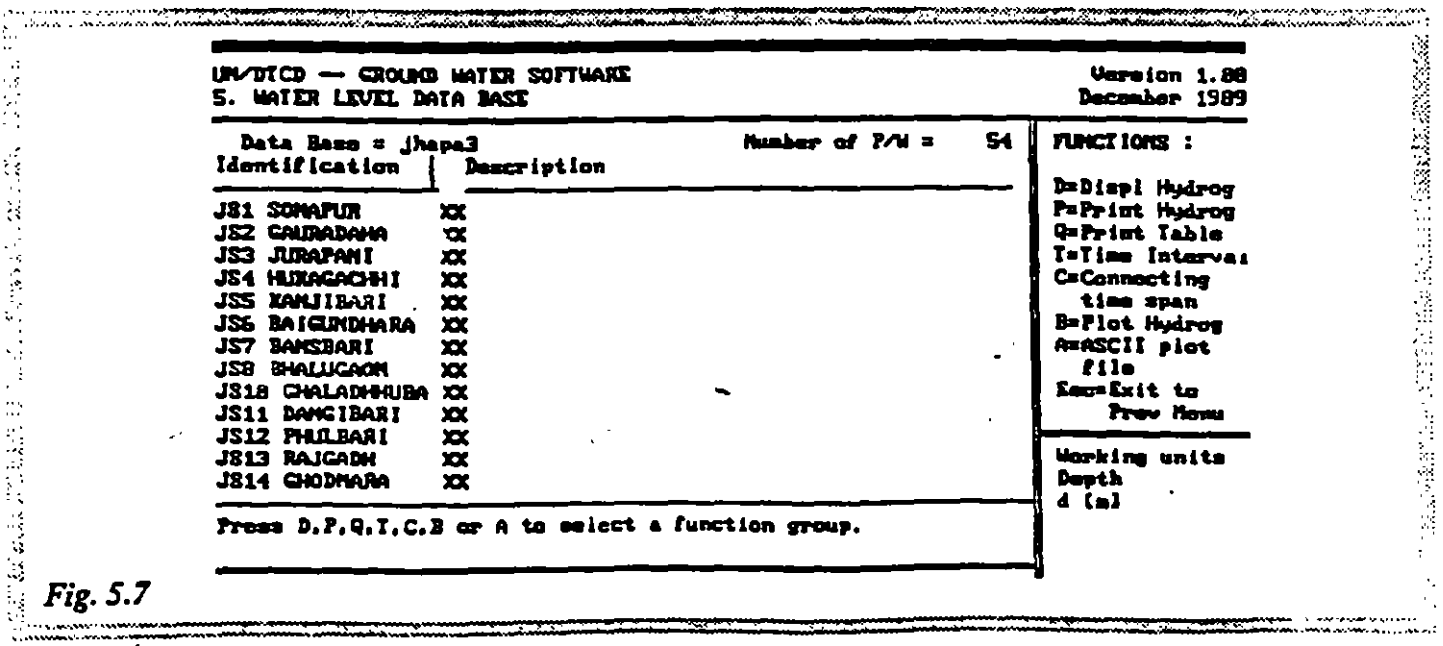


Fig. 5.7

5.6. Example

To run this example, create a data base from the keyboard containing one data file. The data are real (Nepal, UNDP project NEP/86/025, executed by Department of Technical Co-operation for Development, Water Resources Branch).

Type GW and press RETURN. Wait for the opening screen, press any key except Esc. Read, if you wish, the copyright notice and press any key except Esc. Select the module 5. Hydrographs, and press RETURN. When prompted for Data Base File type NEPAL. The cursor is now on the Project. Type NEP/86/025 GROUND WATER IN TERAI. Press RETURN. For Organization type GWRDB, UNDP, UN/DTCD. The screen is as shown in Fig. 5.8. The line (m) is highlight ed. Press RETURN. The screen Define the Working Time Interval appears next. Type 1988 for the starting year, 5 for the starting month, 1 for the day, press twice RETURN bypassing starting hour and minute. Type 1989 for the ending year, 2 for month, 28 for day, press RETURN followed by Esc.

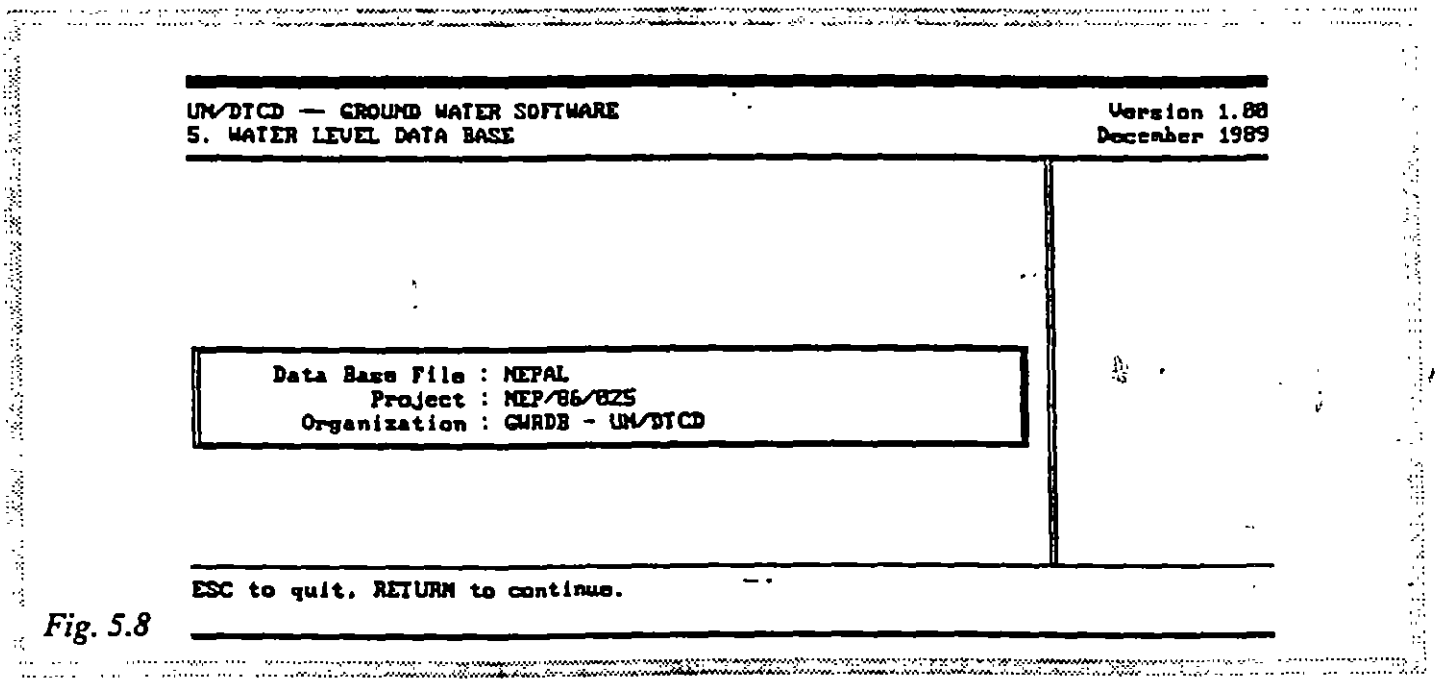


Fig. 5.8

You are now on the main menu. Type D for data input, and select N for new data. Answer the Identification prompt with STW-3 PARASI UN and press RETURN. The screen as in Fig. 5.5 will appear. On the line Description type "Shallow, 38.4 m, drilled Jan. 88" and press RETURN. Type "Quaternary" at the Aquifer prompt. Press RETURN. Type for X 762900, and for Y 3048000. For LS Elevation Z type 111.39, and for MP Elevation Z1 type 112.03. LS and MP are abbreviations for land surface and measuring point, respectively. Press Esc. Modify the year 1989 offered by the program to 1988. Press RETURN and wait a while until another table with columns for time and level is displayed. The cursor is in the first row, first column. We start with May 1988, actually the level on 2 May 1988 is 3.08 m. Type 5, press RETURN, type 2, followed by two returns (or several cursor right-arrow keys). Type 3.08 in column Depth. Press RETURN. You are now on the second line. Type 6 (June), 9 (day), RETURN for hour and minute, 3.6 for depth to water table from measuring point. After all months in 1988 are processed the table will look as follows:

5	2	0	0	3.08
6	9	0	0	3.6
7	1	0	0	1.8
8	3	0	0	0.7
9	2	0	0	0.62
10	3	0	0	1.95
11	3	0	0	2.12
12	15	0	0	2.28

Do not forget to press RETURN after typing 2.28. The cursor must be in column 1 on the blank line. Press Esc. Notice that the program updates the year to 1989. Confirm that year by pressing RETURN. Type 1 for month; 15 for day, two returns for hour and minute, and 2.57 for depth. Press RETURN. On the second line type 2 for month, 3 for day, press twice RETURN, and type 3.36 for depth. Press RETURN. Do not forget this! Press Esc. All data are now in the file STW-3 PARASI UN.

Type A. to select data analysis. Type T to confirm the time interval. If you select the time interval to start with May 1988 and terminate with December 1988, the hydrograph will be as shown in Fig.5.9. View the hydrograph by pressing D. Print it by typing P. Print the data in table form by typing Q. The data are printed in the table as shown in Fig. 5.10. You may also plot this graph. Press letter B.

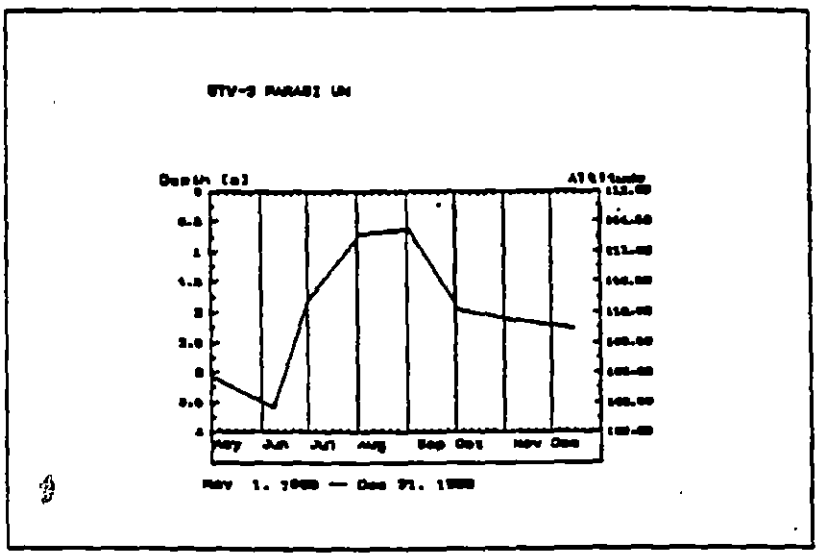


Fig. 5.9

```
F1 - Help     Esc - Exit        SHOW text                          Version 1.1
      GWRDB - UN/DTCD
      MEP/86/BZS

      Identification : STW-3 PARASI UN
                       Shallow, 38.4 m deep, drilled Jan. 88
            Aquifer : Quaternary
        Coordinates [m]
                    X =   762900.88
                    Y =  3848888.88
                    Z =  113.39
                   Z1 =  112.83

                Period : May 1988 - Dec 1988

      ---- May, 1988 ----
        2  8: 0     3.88
      ---- Jun, 1988 ----
        9  8: 0     3.68
      ---- Jul, 1988 ----
        1  8: 0     1.88
      ---- Aug, 1988 ----
        3  8: 0     0.78
      ---- Sep, 1988 ----
        2  8: 0     0.62
```

Fig. 5.10

Well Logs and Lithological Cross-sections

6.1. Program Overview

The program GW6 is Lithological Data Base, which includes several retrieval subprograms: (1) Well construction data with lithological column in graphical form; (2) Lithological cross-sections; (3) Table with all wells in data base, including well name, x,y,z, depth, and screened interval; (4) Calculation of the percentage of permeable intervals; (5) Map showing the location of all wells in the data base. The program has built-in many graphical symbols for lithological units (sand, clay, gravel, hard rock, etc.), but you may also design almost any kind of symbols and assign to them different names. You may edit all data from inside the program using your favorite editor. You may view on the screen individual well logs and whole cross sections. You may also use a mouse and select the lines of cross sections directly from the screen map. You may print or plot well logs and cross-sections.

The GW6 program contains the following files:

GW6.EXE – run file, command file, executable file

UN6.CMN – communication file

UN6.WND – windows

UN6.MST – menu structure

GW6.GEN – general data file (MUST BE EDITED BEFORE STARTING NEW PROJECT)

GW6.DLT – description of lithology file, with various symbols preprogrammed and/or designed by the user

GW6.STM – codes for permeable members

DIGXSC.EXE – file called from main program to create coordinate system with map of wells

GW6CF.EXE – file called from main program (GW6.EXE) which is used in creating new files in lithological data base

BL#.LTH – examples from a recent project in Nepal, where # is the number of the well

The following files must be copied to the \GW directory: GW6.EXE, UN6.MST, UN6.CMN, UN6.WND, GW6CF.EXE, DIGXSC.EXE, GW6.DLT, GW6.STM. They occupy about 330,000 bytes of disk storage. The minimum memory requirement for the GW6.EXE program is about 430 Kilobytes, but, with screen and printer drivers, the maximum memory requirement is about 580 KB. This means that you must eliminate any memory-resident program, and even reduce your CONFIG.SYS file, if you wish to use screen display and printing capabilities of the program.

You will need a video graphics adapter, if you wish to view well logs, well map, and cross sections on the screen. A mathematical co-processor is optional, but it is highly recommended. The graphics on the screen is very much computer-time demanding, and the speed and efficiency of screen presentation is greatly improved by running the program on a fast microcomputer, preferably the one with clock speed of 12 megahertz or more. A typical well log is calculated and displayed on the screen in about 35 seconds on a 25 MHz computer equipped with a 25-MHz co-processor. It may take 5 minutes if the program is run on a computer running at 8 MHz, without a co-processor. You may find a mouse useful in selecting the lines of cross sections directly from the screen map.

In this manual you will be instructed to create the data base, to run the program, to design additional lithological symbols.

The program is written in such a way that it can be installed on a hard disk drive other than C. However, should you select a hard disk partition other than the boot disk C, you must copy the COMMAND.COM file into the root directory of the hard disk partition where your data base shall reside. The COMMAND.COM file is used by the program to read other files (GW6.GEN, lithological files, etc.).

You do not need to have your text editor in the same subdirectory (e.g. \gw\gw6). However, be careful, if you specify the path to the editor correctly, this still does not mean that the program will be able to use that editor. Almost every text editor or word processor has, in addition to one EXE file, speller and thesaurus, several message or overlay files. These cannot be found by the program with ordinary DOS PATH utility. You need something like "SEARCH" utility which will search specified subdirectories and find any required file, no matter what is its extension. If you are an inexperienced computer user, it is advisable that you copy your text editor files into the \GW\GW6 subdirectory (without speller checker, thesaurus, or printer files). However, data files (data base) can be physically separate from the program subdirectory. When you are asked by the program to select files, specify the complete path. E.g., if your data base files are on hard disk subdirectory called NEPAL and each well file is terminated with extension *.lth, specify the path C:\NEPAL*.lth.

The maximum number of individual data files (well logs) is 300.

6.2. General Program Files

6.2.1. General Data File, GW6.GEN

The first step in running the program is to tell the computer which text editor you want to use and where it is located. This information is contained in the file GW6.GEN. The file GW6.GEN must be in the current n directory. Since you must have the files such as GW6.EXE, all three UN6 files, and GW6.DLT, GW6.STM, GW6CF.EXE, in the \GW directory, you may opt to create a data base directory in which you will have all your data base files (we recommend the extension *.lth for each) plus the file GW6.GEN.

It is important and MANDATORY that you log onto that directory in which your GW6.GEN file is located before you run the program GW or GW6.

This file contains the information identifying the project (two lines), vertical and horizontal scale for cross sections, and most of all, the path to your text editor. The project identifications are not that critical, neither are the scales for cross sections. But the path to the text editor is crucial, whether you want to use that editor or not. Take note now, that the name of the executable text processor file must be typed with extension. If this is WordStar, type WS.COM. If this is WordPerfect, type WP.EXE, etc. You may edit this file independently from the program using any screen editor, or, you may do it from inside the program. Before you use the program for the first time, you must edit the GW6.GEN file with a screen editor outside the program. The file GW6.GEN, as supplied on the distribution diskette, looks as follows:

```
PROJ:  NEP/86/025
ORG:  GWRDB - UN/DTCD
EDITOR:  C:\UTIL\PE.EXE
HSCALE:  100000
VSCALE:  1000
```

There are five lines in this file. You supply the information starting with column 11. Do not change words before a colon. The first two lines are project name or symbol and organization. In this version of the program, these two lines are used to identify well logs only. (In earlier version they were also identifying lithological cross section. This was eliminated to make more space for real cross section. Titles and identifications can be added by printer later!)

On the third line you should provide the path to and the name of text editor that program will use. In this example, IBM's Personal Editor is used, and it is located in the hard disk subdirectory \UTIL (for utilities). Again, be careful. If your text editor's main executable file is in this subdirectory, the program will find it, but

not its overlay or message files, unless you have some "SEARCH" utility in your autoexec.bat file. (Some editors need only one executable file, such as Borland's SideKick, Norton's Editor, etc.)

The last two lines specify the scale for cross sections, horizontal and vertical. The horizontal scale of 100000 means that 1 cm on the printout will represent 1000 m in nature. The horizontal scale of 1000 means that 1 cm on the printout will represent 10 m in nature. The scale is for lithological cross-sections. You have a choice of having lithological cross section printed on A4, A3 format, or user-specified format. In A4 format the maximum length of a cross-section is 26 cm, and the maximum height is 16.5 cm. Thus, with horizontal scale 100,000, one may display a cross-section of maximum length 26 km; with scale 200,000 the length can be as big as 52 km; with scale 50,000, the maximum length of the section can be 13 km. Vertical scale of 2000 is used for cross-sections up to 332 meters or feet vertical difference; scale of 1000 can display up to 165 m or feet. In A3 format the maximum length of the cross section (along horizontal) is 36 cm, and the maximum height is 21.9 cm. Thus, in A3 format in 100,000 horizontal scale, the total length of cross section can be as much as 36 km. (If you select A3 format, paper should be placed into printer with shorter side horizontal.)

6.2.2. Lithological Symbols Default File, GW6.DLT

The file GW6.DLT contains preprogrammed symbols for various lithological units (about 30). You can use these symbols without modification, or you can make your own. One part of the file is reproduced here belo

```
CLAY Clay
3 1.5
2 0.00 0.75
0 0.75 1.50
1 1.50 0.75
0 2.25 0.00
1 3.00 0.75
•
SILT Silt
2 2
2 0.0 0.0
1 1.0 1.0
•
ROCK1 Hard rock
2 2
2 0.00 1.00
1 2.00 1.00
•
```

The list of all symbols and instructions to prepare additional symbols are contained in Appendix A. The symbols can be simple (horizontal line, diagonal line, etc.) or very complicated (e.g., mixture of fine sand with gravel).

Each symbol is defined with symbol name, which is the first word in the GW6.DLT file (CLAY, SILT; up to 10 characters, sensitive to the case of letters, that is upper case and lower case are not the same), and description which will show on the printed well log. This is one or more words after the symbol name (with maximum of 100 characters). In the above example the description of clay and silt is the same as the name of the symbol, but for the symbol ROCK1 the description is "Hard rock". You may modify in this file the symbol name, or description, to suit your project better. You may also add to this list new symbols using the procedure explained in Appendix A.

The important thing to remember is that in data files to be created by you, one file for one well, symbol names are matching with symbol names in this file. If the program does not find a symbol name specified by you in data files, that portion of the lithological log will remain blank (no symbols). In lithological cross-sections, a message shall be displayed that error was noticed in reading lithology. (The name of the file with error shall be also displayed.)

You have also the option to have the default description of lithology typed on the well log (such as Clay, Rock1, or Silt), or to type something different and/or expanded. If in the well log data you type only the name

of the symbol next to the depth, e.g. CLAY, the program will use the default description (Clay). If you type something else, the program will reproduce this "something else". Thus, next to CLAY symbol the following can be typed: Clay hard with some silt and sand.

6.2.3. File with Codes for Permeable Units, GW6.STM

One more file must reside in the \GW directory. This is the file which contains the codes for permeable units or members. It is used in several application routines: (a) for displaying permeable units in blue, and all other units (interpreted as impermeable) as yellow, in well logs and Lithological cross sections; (b) for creating a table with percentages of permeable versus impermeable layers in each and all wells in the data base. The current GW6.STM file looks as follows:

```
SAND
SANDV
SANDF
SANDM
SANDC
SCWG
GRAVEL
GRAVELF
GRAVELC
GWS
SRGRAV
```

6.2.4. New File-Creating File, GW6CF.EXE

This file must reside in the \GW directory. It is needed only if and when you want to add new files to the data base.

6.2.5. Digitizing Coordinates File, DIGXSC.EXE

This file, which must also reside in the \GW directory, is needed for digitizing the wells' coordinates, displaying a map with wells, and supporting the mouse-defined cross section lines. Without this file, you may specify the beginning and end coordinates of a cross-section line manually, without using a mouse.

6.3. Running the Program

Copy the files GW6.EXE, UN6.MST, UN6.CMN, UN6.WND, GW6.DLT, GW6.STM, GW6CF.EXE, DIGXSC.EXE into the \GW directory. Create a subdirectory, say GW6, and copy the GW6.GEN file plus all .LTH files into that subdirectory. Log into the GW6 subdirectory (*the one in which is your GW6.GEN file!*). Type GW to start the whole package, or GW6 to start only the lithology program.

After you select the module "6. Well Lithology" press RETURN. The next screen displays two lines with Project and Organization identification, Fig. 6.1. This information is read from your GW6.GEN file. If there is any error you will see either a message "Please, edit file GW6.GEN first, then call again." or "Text editor given in \GW\GW6.GEN does not exist. Prepare \GW\GW6.GEN and call again." The first message appears if you do not have any GW6.GEN file in your currently logged directory. The second message is displayed if the path to the text editor is wrong or its executable file name is not complete, i.e. without extension. (The list of error messages is appended in Appendix B.)

If you do not see these messages, and the project name and organization appear on the screen, you may edit these two lines now or modify them by editing the GW6.GEN file. The changes you make shall be reflected

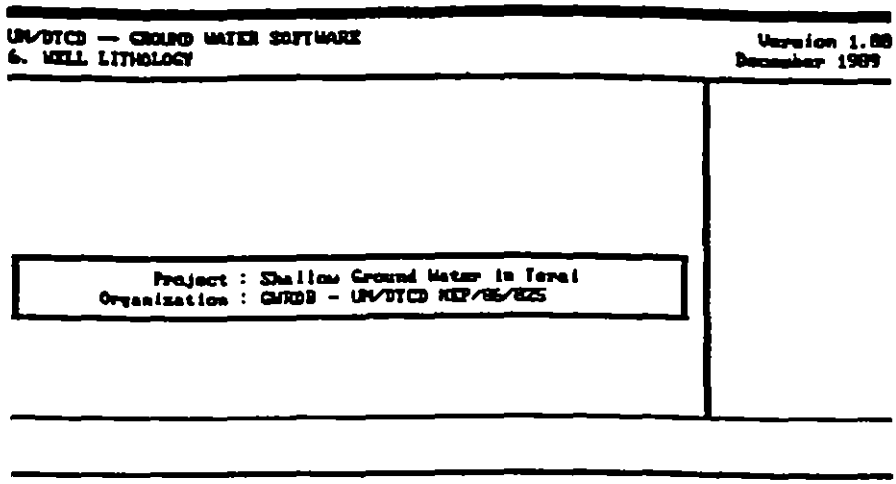


Fig. 6.1

not only in the headings of your printout (well logs, cross-sections) in the current run, but will also be copied to your GW6.GEN file.

Press RETURN twice. The main opening screen with the main menu will appear (Fig. 6.2). On the right side of the screen are shown various functions available in this program.

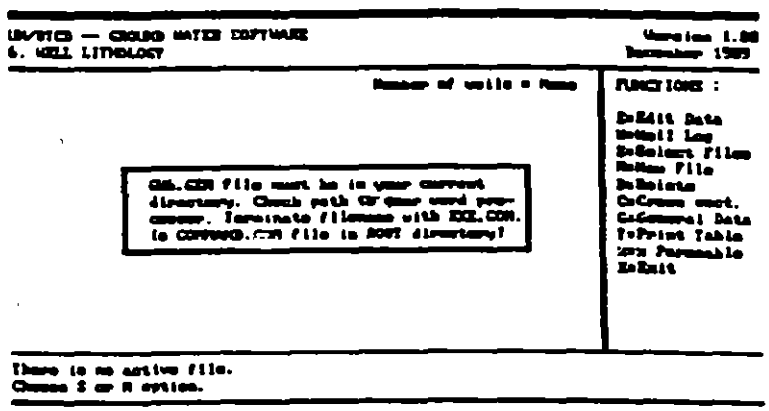


Fig. 6.2

E=Edit Data.

This is used for editing existing data files. You will normally first select one or more files, place the cursor on the name of the file that you wish to edit, and type the key E for editing. Then your selected screen editor will be activated (in this case Personal Editor) and the file contents are displayed automatically.

W= Well Log.

This function is used for displaying/printing/plotting a well log from the data file which is currently highlighted. In order for this to work properly, the printer driver in CONFIG.CNF must be correctly selected (9-pin or 24-pin printer) and its EXE file must be in the \GW directory (options: DVIRX120.EXE and/or DVILQ180.EXE, see Introduction). Likewise, a correctly selected screen driver must be present in the \GW directory (options: CGA, EGA, VGA, ATT, HGC, WYSE). You cannot plot the log unless you have the plotter driver in \GW directory. The plotter driver executable file is DVIHPGLF.EXE for plotting through the COM1 serial port, and/or for creating an ASCII plot file to be used later, in edited form, when a plotter becomes available.

S=Select Files.
This will normally be the first process to perform after the general data file (GW6.GEN) is edited. After S is typed, the program will prompt you for the form of data file names. If you have prepared all data with the same extension, say .LTH, the answer to the prompt can be *.LTH. The program searches through directory and reads all data files with the matching extension .LTH. Alternatively you may add file names one by one.

N=New File.
To create the data base, you must use this function. The program prompts for file name, and displays the default (preprogrammed) list of entries to which you must supply answers. In order that this portion of the program works correctly, there must be the file GW6CF.EXE in the \GW directory.

D=Delete.
Place the cursor on the file name to be deleted and type D. Warning! The file with that name will be deleted not only from the data base but from the computer directory. This is actually the DOS command which is incorporated into this program. Unerase accidentally erased file using one of commercially available utilities (Norton Utilities or PC-Tools, e.g.). A recommended practice is to have a copy of your data base on a diskette.

C=Cross Section.
If more than one well data file is available in the data base pressing the C key will initiate the processing of cross sections through the project area. You will be asked for the title of cross section, for the initial x coordinate, the ending x coordinate, the initial y coordinate, the ending y coordinate. The final question is how far from the cross section line eventually existing wells should be projected onto the line. If you have a mouse you will be able to select the cross-section line with the mouse. If you have a graphics adapter you may also create a map with all selected wells and view it on the screen. Lithological cross sections can be viewed on the screen, printed, plotted.

G=Edit General Data.
You may edit general data in this file at any time during the program execution. Once the general data are correctly selected, the only changes that may be required by the program or user are horizontal and vertical scales for cross sections.

T=Table of Data.
This is used to write to a file, from which you can print the data, the basic data identifying the data base: well name, x and y coordinates, elevation, total drilled depth, screened metrage (footage). At the bottom of the file you will find the basic statistics: (a) total number of wells, (b) total drilled metrage or footage, (c) total screened intervals, (d) percentage of screened interval with respect to total drilled metrage (footage). The same final statistics will be displayed on the screen.

%=Percentage of permeable
materials in selected interval of depth. As in the previous table, the information is copied to a disk file, with the summary displayed on the screen.

X=Exit to Main program.
As in any other program in this Ground Water series, typing X will return you to the Main Program.

6.4. Example

6.4.1. Start the Program

By running the example supplied on the distribution diskette you will master the program and understand its features. Log to the subdirectory in which your data files are located. The file GW6.GEN must also be there. Type GW, press RETURN twice, move the cursor to the line "6. Lithology". Press RETURN again. The following screen will appear:

Project: Shallow Ground Water In Teral
Organization: GWRDB – UN/DTCD NEP/86/025

The program gets this information from the first two lines in GW6.GEN. Press RETURN twice. The main menu with available functions comes next. On the right side of the screen the display is as follows:

FUNCTIONS:
E=Edit Data
W=Well Log
S=Select Files
N=New File
D=Delete (for deleting file)
C=Cross Sect. (for cross-section)
G=Edit General Data
T=Table of Data
%=% of Permeable (for percentage of permeable materials)
X=Exit to Main Program or DOS

Press S to select data files. The program prompts for file name format. Type *.LTH. This is interpreted by the program "look in data directory and find all files with extension LTH. Then transfer these files into computer memory". After a few seconds the screen will display the first 13 data files and show the total number of wells in the data base (Fig. 6.3). In this example the number is 15. The cursor is on the first line. Move the cursor to file BR4.LTH and press E to edit data. (You may need to answer the prompt of your text editor. E.g., if you are using IBM's Personal Editor, you must press RETURN.)

The following is displayed:

WELL: BLII/4
LOC: MAHADEVA
ELEV: 99.3
X: 730240
Y: 3050000
SCREEN: 51.8,56.9,65.1,68.1,76.2,81.3,87.4,90.5,104.1,113.3,117.9,120.9,154.4,157.5,178.9,184.9,191.0,197.1
DR.METH: RIG
DR.DATES: 16.2.87 - 9.3.87
COMM: WELL SIZE:16"/10";M.P:0.6m;SCRN:W.WRAPED\SCREEN POS:51.8-56.9,65.1-68.1,76.2-81.3\87.4-90.5,104.1-113.3,117.9-120.9\154.4-157.5,178.9-184.9,191.0-197.1\DRILLED UNDER BLGW PROJ.
PT.DATE: 3-4.4.87
Q: 111 l/s
DUR: 20 h
TRAN: 1780 m2/d
METHOD: THEIS
STORAGE:
SWL: 8.48 m(A.GR.L)
DWL: 9.0 m(B.GR.L)
PT.COMM:
LITH:
11.0 CLAY
22.0 SAND
43.0 CLAY Clay with thin\gravel layer
68.0 GRAVEL Gravel with thin\clay layer
75.0 CLAY
81.0 GRAVEL Gravel
86.0 CLAY
91.0 GRAVEL Gravel
103.0 CLAY
134.0 GRAVEL Gravel with thin\clay layer
152.0 CLAY
173.0 CWIOS Clay with sand\& gravel
198.0 SCWG Gravel and sand\with thin clay\layer
203.0 CLAY

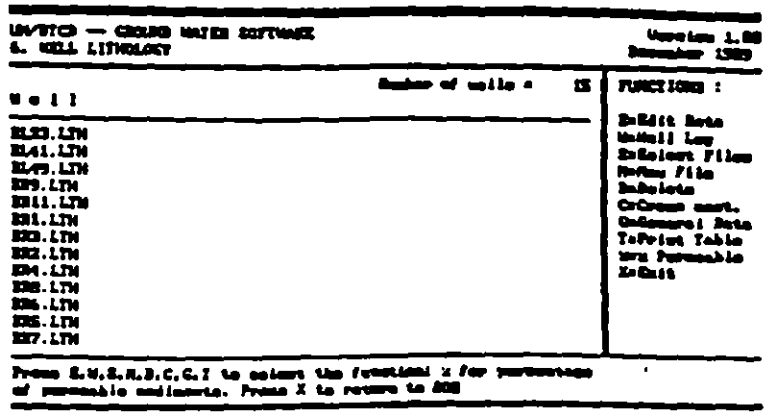


Fig. 6.3

Abbreviations are for the following:

LOC	– location
ELEV	– elevation
DR.METHOD	– drilling method
DR.DATES	– drilling dates
COMM	– comments
PT.DATE	– pumping test date
DUR	– duration of pumping test
TRAN	– transmissivity value
SWL	– static water level
DWL	– dynamic water level
PT.COMM	– pumping test comments
LITH	– lithology

Some of the fields must be input in correct format, some are just for the record and can contain anything. That "anything" will be printed on the well log, however. The first field, WELL, is important because its content will be printed on the cross section exactly as it is typed. If you want number to be shown on your lithological cross section, type the number. Type the name if this is what you want.

Elevation and coordinates must be correct, that is only numbers without blanks or any textual character. A typical mistake is to type elevation with m (meters) or ft (feet). This will not create a problem in printing the well log, but it will be noticed by the program when a cross-section is attempted, or when a table of data printed.

Several comments are in order.

(1) All data in data files are typed from column 11 on, although you may start at any column after the tenth.

(2) You may specify several well screen sections in one well by typing beginning and ending depths of the first section, followed by the beginning and ending depths of the second section, etc., with each value separated by a comma. In the above example (BR4.LTH) there are nine screen sections, the first at 51.8-56.9, and the last at 191.0-197.1 m. Typing the interval such as 24.5-30.5 will create error. Likewise, you must not type textual comment such as "Uncased", or "Screen position unknown". Only numbers separated by commas are allowed!

(3) The "total depth" information does not appear explicitly in the data form or file. The final depth of the last lithological unit is interpreted by the program as equivalent to the total depth. You may write in "Comments" if this is not the case.

(4) On "Comments:" line in data form (file), five lines of information can be accommodated. The instruction marker for the program to start with next line is the backslash character "\". For example, if you want the following comments to appear:

Screen: 40.2–45.5 m.
Type: Wire-wrapped, slots 0.5 mm.
M.P.: 96.95

the comment line should be typed as follows:

Screen: 40.2-45.5 m.\Type: Wire-wrapped, slots 0.5 mm.\M.P.: 96.95

(5) Exactly the same principle is used in typing lithological descriptions for various units (layers) for which you want to use a description other than the default. For example, for the description "Alternate bands of clay and gravel" you may type "Alternate\bands of clay\and gravel" next to the symbol selected to represent such lithology. In order not to type over the vertical line ending the well log, you should not have lines longer than 20 characters in the lithological description. Lithology may be typed with the default values for symbols, or with additional text of your own.

View the data with your editor, and quit editing by using your editor's command to quit and return to the main program. Instead returning to the main program you will be back in the main menu ready for further action. You will see the message "Error in file edit" if the program discovers that something is wrong.

Before you continue, it is good practice to write the table with all general data to a disk file. This routine will detect most of errors in your input. Type the letter T. Supply a file name as an answer to the program prompt: "File name to accept data". As an example type "TABLE". The program will inform you what it is doing. Also if the program detects an error, it will display the name of the file in which the error was detected. If no errors are detected, you may view this table by exiting the program (letter X) and using the DOS command "TYPE TABLE". The table shall look as follows:

No.	WELL NAME	X		Y	Z	DEPTH SCREEN
1	BR1.LTH	730560.	3045600.	95.95	193.00	48.7
2	BR2.LTH	728000.	3044160.	92.80	194.00	48.7
3	BR3.LTH	730560.	3047040.	97.30	163.10	16.5
4	BR4.LTH	730240.	3050000.	99.30	203.00	43.7
5	BR5.LTH	727600.	3044720.	94.80	180.10	56.2
6	BR6.LTH	728480.	3048960.	98.98	182.00	31.2
7	BR7.LTH	729280.	3047280.	100.70	163.00	45.5
8	BR8.LTH	729120.	3048720.	98.70	167.00	43.7
9	BR9.LTH	728480.	3047120.	98.10	166.10	38.6
10	BR10.LTH	727920.	3045920.	95.99	195.00	43.5
11	BR11.LTH	728480.	3046320.	96.90	222.00	39.8
12	BL32.LTH	734320.	3057920.	119.40	136.00	47.3
13	BL33.LTH	733360.	3056640.	115.90	143.30	49.8
14	BL41.LTH	732400.	3054000.	110.30	176.00	58.8
15	BL49.LTH	731280.	3052240.	109.80	168.00	49.3

Number of wells in data base:	15
Total drilled depth in data base:	2651.6
Average depth per well:	176.8
Total screened interval:	661.3
Average screened interval:	44.1
Number of wells with screen:	15
Number of wells w/out screen:	0

Now you may check the percentage of permeable materials in each well and in the whole area (data base). Select "%". You will be asked for a depth down to which you wish to calculate this percentage. If you wish to get the percentage of permeable versus impermeable materials for all wells, regardless the depth, answer this prompt by a number greater than maximum drilled depth. In our case type 230. Supply the name for the file to receive this information as "PERCENT". The program now offers you an opportunity to select a certain portion of the area with wells in which you might be interested. For example you may want to obtain average percentage of permeable materials in a certain quadrant. Supply initial X and Y coordinates, and final X and Y coordinates. Actually you are specifying the coordinates of the lower left corner and the upper right corner of a rectangle, respectively. You may override this option by pressing RETURN four times. While processing, the program will inform you what is it doing. After a while, the following table shall be written to the disk file PERCENT:

WELL NAME	DEPTH	PERMEABLE	PERCENT
BR1.LTH	193.0	49.0	25.4
BR10.LTH	195.0	35.0	17.9
BR11.LTH	222.0	94.0	42.3
BR2.LTH	194.0	110.0	56.7
BL32.LTH	136.0	88.5	65.1
BR3.LTH	163.1	54.0	33.1
BL33.LTH	143.3	82.7	57.7
BR4.LTH	203.0	103.0	50.7
BR5.LTH	180.1	82.1	45.6
BR6.LTH	182.0	74.0	40.7
BR7.LTH	163.0	88.0	54.0
BR8.LTH	167.0	50.0	29.9
BR9.LTH	166.1	79.0	47.6
BL41.LTH	176.0	107.0	60.8
BL49.LTH	168.0	113.0	67.3

DEPTH OF CALCULATION: 230.0
Cumulative depth down to selected range: 2651.6
Total permeable thickness in selected range: 1209.3
Average percentage of permeable materials: 45.6%

However, it may be of interest to calculate the percentage of permeable materials to a depth less than the one reached by the deepest well. Say, you are interested in upper 60 m. Without exiting the program, select % again, and answer with the depth of 60. Supply the file name as PERC60. Type this file after exiting the program. It looks as follows:

WELL NAME	DEPTH	PERMEABLE	PERCENT
BR1.LTH	60.0	0.0	0.0
BR10.LTH	60.0	0.0	0.0
BR11.LTH	60.0	16.0	26.7
BR2.LTH	60.0	0.0	0.0
BL32.LTH	60.0	33.9	56.5
BR3.LTH	60.0	26.0	43.3
BL33.LTH	60.0	26.5	44.2
BR4.LTH	60.0	28.0	46.7
BR5.LTH	60.0	9.0	15.0
BR6.LTH	60.0	27.0	45.0
BR7.LTH	60.0	33.0	55.0
BR8.LTH	60.0	6.0	10.0
BR9.LTH	60.0	43.0	71.7
BL41.LTH	60.0	38.0	63.3
BL49.LTH	60.0	37.0	61.7

DEPTH OF CALCULATION: 60.0
Cumulative depth down to selected range: 900.0
Total permeable thickness in selected range: 323.4
Average percentage of permeable materials: 35.9%

The program has given you an analytical tool that will tell you which interval contains the most permeable materials. In our case, all wells down to 60 m depth display an average percentage of permeable materials of only 35.9, while going deeper, to 230 m, this percentage becomes higher, 45.6. Likewise you may analyze a certain area, not only a certain depth interval.

However, it is important to understand how the program distinguishes between permeable and impermeable materials. The program checks each layer in each well and evaluates against all lithological symbols in the file GW6.DLT. If the interval is described by one of the following 13 codes, the interval is permeable:

SAND, SANDV, SANDF, SANDM, SANDC, SCWG, GRAVEL, GRAVELF, GRAVELC, GWS, PEBBLE, BOULDER, GWS.

(You may redefine some of descriptions for these 13 codes, but keep the same codes in the file GW6.DLT. You will notice that SCWG means "Sand Coarse with Gravel", that GWS stands for "Gravel with Sand", etc.)

6.4.2. Display, Print or Plot Well Log

Press W to display and/or print a well log. You will be offered four choices: (1) to display log (letter D), (2) to print log (letter P), (3) to plot log directly through the COM1 serial port to plotter (letter A), (4) to create a plot file in ASCII format to be edited and/or used by another commercial graphical program (letter B).

Whatever you select, there will be a message: **Change Length of Log [Y/N]:**. You will see also the following text to remind you what you may do.

> The default vertical size of well log is 16 cm. You may increase the size by pressing Y and supplying any length between the default and 40 cm. However, display shall be impaired, letters will become squeezed, and it will take time to display and/or prepare for printing. Use mouse to zoom. Use continuous computer paper to print long logs.

This option gives you the possibility to create larger well logs than A4 format. As an exercise press Y. The new message will be: **Type new log length (max. log length = 40 cm)**. Type 20 and press RETURN. You will be prompted to change scale that otherwise will be automatically selected by the program. (The program always selects the scale in such a way that the whole space allocated for the log, normally 16 cm or whatever you specify, is filled with the log.) The message is: **Your Scale [Y/N]**. There is also a text displayed on the screen to inform you about this possibility. The text is as follows.

> Answer with Y if you wish to override automatic scale selection. Program normally uses a scale such that whole 16 cm, or whatever you defined one step before, is filled with lithology. Type only denominator of scale. E.g., for 1:1000 type only 1000. You may check maximum scale by typing small number. Program will display maximum scale.

Type Y and press RETURN. The message is **Type your scale. Remember well log length = 20.0 cm**. Now you may find out what would be the program-selected scale that would fill in the whole space. Type 10 and press RETURN. The program displays **Scale greater than max permitted: 742.49. Any key to try again.** When prompted again for your scale press N and accept the program's scale.

If everything is in order, your lithological symbols correctly typed and selected, and your printer or plotter properly connected to the computer, after a few seconds the message line at the screen bottom will display the message "Creating page layout ...", followed by another message "Rasterizing and printing ...". Remember this is a graphics program and the whole page must be laid out, and rasterized for displaying and/or printing. This takes time - on Toshiba 1600, which is equipped with 12 MHz 80286 processor and 10 MHz 80287 co-processor, it takes about 2 minutes to set up and print well log; on AST Premium, running at 25 MHz and equipped with INTEL 80386 processor, it takes only 35 seconds to display a well log). If there is an error, notably in lithological part, the program displays the message "Error in log print". The typical error will be if you have in your data file (well file) some lithological codes that do not match the list in the program file GW6.DLT.

If you opt to display the log on the screen you will notice that the screen resolution is insufficient to allow you to see details. Yet, with a mouse connected to the system, you have an opportunity to zoom a portion of the log and see all details clearly before you decide to print or plot the log. Type Z for zoom; move the cursor to the lower left corner of the rectangle you wish to enlarge. Press the left mouse button. Move the cursor to the right upper corner to define the rectangle. Press the left mouse button again. The screen may look as in Fig.6.4A.

On the color monitor, you may note that all permeable layers are shown in blue, while impermeable parts are yellow.

The printer prints first two lines of project identification (Project and Organization), followed by General Well Data, Well Construction and Lithological Log, and pumping test data (Fig. 6.4). In the Pumping Test portion only information that is available will be printed. The plotter will plot everything except the first two identification lines.

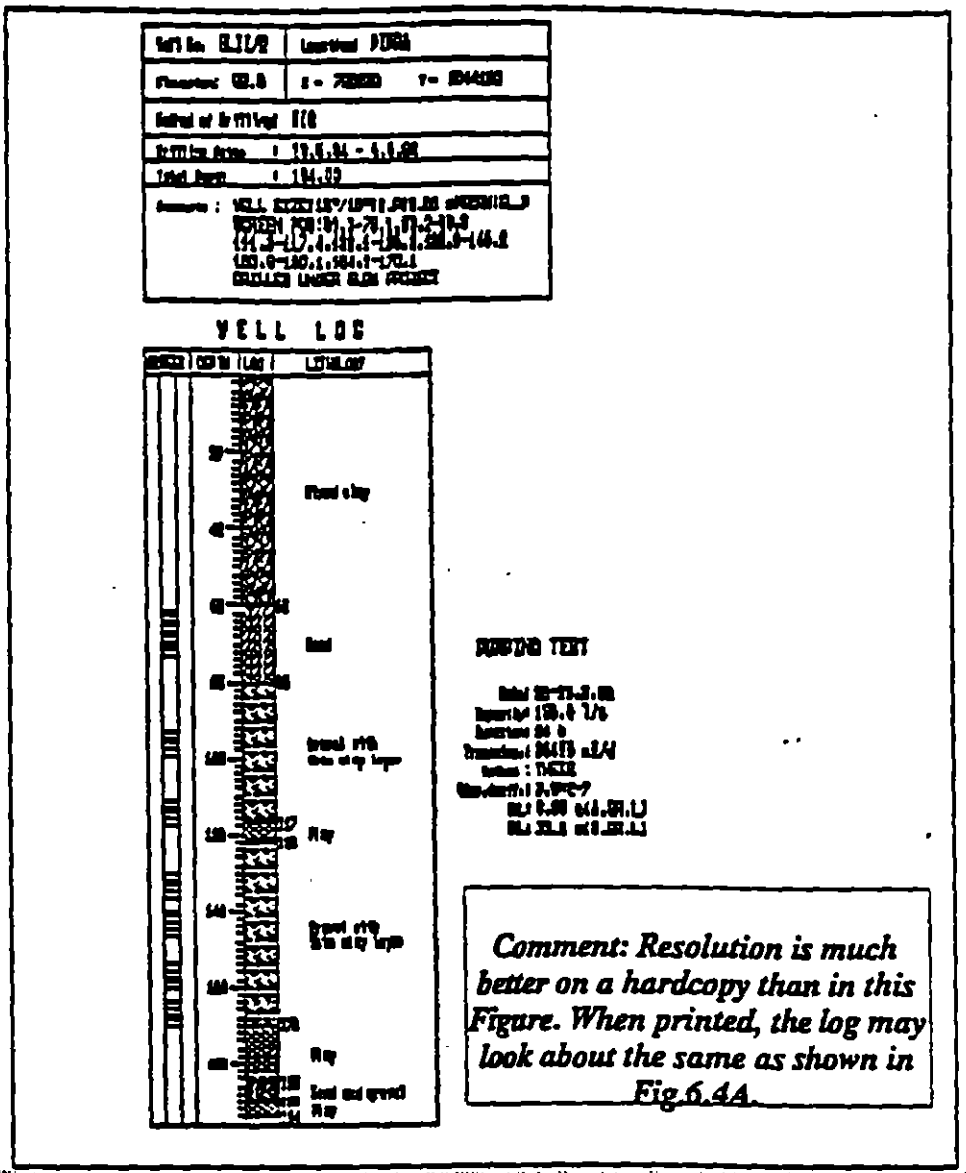


Fig.6.4

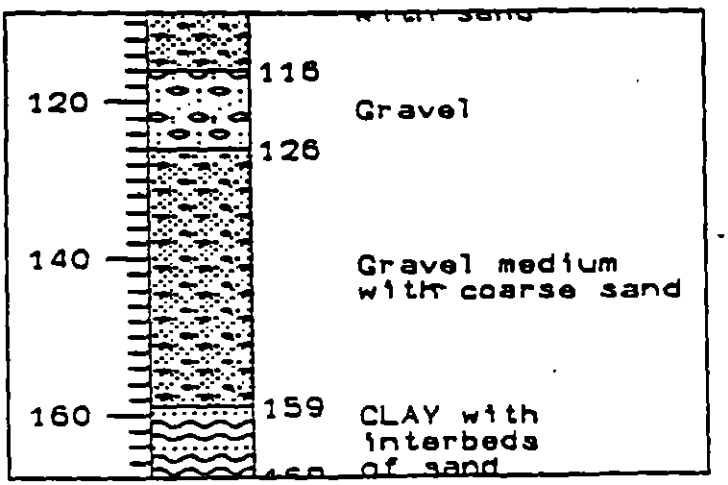


Fig. 6.4A

6.4.3. Display and Print Cross-Section

Select C for cross section. At the very beginning of this portion of the program you are asked the followin "Save well positions for plotting [Y/N]". If you answer Y (Yes), the program will use the DIGXSC.EXE fi in \GW\GW6 to create a map of well locations in the actual coordinate system. Type Y. The following promp follow. Answers are shown to the right.

Output file	Example
Plot well labels? [Y/N]	Y
Circle diameter (cm)	0.10
Cross height [cm]	0.0
Symbol color	4 (red)
Label height [cm]	0.1
Text color	6 (yellow)
Label x-offset [cm]	RETURN
Label y-offset [cm]	RETURN

When you select to plot well labels, you should supply the size (label height) and color of the label. The colc numbers are the following: 0-black, 1-blue, 2-green, 3-blue/green, 4-red, 5-pink, 6-yellow, 7-white.

Label offset means the shift of writing labels with respect to the location of circles.

The program starts reading coordinates and elevations of all wells, and displays the message to that effec "Reading coordinates and elevations. ESC to stop." After all wells are checked for coordinates and elevations provided that errors are not detected, the program prompts for the format of printout:

"What is the format of the paper you use?. Press 4 for A4, or 3 for A3, or [ENTER] for other format."

Type 4 and RETURN. Wait a little bit, while the program creates a map of well locations. The next promp is for the cross-section title that will be displayed/printed "Enter cross-section title". Type "CROSS-SECTIOI II-II' RUPANDEHI DISTRICT", or skip the title by pressing ENTER.

The program now asks you to select the cross-section line. You may do it in two ways: (a) with a mouse, o (b) by supplying coordinates for the beginning and terminating points of the line. The prompt is as follows

Do you want to digitize ending points? [Y/N]

If you answer Y, the map will be displayed with location of all wells in the data base. You will notice a cros which you can move with mouse to the beginning point of the cross-section line. Press the left mouse buttor at the beginning point. Move the mouse away. You will notice a "rubber-band". Press the left mouse buttor at the ending point of the cross-section line.

In this example you should answer N. The dialog between the program and you will be as follows:
"X-coordinate for STARTING point"... Type 735000.

"X-coordinate for ENDING point" ..... Type 725000.

Note that program suggest the same number for ending point as for the initial point. This is for the case o north-south cross-section, in which both X coordinates are the same.

"Y-coordinate for STARTING point" ... Type 3060000
"Y-coordinate for ENDING point" ..... Type3040000.

After the program "learns" from you which cross-section line you want to make, either with a mouse or b typing the coordinates, there will be one more prompt:

Max. distance of cross section line

The number you supply is interpreted by the program as the spacing on either side of the cross-section lin within which the wells will be used and projected onto the section line. Type 400. This means that all well that are less than 400 m far from the cross-section line will be projected onto the line. Always press RETURN after each number. The program scans coordinates, elevations, and distance from the cross-section line, an displays selected wells on the right side of the screen, writes a message at the bottom "Confirm or edi minimum elevation", and shows in a rectangle in the middle of the screen the following (Fig. 6.5):

Horizontal Scale:	100000.0
Vertical Scale:	500.0
Cr. Sect. Length:	22360.7

Required "cm" H:	24.4
Required "cm" V:	53.0
A4 format (HxV):	26x15.5 cm;A3:36x22 cm

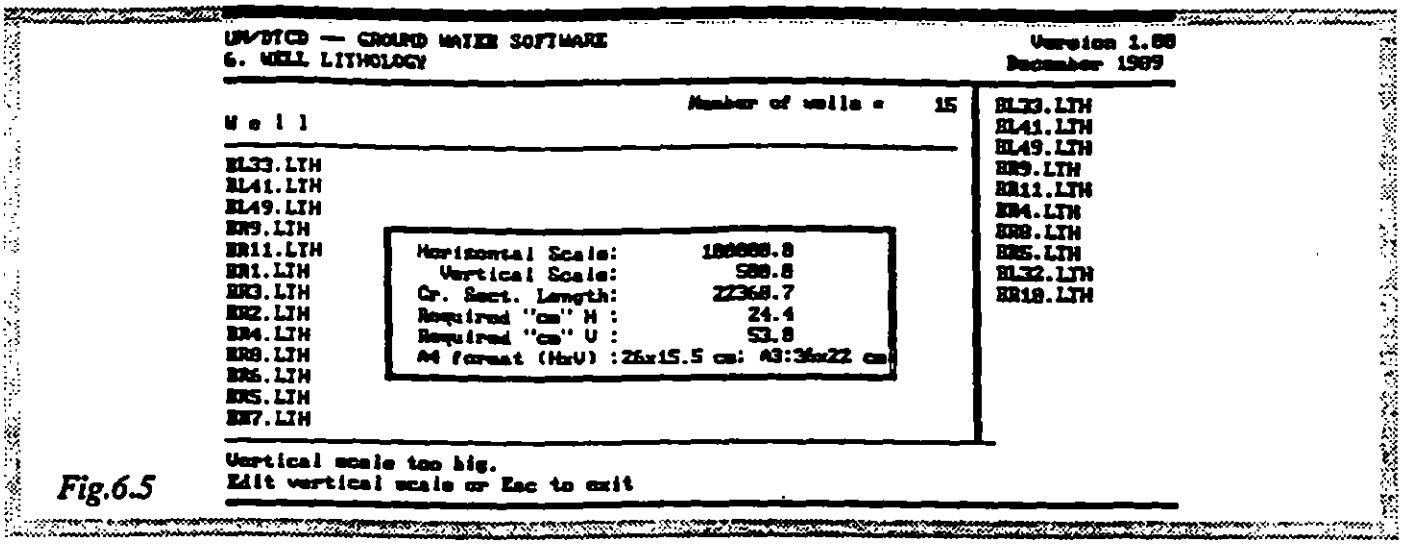


Fig.6.5

The first message "Confirm or edit minimum elevation" informs you that you may select a portion of the cross section, down to a certain depth specified by you, or the whole depth controlled by the bottom of a well which is at the lowest elevation. This is important if you wish to get details for shallower part of the cross section. In your example the minimum elevation of the cross section will be -125.10. The program automatically checks the scale (the one you have input in GW6.GEN file). If the scale, either horizontal or vertical, is too large, a message to that effect will be displayed, and you will be given a chance to modify the scale, until you find the size of the drawing that suits you best. You may experiment with scales. If you select 1000 for vertical scale the vertical size of the graph will be 28.0 cm, which is more than the A4 format. You will notice that th appropriate scales shall be 2100 for vertical, and 100,000 for horizontal.

In this example 10 out of 15 wells will be plotted on the cross-section: BL32, BL41, BL49, BL33, BR4, BR10, BR11, BR5, BR8, BR9. The names of all files to be plotted are shown in the right window. Due to limited space on the screen the maximum number of files to be displayed is 18. (Hardly ever you will have more than 18 wells on one cross section. Wells would overlap one on the other.)

If the program notices any error in lithological description (code, depth) there will be a corresponding message and the file name will be displayed. Thus you can locate the error and correct it. Should you decide to stop the processing, you may do so by pressing ESC. However, wait until the processing comes to next well. It may take a while, depending on the speed of your processor, and number of layers in the well that is being read!

In this portion of the program, lithology is checked for files to be shown on the cross section. The message displayed in the first "message line" is the following:

"Reading lithological description. Selected wells are shown above right."

The second line displays file names:

"Now reading ... BL32.LTH .... ESC (and wait!) to quit."

If everything is in order there will be a message "Display [D], print [P], plot [A], or create ASCII plot file [B] of this X-section?" If your computer is equipped with a graphics adapter, you should select "D" to view the cross-section. Notice that all permeable layers are shown in blue, while all impermeable layers are in yellow. Thus on a glance you may notice which parts of the cross section are more permeable. You may zoom a portion of the cross section to see details. Follow the instructions as discussed in the **Introduction.**

After viewing the cross section press ESC to escape. There will be a message "Print or plot this X-section [Y/N]". If you select "Y", you will have to direct the output to either printer [P], plotter [A], or ASCII plot file [B]. The output shall be of the size as selected earlier by modifying the vertical and horizontal scales. During the printing there will be a message "Rasterizing and printing ..." which stays on the screen as long as the real printing is done.

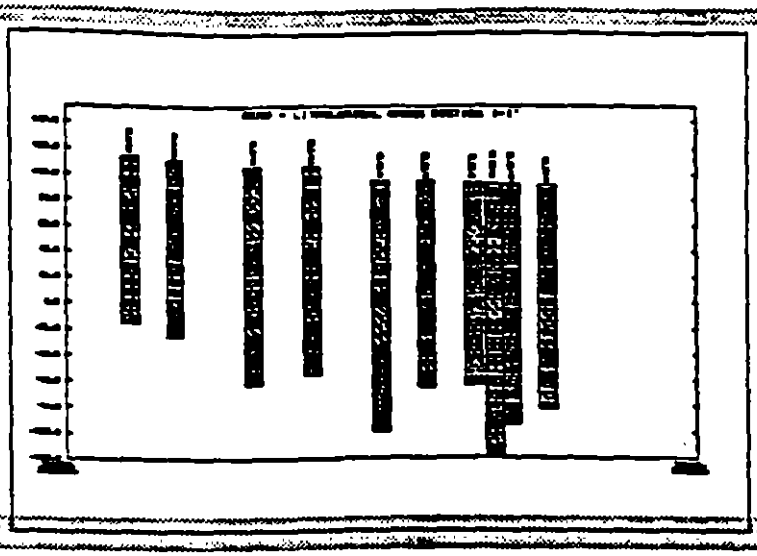


Fig.6.6

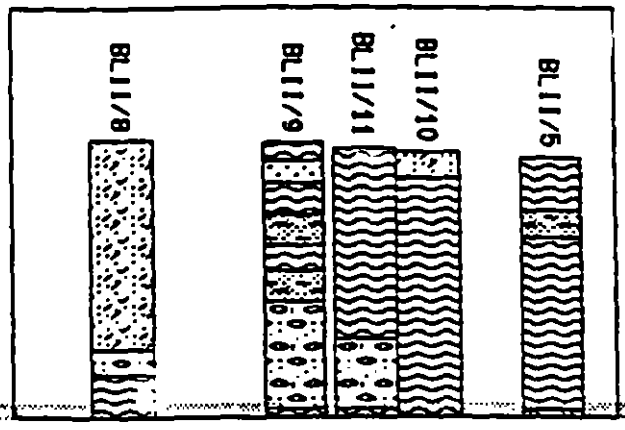


Fig. 6.6A

The cross section looks as shown in Fig. 6.6. You must draw a land surface line, either directly connecting wells, or by consulting the topographic map and interpolating correct elevations. In addition to vertical scale shown on the left, the cross section is identified with X and Y pairs of coordinates for beginning and ending points. Each well is identified by the description supplied by you in the first line in data form (WELL:).

Same as in the case of well log, you may use the mouse to enlarge a detail. Type Z. Move the cursor to the lower left corner of the rectangle you wish to enlarge. Press the left mouse button. Move the cursor to the upper right corner to define the rectangle. Press the left mouse button again. The screen may look similar to Fig.6.6A.

After one cross section is printed, the prompt is back at "Enter cross section title".

Now, type anything on this prompt and press RETURN. To the next prompt "Max. distance of cross-section line" type 1000. Select Y to digitize ending points. Wait until the well map appears on the screen, Fig. 6.7.

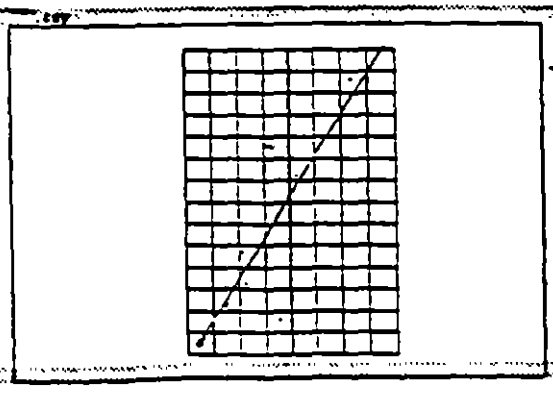


Fig.6.7

Use the mouse to select the line from the southwest to northeast.Experiment with different scales, view the cross-section on the screen, and print or plot when you are satisfied.

6.5. Create Data File

To create a data file using your text processor, type the letter N from the main menu. The program responds with "Enter new file name". Type "TEST.LITH" and press RETURN. After a few seconds your editor's familiar logo will appear and well format data input will be displayed. The cursor will be on the W in the line Well:. Move the cursor to column 11 in this line and type the well identification. What you type here will appear on top of the well when it is shown in cross sections. Restrict the WELL NO. to a maximum of 8 characters. Type "Well 1". Press the down arrow to move the cursor down. The cursor is set at column 11 (if you use WordStar) or under the last character of the previous line (if you use Personal Editor) in the second line defined with LOC:. Type for well location "Kapilvastu". Keep in mind that not more than 20 characters can fit the printout. Press the cursor down key. Type 96.68. Press cursor down. Type 696500 for X, press cursor down; type 3046750 for Y and press cursor down. On SCREEN line type 15.5,21.0,40.0,45.5. This means that this well has two screen sections; one from 15.5 to 21.0, and another from 40.0 to 45.5. Press cursor down key. On DR.METH: line (drilling method) type ROTARY RIG. Press cursor down. On DR.DATES: line (drilling dates) type 15/3/89 – 18/3/89. After pressing cursor down key you will be on COMM: line. Here type several comments, all on one line, separated by backslash. For example, start with "Screens at 15.5–21.0 m and 40.0–45.5 m.\Measuring point +0.5 m above LS.\Screen type: Wire-wrap with 1.5 mm openings. The space reserved for comments permits five lines to be printed. Press cursor down key. On PT.DATE line (stands for Pumping Test Date) type 22/4/89. Press cursor down key. For Q type 5 l/sec. For DUR: (duration of pumping test) type 60 minutes. Next line is TRAN: (transmissivity), followed by METHOD: (test interpretation method), and STORAGE: (storage coefficient). Type one after another: 125 m2/day, THEIS, 0.004, and press cursor down key after each entry. For SWL: and DWL: (static and dynamic water levels, respectively) type 3.45 m and 5.65 m. After SWL the form contains one additional "comments" line, PT.COMM:. The information you supply shall be printed in one or more line, depending whether you split the comments with backslash "\". Type the following under PT.COMM: Discharge fluctuates\Level unsteady\Test interrupted.

The final query is LITH:. Go to one line below the LITH: line. It is not important whether you start in column 1,2 or any. Suppose your lithological log looks as follows:

0–3.4	m	CLAY
3.4–6.3	m	SAND fine-grained
6.3–9.2	m	SILT mixed with some sand
9.2–13.3	m	Sand coarse with coarse gravel
13.3–16.2	m	CLAY hard, layered
16.2–21.2	m	Metamorphic rocks, dense, hard

If you do not want to create your own symbols for lithology (for explanation see Appendix A), select for "CLAY" the symbol from GW6.DLT file also labeled as CLAY, for "SAND fine-grained" symbol SANDF, for "SILT" symbol labeled SILT, for "Coarse sand with gravel" symbol SCWG, and for "Metamorphic rock" the symbol ROCK7. However, the description of lithology that you want to appear on the log is not the same as default in GW6.DLT, except for CLAY. Type your own description in data file after the symbol code, separating lines of text with backslash "\".

After LITH: line, type as follows:

```
3.4 CLAY
6.3 SANDF SAND fine-grained
9.2 SILT SILT mixed\with some sand
13.3 SCWG SAND coarse with\coarse gravel
16.2 CLAY CLAY hard,\layered
21.2 ROCK15 Metamorphic\rocks, dense,\hard
```

After each line press RETURN. Before exiting check that the cursor is on the line below the last lithological layer.

The program is prepared in such a way that it checks for code for lithology, and uses its own description from GW6.DLT if there is nothing typed after the code, or it uses your own definition if there is something afte the code. Only in the case of the first layer, CLAY, there is nothing typed and the definition "Clay" from th GW6.DLT file is used. In every other line, you have supplied your own definitions. Make note that no mor than 20 letters can fit the space on the log and split the text into two or more lines, provided that scale an thickness of a layer permits it. Notice also that the program is case sensitive, i.e. lower case letter is differen than the upper case letter.

Save this file in the way you would normally use your editor. Read explanation for various text editors in tex to follow. If everything was correct, press P to print this well log.

6.5.1. Work with Various Editors

This program was tested with the following editors: WordStar release 4, IBM's Personal Editor (PE), WordPerfect version 4.2, PFS Write, Norton Editor. Theoretically every editor should work. The important thing to remember is that before returning to the program's main menu, the file created by any editor must be converted to DOS text format or ASCII. With Personal Editor and Norton Editor there were no problems. since both create automatically an ASCII format. With other three editors a conversion was required. If you do not convert the file, you will have some incompatible characters, usually from ASCII set above 128. Should such a character occur the program either displays the message "Error in well log", or hangs. Should this occur, exit the program (or reboot the system), use the SHOW "filename" program supplied on the distribution diskette, and detect such characters. Or, alternatively, type the DOS command GRAPHICS, and use the standard DOS command TYPE "filename" to view the data file which is corrupted. Remember the corrupted characters, return to your text editor and correct them. Run the GW6 program again. Yet it is better to avoid the problem by following the procedure outlined here below.

Wordstar 4.0

Fill-in the form on the screen, or edit data, in a standard way. Do not exit by typing CONTROL+K,X but save the file by CONTROL+K,D. On WordStar prompt type P for "Print file", and supply the name of your data file which you just have created. Suppose that you supplied the name TEST1 after pressing N from Main Menu. Now reply to WordStar prompt "Document to print?" with TEST1, and press several returns to come to the prompt "Name of printer?". Type ASCII. There will be a message in the upper right corner of WordStar menu "Printing". When it disappears rename the file ASCII.WS, which was created by WordStar (and which is your file!). Press E (for rename file), supply the name of the file to be renamed ASCII.WS, press RETURN, and supply the name of the new file (converted), say TEST2.LTH. Now press X to exit from WordStar and to return to the main menu of the GW6 program. The list of files still does not display this newly created file. Press S to select a file, and supply the name TEST2.LTH. Now everything is in order and you can print the well log, or continue with input of other wells. WordStar has a rather awkward way to create an ASCII file.

WordPerfect, ver. 4.2.

With WordPerfect it is much easier to create an ASCII file. In your GW6.GEN file on EDITOR: line type the path to your Wordperfect directory, say \WP\WP.EXE. Press N to create a new data file, give the name TEST3, and fill in the form automatically displayed on the screen. After you finish do not exit the WordPerfect. Press CONTROL+F5, followed by number 1. Confirm the name of your new data file with Y (YES), press F7 to exit WordPerfect, and answer the options with N (NO). You will be back in the GW6 program, and your data file will be replaced by a good ASCII version. You may print TEST3 well log, or continue with the work.

PFS WRITE

There is also an integrated software package, PFS First Choice, which in addition to text editor has spreadsheet, calculator, and data base. GW6 will not work with this program because of memory problem (there will be a message "not enough memory"). With PFS it is simple to create an ASCII data file. Select F2 to save file, and supply the name of the data file with extension not displayed. Use S to select file, and supply the name TEST4.ASC.

NORTON EDITOR, XTPRO and many other editors create directly an ASCII file.

Appendix A.

Creation of Lithological Symbols

List of Lithological Symbols (see Figures 6.8, 6.9, 6.10, 6.11)

ROCK1	Rock1
ROCK2	Rock2
ROCK3	Rock3
ROCK4	Rock4
ROCK5	Rock5
ROCK6	Rock6
ROCK7	Rock7
ROCK8	Rock8
ROCK9	Rock9
ROCK10	Rock10
ROCK11	Rock11
ROCK12	Rock12
ROCK13	Rock13
ROCK14	Rock14
ROCK15	Rock15
CLAY	Clay
CLAYH	Clay hard
SAND	Sand
SANDV	Sand very fine
SAND	Sand
SANDF	Sand fine
SANDM	Sand medium
SANDC	Sand coarse
SCWG	Sand coarse\with gravel
GRAVEL	Gravel
GRAVELF	Gravel fine
GRAVELC	Gravel coarse
GWS	Gravel with sand
MIXED	Mixed sand\and silt
SILT	Silt
CWIOS	Clay with\interbeds\of sand
SRGRAV	Semi-rounded gravel
CWG	Clay with thin\gravel layer(s)
LIME	Limestone
DOLO	Dolomite
GWC	Gravel with thin\clay layer(s)

The creation of symbols shall be explained first using simple examples from the default file GW6.DLT. Take for example the symbol for SILT. The block for silt is copied here below.

```
SILT Silt
2 2
2 0.0 0.0
1 1.0 1.0
```

The first line contains the code for silt "SILT", and the default description that will be typed in well log if you do not override the default. (You can also modify this default file by adding a word or more to Silt to better identify the unit. This will than become the default for SILT) The code may have up to 10 characters. Upper case and lower case letters are not the same. In other words, the program is sensitive to the case of lette The description may be any combination of up to 100 characters.

The second line contains two numbers which define the size of a block. The philosophy of creating symbols is related to the size of blocks. One block is repeated in both horizontal and vertical direction in the log. One may think of small building blocks, such as bricks of exactly the same size and shape, which are laid on top and side one from the other to fill the whole space. The numbers 2 2 imply a square, so that any symbol defined in such a square shall be symmetrically repeated horizontally and vertically. We will demonstrate this concept later!

The block for silt, as well as for any other symbol, terminates with "*". Between the first line and the asterisk sign, there may be one or many lines. The first number in each such line can be 2, 1 or 0. The number 2 defines the starting point, number 1 means "connect this point with the previous", number 0 means "make an arc through this point without actually passing through it". In the third line of the SILT block, the remaining two numbers (0,0) define X and Y coordinates of the starting point within the block defined by 2 by 2. The number 1 in the next line is interpreted as "connect the starting point with this point", and the coordinates of this second point are 1.0 and 1.0. When this is interpreted, the diagonal line appears in the lower one half of the square, connecting the point with coordinates (0,0) with the point with coordinates (1,1). Since the small block which defined the symbol is repeatedly used, the final appearance of this symbol is as is usually used for SILT. If one wants to create a symbol for horizontal lines widely spaced, such as the default symbol ROCK1, the design would be as follows:

```
ROCK1 Rock1 (you may type something else)
2 2
2 0.0 1.0
1 2.0 1.0
*
```

This is equivalent to saying "draw a straight line from starting point with X,Y coordinates (0,1) to ending coordinates (2,1)", which is along the middle of the block of size 2,2. If one wants denser horizontal lines, tl block to define should be smaller, and so will be the spacing between repeating blocks. For example,

```
ROCK2 Rock2
1 1
2 0.0 0.5
1 1.0 0.5
*
```

Very narrowly spaced horizontal lines can be obtained by assigning even smaller size to the block, say 0.5 by 0.5. Thus the design for ROCK3 may be as follows:

```
ROCK3 Rock3
0.5 0.5      This is interpreted as "connect the point with
2 0.00 0.25  coordinates 0.00,0.25 with point coordinates 0.50,0.25".
1 0.50 0.25
*
```

In addition to connecting two points with straight lines, you may create an arc between two points. This is done by inserting a line with the first number 0 between two lines starting either with the number 2 or 1. Suppose we want to create a sinusoidal line with amplitude 1.5 and period 3.0. The block to define shall be 3 by 1.5. The fixed points should be at coordinates (0,0.75), (1.5,0.75), (3,0.75). These will be the three lines defined with starting number either 2 (for the first point) or 1 (for the remaining two points). The top of arc shall be at the point (0.75,1.5), and the bottom of arc at the point (2.25,0). Thus the block to define a sinusoidal line, which may be used to describe clay, may look as follows:

```
CLAY Clay
3 1.5
2 0.00 0.75
0 0.75 1.50
1 1.50 0.75
```

0 2.25 0.00
1 3.00 0.75
*

By reducing the height of the block from 1.5 to 1.0 the waves will become more "ironed" and lines closer. For example, one may design the following block for schist or shale:

SCHIST Schist
3 1.0
2 0.00 0.50
0 0.75 1.00
1 1.50 0.50
0 2.25 0.00
1 1.50 0.50
*

You may connect several points to create a circle, or any rounded or semirounded object. Let us create a design for semirounded fine gravel. Define the block as 3 by 2.

SRGRAV Semi-rounded gravel
3 2
2 0.70 0.40
1 0.70 1.50
0 1.40 1.90
1 1.90 1.40
0 2.00 1.00
1 1.60 0.50
0 1.15 0.20
1 0.70 0.40
*

As an exercise, double the size of this block and create gravel grains in checkered position, i.e. second line shifted to middle between two grains in lines above and below.

Now we will create a symbol for "Clay alternating with fine sand". Define block as 3 by 2.5, and use the upper 1.5 units for clay (actually, duplicate the design of CLAY), and lower one unit for sand. Start with "Clay line" in the upper 1.5 units. The starting point will be at coordinates (0.00,1.5), and fixed points at (1.50,1.75) and (3.00,1.75). The arc should pass through the points (0.75,2.50) and (2.25,1.00). Thus, the first part of the block would be as follows:

3 2.5
2 0.00 1.75
0 0.75 2.50
1 1.50 1.75
0 2.25 1.00
1 3.00 1.75

The "sand" portion of the design will be in the lower 1.0 unit, i.e. within the block defined by coordinates 0,0; 0,1; 3,1; 3,0. The sand "grains" are created by connecting points through small distance. For example,

2 0.00 0.00
1 0.10 0.00
2 0.50 0.00
1 0.60 0.00
2 1.00 0.00
1 1.10 0.00
etc.

The final design for "Alternating bands of clay with fine sand" could be as shown here below. (In your file, this should be typed line after previous line, continuously, not in three columns.)

```
ABOCWFS Alternating\bands of clay\with fine sand
3 2.5
2 0.00 1.75    2 2.50 0.00    2 0.00 0.80
0 0.75 2.50    1 2.60 0.00    1 0.10 0.80
1 1.50 1.75    2 0.20 0.40    2 0.50 0.80
0 2.25 1.00    1 0.30 0.40    1 0.60 0.80
1 3.00 1.75    2 0.70 0.40    2 1.00 0.80
2 0.00 0.00    1 0.80 0.40    1 1.10 0.80
1 0.10 0.00    2 1.20 0.40    2 1.50 0.80
2 0.50 0.00    1 1.30 0.40    1 1.60 0.80
1 0.60 0.00    2 1.70 0.40    2 2.00 0.80
2 1.00 0.00    1 1.80 0.40    1 2.10 0.80
1 1.10 0.00    2 2.20 0.40    2 2.50 0.80
2 1.50 0.00    1 2.30 0.40    1 2.60 0.80
1 1.60 0.00    2 2.70 0.40    *
2 2.00 0.00    1 2.80 0.40
1 2.10 0.00
```

If you wish to have two lines of clay before a small interbed of sand, extend the "clay" part for one more unit. For example, the design such as follows creates the shape used in Figure 6.5 for "CLAY with interbeds of sand".

```
CWIOS CLAY with\interbeds\of sand
3 4
2 0.00 3.25
0 0.75 4.00
1 1.50 3.25
0 2.25 2.50
1 3.00 3.25
2 0.00 1.75
0 0.75 2.50
1 1.50 1.75
0 2.25 1.00
1 3.00 1.75
2 0.20 0.40
1 0.40 0.60
2 1.20 0.40
1 1.40 0.60
2 2.20 0.40
1 2.40 0.60
*
```

All symbols currently contained in the GW6.DLT file are shown in Figures 6.8, 6.9, 6.10 and 6.11.

Well No.	Location:
Elevation:	X = Y =
Method of Drilling:	
Drilling Dates :	
Total Depth :	80.00
Comments :	

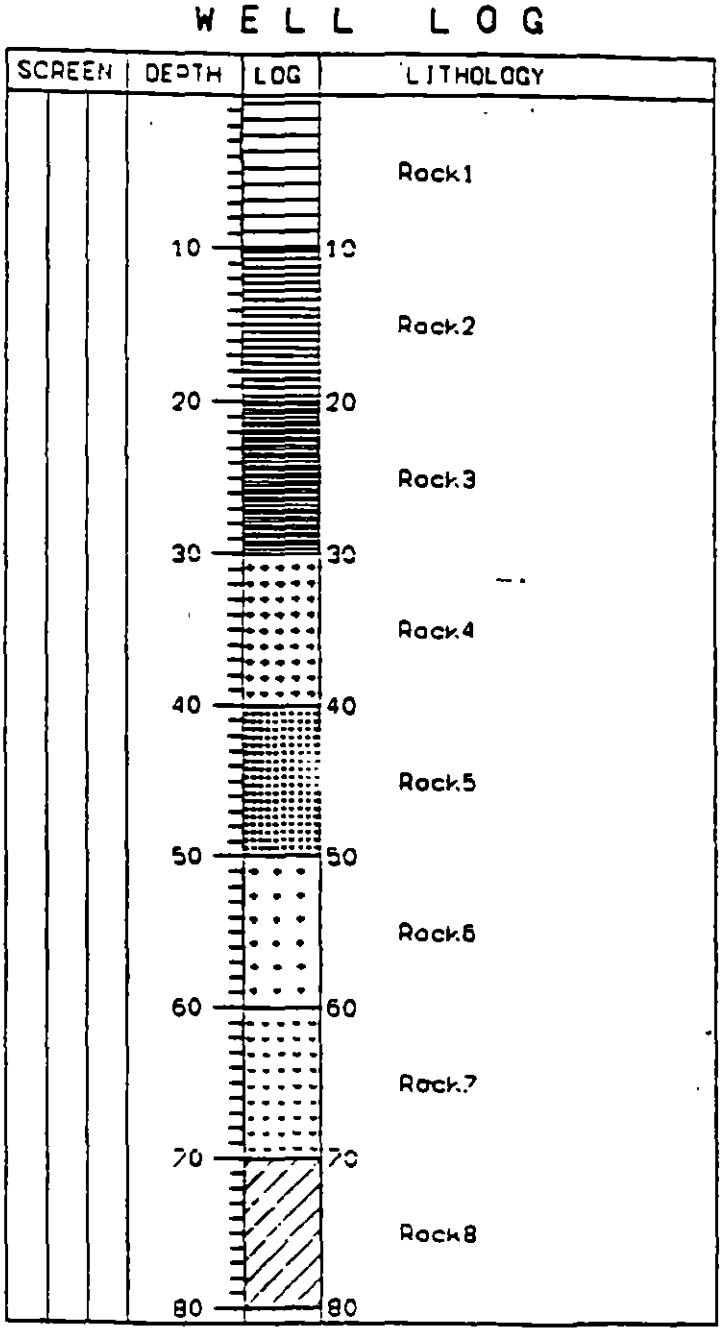


FIGURE 6.8

Well No.	Location:
Elevation:	X = Y =
Method of Drilling:	
Drilling Dates :	
Total Depth :	80.00
Comments :	

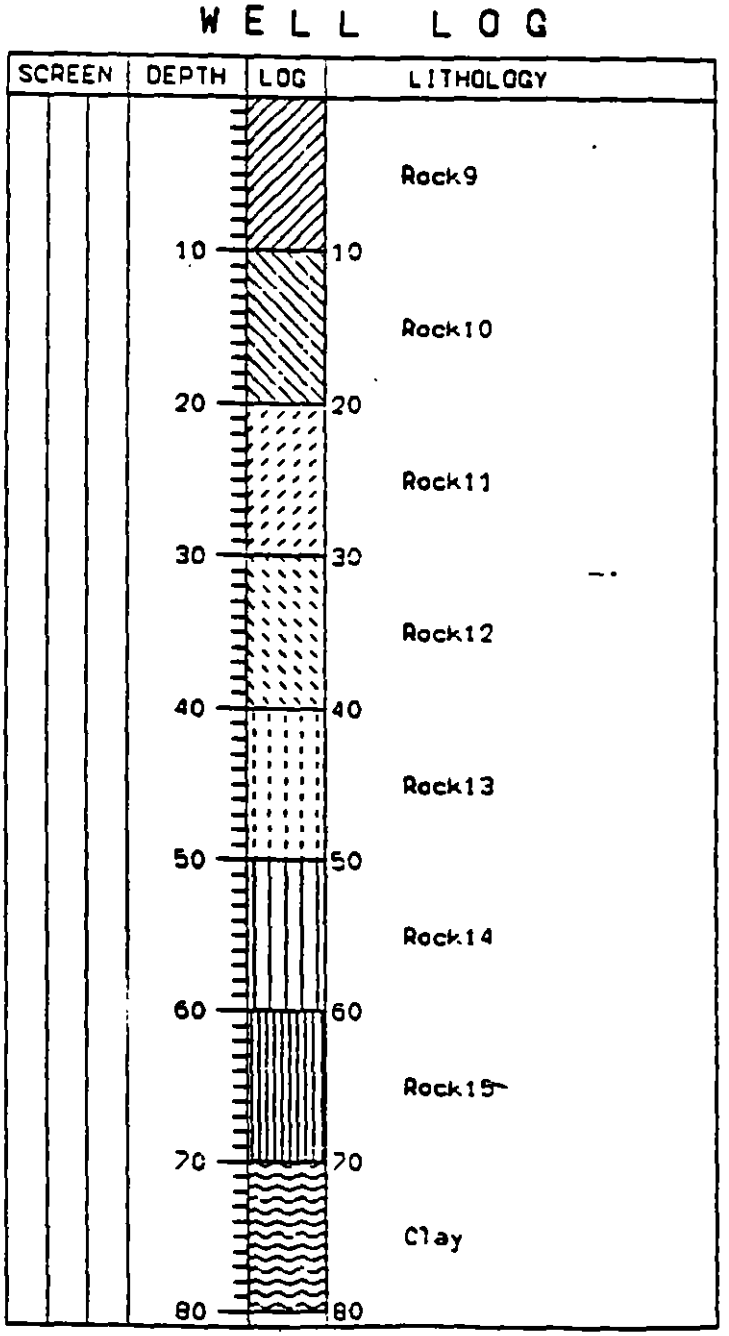


FIGURE 6.9

Well No.	Location:
Elevation:	X = Y =
Method of Drilling:	
Drilling Dates :	
Total Depth :	80.00
Comments :	

W E L L L O G

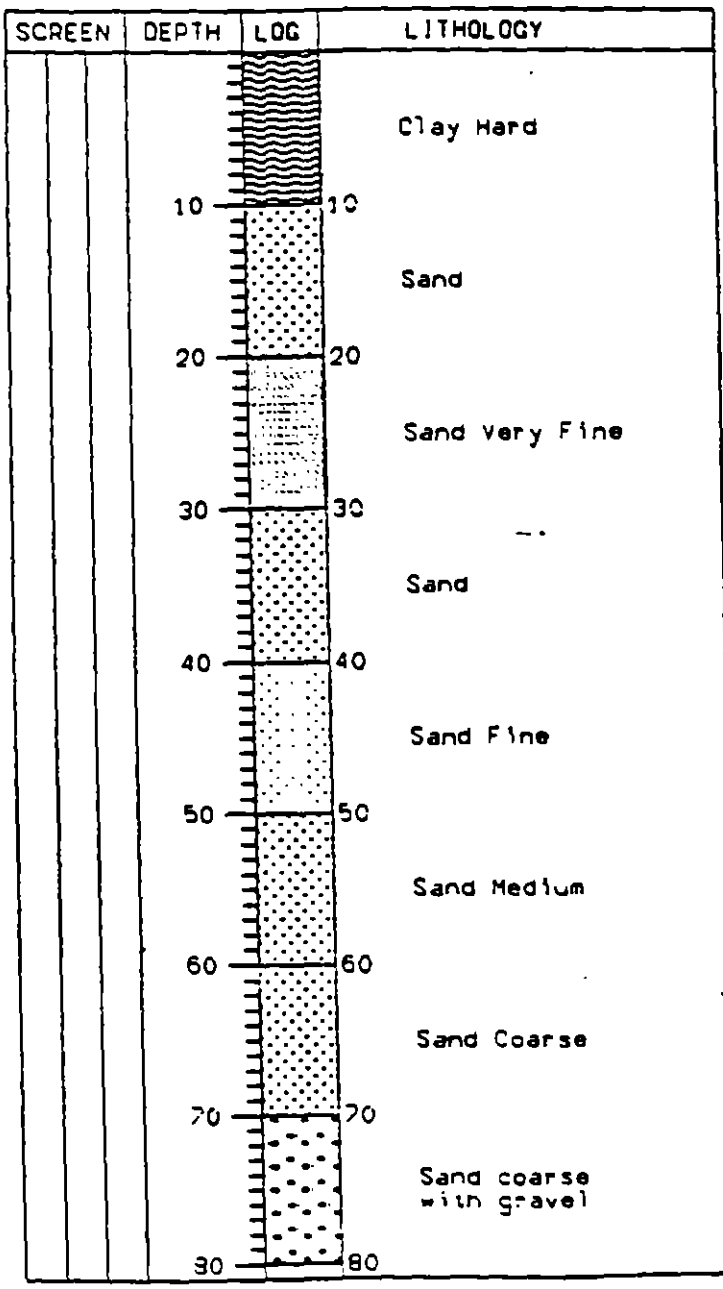


FIGURE 6.10

Well No.	Location:
Elevation:	X = Y =
Method of Drilling:	
Drilling Dates :	
Total Depth : 100.00	
Comments :	

WELL LOG

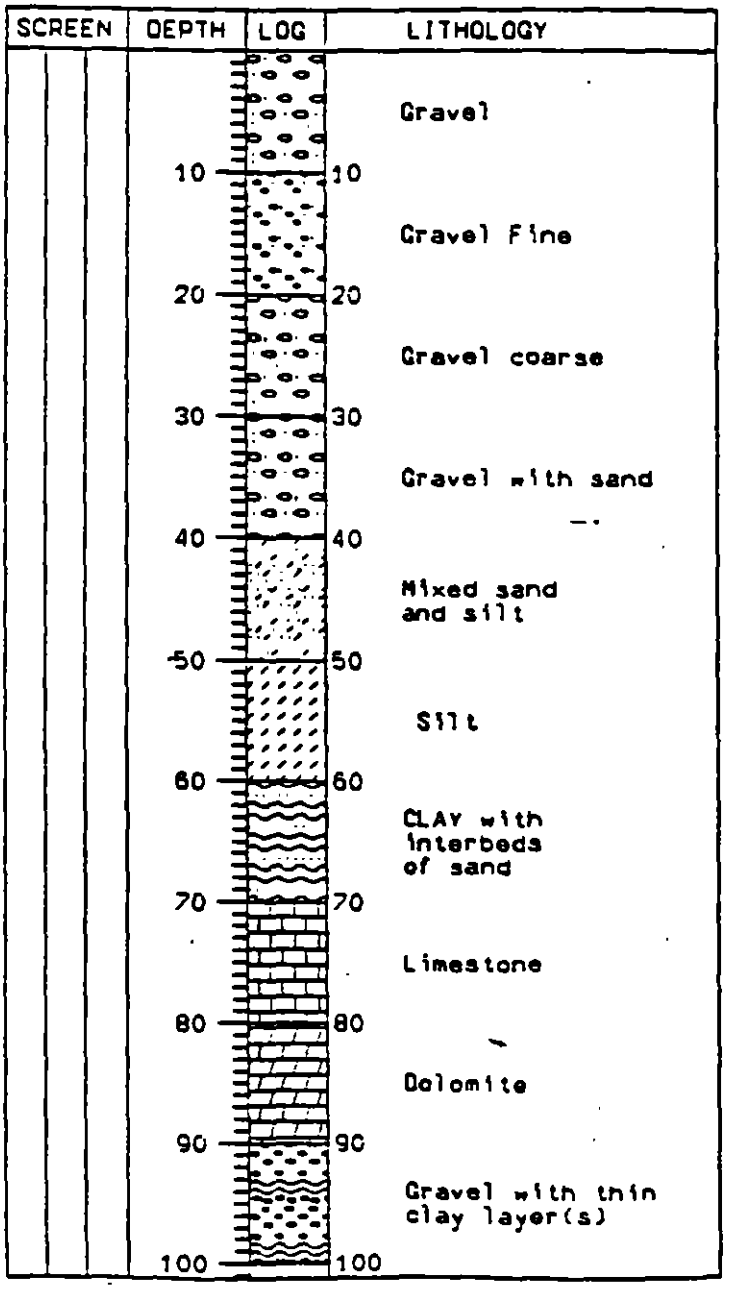


FIGURE 6.11

Appendix B

ERROR MESSAGES

Message: Unable to load comm. group.
Cause: Error in UN6.*.
Action: Copy original UN6.* files from distribution disk.

Message: Unable to load window.
Cause: Error in UN6.WND
Action: Copy original UN6.WND file from distribution disk.

Message: There is no open comm group.
Cause: Error in UN6.CMN.
Action: Copy original UN6.CMN file from distribution disk.

Message: Unknown port.
Cause: Error in UN6.*.
Action: Copy original UN6.* files from distribution disk.

Message: Please, edit file GW6.GEN first, then call again.
Cause: GW6.GEN file is missing in current directory, or path to text editor is incorrect.
Action: Check your GW6.GEN file, establish correct path to text editor.

Message: Text editor is not defined in GW6.GEN.
Cause: There is no text editor specified in GW6.GEN
Action: Check the path and name of text editor in GW6.GEN.

Message: Text editor given in GW6.GEN does not exist.
Cause: Incomplete or wrong definition of text editor.
Action: Type the text editor file name with extension (EXE or COM).

Message: Invalid format or value of horizontal scale.
Cause: Wrong information in GW6.GEN.
Action: Correct the input in GW6.GEN.

Message: Invalid format or value of vertical scale.
Cause: Wrong information in GW6.GEN.
Action: Correct the input in GW6.GEN.

Message: Unsuccessful coordinate digitization.
Cause: File DIGXSC.EXE is not in \GW directory.
Action: Copy DIGXSC.EXE to \GW directory.
Message: Unsuccessful well map plotting.
Cause: File PLTCSY.EXE is not in \GW directory.
Action: Copy PLTCSY.EXE to \GW directory.

Message: There is no active file.
Cause: You have not selected any lithological file.

Action: Select existing data file or create new file.

Message: Lithology description file \GW\GW6.DLT does not exist.

Cause: File GW6.DLT is not in \GW directory.

Action: Copy GW6.DLT file to \GW directory.

Message: Premature end of file \GW\GW6.DLT

Cause: Last line in GW6.DLT not terminated with RETURN

Action: Edit GW6.DLT file. Cursor must be in column 1 of the first blank line.

Message: Maximum number of active files surpassed.

Cause: More than 300 data files selected and copied to current directory.

Action: Reduce the number of selected files to 300.

Message: Error in log print.

Cause: In creating Well Log some information missing or wrong. This is normally in lithological codes and descriptions which do not match with codes in GW6.DLT. Characters other than ASCII (1-128) discovered.

Action: Edit data files. Use ASCII version of a data file.

Message: Error in file selection.

Cause: Wrong name, or file is not an ASCII file in required format.

Action: Check the file name or file format.

Message: Computer hangs when attempting to display well log.

Cause: Insufficient memory for both program (430 KB) and screen display (140 KB)

Action: Eliminate all memory-resident programs; reduce, if necessary, CONFIG.SYS file; check AUTOEXEC.BAT file.

Message: Computer hangs when attempting to print well log or cross section.

Cause: Insufficient memory for both program (430 KB) and printing driver (140 KB).

Action: Eliminate all memory-resident programs; reduce, if necessary, CONFIG.SYS file; check AUTOEXEC.BAT file.

Message: Computer hangs when attempting to run GW6 program.

Cause: Insufficient memory for program (430 KB).

Action: Eliminate all memory-resident programs; reduce, if necessary, CONFIG.SYS file; check AUTOEXEC.BAT file.

CHAPTER 7.

Graphics

7.1. General

This is a utility program that, in this Ground Water Software Package, is used by the GW6 module, Lithology to create maps with wells, boundaries, rivers, roads, and other features. The following files must be copied to the \GW directory: GW11.EXE, UN11.CMN, UN11.MST, UN11.WND. There are several executable files which are used by certain portions of the graphics program. These files are the following:

PLTCSY.EXE ... for Plotting coordinate system
PLTPTS.EXE ... for Plotting points
PLTTXT.EXE ... for Plotting text
PLTLIN.EXE ... for Plotting line
PLTCNT.EXE ... for Plotting contours

The total disk space for all files in this module is about 514,000 bytes, out of which the five executable graphics files (PLT...) occupy a total of 284,610 bytes.

The graphics package is flexible. You may display (print or plot) a coordinate system only, or well locations superposed onto the coordinate system. You build up your final graph by superposing individual parts. You may add individual lines (district boundary, rivers, roads, etc.), add text, add some other points. You may add contour lines, but the contouring is not a part of this package. Some of drawing elements, such as well points and lines, may be prepared beforehand, by a text processor. Well points may be also prepared by the GW6 program (lithology). Contours are prepared by modeling programs.

7.2. Coordinate System

After you select the Graphics Module from the Main Program Menu and press RETURN, the program checks in your current directory whether there is a coordinate file in that directory. A coordinate file has an extension .CSY. If a coordinate file exists, the program lists all .CSY files on the left side of the screen, while the usual Function window contains the following options, as shown in Fig. 7.1:

N=New Coords
D=Display
P=Print/Plot
E=Edit Coordinates
C=Copy
K=Contours
L=Plot line
T=Plot text
S=Plot points
R=Clear
Y=Delete
ESC=Exit

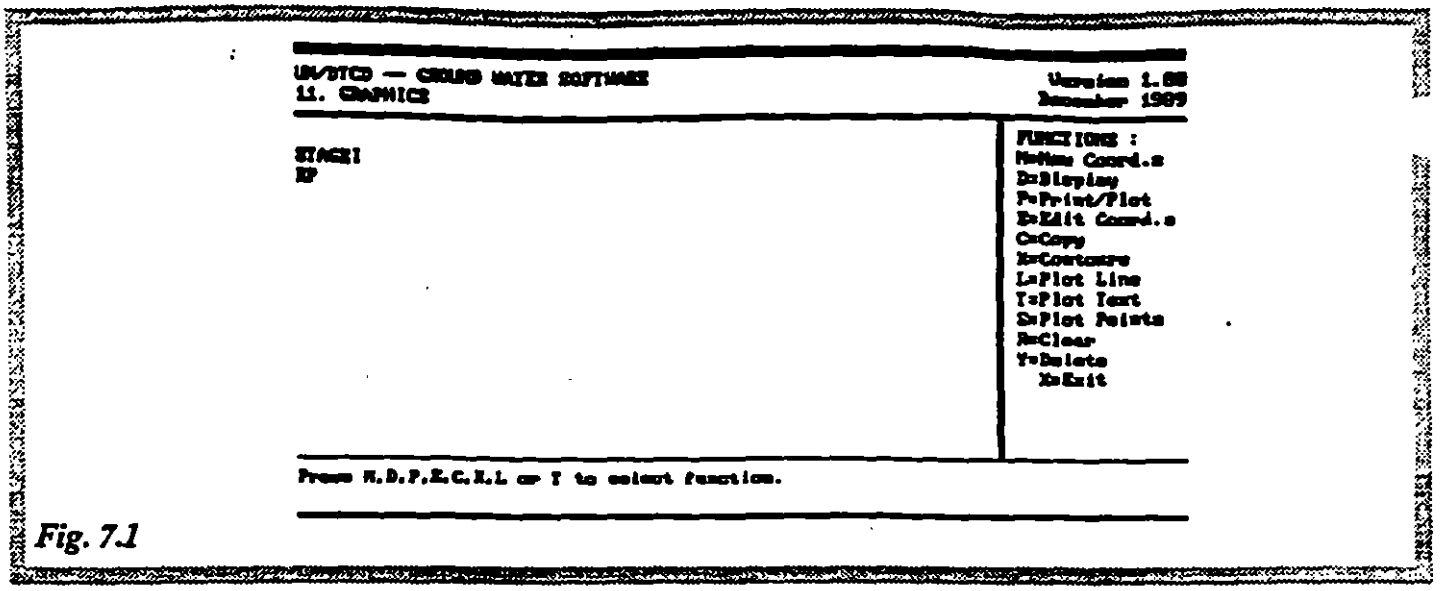


Fig. 7.1

However, if there is not a single coordinate file, there will be a message: "Enter coordinate system name (8 chrs). Esc to quit!" You are expected to provide a name for a new coordinate system file, after which there will be a message: "To edit coordinate system description press RETURN. ESC to abandon.", which gives you a chance to skip editing and exit. Should you decide to continue with editing, press RETURN, after which the following is displayed (Fig. 7.2):

Minimum Y =
Maximum X =
Maximum Y =
Scale =
Heading =
Axis Labeling Distance =
Lines Color = 7
Axis Labeling Color = 3
Heading Color = 15
Coordinate Grid Color = 1
Grid Cross Height [cm] = 0.2

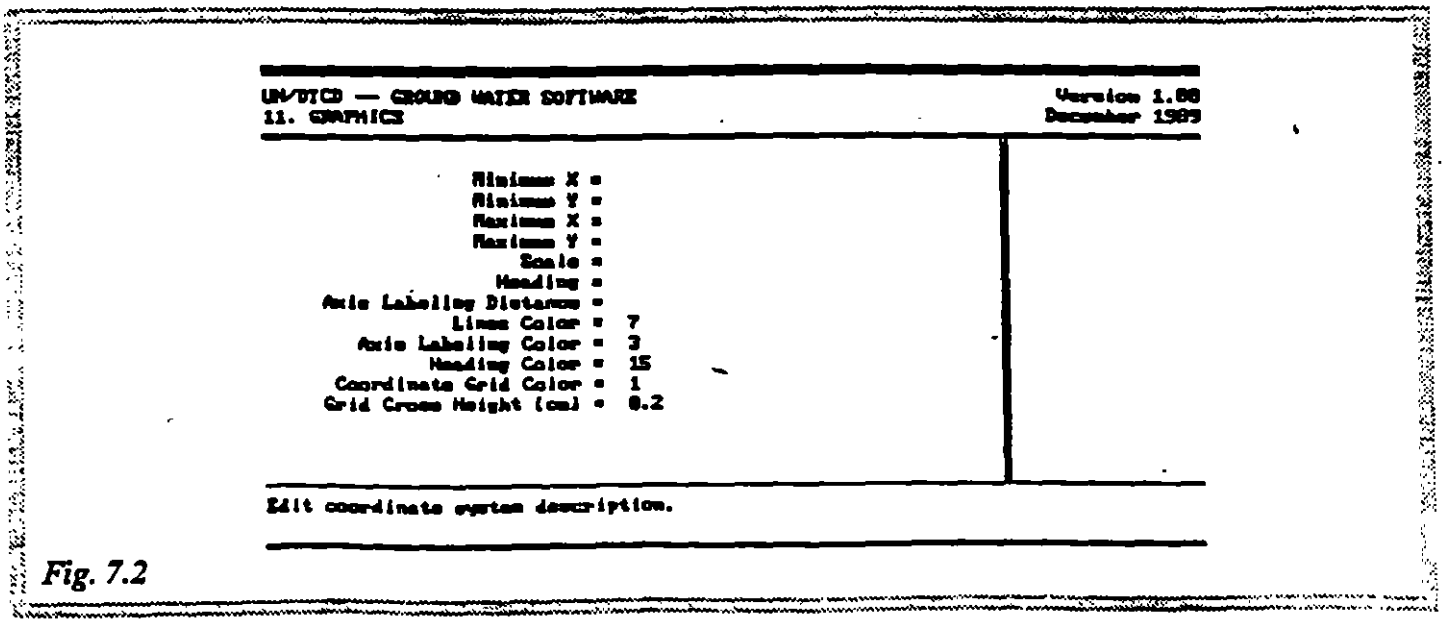


Fig. 7.2

You may select the coordinate system size, scale of printout, and the heading of printout. Axis labeling distance is the distance in real coordinates, for example, 5000 m, after which the label will be shown and/or printed. The program offers by default the colors for lines (frame) of the coordinate system 7 (white), for axis labels 3 (red/green), for heading 15 (intensive white), for coordinate grid 1 (dark blue). You may change this if you wish.

Whenever you select in the GW6 program to "Save well positions for plotting", a file with wells' coordinates will be created with the file name that you supply. You may read again Chapter 6, and notice that your answer to that prompt should have been "Y" followed by the file name "EXAMPLE".

For the present example, you may create a new coordinate system as follows. Select N from the menu. Enter the name TEST. Type 717000 for minimum X, 3024000 for minimum Y, 761000 for maximum X, 3073000 for maximum Y, 100000 for scale, RUPANDEHI DISTRICT for heading, and 5000 for axis labeling distance. Change the color for lines color from 7 to 2. After you finish, you will notice that the size of the printout is 48 by 53 cm. You are prompted to confirm the scale or to modify it. Press Y and change scale to 200000. Move to the last line by repeatedly pressing the RETURN key. You will notice that the size of the printout is now 26 by 28.5 cm. Press RETURN. After that a graph with the new coordinate system will be displayed. Notice the colors that you have selected. Press ESC. Type S from the main menu and supply the file name EXAMPLE. Wait a while and type D to display the drawing. You will notice that 15 wells are superimposed onto the coordinate grid. A coordinate system file may look as shown in Fig. 7.3. After editing is completed and RETURN pressed on the last line, the program displays the following message (Fig. 7.4):

Drawing dimensions [cm]: 20.0 (H) 21.8 (V)
To change data press Y; otherwise press any key

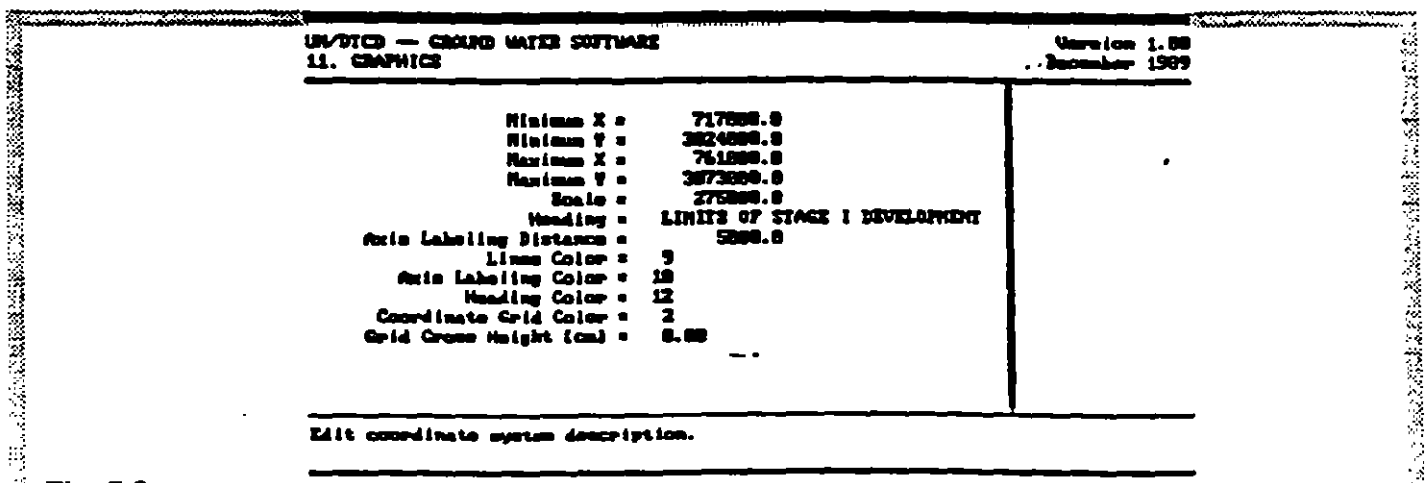


Fig. 7.3

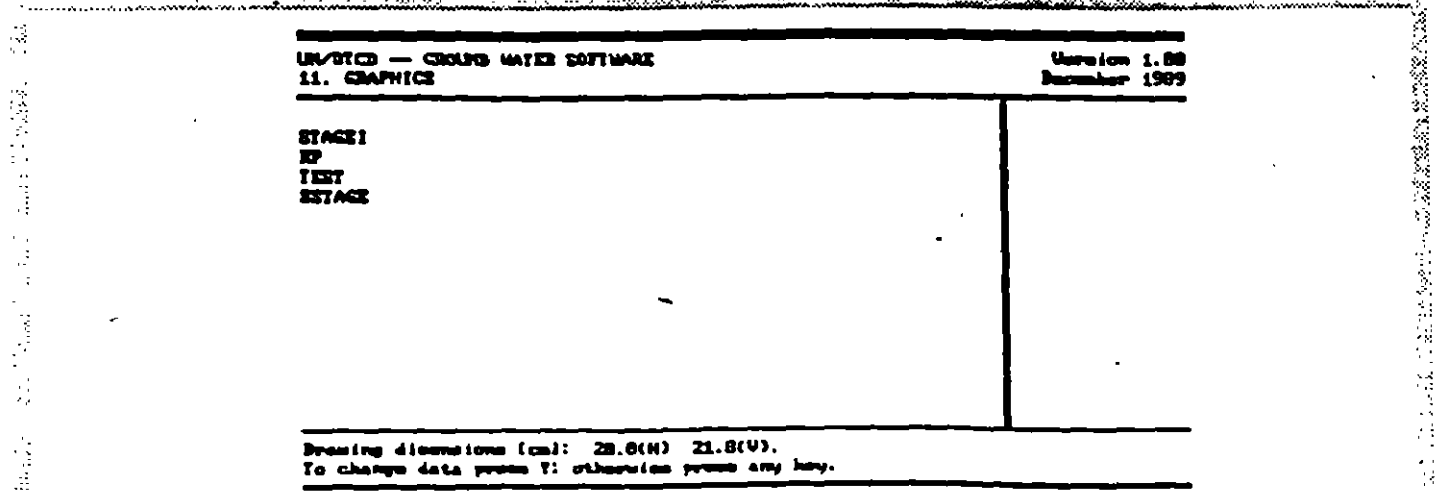


Fig. 7.4

This is an indicator to you how big the drawing will be. If this is not what you would like, or your printer/plotter can support, answer with Y and modify the scale.

WARNING: Whenever you select to edit a coordinate system file, the whole content of the file, except the coordinate system, will be erased. Be careful, if you wish to save the drawing, copy it first to another file, before editing the coordinate system.

7.3. Composite Drawings

Several data files that demonstrate the use of this graphics package are included with the GW11 files on the distribution diskette. The file names are BOUNDARY for the district boundary, RIVER for one of major rivers in the district, ROAD for major roads. There are also files named BLWELLS, BRWELLS, and USWELLS, each with different groups of wells. Try to build a composite drawing by adding points, lines and text onto your coordinate system.

Remember that the coordinate system is duplicated in a file with the name same as the name of the coordinate system file, but with a PLT extension, meaning a plot file. The content of this file may be eliminated by typing R to clear. It may be copied to another file by pressing C and supplying another file name.

For this exercise type GW11, move the cursor to TEST, press R to clear TEST.PLT. After a while you will see the coordinate system displayed on the screen. Edit the file TEST by pressing E. Change only the color of "coordinate grid". Replace the default color 1 with 9 (light blue). Press RETURN several times, and wait until the coordinate system is displayed. Press ESC. Press L and supply the file name BOUNDARY. Answer the prompt "Color" with 6, and answer the next prompt "Enter line thickness" with 3. Wait until the plot is created. See the result by typing D (display). You will notice that the boundary of the district has been added in brown. Press ESC to return to the main menu. Add the river by typing L again and supplying the file name RIVER, followed by the color 1, and thickness 1. You may see the river added to the previous drawing by typing D, or you may continue with adding the content. Type L again. Type ROAD. For color type 4, fr thickness confirm 1. See the plot by typing D. You have now the boundary, river, and roads.

Now you may add some wells. There are three groups of wells: US wells (drilled by USGS), BL and BR wells (first and second stage of an irrigation system). Each well position group has been created during the lithological processing (program GW6), and three files have been created: USWELLS, BLWELLS, and BRWELLS. These files are ordinary ASCII files. The USWELLS file looks as shown below:

```
0.00   0.1   0.3   6 14 -0.07   0.02
    738375.   3042500. US5/3
    731500.   3041750. US6/7
    732375.   3057625. US6/12
    732875.   3063750. US6/13
    722625.   3064000. US 8/6
    722125.   3056750. US8/5
    721625.   3048500. US8/4
    720625.   3042125. US8/3
    752750.   3041250. US4/1
    752375.   3048500. US4/3
    755875.   3059250. US4/6
    742500.   3043625. US5/4
    752000.   3052375. US4/5
    742625.   3048500. US5/10
    743125.   3056625. US5/14
    742875.   3061875. US5/18
    743375.   3064000. US5/19
    730500.   3026500. US6/2
    731250.   3035375. US6/5
```

The numbers in the first line of this file have the following meaning:

Cross height	_ 0.0
Circle diameter	_ 0.1
Label height	_ 0.3
Symbol color	_ 6
Text color	_ 14
Label x-offset	_ -0.07
Label y-offset	_ 0.02

From the second line, the values are as expected: x coordinate, y coordinate, label. Although the program GW6 creates this file, you may make it on your own, using a text processor. Likewise, you may edit and modify it if you wish. For example, you may alter the symbol: from circle (diameter 0.1) to a cross. Change the first value (0.0) to 0.1, and change the second value (0.1) to 0.0.

Add groups of wells, one by one, by typing S (Plot points), and supplying file name USWELLS. Repeat by typing S and BLWELLS, S again and BRWELLS. Now see the whole drawing. Type D.

Add some text by typing T (for text). Type TINAU RIVER, press RETURN, and confirm the height of letters to be 0.25. For angle type 52, for color 15 (intensive white), and for thickness 2. You will establish the position of the text string by pressing ENTER (RETURN) when prompted by the program, and supplying for X 728000 and for Y 3055000.

Another text string is prepared as follows:

Text	BUTWAL
Height	0.40
Angle	0
Color	14 (yellow)
Thickness	2
Coordinates	RETURN
X	743000
Y	3070500

Type D to display the composite drawing. It should look as in Fig. 7.5. You may enlarge a detail by pressing Z. Move the mouse and place the cursor on the left corner of the rectangle to zoom. Press the left button. Move the cursor to the right upper corner of the rectangle and press the left button again. The screen may look as shown in Fig.7.6. Repeating the zooming procedure, even larger detail is produced as shown in Fig.7.7.

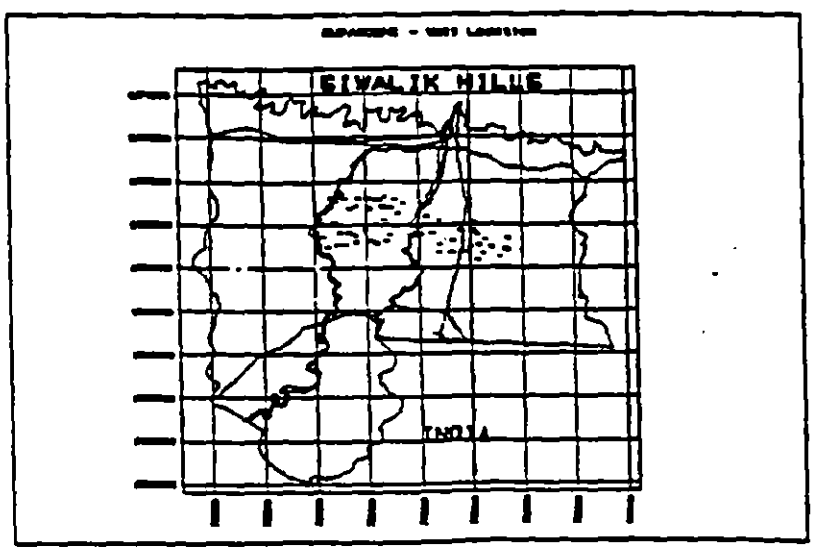


Fig. 7.5

FACULTAD DE INGENIERIA U.N.A.M.
DIVISION DE EDUCACION CONTINUA

VII CURSO INTERNACIONAL DE CONTAMINACION DE ACUIFEROS

MODULO III. MODELOS EN GEOHIDROLOGIA Y CONTAMINACION DE ACUIFEROS

TEMA:

MODELO DE FLUJO PLASM

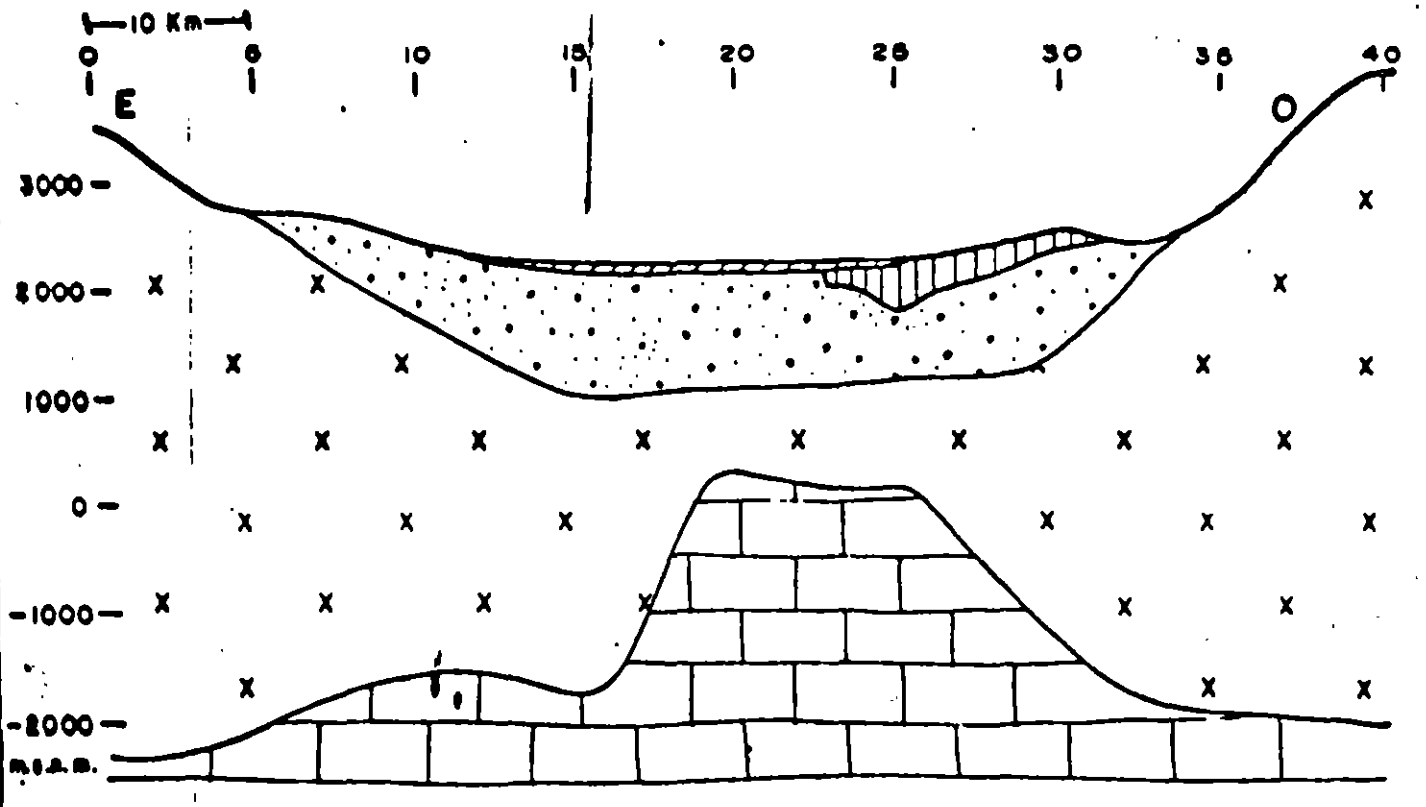
ING. DAVID GONZALEZ

INFORMACION BASICA PARA LA IMPLANTACION DE UN MODELO

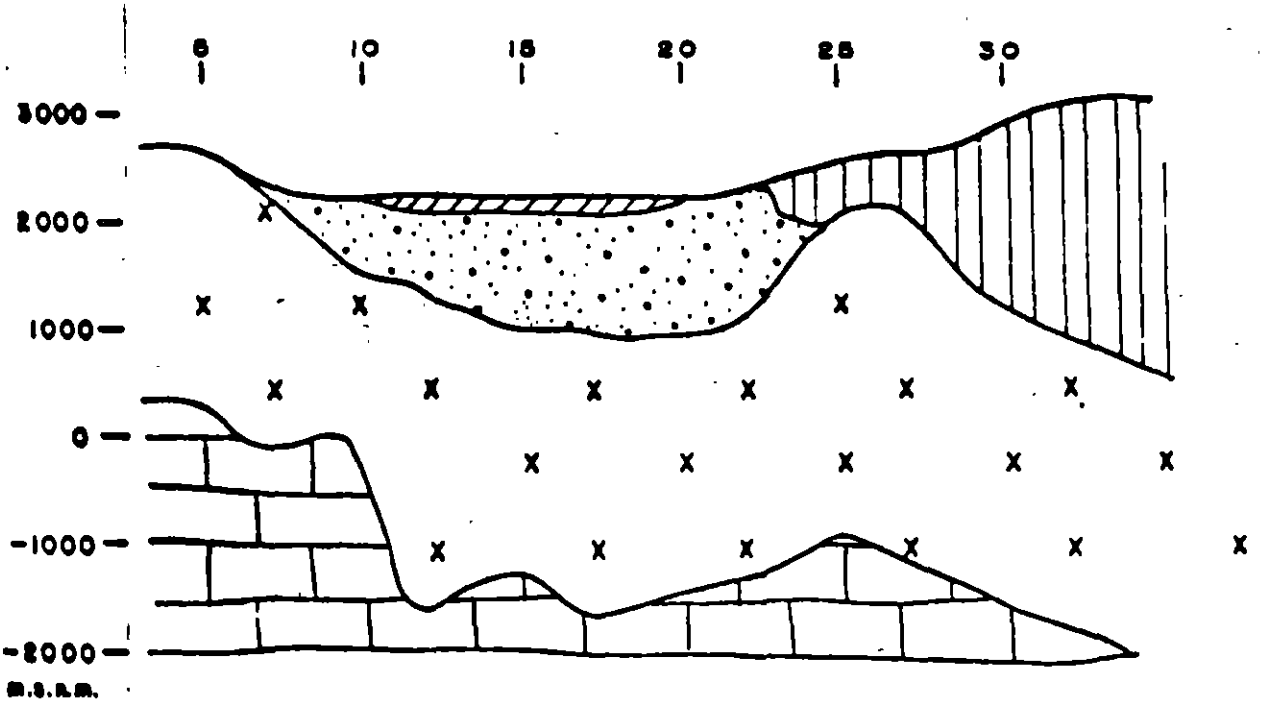
1.- DISCRETIZACION

- Planos Topográficos. Parteaguas.
- Plano Geohidrológico.
- Delimitación del Area
- Geología Subterránea. Cortes Litológicos.
- Registros Eléctricos. Perfiles Geológicos.
- Geofísica. Geometría de las Formaciones en el Subsuelo.
- Censo de Aprovechamientos. Localización de Pozos Piloto.
- Selección de la Malla. Areas de Concentración de Información.

CORTE TRANSVERSAL ESQUEMATICO A LO LARGO DEL RENGLON 17

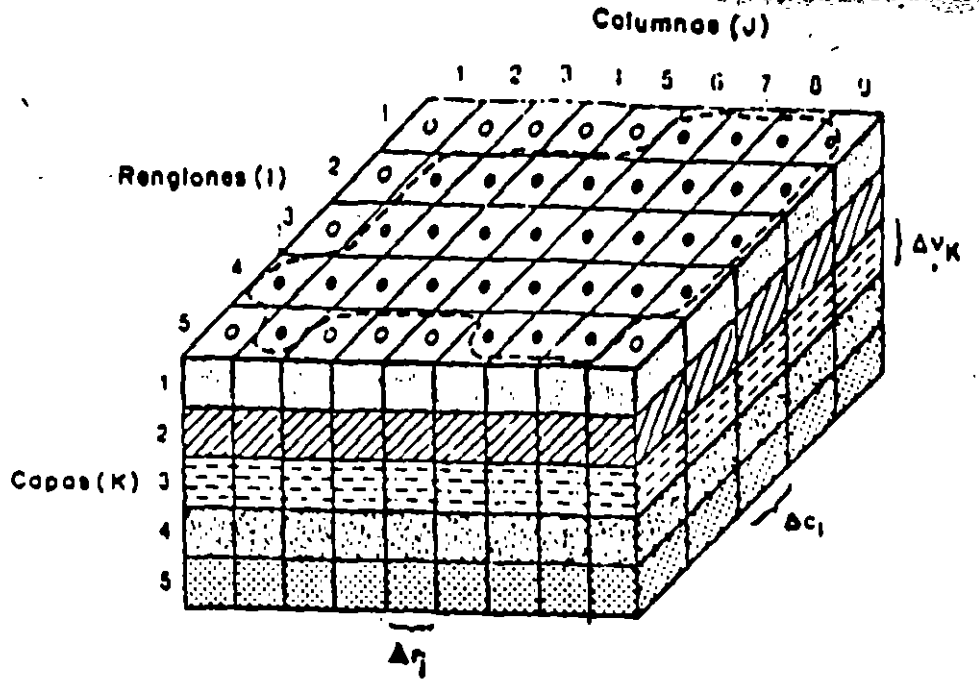


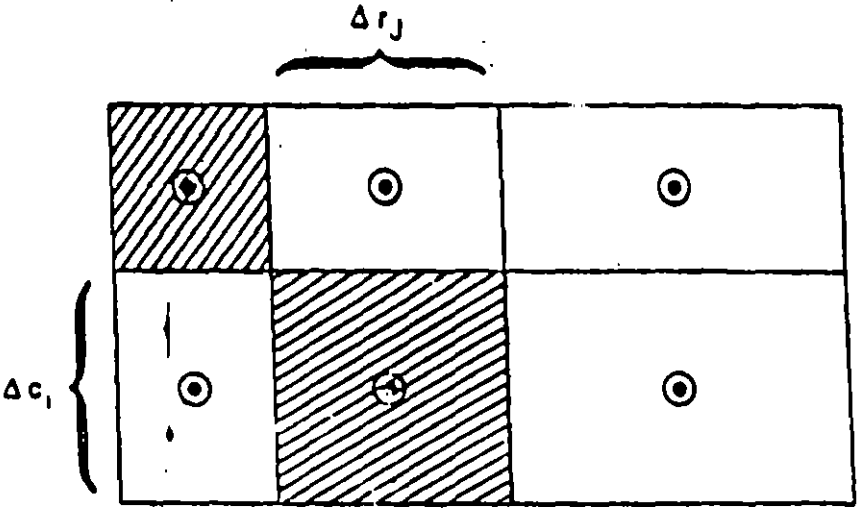
CORTE TRANSVERSAL ESQUEMATICO A LO LARGO DE LA COLUMNA 15



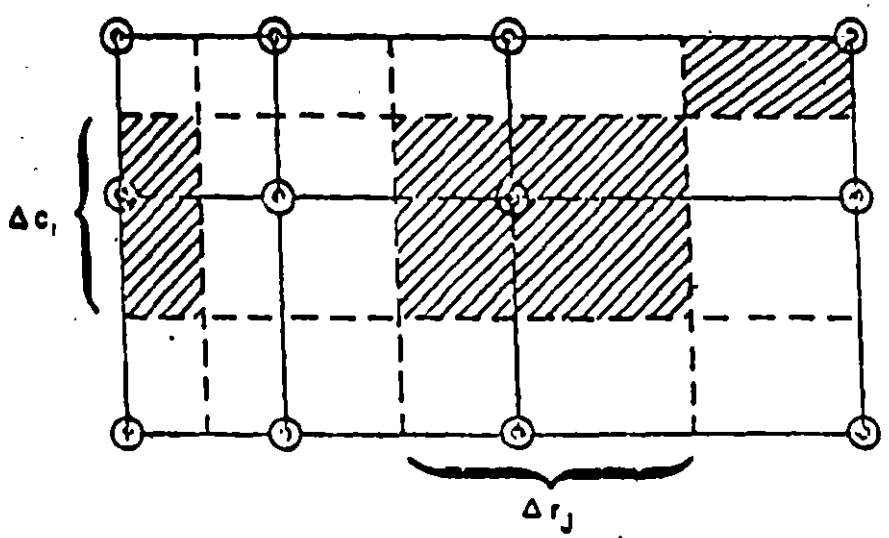
ACUITARDO SUPERIOR
BASALTO CUATERNARIO
ACUIFERO GRANULAR
ACUIFERO VOLCANICO
ROCAS CARBONATADAS SEDIMENTARIAS

FIG. 4. CORTES TRANSVERSALES ESQUEMATICOS





Sistema de Celda Centrada



Sistema de Nodo Centrado

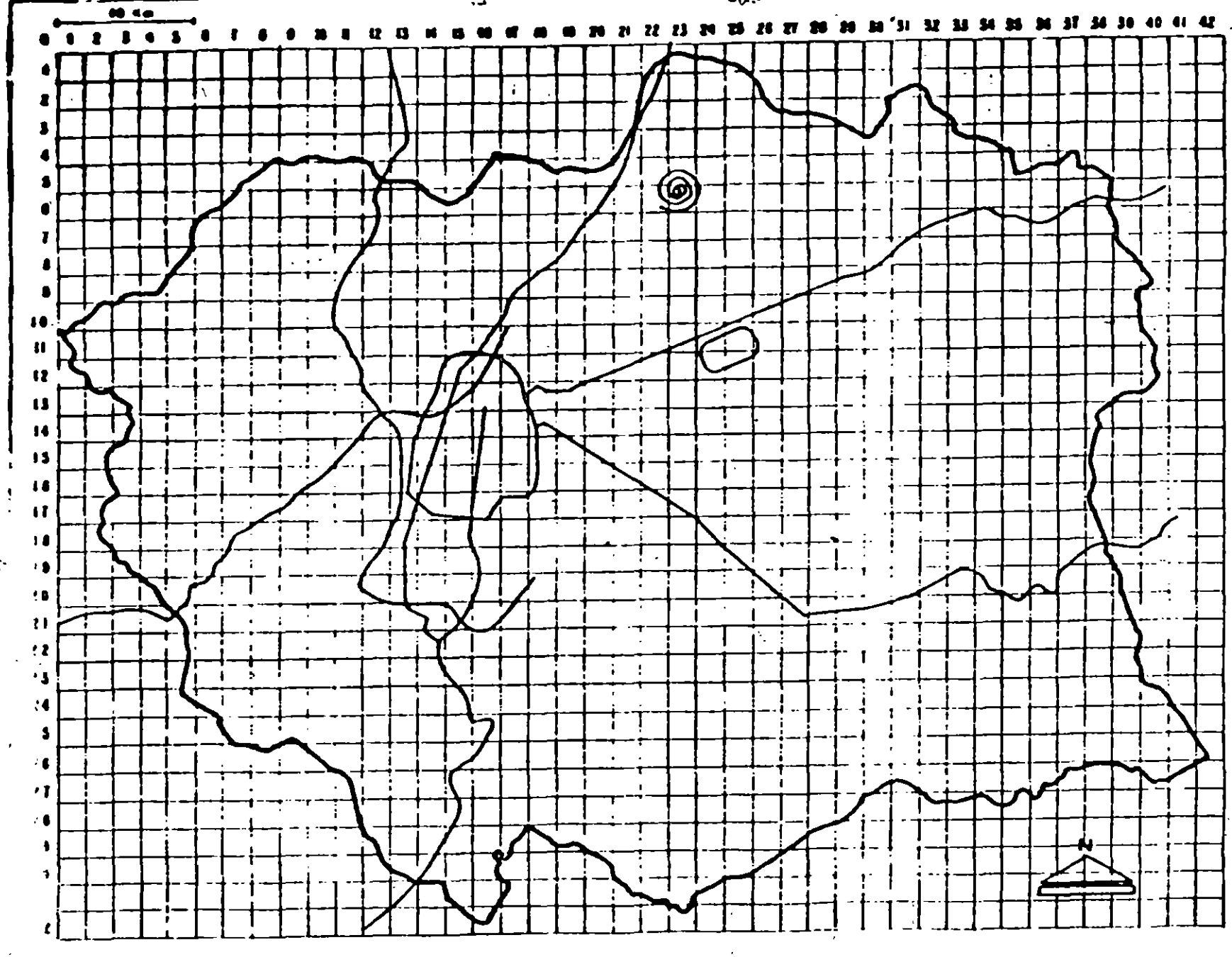


FIG. 3 . ILUSTRACION EN PLANTA DE LAS CELDAS DEL MODELO

INFORMACION BASICA PARA LA IMPLANTACION DE UN MODELO

2.- PARAMETRIZACION

- Pruebas de Bombeo. Aforos en pozos.
- Interpretación de Caracteristicas
  T, S, b, K, Ss, K',
- Distribución espacial de Caracteristicas
  Hidrodinámicas.
- Adaptación de Caracteristicas por Celdas.
- Construcción de Matrices de Parámetros.

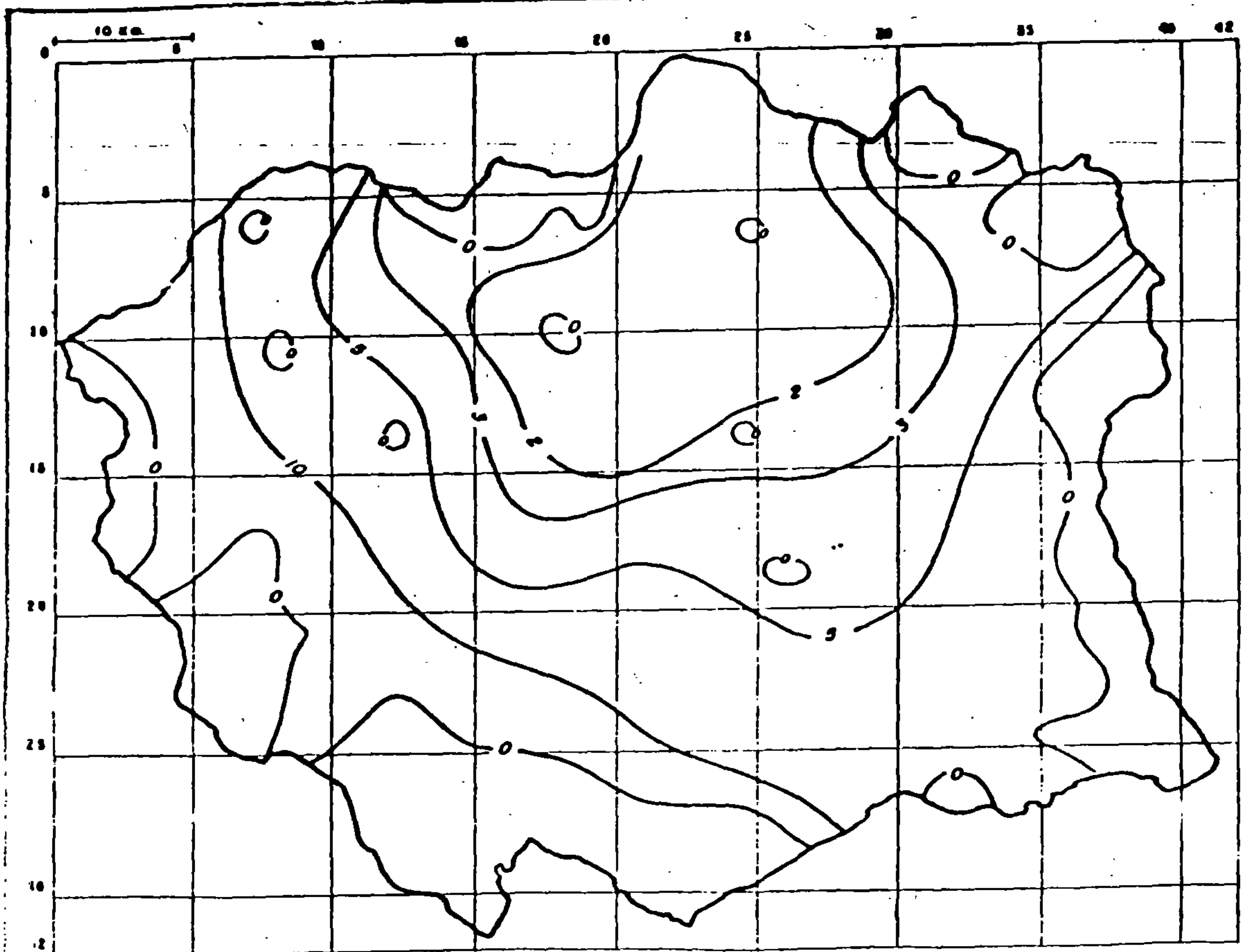


FIG. 7. COEFICIENTE DE ALMACENAMIENTO ESPECIFICO DEL ACUIFERO GRANULAR. $10^{-6} m^{-1}$

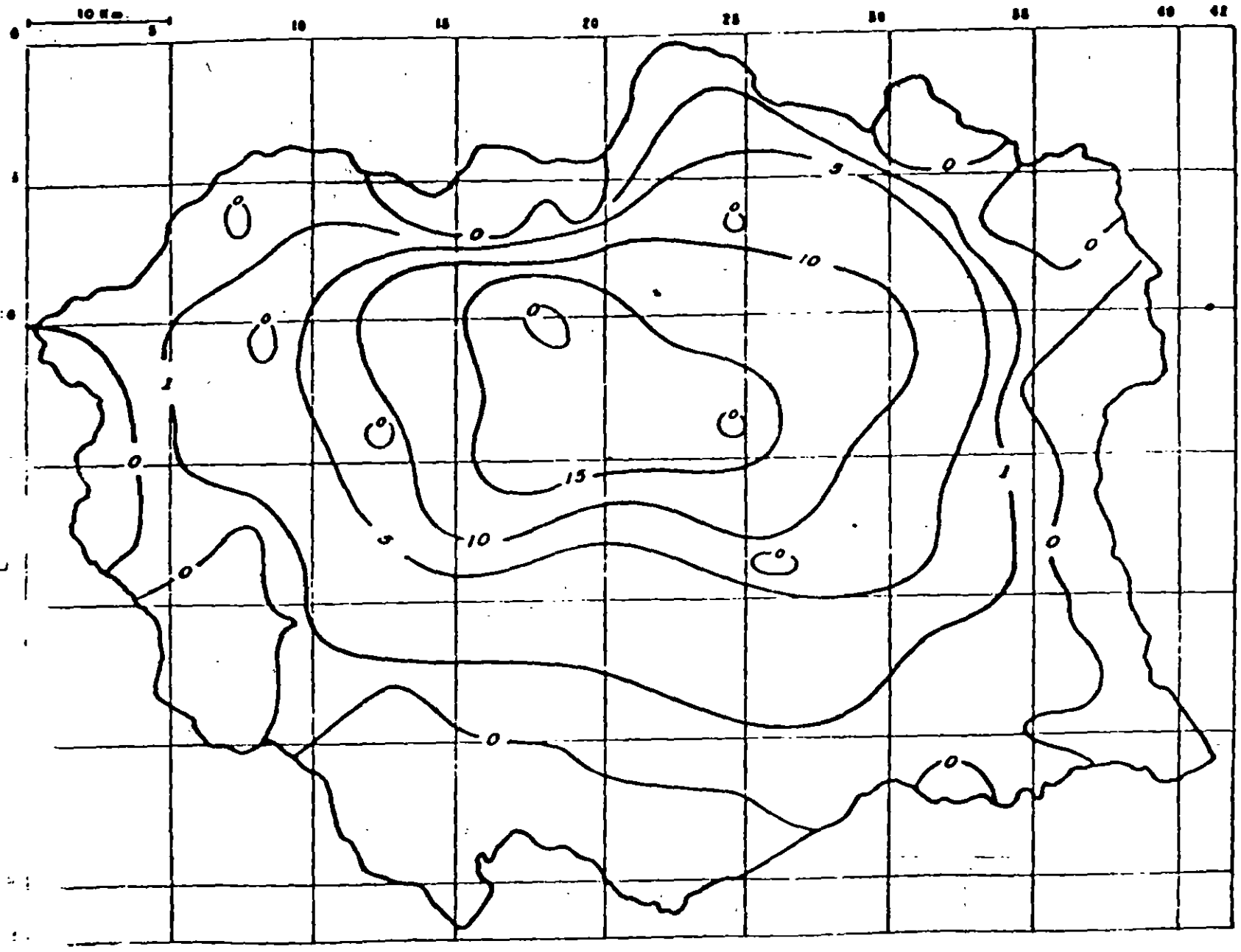


FIG. 6 CONDUCTIVIDAD HIDRAULICA HORIZONTAL DEL ACUIFERO GRANULAR 10^{-5} m/seg.

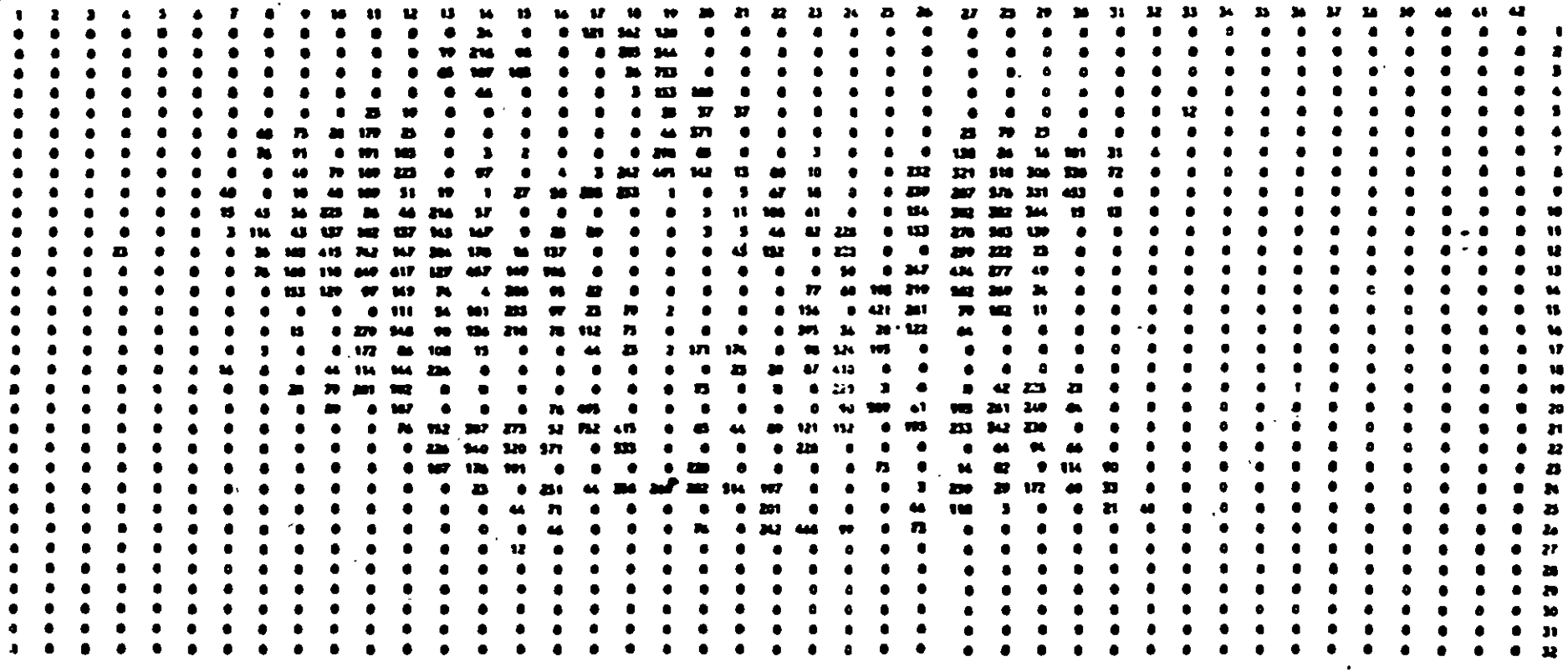


FIG. IO EXTRACCION DE AGUA SUBTERRANEA $m^3/seg. \times 10^{-3}$

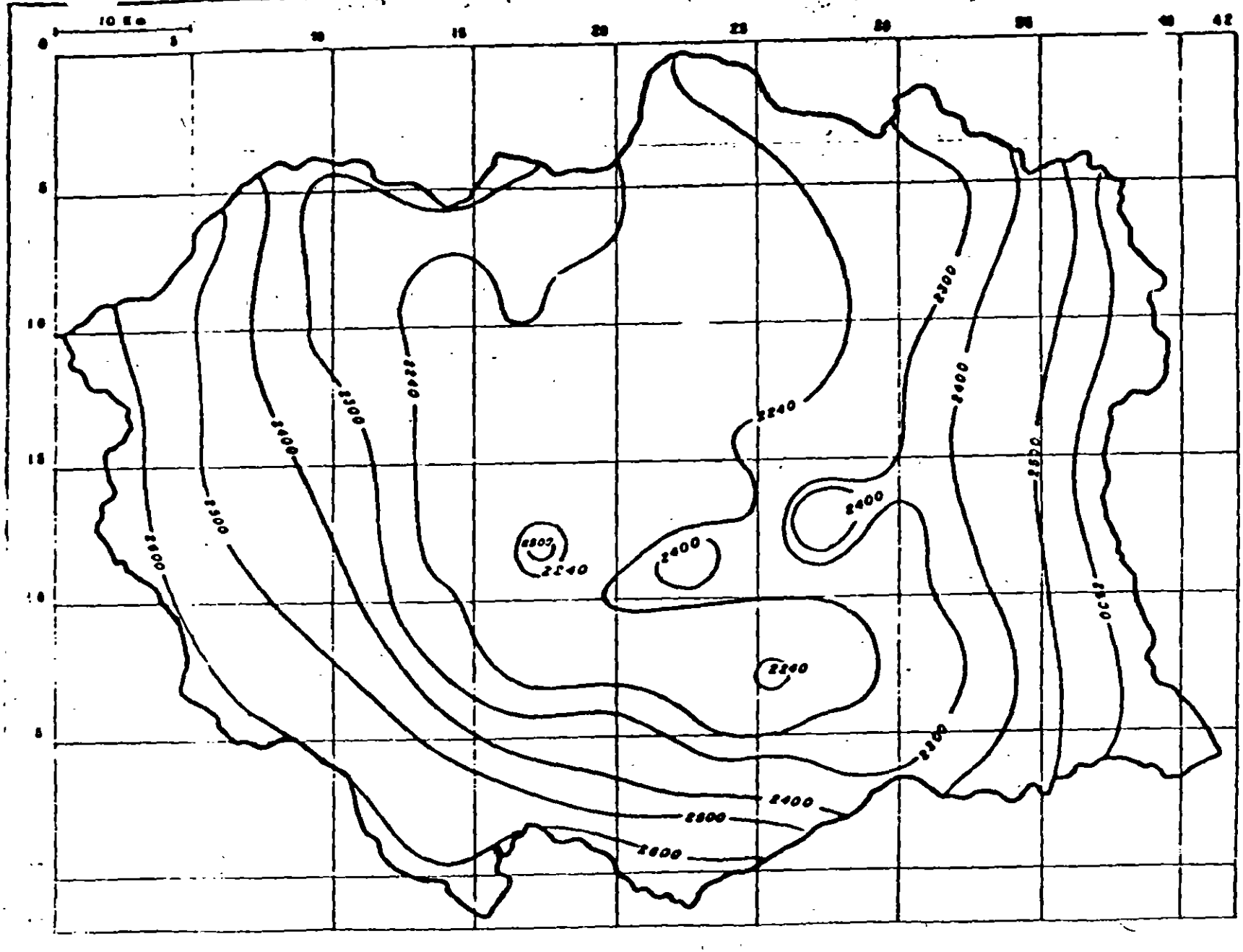


FIG. 8 . ELEVACION INICIAL DEL NIVEL PIEZOMETRICO. m.s.n.m. 1940

INFORMACION BASICA PARA LA IMPLANTACION DE UN MODELO

3.- CONCEPTUALIZACION

- Modelo Conceptual de Funcionamiento.
  Definición de Entradas y Salidas.

- Distribución de la Lluvia por Periodos.
  Volumen de Lluvia por Celda. Adjudicación de Coeficientes de Infiltración.

- Cálculo del Caudal de Infiltración.

- Infiltración y/o Drenaje de Ríos y Arroyos
  Cálculo del Caudal por Celda.

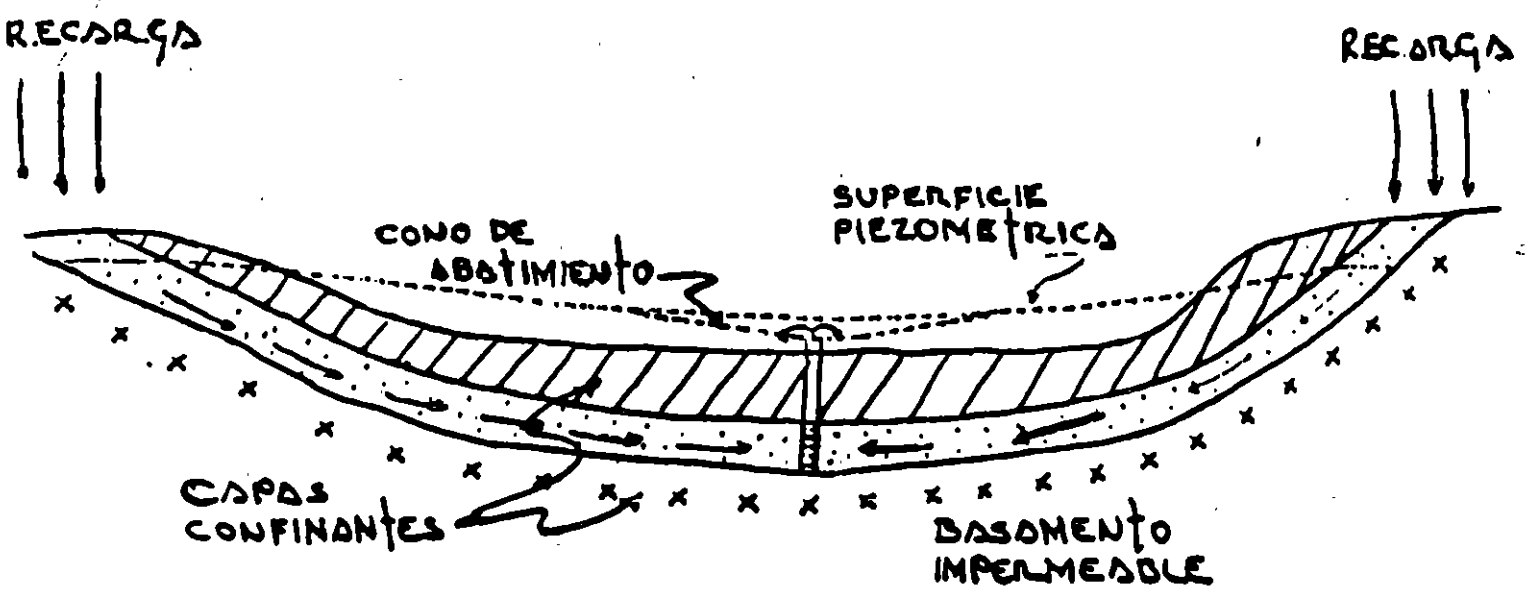
- Definición de Areas de Salidas del Acuífero por Evapotranspiración.

- Volúmenes de Extracción por pozo.
  Cálculo de la Extracción por Celda.
  Separación de Extracciones por Riego, Industrial y Potable. Cálculo de Láminas de Riego y Retornos al Acuífero.

- Piezometría. Red de flujo en Condiciones Iniciales, Intermedias y Actuales. Hidrógrafos de Pozos.
  Evoluciones Piezométricas por Períodos.

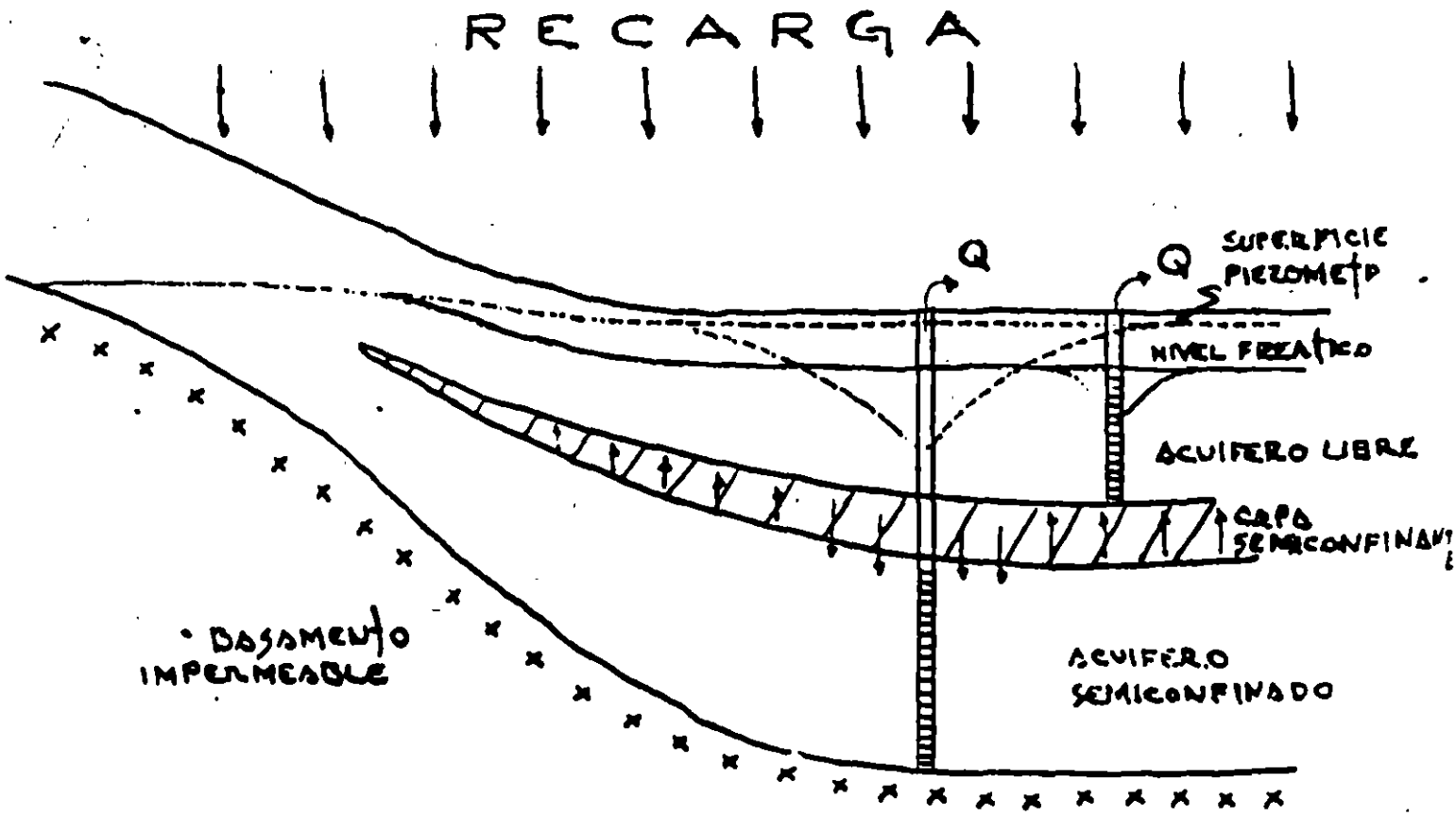
- Condiciones de Frontera. Definición de Celdas de no Flujo (Inactivas).
  Celdas de Carga Constante. Celdas de Carga Variable. Celdas de Flujo Constante.
  Alimentación por Semiconfinamiento.
  Otras Celdas.

ACUIFERO CONFINADO

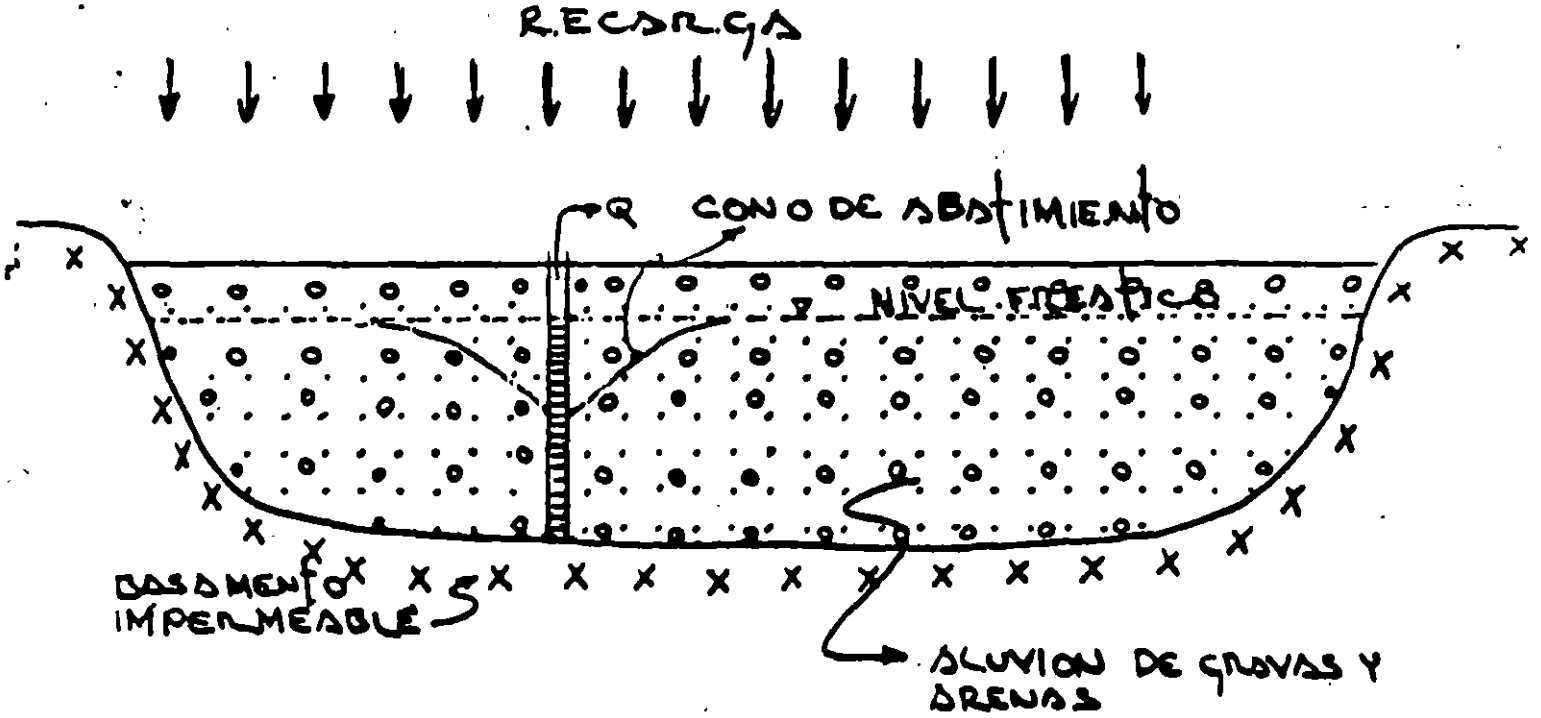


II

ACUIFERO SEMICONFINADO

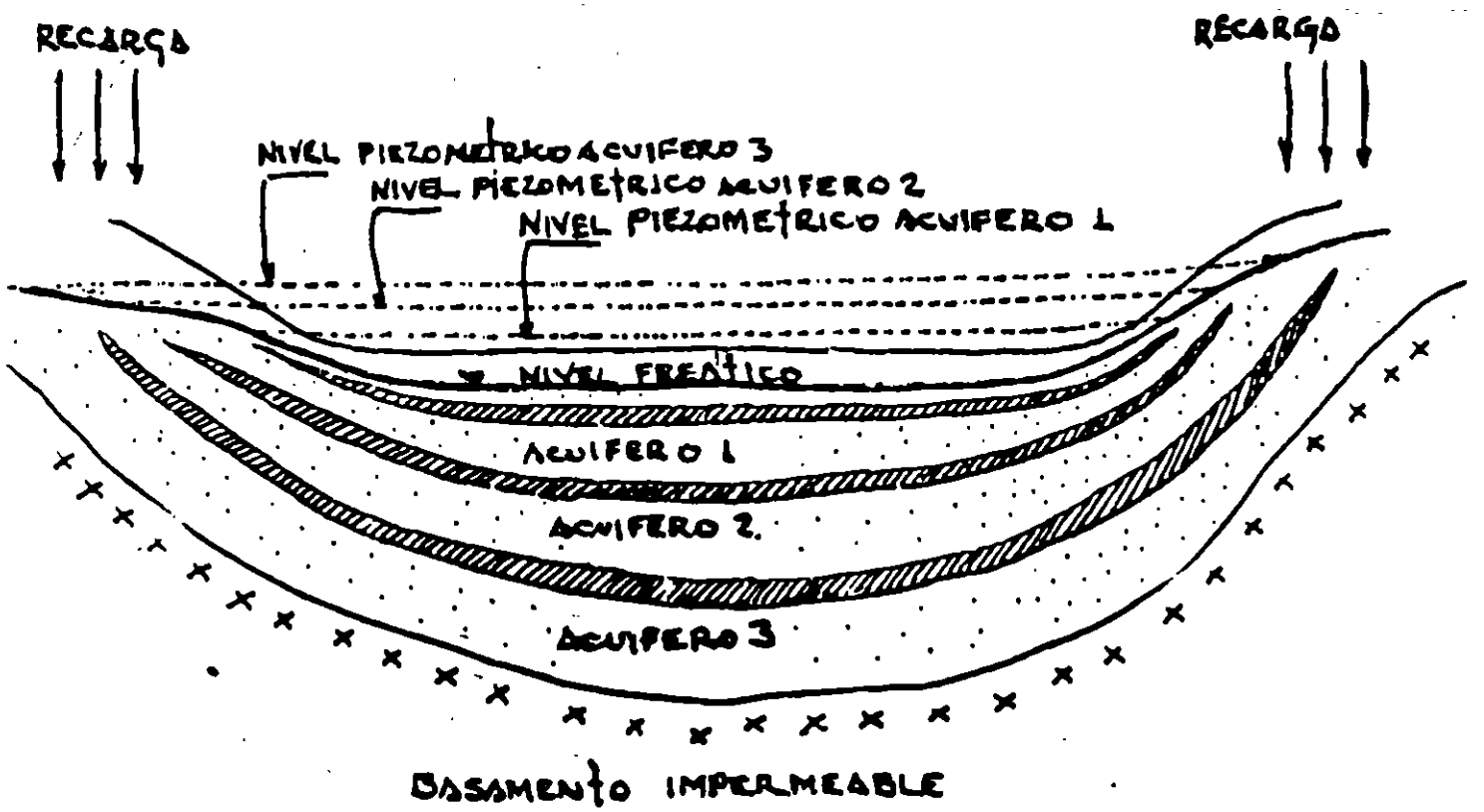


ACUIFERO LIBRE



I

ACUIFEROS MULTIPLES



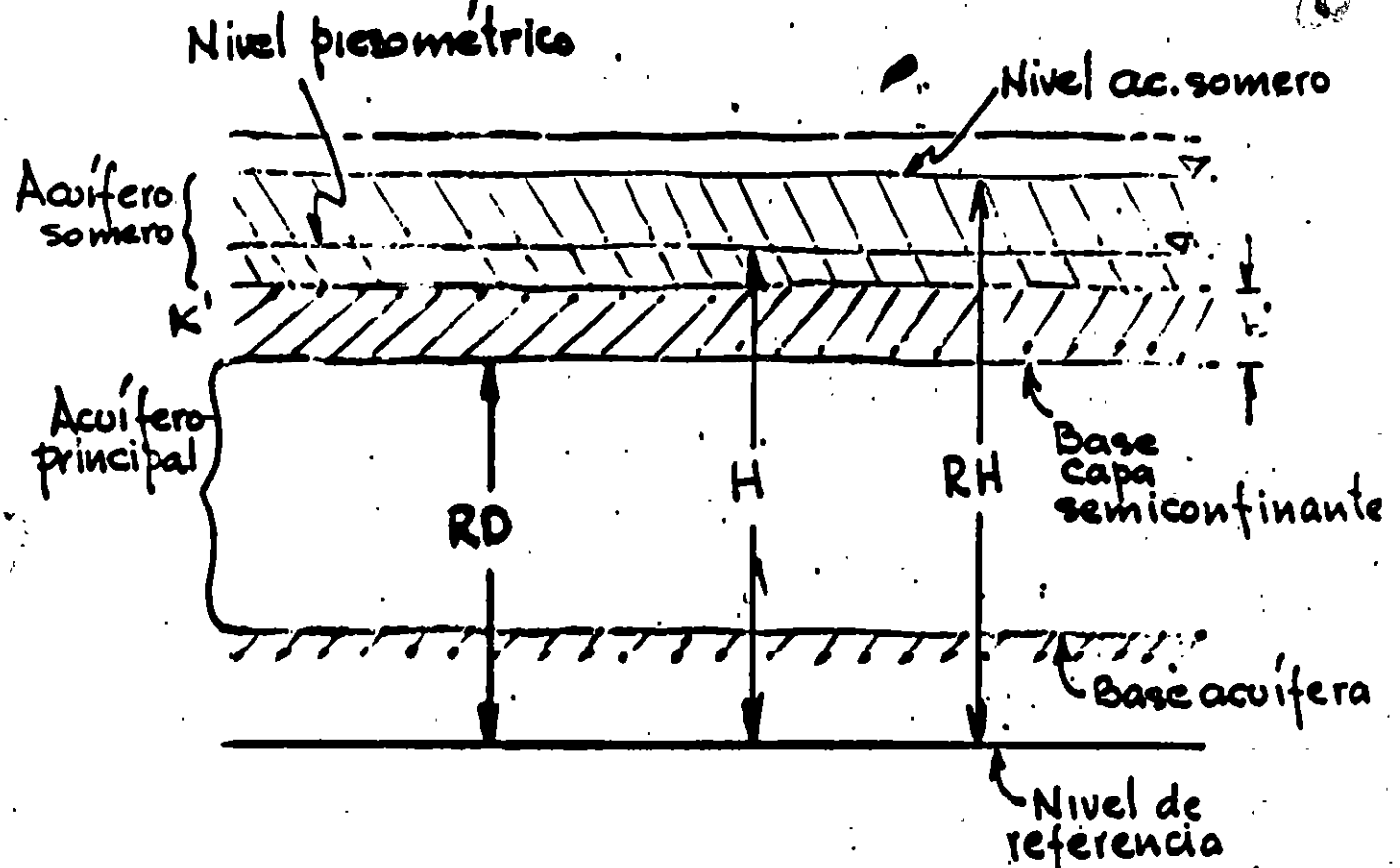
nombre: TOLDCAIO. ARCHIVO EXTERNO PARA EL PROGRAMA PLASM_CT

```
1
s
s
 20

DC
 1   2190   .45   1
25   18   0   0   0
 1   1   0   0   .01   900   0   0   0   0   395   0   0
 1   2   0   0   .01   860   0   0   0   0   452   0   0
 1   3   0   0   .01   830   0   0   0   0   450   0   0
 1   4   0   0   .01   800   0   0   0   0   511   0   0
 1   5   931   931   .1   770   -.0001   0   0   0   500   0   0
 1   6   650   650   .1   750   -.0044   0   0   0   500   2   2
 1   7   600   600   .1   730   -.0001   0   0   0   500   2   2
 1   8   500   500   .1   700   -.0001   0   0   0   500   2   2
 1   9   500   500   .1   650   -.0001   0   0   0   500   2   2
 1   10   1000   1000   .20   600   -.0001   0   0   0   400   5   5
 1   11   1000   1000   .20   600   -.0001   0   0   0   450   5   5
 1   12   1150   1150   .2   630   -.0015   0   0   0   390   5   5
 1   13   1000   1000   .2   600   -.0020   0   0   0   300   5   5
 1   14   1000   1000   .25   600   -.0020   0   0   0   420   5   5
 1   15   1200   1200   .25   630   -.0020   0   0   0   410   5   5
 1   16   1200   1200   .25   650   -.0020   0   0   0   410   5   5
 1   17   0   0   .25   650   0   0   0   0   380   0   0
 1   18   0   0   .25   650   0   0   0   0   380   0   0
 2   1   0   0   .01   900   0   0   0   0   395   0   0
 2   2   0   0   .01   860   0   0   0   0   452   0   0
 2   3   0   0   .01   830   0   0   0   0   450   0   0
 2   4   0   0   .01   800   0   0   0   0   511   0   0
 2   5   700   700   .1   770   -.0001   0   0   0   500   0   0
 2   6   650   650   .1   750   -.0044   0   0   0   500   2   2
 2   7   520   520   .1   730   -.0001   0   0   0   500   2   2
 2   8   500   500   .1   700   -.0001   0   0   0   500   2   2
 2   9   500   500   .1   650   -.0001   0   0   0   500   2   2
 2   10   600   600   .2   600   -.00007   0   0   0   450   4   4
 2   11   700   700   .2   590   -.0001   0   0   0   390   4   4
 2   12   1150   1150   .2   600   -.0001   0   0   0   390   5   5
 2   13   1000   1000   .2   580   -.0001   0   0   0   400   5   5
 2   14   1000   1000   .25   560   -.0001   0   0   0   370   5   5
 2   15   1000   1000   .25   590   -.0001   0   0   0   410   5   5
 2   16   2000   2000   .3   600   -.0001   0   0   0   410   10   10
 2   17   2000   2000   .3   600   -.003   0   0   0   420   10   10
 2   18   0   0   .3   630   0   0   0   0   380   0   0
 3   1   0   0   .01   900   0   0   0   0   395   0   0
 3   2   0   0   .01   860   0   0   0   0   452   0   0
 3   3   0   0   .01   830   0   0   0   0   450   0   0
 3   4   0   0   .01   800   0   0   0   0   511   0   0
 3   5   600   600   .1   770   -.0001   0   0   0   500   0   0
 3   6   500   500   .1   750   -.0044   0   0   0   500   2   2
 3   7   460   460   .1   730   -.0001   0   0   0   500   2   2
 3   8   460   460   .1   700   -.0001   0   0   0   500   2   2
 3   9   500   500   .08   650   -.000004   0   0   0   450   2.5   2.5
 3   10   500   500   .2   600   .0001   0   0   0   400   4   4
 3   11   500   500   .2   585   -.0001   0   0   0   380   4   4
 3   12   700   700   .2   580   -.0001   0   0   0   390   4   4
 3   13   700   700   .25   560   -.0001   0   0   0   390   4   4
 3   14   900   900   .25   550   .0066   0   0   0   348   4.5   4.5
 3   15   1000   1000   .25   550   -.0001   0   0   0   410   5   5
 3   16   2000   2000   .3   555   -.0001   0   0   0   380   10   10
 3   17   2000   2000   .35   560   -.0051   0   0   0   390   10   10
```

15

ACUIFERO PARCIALMENTE CONFINADO



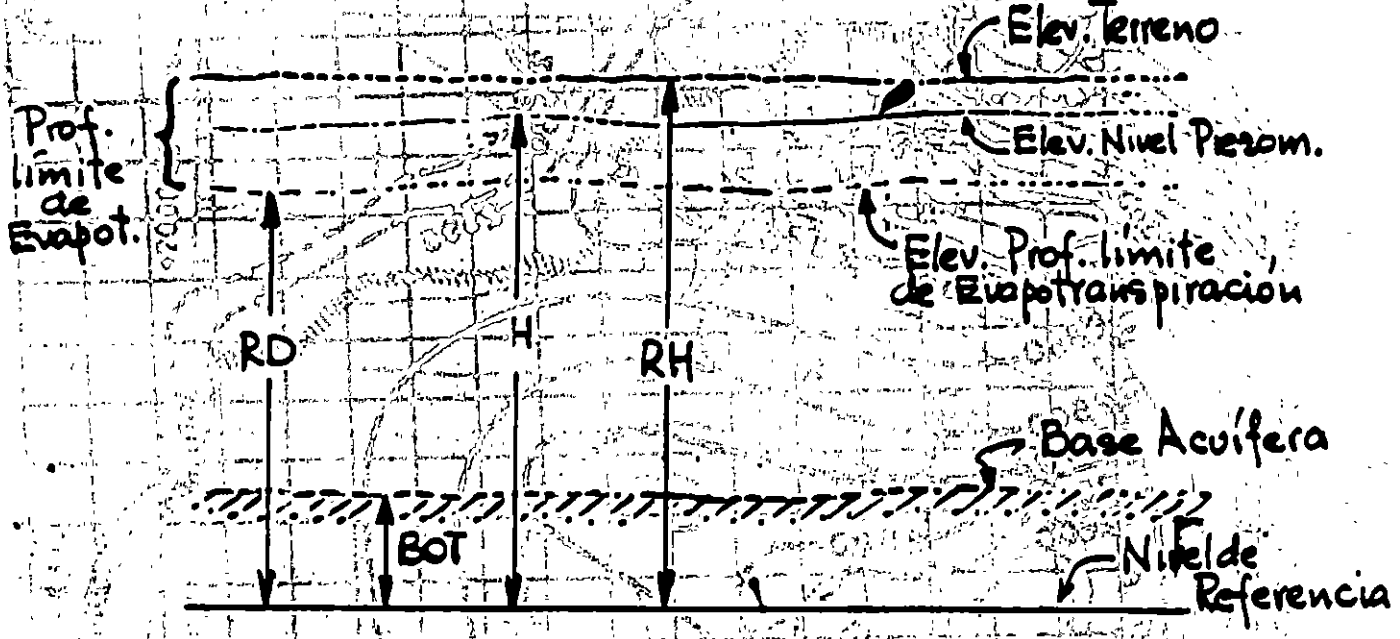
$R = K'/b'$ [1/d] Coeficiente de filtración

Filtración vertical: F

$F = R \cdot (H - RH)$, $H > RD$

$F = R \cdot (RD - RH) = cte$, $H \leq RD$

EVAPOTRANSPIRACION



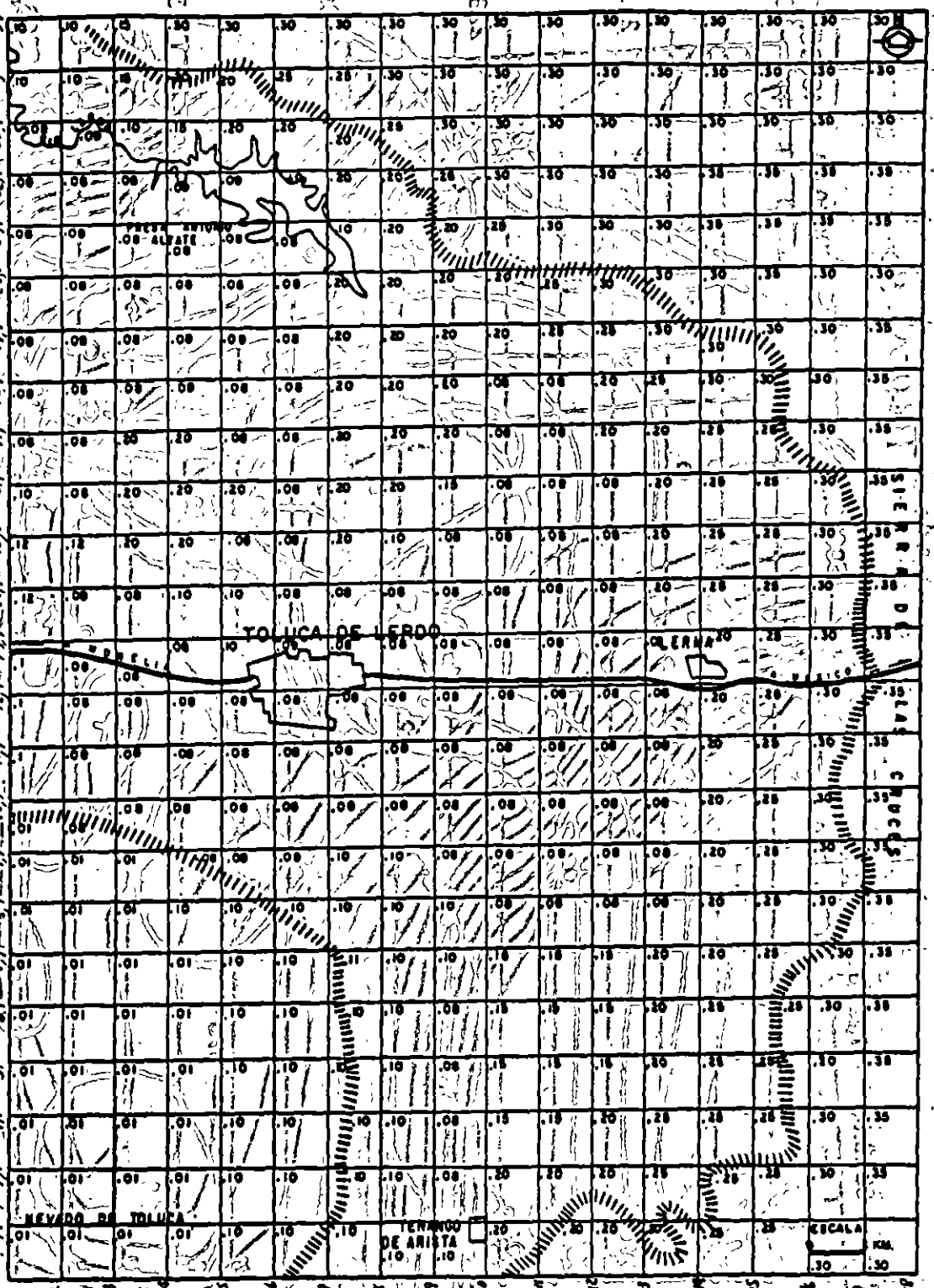
$$R = \frac{\text{Evap. media diaria (m)/d}}{\text{Prof. límite de Evapot. (m)}} = \left[\frac{1}{d}\right]$$

Evap. media diaria = Evap. anual x 0.75 / 365d

Arreglo Columnas Archivo

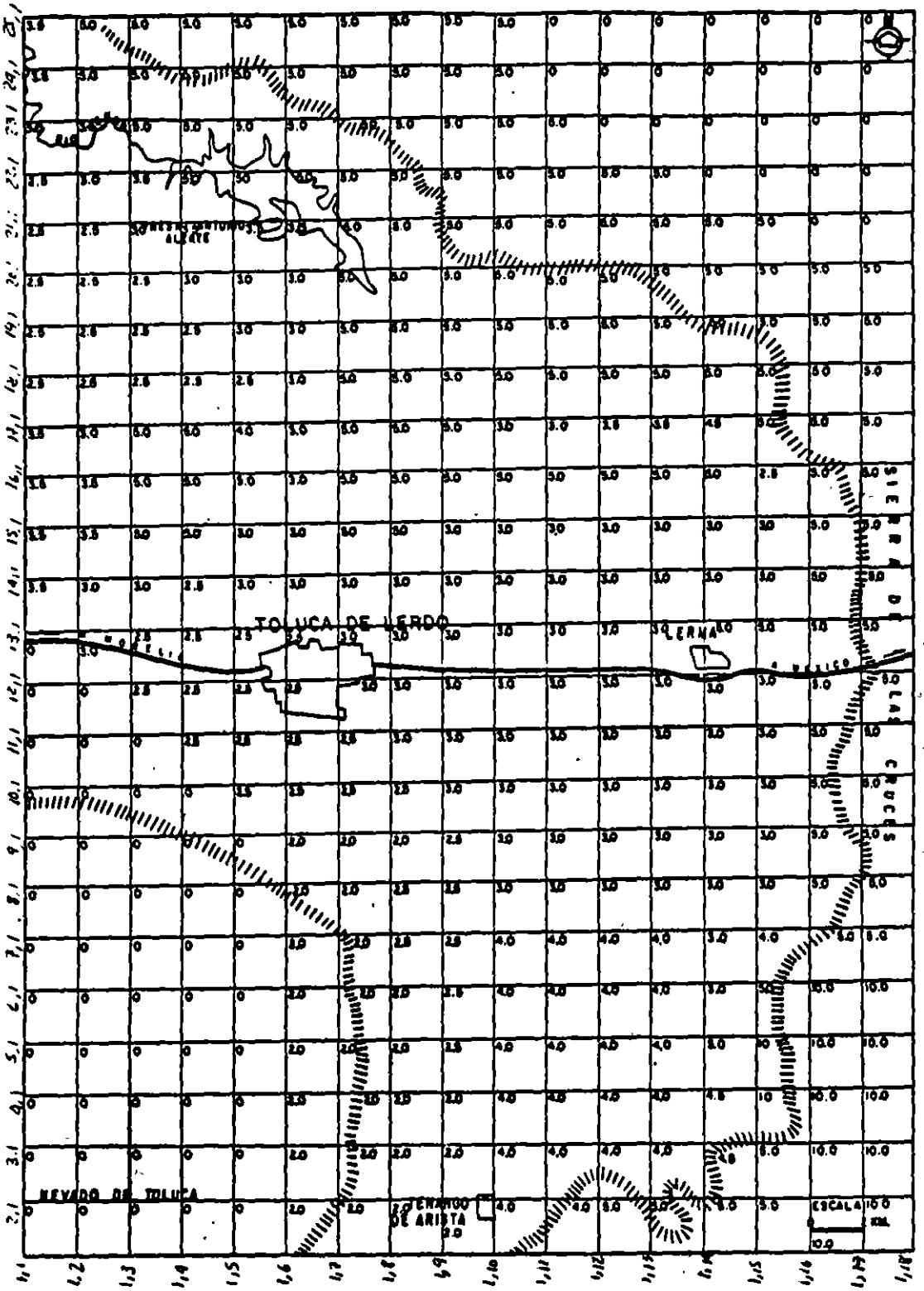
I, J, TI, TJ, SC, H, Q, R, RH, RD, BOT, PERM I, PERM J

Q = Evap. media diaria (m/d) + Extracción - Recarga



COEFICIENTE DE ALMACENAMIENTO

FIGURA 8.3



CONDUCTIVIDAD HIDRAULICA EN m/dia

FIGURA 8.2

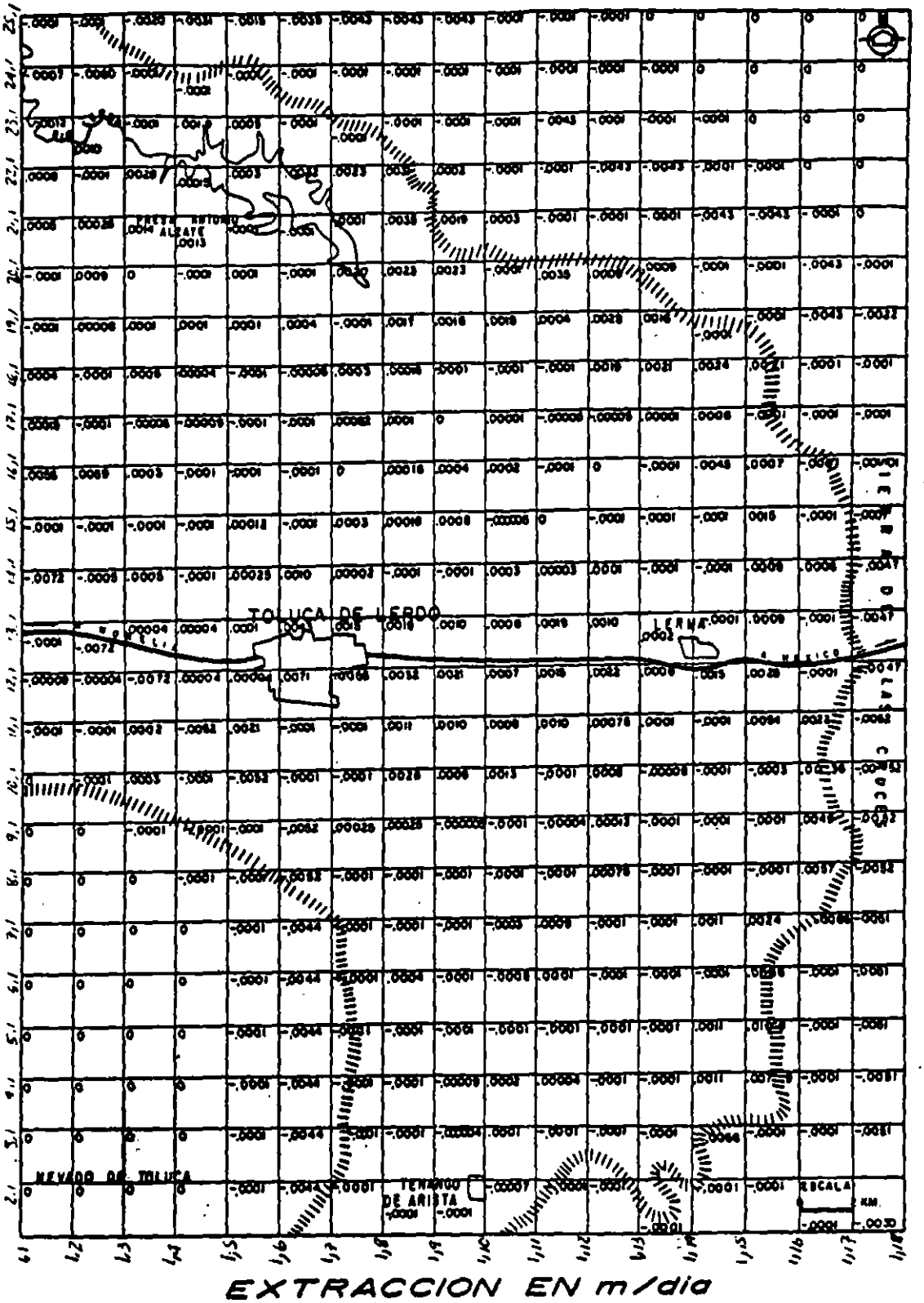

TOLUCA DE LERDO
LERMA
NEVADO DE TOLUCA
TENANGO DE ARISTA
ESCALA
KM.
EXTRACCION EN m/dia

FIGURA 8.6

- PRICKETT LONNQUIST AQUIFER MODEL SYSTEM (PLASM)

MODELO MATEMATICO PARA SISTEMAS ACUIFEROS

DESCRITO POR EL METODO DE DIFERENCIAS FINITAS PARA RESOLVERSE POR (METODO NUMERICO) UNA VARIANTE DE METODO IMPLICITO EN DIRECCION ALTERNANTE.

AUTORES. T.A. PRICKETT Y C.G. LONNQUIST
ILLINOIS STATE WATER SURVEY
U.S.G.S. BULLETIN 55, 1971.

FUNDAMENTOS MATEMATICOS.

LA ECUACION DIFERENCIAL EN DERIVADAS PARCIALES (BITTINGER Y OTROS, 1967) QUE DESCRIBE EL FLUJO BIDIMENSIONAL EN REGIMEN TRANSITORIO, EN UN ACUIFERO CONFINADO, HETEROGENEO E ISOTROPO ES:

$$\frac{\partial}{\partial x}\left(T\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(T\frac{\partial h}{\partial y}\right)=S\frac{\partial h}{\partial t}+Q$$

DONDE:

T= TRANSMISIVIDAD
h= ALTURA PIEZOMETRICA
t= TIEMPO
S = COEFICIENTE DE ALMACENAMIENTO
Q= DIFERENCIA DE CAUDALES (EXTRAIDOS Y RECARGADOS) POR UNIDAD DE AREA.
X.Y= COORDENADAS RECTANGULARES

PLANTEAMIENTOS DE LAS ECUACIONES.

CONDICION DE CONTINUIDAD O CONSERVACION DE MASA

CAMBIO EN EL ALMACENAMIENTO	=	FLUJOS DE ENTRADA	-	FLUJOS DE SALIDA

$$Q5 = Qn + Q1 + Q3 - Q6 - Q4 - Q2$$

Q1 a Q4 => TRANSFERENCIAS DE AGUA DE UN NUDO A OTRO. FLUJOS DEL ACUIFERO.
Qs => CANTIDAD DE AGUA INCORPORADA O LIBERADA DELALMACENAMIENTO POR UNIDAD DE TIEMPO. POSITIVO CUANDO SE LIBERA AGUA.

FLUJOS DEL ALMACENAMIENTO

Q6 => CAUDAL CONSTANTE DE BOMBEO
Q(I,J) = SALIDA (+) ENTRADAS (-)
Q(I,J) = EXTRACCIONES - RECARGA ART.

Qm => ACCIONES ESPECIALES: INFILTRACION INDUCIDA; EVAPOTRANSPIRACION; REZUMEN (INFILTRACIONES)

TRES CONSIDERACIONES:

1) DEFINIR LA PARTE DEL ACUIFERO QUE INTERVIENE EN CADA TERMINO

2) LOS CAUDALES ESTAN RESTRINGIDOS A LAS COORDENADAS X y Y, POR LO QUE SE TOMAN LAS PROYECCIONES ORTOGONALES.

3) BALANCE INSTANTANEO

PROCEDIMIENTO DE TRABAJO PARA EL PLASM.

1) DISCRETIZACION DE LAS PROPIEDADES FISICAS (SUPERPOSICION DE UNA MALLA)

NC (NUMERO DE COLUMNAS)
NR (NUMERO DE RENGLONES)

2) ASIGNACION DE VALORES COMUNES
T, FACTOR DE ALMACENAMIENTO (S)
ho (NIVEL INICIAL) Y Q DE BOMBEO

3) ZONAS ESPECIALES

A) BORDE DEL ACUIFERO -> T = 0
NO SE PUEDE S=0 (DIVISION CERO)

B) ADEMAS DE AGUAS SUPERFICIALES
LAGOS, MARES => S = 1

(FIG. NO. 10 p 33. DIAGRAMA DE FLUJO)

EJEMPLOS:

- SOLUCION TEORICA

MALLA DE TAMANO UNIFORME
ACUIFERO PROPIEDADES HOMOGENEAS E ISOTROPIAS
NIVELES PIEZOMETRICOS INICIALES = CERO
INCREMENTOS DE TIEMPOS IGUALES

CASO DE ACUIFERO ILIMITADO

1) NR y NC = 31 ; LADO DE MALLA 300 m
2) T = 100 m2/dia
   S = 0.01
   W = 900 m3/m
   H = 0
   Qo = 0 m3/dia

3) DELTA = 0.5 dias
   NSTEPS = 40

4) Q(16,16) = 4000 m3/dia

FACULTAD DE INGENIERIA U.N.A.M.
DIVISION DE EDUCACION CONTINUA

VII CURSO INTERNACIONAL DE CONTAMINACION DE ACUIFEROS

MODULO III. MODELOS EN GEOHIDROLOGIA Y CONTAMINACION DE ACUIFEROS

TEMA:

MANUAL DE USUARIO PARA EL PROGRAMA DE SOLUCION DIRECTA E INVERSA EN LOS SONDEOS ELECTRICOS VERTICALES (SEV)

ING. ALFONSO ALVAREZ MANILLA

1. INTRODUCCION:

Para la solución en la interpretación de las curvas de resistividad aparente en los sondeos eléctricos verticales (SEV) se ofrecen dos opciones: "directa" e "inversa".

La solución directa calcula la curva de resistividad aparente de un corte geoeléctrico teórico, mientras que la solución inversa encuentra el corte geoeléctrico de la curva de resistividad aparente obtenida en campo.

La solución directa es por medio de la teoría del filtrado lineal desarrollada por Ghosh, 1971. El programa inverse aplica el algoritmo de Marquart, 1963 para iniciar la obtención del modelo, lo modifica mediante iteraciones hasta que produce el mejor ajuste entre las curvas de campo y teóricas.

Los programas fueron modificados del artículo técnico de Philip A. Davis de la Minnesota Geological Survey por J. Cuauhtémoc Orendain M y Alfonso Alvarez Manilla A (1978).

El modelo se basa en un semiespacio dividido en un total de Ei capas horizontales, electricamente homogéneas e isotrópicas y de extensión infinita (figura 1), los parámetros incluyen a la resistividad (Ri) y espesores (Hi-1) de cada capa.

Los errores producidos pueden ser todavía disminuios con un proceso de retroalimentación; la interpretación con el programa inverse no manipula los problemas de equivalencia y supresión, los cuales deben ser observados por separado.

2. DESCRIPCION DE LOS PROGRAMAS

El programa en el disco, presenta cuatro archivos principales:

RES_APRT.EXE que es el que contiene los ejecutables de los subprogramas CAPTURA, INVERSE Y RESIST.

FILTRO1 y FILTRO 2 contiene los filtros de Ghosh, los cuales pueden ser cambiados por los de Oneil, u otros.

NO87.BAT es un subprograma para simular la existencia de coprocesador matemático en caso de que no tenga el propio la máquina donde opere.

2.1 INICIO (RESIST)

Con el programa en la unidad de disco correspondiente, se teclea:

NO87 RETURN

y se visualiza el MENU PRINCIPAL con las opciones de:

1. CAPTURA
2. RESIST
3. INVERSE
4. FIN DE CAPTURA

PROGRAMA SELECCIONADO:_

primero es necesario capturar los datos, por le que se teclea (1) RETURN

observando PROGRAMA CAPTURA con las opciones de:

1. RESIST
2. INVERSE
0. FIN DE PROGRAMA

PROGRAMA SELECCIONADO_

2.1a si se tiene la interpretación o presunción de un corte geoeléctrico determinado se oprime (1) RETURN

donde la pantalla muestra DATOS PARA EL PROGRAMA RESIST

NOMBRE DEL ARCHIVO DONDE SE ALMACENAN LOS DATOS:_

se teclea el nombre del archivo dónde son guardados los datos, por ejemplo

DUAQ RETURN

aparece DATOS PARA EL PROGRAMA RESIST

TIPO DE ARREGLO: 1. SCHLUMBERGER
2. WENNER
3. BIPOLO-BIPOLO
0. FIN DE CAPTURA

NUMERO DEL ARREGLO DESEADO:

se teclea el número al arreglo electródico correspondiente:

(1) RETURN

ESPACIAMIENTO (AGREGAR PUNTO DECIMAL):

El espaciamiento de AB/2 con el que se desea iniciar, asumiendo que fuera
1. RETURN

NUMERO DE CAPAS (ENTERO SIN PUNTO DECIMAL) 3 RETURN

NUMERO DE LECTURAS (ENTERO SIN PUNTO DECIMAL)
el número de lecturas corresponde a los espaciamientos generados
por la regla de correspondencia A = Ai10**(k/6) con 0= k =M
donde Ai es el espaciamiento inicial, k un entero y M el total de
espaciamientos deseados 10 RETURN

aparece ahora == AGREGAR PUNTO DECIMAL A LOS SIGUIENTES VALORES ==

ESPESOR (1) =_ 1. RETURN
ESPESOR (2)=_ 10. RETURN

RESISTIVIDAD (1)=_ 1. RETURN
RESISTIVIDAD (2)=_ 10. RETURN
RESISTIVIDAD (3)=_ 0.1 RETURN

pregunta en la pantalla: ESTAN BIEN TUS DATOS? (S/N):_

Si fue cometido algún error en la captura de cualquier dato debe teclearse N, exclusivamente este SEV no será codificado; caso contrario oprimir S RETURN

aparece: DATOS PARA EL PROGRAMA RESIST

TIPO DE ARREGLO: 1. SCHLUMBERGER
2. WENNER
3. BIPOLO-BIPOLO
0. FIN DE CAPTURA

NUMERO DEL ARREGLO DESEADO:_

como la captura de datos para el programa Resist ha concluido, se tecla 0 RETURN

pregunta si QUIERES OTROS DATOS (S/N)_

si se desea conocer las curvas de resistividad aparente de otros cortes, deberá continuar con la secuencia inicial oprimiendo S RETURN, caso contrario N RETURN

aparece el MENU PRINCIPAL

OPCIONES DE PROGRAMAS

1. CAPTURA
2. RESIST
3. INVERSE
0. FIN DE PROGRAMA

PROGRAMA SELECCIONADO:_

como los datos capturados son del programa Resist, el número seleccionado debe ser el 2 RETURN

PROGRAMA RESIST

ARCHIVO DE DATOS: teclear DUAQ RETURN

ARCHIVO DE REPORTE: teclear un nombre diferente a DUAQ; RUAQ RETURN

aparece FAVOR DE ESPERAR UNOS MOMENTOS

al ser concluido el proceso, el MENU PRINCIPAL es mostrado en la pantalla

debiendo teclear 0 RETURN

Para observar los datos en la pantalla, teclear

TYPE RUAQ RETURN y detener con la tecla de PAUSA

para impresión de los datos teclear

TYPE RUAQ>LPT1:

2.2 INICIO (INVERSE)

El modelo de inversión contiene errores significativos al no considerar el principio de equivalencia y supresión de capas, lo cual hace a la "resolución única" imposible de existir.

La solución de la inversión no representa el modelo geológico real, lo que debe ser calibrado con los conocimientos de geología.

El método de inversión fue originalmente desarrollado por Merrick en 1977, se han hecho algunas modificaciones para incrementar la flexibilidad propia del programa.

Con el programa en la unidad de disco correspondiente, se teclea:

NO87 RETURN

y se visualiza el MENU PRINCIPAL con las opciones de:

1. CAPTURA
2. RESIST
3. INVERSE
4. FIN DE CAPTURA

PROGRAMA SELECCIONADO:_

primero es necesario capturar los datos, por le que se teclea (1) RETURN

observando PROGRAMA CAPTURA con las opciones de:

1. RESIST
2. INVERSE
0. FIN DE PROGRAMA

PROGRAMA SELECCIONADO_

2.2a si se tiene la interpretación o presunción de un corte geoeléctrico determinado se oprime (2) RETURN

donde la pantalla muestra DATOS PARA EL PROGRAMA INVERSE

NOMBRE DEL ARCHIVO DONDE SE ALMACENAN LOS DATOS:_

se teclea el nombre del archivo dónde son guardados los datos, por ejemplo

DAUAQ RETURN

aparece DATOS PARA EL PROGRAMA INVERSE

TIPO DE ARREGLO: 1. SCHLUMBERGER
2. WENNER
3. BIPOLO-BIPOLO
0. FIN DE CAPTURA

NUMERO DEL ARREGLO DESEADO:

se teclea el número al arreglo electródico correspondiente:
(1) RETURN

ESPACIAMIENTO (NUMERO REAL, AGREGAR PUNTO DECIMAL):

El espaciamiento de AB/2 con el que se desea iniciar, asumiendo que fuera
1. RETURN

NUMERO DE CAPAS (ENTERO SIN PUNTO DECIMAL) 3 RETURN

NUMERO DE LECTURAS (ENTERO SIN PUNTO DECIMAL)
el número de lecturas corresponde a los espaciamientos generados por la regla de correspondencia A = Ai10**(k/6) con 0= k =M donde Ai es el espaciamiento inicial, k un entero y M el total de espaciamientos deseados 10 RETURN

NUMERO DE PARAMETROS FIJOS (NUMERO ENTERO):
Si se tienen conocimiento de algún estrato, sus valores de espesor y resistividad quedan fijados y el programa no los manipula; información adicional es pedida subsecuentemente. Si no se tienen datos teclear 0 RETURN

PORCENTAJE DE ERROR (NUMERO REAL):
Es el error en la aproximación numérica deseado 1. RETURN

TIPO DE LECTURAS

1. SI LAS LECTURAS SON LOGARITMICAS
2. DE OTRO MODO

si las lecturas están tomadas en función a la regla de correspondencia A = Ai10**(k/6) con 0= k =M son logarítmicas y se debe teclear 1 RETURN, caso contrario en la pantalla aparecerán preguntas acerca del espaciamiento y resistividad aparente para cada estación de medida, en esta última opción debe ser tecleado el número 2RETURN 1 RETURN

aparece === TECLEAR SOLO NUMEROS CON PUNTO DECIMAL ===

RESISTIVIDAD APARENTE No 1:
los datos de resistividad aparente correspondientes a los
diez espaciamientos y lecturas son introducidos, aparece
al final

PARAMETROS DE LA CAPAS (TOTAL 5)

ESPESOR (1)=
ESPESOR (2)=

RESISTIVIDAD (1)=
RESISTIVIDAD (2)=
RESISTIVIDAD (3)=

pregunta en la pantalla: ESTAN BIEN TUS DATOS? (S/N):_

Si fue cometido algún error en la captura de cualquier dato debe teclearse N, exclusivamente este SEV no será codificado; caso contrario oprimir S RETURN

aparece: DATOS PARA EL PROGRAMA RESIST

TIPO DE ARREGLO:
1. SCHLUMBERGER
2. WENNER
3. BIPOLO-BIPOLO
0. FIN DE CAPTURA

NUMERO DEL ARREGLO DESEADO:_

como la captura de datos para el programa Resist ha concluido, se tecla 0 RETURN

pregunta si QUIERES OTROS DATOS (S/N)_

si se desea conocer las curvas de resistividad aparente de otros cortes, deberá continuar con la secuencia inicial oprimiendo S RETURN, caso contrario N RETURN aparece el MENU PRINCIPAL

OPCIONES DE PROGRAMAS

1. CAPTURA
2. RESIST
3. INVERSE
0. FIN DE PROGRAMA

PROGRAMA SELECCIONADO:_

como los datos capturados son del programa Inverse, el número seleccionado debe ser el 3 RETURN

ARCHIVO DE DATOS: teclear DAUAQ RETURN

ARCHIVO DE REPORTE: teclear un nombre diferente a DAUAQ;
REUAQ RETURN

aparece FAVOR DE ESPERAR UNOS MOMENTOS

al ser concluido el proceso, el MENU PRINCIPAL es mostrado en la pantalla

debiendo teclear 0 RETURN

Para observar los datos en la pantalla, teclear

TYPE REUAQ RETURN y detener con la tecla de PAUSA

para impresión de los datos teclear

TYPE REUAQ>LPT1:

BIBLIOGRAFIA

Davis, P.A., 1979, Development and aplications of resistivity sounding inversion for several field arrays: M.S. thesis, University of Minnesota, Minneapolis.

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Ghosh, D., 1971, Inverse filter coefficients for computation of apparent resistivity standar curves for horizontally layered earth. Geophysical Prospecting, v.19.

GEO INGENIERIA ALFVEN, SA DE CV
GEOFISICA, GEOHIDROLOGIA, GEOLOGIA, GEOQUIMICA Y GEOTECNIA

MANUAL DE USUARIO PARA EL PROGRAMA REDUCCION DE DATOS DE GEOELECTRICOS

RESISTIVIDAD APARENTE
RESISTIVIDAD MEDIA CUADRATICA
RESISTIVIDAD SERIE NATURAL
RESISTIVIDAD EN PARALELO NATURAL

PARA

UNIVERSIDAD AUTONOMA DE QUERETARO
DIVISION DE ESTUDIOS DE POSTGRADO
FACULTAD DE INGENIERIA

POR

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1. 0 GENERALIDADES

La reducción de datos geoeléctricos es de suma importancia, de ellos es obtenida la curva de resistividad aparente de donde será interpretado el corte geoeléctrico; de acuerdo a la distribución del potencial, las anomalías detectadas con los sondeos eléctricos verticales (SEV) con cualquiera de sus arreglos electródicos -Schlumberger, Wenner, Bipolo-Bipolo- no ubican correctamente en el subsuelo a los eventos geológicos que las producen ocasionando " pifias ".

En el programa que fue desarrollado por J. Cuauhtémoc Orendain Munguía con algoritmo de A.A. Manilla (1983), se presenta la reducción de datos de geoelectricidad basado en el artículo de G. Hernández Moedano (1983) de nombre: CALCULO DE LA RESISTIVIDAD MEDIA PARTIENDO DE LAS MEDICIONES DE CAMPO DE SONDEOS ELECTRICOS VERTICALES PARA INTERPRETACION GEOLOGICA CUALITATIVA CERCANA A LA REAL, en el es descompuesta la resistividad aparente de un volumen de masa en sus componentes: serie, paralelo y media cuadrática, obteniendo de igual manera los valores de anisotropía y profundidad real de investigación.

El programa está compuesto de cuatro archivos, dos corresponden al sistema operativo y son:

COMMAND.COM
GWBASIC.EXE

en tanto que los programas que se refieren a la reducción de datos son:

SCHLUMB.BAS
DIPDIP.BAS

El primero reduce los datos del arreglo electródico Schlumberger y el segundo al arreglo Bipolo-Bipolo. Con la misma secuencia y de manera amistosa en la comunicación entre la computadora y usuario.

2.0 USO DEL PROGRAMA

Con el programa en la unidad de disco correspondiente, se teclea

GWBASIC RETURN

la pantalla mostrada es típica de basic, se oprime la tecla F3, y pide el nombre del programa a cargar

LOAD" SCHLUMB RETURN

aparece

OK, la tecla F2 debe ser oprimida y el programa ha dado inicio mostrando la pantalla de presentación y segundos después da inicio a:

CALCULO DE RESISTIVIDADES APARENTES

VALOR DE LA CORRIENTE:_

el valor de la corriente del transmisor debe ser introducida y ser consistente con la unidades del receptor, esto es: voltios-amperios, milivoltios-amperios, etc....

10 RETURN

pide

VALOR DE 'A':_

que es la distancia entre los electrodos de potencial MN,

5 RETURN

pide inmediatamente los valores de las L's o espaciamientos de AB/2 referentes a las estaciones de medida hechas en campo y los valores del voltaje.

LECTURA	L's	DV/I
1	10 RETURN	10 RETURN
2	21 RETURN	2 RETURN
3	32 RETURN	0.8 RETURN
4	46 RETURN	0.2 RETURN
5	si no se tienen mas datos debe ser tecleado RETURN apareciendo	

REPORTE EN PANTALLA O IMPRESORA (P/I)_

si se desea visualizar exclusivamente los datos debe ser tecleado una P, si es imprimir solo se oprime I seguido de un RETURN.

En la presentación de datos aparece

A= 5 que es la distancia entre los electrodos de potencial MN

L	Espaciamiento electródico AB/2
K	Factor geométrico
DV	Diferencia de potencial observada en M,N
RHOA	Resistividad aparente
RMCN	Resistividad media cuadratica natural
RSN	Resistividad serie natural
RPN	Resistividad paralelo natural
AAN	Coeficiente de anisotropía
IRR	Intervalo y profundidad real investigada

QUIERES OTROS CALCULOS (S/N)

en el caso de no tener mas datos que procesar oprimir N, situación contraria volver a empezar.

Para el Arreglo Bipolo-Bipolo, que aparece en la figura 1b, n corresponden a las distancias x que separa al dipolo de potencial del de corriente, x es la distancia entre los electrodos de potencial y los de corriente, son siempre números enteros.

BIBLIOGRAFIA

Barnes Layer Method Technical Memo No. 6 Instruction for use whit Bison Earth Resistivity Meter.

Orellana E., Prospección Geoeléctrica en corriente contínua, 1972.

Hernández Moedano G., 1983. Calculo de la Resistividad Media partiendo de las mediciones de campo de sondeos eléctricos verticales para una interpretación geológica cualitativa cercana a la real. XV Aniversario de la Creación de la Carrera de Ingeniero Geofísico, Palacio de Minería de la UNAM.

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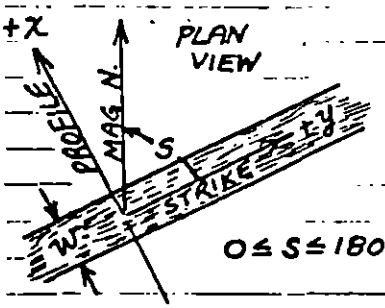
TITLE Magnetic Profiles over Dikes PAGE 1 OF 10 TI Programmable MAG 4

PROGRAMMER D.L. Campbell & D.N. Haines DATE _____ Program Record

Partitioning (Op 17) 4.7.9.5.9 (Standard) Library Module None used Printer Optional Cards 1

PROGRAM DESCRIPTION

Program Description, Equations, Variables, etc. This program calculates magnetic anomaly profiles over a two-dimensional dipping thick or thin dike. Dike is assumed to be infinitely long along strike (±y direction) and its bottom edge is infinitely deep. Anomalies in total field $\Delta T'$, in horizontal field $\Delta H'$, or in vertical field $\Delta V'$ may be calculated. If thickness w is known, program uses "thick dike" equations; if unknown, program uses "thin dike" equations (below).



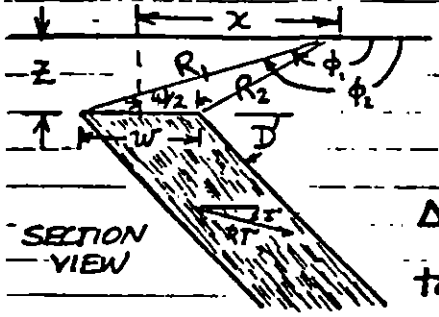
EQUATIONS FOR THICK DIKE:

$\Delta T' = 2kTh^2 \sin D\,[\sin(2I'-D)\cdot\Delta\phi - \cos(2I'-D)\cdot\Delta\ln R]$

$\Delta H' = 2kTh \sin D\,[\sin(I'-D)\cdot\Delta\phi - \cos(I'-D)\cdot\Delta\ln R]$

$\Delta V'$ = same as $\Delta H'$ with $I' \leftarrow I'+90°$

EQUATIONS FOR THIN DIKE:



$\frac{\Delta T'}{w} = 2kTh^2 \sin D\left[\sin(2I'-D)\frac{z}{R^2} - \cos(2I'-D)\cdot\frac{x}{R^2}\right]$

$\frac{\Delta H'}{w} = 2kTh \sin D\left[\sin(I'-D)\frac{z}{R^2} - \cos(I'-D)\cdot\frac{x}{R^2}\right]$

$\frac{\Delta V'}{w}$ = same as $\frac{\Delta H'}{w}$ with $I' \leftarrow I'+90°$

$\Delta\phi = \phi_2 - \phi_1$; $\Delta\ln R = \ln R_1/R_2$; $h^2 = 1-\cos^2 S\cos^2 I$

$\tan I' = \tan I / \sin S$

I = true field inclination

k = magnetic susceptibility

Reference: S. Parker Gay, Jr., 1967, Curves for interpretation of magnetic anomalies, in Mining Geophysics, v. II: Society of Exploration Geophysicists, Tulsa, OK, pps. 512–548.

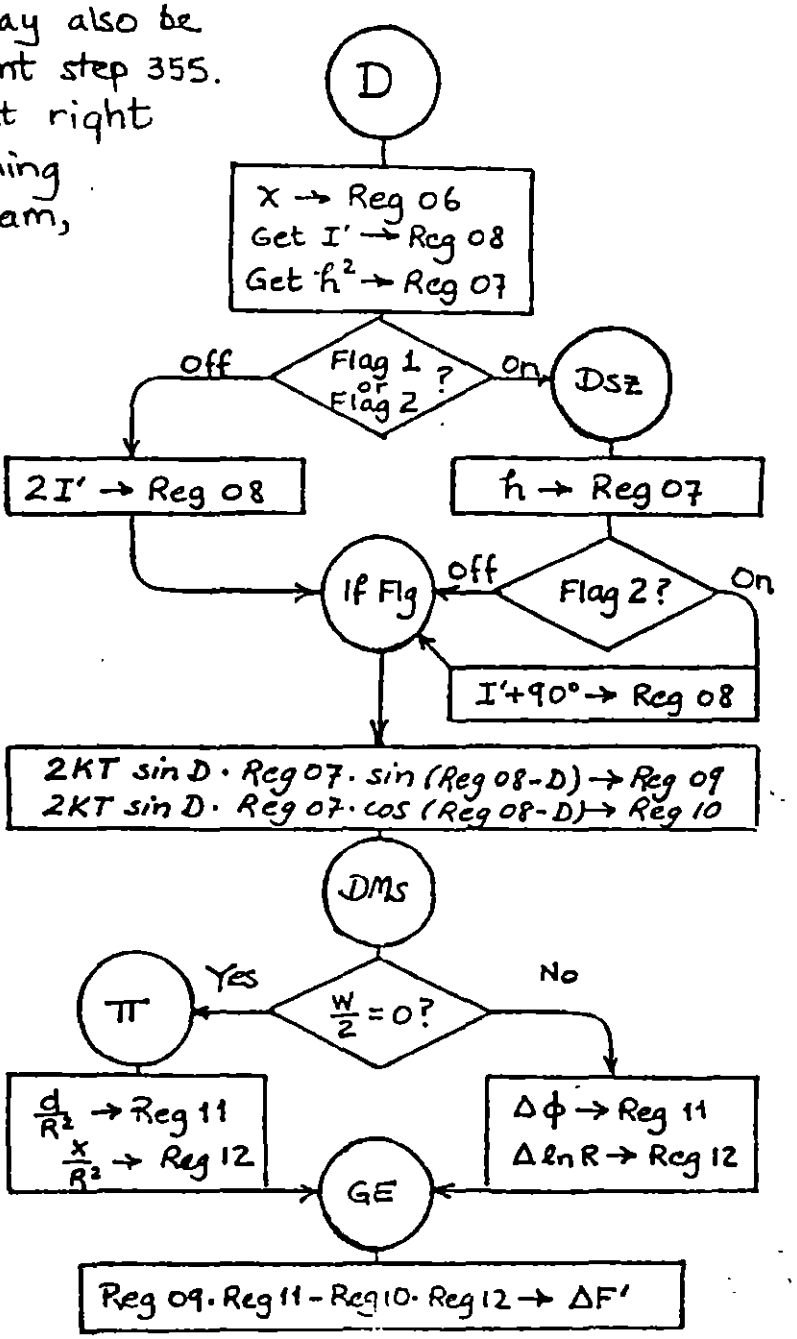
Operating Limits and Warnings GENERAL: Equations used assume negligible demagnetization effect and that $\Delta T' \ll T$. These conditions are usually met if susceptibility $k \ll 1$.

USER DEFINED KEYS	DATA REGISTERS		LABELS (Op 08)
A D	0 RT	10 cos	202 97 DSZ
B z	1 I	11 z/R^2 or $\Delta\phi$	242 87 IFF
C w	2 S	12 x/R^2 or $\Delta\ln$	280 88 DMS
D $X_0 \rightarrow \Delta E'$	3 $w/2$	13 R^2	328 77 GE
E $X_n, \Delta X \rightarrow$ Profile	4 z	14 ΔX	354 86 STF
F RT	5 D	15 X_n	375 91 R/S
G I	6 X_0 or current x	16 F_0	380 89 π
H λ	7 h^2 or h	17 X	410 15 E
I p, X_p	8 I'	18 X_p	417 78 E+
J F_0	9 Sin	19 T^2	

FLAGS Print 10 ΔH' 1 | ΔV' 2 | — 3 | — 4 | — 5 | — 6 | — 7 | - 8 | — 9

1014888-1

PROGRAMMER'S POINTS: Steps 000 through 130 of the program listing only store and echo-print the ribbon parameter values. These steps may be dropped (in favor of initial direct storage of the parameters into the appropriate registers) when altering the program for a calculator with fewer steps. Similarly, if no print cradle is available, all printout steps (marked in the listing with a vertical bar) become superfluous. In this case, some obvious changes may also be made after present step 355. The flow chart at right shows the remaining "bare-bones" program, subroutine D.



TI Programmable **MAG 4**

PROGRAMMER D.L. Campbell & D.N. Haines DATE _____

Program Record

Partitioning (Op 17) 4.7.9.5.9 (Standard) Library Module None Used Printer Optional Cards 1

USER INSTRUCTIONS

STEP	PROCEDURE	ENTER	PRESS	DISPLAY
1	Read in side 1 and side 2 of card.			
2	Set flags as needed			
	(a) To calculate horizontal field, ΔH'		2nd St Flg 1	
	(b) To calculate vertical field, ΔV'		2nd St Flg 2	
	• Default condition (flags 1 and 2 cleared)		calculates total field ΔT'	
	To clear flag n, press...	Inv	2nd St Flg n	
3	Input dike parameters (in any order)			
	(a) Magnetic susceptibility x field strength	kT [nT]	2nd A'	kT
	(b) Inclination of magnetic field	I [deg]	2nd B'	I
	(c) Angle from strike of dike to mag. north	S [deg]	2nd C'	S
	(d) Dip of dike, positive down from +x	D [deg]	A	D
	(e) Depth to top of dike	z	B	z
	(f) Apparent width of dike (Optional)	w	C	w/2
	• If no value of w is input, or if w is subsequently set to zero, the program uses the thin dike equations. These equations give little error as long as w ≤ z. Note in this case output field values are normalized by dike's apparent width w.			
4	Starting value of x for profile	x_0	D	ΔF'
	• You may wish to set display formats at this point. For example, to display only 2 decimal places, press...		2nd Fix 2	
5a	If no print cradle is available, skip the next 2 (starred) lines.			
*	Set flag 0		2nd St Flg 0	
*	Final x for profile	x_n	x⇄t	x_0
b	Increment of x	Δx	E	ΔF'
	• If flag 0 is set printout consists of pairs [x, ΔF'(x)] along the profile, where x ranges from x_0 to x_n in steps of Δx. If flag 0 is not set, the program stops at each profile point with ΔF'(x) in display and x in the t-register. (Press x⇄t to display x.) For next profile point, press...		R/S	
	— Continued next page —			

CARD LAYOUT

Magnetic Profiles over Dikes

RT	I	S	P, x_p	F_0
D	z	w	x_0	x_n, Δx

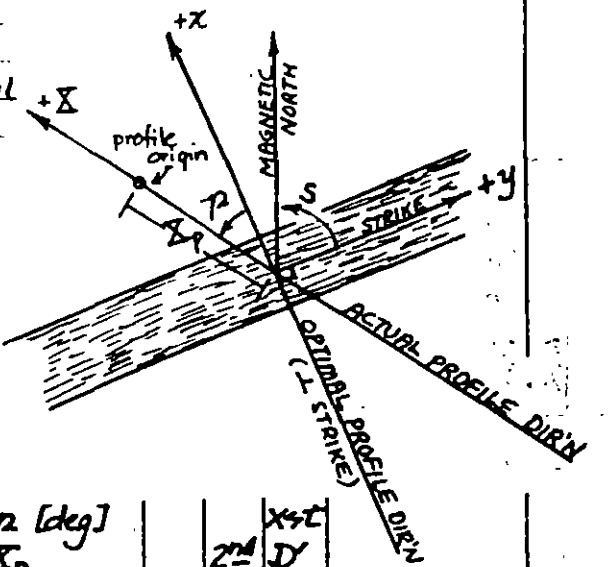
16

MAG 4 WMER D.L. Campbell & D.N. Haines DATE _____ TI Programmable Program Record

Partitioning (Op 17) [ ] Library Module _____ Printer _____ Cards _____

USER INSTRUCTIONS

STEP	PROCEDURE	ENTER	PRESS	DISPLAY
6	(Optional) Some users may wish to attempt to match particular field profiles using this program. Field profiles are likely to have the additional features: • Profile direction is not perpendicular to strike, but at an angle p to this optimal direction. • Profile coordinates X start at an arbitrary origin, a distance X_p from the dike's center-line. • Dike anomaly is superposed on a regional or background magnetic field F_o. These variables may be entered at step 3 (actually, anytime) via the following steps:			
3g	Profile angle	p [deg]		X↔Y
	Profile origin	X_p	2nd	D'
3h	Background field (assumed const.)	F_o [nT]	2nd	E'
	The profile parameters $x_o, x_n, \Delta x$ of Steps 4 and 5 now represent coordinates along the actual profile. The above process allows the user to shift the calculated curve at will; to right or left by changing X_p, and up or down by changing F_o. Note the default values of p, X_p and F_o are all zero: if no values are entered here, the calculated curve is not shifted.			
	COMMENTS: • Parameters of Steps 2 and 3 may be changed between profiles, and in any order. Do not change parameters between steps 4 and 5. • When $s=0$, a flashing display results at Step 4, but the displayed field $\Delta F'$ is correct. Press "CE" to clear the flashing display. • All distances $z, w, x_o, x_n, \Delta x, X_p$ must be in same units. Output $\Delta F'$ is in [nT (=gammas)] for thick dike case, [nT/distance] for thin dike case. • Caution: Calculated $\Delta H'$ is along profile direction. To get ΔH, the anomaly along magnetic north direction, take $\Delta H = \Delta H' \cdot \frac{\sin s}{\cos p}$ • Profile points are on the horizontal datum, z = constant. To calculate profiles on a topographically-varying surface, user must change z and x together, point for point.			



TITLE Magnetic Profiles over Dikes PAGE 5 OF 10 TI Programmab MAG 4

PROGRAMMER D.L. Campbell & D.N. Haines DATE _____ Coding Form

LOC	CODE	KEY	COMMENTS
000	76	LBL	Fcn A':
001	16	A'	
002	42	STO	Store kT
003	00	00	
004	69	OP	
005	00	00	
006	02	2	
007	06	6	"KT"
008	03	3	
009	07	7	
010	69	OP	
011	04	04	
012	43	RCL	
013	00	00	
014	69	OP	
015	06	06	
016	91	R/S	
017	76	LBL	Fcn B':
018	17	B'	
019	42	STO	Store I
020	01	01	
021	02	2	
022	04	4	"I"
023	69	OP	
024	04	04	
025	43	RCL	
026	01	01	
027	69	OP	
028	06	06	
029	91	R/S	
030	76	LBL	Fcn C':
031	18	C'	
032	42	STO	Store s
033	02	02	
034	03	3	
035	06	6	"S"
036	69	OP	
037	04	04	
038	43	RCL	
039	02	02	
040	69	OP	
041	06	06	
042	91	R/S	
043	76	LBL	Fcn D':
044	19	D'	
045	42	STO	Store Xp
046	18	18	
047	04	4	
048	04	4	"XP"
049	03	3	
050	03	3	
051	69	OP	
052	04	04	
053	43	RCL	
054	18	18	

LOC	CODE	KEY	COMMENTS
055	69	OP	
056	06	06	
057	03	3	"p"
058	03	3	
059	69	OP	
060	04	04	
061	32	X:T	
062	42	STO	Store p
063	19	19	
064	69	OP	
065	06	06	
066	92	RTN	
067	76	LBL	Fcn E':
068	10	E'	
069	42	STO	Store F0
070	16	16	
071	02	2	
072	01	1	"F0"
073	03	3	
074	02	2	
075	69	OP	
076	04	04	
077	43	RCL	
078	16	16	
079	69	OP	
080	06	06	
081	92	RTN	
082	76	LBL	Fcn A:
083	11	A	
084	42	STO	Store dip
085	05	05	
086	01	1	
087	06	6	"DIP"
088	02	2	
089	04	4	
090	03	3	
091	03	3	
092	69	OP	
093	04	04	
094	43	RCL	
095	05	05	
096	69	OP	
097	06	06	
098	91	R/S	
099	76	LBL	Fcn B:
100	12	B	
101	42	STO	Store z
102	04	04	
103	04	4	"z"
104	06	6	
105	69	OP	
106	04	04	
107	43	RCL	
108	04	04	
109	69	OP	

LOC	CODE	KEY	COMMENTS
110	06	06	
111	91	R/S	
112	76	LBL	Fcn C:
113	13	C	
114	42	STO	Store w
115	03	03	
116	04	4	
117	03	3	
118	69	OP	
119	04	04	"W"
120	43	RCL	
121	03	03	
122	69	OP	
123	06	06	
124	02	2	
125	22	INV	Replace w
126	49	PRD	by w/2
127	03	03	for
128	43	RCL	calc. of
129	03	03	coords.
130	91	R/S	
131	76	LBL	Fcn D:
132	14	D	
133	42	STO	Store X
134	17	17	
135	75	-	
136	43	RCL	Get x'
137	18	18	
138	95	=	=
139	65	×	
140	43	RCL	(X-Xp)·
141	19	19	
142	39	COS	cos p
143	95	=	
144	42	STO	
145	06	06	
146	42	STO	Set default
147	15	15	Xn.
148	43	RCL	
149	01	01	
150	30	TAN	Get I'
151	55	÷	
152	43	RCL	
153	02	02	
154	38	SIN	=tan⁻¹
155	95	=	
156	22	INV	$\left(\frac{\tan I}{\sin s}\right)$
157	30	TAN	
158	42	STO	
159	08	08	

MERGED CODES

62 [x≥t] [t]		72 (STO) [÷]		83 (STO) [(]	
63 [x<t] [t]		73 (RCL) [×]		84 [)] [=]	
64 [x=t] [t]		74 (SUM) [−]		92 (RTN) (SBR)	

TEXAS INSTRUMENTS

TI-59181

MAG 4 Magnetic Profiles over Dikes PAGE 6 OF 10 TI Programmable Coding Form

PROGRAMMER D.L. Campbell & D.N. Haines DATE _____

LOC	CODE	KEY	COMMENTS
160	69	DP	Clear Print Regs.
161	00	00	
162	43	RCL	
163	02	02	
164	39	COS	
165	65	×	
166	43	RCL	
167	01	01	Get h^2
168	39	COS	
169	95	=	
170	33	X^2	
171	75	-	
172	01	1	
173	95	=	
174	94	+/-	
175	42	STO	
176	07	07	
177	87	IFF	.8125
178	01	01	Are ΔH', ΔV' flags set?
179	97	DSZ	
180	87	IFF	
181	02	02	
182	97	DSZ	
183	43	RCL	If not I'←2I'
184	08	08	
185	44	SUM	
186	08	08	
187	04	4	
188	04	4	
189	05	5	Write
190	07	7	
191	03	3	"X,TOT"
192	07	7	
193	03	3	in print
194	02	2	block #2
195	03	3	
196	07	7	
197	69	DP	
198	02	02	
199	61	GTO	
200	87	IFF	
201	76	LBL	DSZ: Come
202	97	DSZ	here if ΔH',
203	34	FX	ΔV' field is
204	42	STO	to be calculated, &
205	07	07	store h
206	04	4	in place of
207	04	4	h^2
208	05	5	
209	07	7	
210	02	2	Write
211	03	3	"X,HOR"
212	03	3	in print
213	02	2	block #2
214	03	3	

LOC	CODE	KEY	COMMENTS
215	05	5	
216	69	DP	
217	02	02	
218	22	INV	Is ΔV' flag
219	87	IFF	set?
220	02	02	
221	87	IFF	
222	09	9	If so,
223	00	0	I'←I'+90°
224	44	SUM	
225	08	08	
226	22	INV	A precaution
227	86	STF	to avoid trouble
228	01	01	at step 344.
229	04	4	
230	04	4	
231	05	5	Overwrite
232	07	7	
233	04	4	"X,VER"
234	02	2	
235	01	1	in print
236	07	7	block #2
237	03	3	
238	05	5	
239	69	DP	
240	02	02	
241	76	LBL	Iff:
242	87	IFF	
243	98	ADV	
244	69	DP	Print
245	05	05	title
246	69	DP	
247	00	00	
248	43	RCL	
249	05	05	Get I'-D
250	22	INV	
251	44	SUM	
252	08	08	
253	43	RCL	
254	08	08	Sin(I'-D)
255	38	SIN	→Reg 09
256	42	STO	
257	09	09	
258	43	RCL	
259	08	08	cos(I'-D)
260	39	COS	→Reg 10
261	42	STO	
262	10	10	
263	43	RCL	Get
264	05	05	factor
265	38	SIN	
266	65	×	Sin D
267	02	2	
268	65	×	×2KT
269	43	RCL	

LOC	CODE	KEY	COMMENTS
270	00	00	× h
271	65	×	
272	43	RCL	
273	07	07	
274	95	=	
275	49	PRD	factor x sin →Reg 09
276	09	09	
277	49	PRD	factor x cos →Reg 10
278	10	10	
279	76	LBL	Dms: Entry
280	88	DMS	for profile
281	29	CP	calculation.
282	43	RCL	
283	03	03	If W=0, do
284	67	EQ	thin dike
285	89	π	calc. at
286	70	RAD	Lbl π
287	43	RCL	
288	06	06	Otherwise,
289	85	+	
290	43	RCL	
291	03	03	
292	95	=	
293	32	X:T	
294	43	RCL	
295	04	04	
296	22	INV	
297	37	P/R	
298	94	+/-	
299	42	STO	ϕ_1 →Reg 11
300	11	11	
301	32	X:T	
302	42	STO	R_1 →Reg 12
303	12	12	
304	43	RCL	
305	06	06	
306	75	-	
307	43	RCL	
308	03	03	
309	95	=	
310	32	X:T	Get
311	43	RCL	ϕ_2, R_2
312	04	04	
313	22	INV	
314	37	P/R	
315	44	SUM	
316	11	11	$\phi_2 - \phi_1$ in
317	32	X:T	Reg 11
318	22	INV	
319	49	PRD	

MERGED CODES

62		72 (STO)		83 (GTO)	
63		73 (RCL)		84	
64		74 (SUM)		92	

TEXAS INSTRUMENTS INCORPORATED

TI 59101

TITLE Magnetic Profiles over Dikes PAGE 7 OF 10 TI Programmable MAG 4

PROGRAMMER D.L. Campbell & D.N. Haines DATE _____ Coding Form

LOC	CODE	KEY	COMMENTS
320	12	12	
321	60	DEG	
322	43	RCL	
323	12	12	$\ln \frac{R_1}{R_2}$ in
324	23	LNX	
325	42	STO	Reg 12
326	12	12	
327	76	LBL	GE: Entry
328	77	GE	from π.
329	43	RCL	
330	11	11	
331	65	×	
332	43	RCL	
333	09	09	
334	75	-	
335	43	RCL	
336	12	12	
337	65	×	
338	43	RCL	
339	10	10	
340	85	+	
341	43	RCL	
342	16	16	
343	95	=	$\Delta F'$
344	22	INV	
345	87	IFF	
346	01	01	
347	86	STF	Project ΔF'
348	65	×	
349	43	RCL	onto line
350	19	19	
351	39	COS	of profile
352	95	=	
353	76	LBL	
354	86	STF	
355	32	X:T	
356	43	RCL	
357	17	17	
358	99	PRT	Print
359	32	X:T	
360	99	PRT	x, ΔF'
361	98	ADV	
362	22	INV	
363	87	IFF	If flag 0
364	00	00	not set,
365	91	R/S	stop for
366	43	RCL	manual
367	15	15	output
368	32	X:T	
369	43	RCL	
370	17	17	Otherwise,
371	22	INV	increment
372	77	GE	Σ at Lbl
373	78	Σ+	Σ+ and
374	76	LBL	go on.

LOC	CODE	KEY	COMMENTS
375	91	R/S	R/S:
376	91	R/S	
377	61	GTO	
378	78	Σ+	
379	76	LBL	π: Thin
380	89	π	dike calc.
381	42	STO	
382	04	04	
383	33	X²	
384	85	+	
385	43	RCL	
386	06	06	
387	33	X²	
388	95	=	
389	42	STO	R^2 in Reg 13
390	13	13	
391	43	RCL	
392	04	04	
393	55	÷	
394	43	RCL	
395	13	13	
396	95	=	
397	42	STO	$\frac{z}{R^2}$ in Reg 11
398	11	11	
399	43	RCL	
400	06	06	
401	55	÷	
402	43	RCL	
403	13	13	
404	95	=	
405	42	STO	$\frac{x}{R^2}$ in Reg 12
406	12	12	
407	61	GTO	
408	77	GE	
409	76	LBL	Fcn E:
410	15	E'	
411	42	STO	
412	14	14	ΔΣ
413	32	X:T	
414	42	STO	
415	15	15	Σ_n
416	76	(LBL)	
417	78	Σ+	Σ+:
418	43	RCL	
419	14	14	
420	44	SUM	Increment
421	17	17	X'
422	65	×	
423	43	RCL	
424	19	19	
425	39	COS	
426	95	=	
427	44	SUM	
428	06	06	
429	61	GTO	

LOC	CODE	KEY	COMMENTS
430	88	DMS	
431	00	0	
432	00	0	
433	00	0	
434	00	0	
435	00	0	
436	00	0	
437	00	0	
438	00	0	

MERGED CODES

62 [P↑] [A] 72 [STO] [P↑] 83 [GTO] [P↑]
63 [LRN] [A] 73 [RCL] [A] 84 [A] [P↑]
64 [P↑] [A] 74 [SUM] [A] 92 [INV] [SBR]

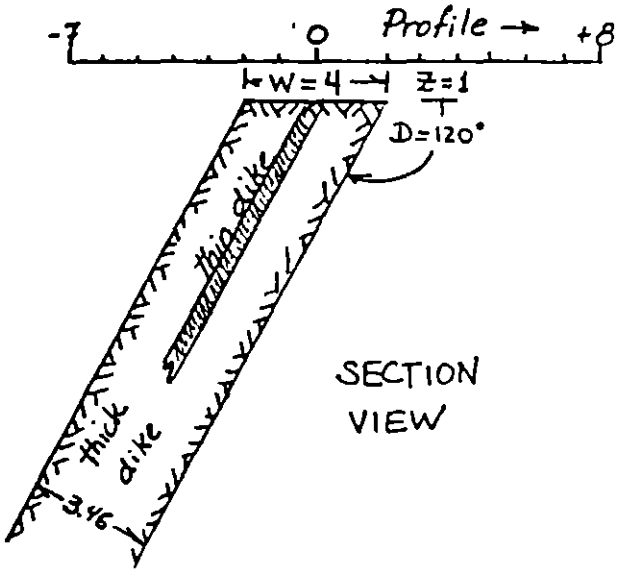
TEXAS INSTRUMENTS INCORPORATED

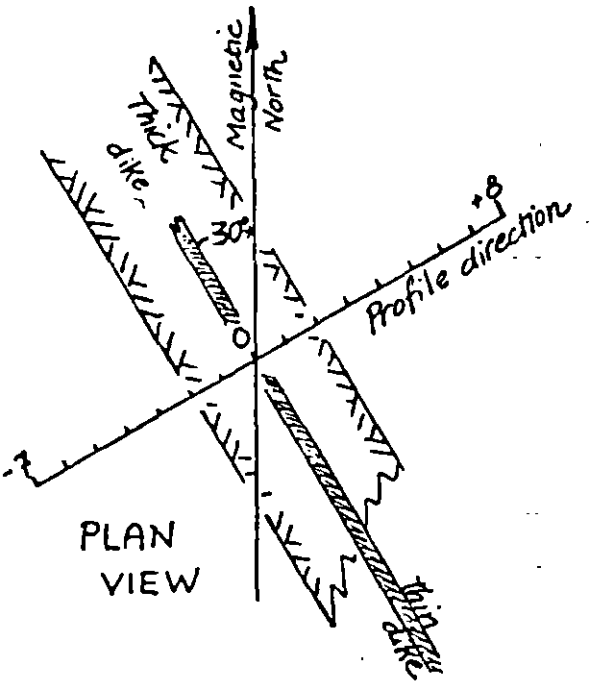
TI-84181

EXAMPLE: Calculate total, horizontal, and vertical magnetic field anomalies for a dike with $\mathcal{H}T = 50$ nT, $I = 60°$, $\lambda = 30°$, $D = 120°$ (= 60° down from the $-x$ direction), and $d = 1$ unit. Do both cases

(i) thick dike with $w = 4$ units (true thickness 3.46 units),

(ii) thin dike with $w < z$.





SOLUTION:

STEP	VARIABLE	KEY	DISPLAY	PRINTOUT (con't next page)
● Thick dike case, total field:				
3a	$\mathcal{H}T = 50$	2nd A	50.	50. KT
b	$I = 60$	2nd B	60.	60. I
c	$S = 30$	2nd C	30.	30. S
d	$D = 120$	A	120.	120. DIP
e	$z = 1$	B	1.	1. Z
f	$w = 4$	C	2.	4. W
4	$X_0 = 7$, +/- (Optional)	D	$\Delta T = 38.59444275$	X: TOT -7.
		2nd Fix 2	38.59	38.59444275
5a		2nd StFlg 0		
	$X_n = 8$	x⇄t	-7.00	-6.00 45.70
5b	$\Delta x = 1$	E	tape output: at end display shows 8.00	

SOLUTION (continued)

STEP	VARIABLE	KEY	DISPLAY	PRINTOUT
• horizontal anomaly:				
2a		2nd StFlg 1		
4	$X_0 = 7$, +/-	D	-7.00	
5a	$X_n = 8$	x⇄t	-7.00	
b	$\Delta X = 1$	E	8.00	
• vertical anomaly:				
2b		2nd StFlg 2		
4	$X_0 = 7$, +/-	D	-7.00	
5a	$X_n = 8$	x⇄t	-7.00	
b	$\Delta X = 1$	E	8.00	
• Thin dike case:				
3f	$W = 0.$	C	0.00	
• total field anomaly:				
		RST	(Clears all flags)	
4	$X_0 = 7$, +/-	D	$\Delta T' = 9.37$	
5a		2nd StFlg 0		
	$X_n = 8$	x⇄t	-7.00	
5b	$\Delta X = 1$	E	8.00	
• horizontal anomaly:				
2a		2nd StFlg 1		
4	$X_0 = 7$, +/-	D	-7.00	
5a	$X_n = 8$	x⇄t	-7.00	
b	$\Delta X = 1$	E	8.00	
• vertical anomaly:				
2b		2nd StFlg 2		
4	$X_0 = 7$, +/-	D	-7.00	
5a	$X_n = 8$	x⇄t	-7.00	
b	$\Delta X = 1$	E	8.00	
Comments: (i) For manual output (no PC available), skip all steps 5a. That is, do this —				
4	$X_0 = 7$, +/-	D	$\Delta F'(x_0)$	
5b	$\Delta X = 1$	E	$\Delta F'(x_0+\Delta X)$	
		x⇄t	$x_0+\Delta X$	
		R/S	$\Delta F(x_0+2\Delta X)$	
		etc...		

```
-5.00
55.99

-4.00
72.09

-3.00
99.12

-2.00
131.68

-1.00
116.85

0.00
72.66

1.00
16.66

2.00
-44.67

3.00
-60.53

4.00
-52.50

5.00
-44.19

6.00
-37.78

7.00
-32.90

8.00
-29.11
```

End of thick dike, total field printout. Remaining printout continued on next page.

- SOLUTION (continued)

(ii) Fixing display formats usually garbles all subsequent alpha output. (In this case, the "FIX 2" shifted the headings — "X, HOR", etc. — to the left.) For correct alpha headings, it is best to press "INV 2nd FIX" before repeating any of steps 3 or 4, and then refix the display format again after step 4.

Remaining printout tapes:

X: HOR	Y: VER	0.00 U Y: TOT	X: HOR	X: VER
-7.00 26.21	-7.00 37.00	-7.00 9.37	-7.00 6.45	-7.00 8.96
-6.00 29.51	-6.00 44.25	-6.00 10.98	-6.00 7.26	-6.00 10.58
-5.00 33.44	-5.00 55.00	-5.00 13.23	-5.00 8.25	-5.00 12.90
-4.00 37.38	-4.00 72.45	-4.00 16.58	-4.00 9.43	-4.00 16.42
-3.00 36.34	-3.00 103.97	-3.00 21.95	-3.00 10.61	-3.00 22.29
-2.00 2.10	-2.00 151.45	-2.00 31.46	-2.00 10.40	-2.00 33.33
-1.00 -70.88	-1.00 155.38	-1.00 47.53	-1.00 -1.06	-1.00 55.19
0.00 -124.55	0.00 119.85	0.00 32.81	0.00 -56.25	0.00 54.13
1.00 -157.99	1.00 64.85	1.00 -14.72	1.00 -55.19	1.00 -1.06
2.00 -151.25	2.00 -7.92	2.00 -18.34	2.00 -32.90	2.00 -11.67
3.00 -102.49	3.00 -40.31	3.00 -15.39	3.00 -21.86	3.00 -11.46
4.00 -70.96	4.00 -40.13	4.00 -12.72	4.00 -16.04	4.00 -10.05
5.00 -53.67	5.00 -35.53	5.00 -10.71	5.00 -12.57	5.00 -8.74
6.00 -43.08	6.00 -31.19	6.00 -9.21	6.00 -10.30	6.00 -7.66
7.00 -35.96	7.00 -27.61	7.00 -8.06	7.00 -8.70	7.00 -6.79
8.00 -30.96	8.00 -24.70	8.00 -7.16	8.00 -7.53	8.00 -6.09

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FACULTAD DE INGENIERIA U.N.A.M.
DIVISION DE EDUCACION CONTINUA

VII CURSO INTERNACIONAL DE CONTAMINACION DE ACUIFEROS

MODULO III MODELOS MATEMATICOS EN GEOHIDROLOGIA Y CONTAMINACION DE ACUIFEROS

TEMA

MODELO DE FLUJO " PLASM"

MODELACION NUMERICA DEL TRANSPORTE DE CONTAMINANTES EN EL SUELO (CONCEPTOS BASICOS)

PONENTE:
ING. DAVID GONZALEZ POSADAS

MODELACIÓN NUMÉRICA DEL TRANSPORTE

DE CONTAMINANTES EN EL SUBSUELO

(Conceptos Básicos)

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Introducción

La contaminación de las aguas subterráneas se ha convertido en uno de los problemas ambientales mas graves en las últimas décadas. Los contaminantes en superficie pueden infiltrarse en el subsuelo y llegar a contaminar los acuíferos. Lo anterior, representa un serio riesgo para la salud y medio ambiente. Dado a que la contaminación no se puede detectar ni medir en forma inmediata, es necesario utilizar herramientas matemáticas, como los modelos numéricos, para estudiar y simular el comportamiento de los contaminantes en el subsuelo.

Los modelos de transporte poseen menor poder predictivo que los modelos de flujo. Lo anterior, se debe a que uno de los parámetros más sensibles es la velocidad promedio en los poros la cual, puede ser determinada solamente dentro de un orden de magnitud. Este problema se torna mas complejo en acuíferos formados por varias capas, donde la velocidad y la concentración de los contaminantes no están homogéneamente distribuidos a profundidad.

En el caso de un balance de agua subterránea, si existe mayor velocidad en una capa que en otra, no tiene importancia ya que la única cantidad relevante es el flujo total en una sección transversal. Por el contrario en un modelo de transporte, se tendrá una gran diferencia si los contaminantes están presentes en una capa de baja o alta velocidad.

Una parte fundamental de un modelo de transporte es la elaboración de un modelo de flujo. Este, constituye la parte más laboriosa por su preparación, calibración y verificación. El modelo de flujo que se utilice de base debe satisfacer un alto grado de exactitud.

Los modelos de transporte requieren mayor información que los modelos de flujo. Esto se debe a que, además de los datos relacionados con el flujo subterráneo se requieren valores del coeficiente de dispersión, porosidad, concentración inicial de contaminantes y factores de retardación y/o atenuación. Esta información se desconoce a priori y tiene que ser estimada. Por ello, los resultados derivados del modelo deben ser tomadas con reserva.

La calibración de los modelos de transporte con los datos de campo es limitada. Los resultados, solo pueden ser comparadas con mediciones promedio de concentración. Si las muestras se obtienen de la parte superficial del subsuelo, como es el caso, la profundidad promedio no es representativa de la

concentración en ese punto. Solamente cuando se tiene un considerable número de observaciones, se pueden comparar los resultados medidos con los calculados. Ver fig.(1).

A pesar de las dificultades mencionadas, los modelos de transporte son una valiosa herramienta para el análisis y solución de problemas de contaminación en el subsuelo. Una primera aplicación puede ser la interpolación de la concentración en pozos de monitoreo. El modelo también puede proporcionar, dentro de los limites, la evolución de la pluma contaminante.

La aplicación más útil de los modelos radica en simular escenarios y métodos para el saneamiento de los acuíferos. Su utilidad radica en predecir el potencial de contaminación creado por una fuente.

Es poco probable que las capacidades predictivas de los modelos mejoren en el futuro, ya que las heterogeneidades a pequeña escala no pueden ser exploradas con suficiente detalle. Por tanto, el desarrollo de los modelos se dirige hacia el desarrollo de modelos estocástico los cuales, agregan a los resultados una medida de las posible variabilidad de estos.

I. Solución Numérica de la Ecuación de Transporte

La ecuación de transporte en una dimensión en un medio poroso homogéneo e isótropo que incluye sorpción y decaimiento, se puede expresar como (Fetter, 1990):

$$\frac{\partial C}{\partial t} = \underset{(dispersión)}{D_L \frac{\partial^2 C}{\partial x^2}} - \underset{(adveción)}{v_x \frac{vC}{\partial x}} - \underset{(sorpción)}{\frac{B_d}{\theta} \frac{\partial C^*}{\partial t}} + \underset{(reación)}{\left(\frac{\partial C}{\partial t}\right)_{rxn}}$$

en donde:

C = concentración del soluto en fase liquida, t = tiempo, Dl = coeficiente de dispersión longitudinal, Vx = es la velocidad lineal, Bd = es la densidad del acuífero, O = porosidad del medio saturado, C * = cantidad de soluto sujeto a procesos de adsorpción o absorpción y rxn = indica reacciones biológicas o químicas.

El primer termino de la ecuación representa la dispersión del soluto, el segundo la advección del soluto, el tercero es la transferencia del soluto de una fase liquida a las partículas solidas por sorpción, y el último termino indica que cambios en la concentración del soluto con el tiempo debido a reacciones biológicas o químicas o por decaimiento radioactivo.

La solución de la ecuación (1) se puede obtener por métodos analíticos o numéricos. Los métodos analíticos brindan soluciones exactas, pero suponen muchas simplificaciones. Por ello, no son utilizados en problemas prácticos ya que no existen soluciones analíticas para geometrías complejas y medios heterogéneos.

Los métodos numéricos permiten obtener soluciones aproximadas de las ecuaciones. Sin embargo, poseen mayor capacidad para representar y resolver problemas hidrogeológicos donde las propiedades del medio varían en el espacio. Los principales métodos numéricos son; diferencias finitas, elementos finitos y de características.

a) El método de diferencias finitas es el método más utilizado, este consiste en:

1. Dividir la región de estudio en celdas rectangulares.
2. Aproximar las derivadas mediante serie de Taylor o balance de masas.
3. Resolver las ecuaciones en diferencias implícitamente.

El método de diferencias finitas es fácil de estudiar y programar. Su principal limitación, es que la solución de la ecuación de transporte produce dispersión numérica y oscilaciones (Ver fig. 2), debidas a errores de truncación en la aproximación del termino de advección. En algunos casos, es posible conjugar soluciones entre la dispersión y las oscilaciones ajustando las aproximaciones en tiempo y en espacio sin embargo, no es posible hacer desaparecer ambas.

b) El método de elementos finitos ha sido utilizado en la modelación de numérica de las aguas subterráneas desde 1970. Actualmente, el método de Garlerking es ampliamente usado, los pasos básicos del método son:

1. Dividir la región en subregiones llamadas elementos.
2. Establecer funciones de interpolación para definir la concentración dentro de un elemento en terminos de la concentración en los nodos de cada elemento.
3. Formular una ecuación integral aproximada en terminos de funciones básicas.
4. Aplicar el teorema de Green de segundo orden a las derivadas de segundo orden.
5. Sustituir los terminos de funciones básicas para formar una ecuación matricial
6. Aproximar la derivada en tiempo por diferencias finitas y resolver el sistema matricial.

El método de elementos finitos (E.F.) es mas difícil de comprender y programar, que el método de diferencias finitas (D.F.). Además, requiere memoria adicional en computo para solucionar del sistema de ecuaciones. Su principal ventaja es la flexibilidad de las formas de los elementos para representar limites hidrogelógicos. El método de elementos finitos genera problemas de dispersión numérica y oscilaciones, en la misma forma que el método de diferencias finitas.

c) El método de las características difiere sustancialmente de los métodos de D.F. y E.F. Este surgió como respuesta a las limitaciones de los métodos anteriores para evitar los problemas de dispersión numérica.

El método consiste en:

1. Resolver la ecuación de flujo usando el método de diferencias finitas
2. Introducir un conjunto de partículas en el sistema desplazandose en una localidad y concentración determinada.
3. Calcular la velocidad en cada punto y mover las partículas acorde con estas.
4. Calcular la concentración promedio en cada celda como el promedio de los puntos en la malla.
5. Modificar las concentración en las mallas y en los puntos para calcular la dispersión.

Este método calcula esencialmente el movimiento por advección de los solutos a través del sistema, y posteriormente le superpone la dispersión. En general, el método no crea dispersión numérica, lo cual constituye su principal atracción. Las características del modelo en dos dimensiones, de transporte de solutos y dispersión en agua subterránea (Konikow y Bredehoeft, 1976), se presentan en el anexo I.

II. Datos para la aplicación del modelo.

Los datos para utilizar un modelo de transporte son considerables. Por ello, la carencia de estos es quizá la mayor limitante para su aplicación. Existen dos tipos de información requerida: las condiciones de frontera y las condiciones iniciales. Las condiciones de frontera, se refieren a la geometría del acuífero, las características del flujo subterráneo, distribución de cargas hidráulicas y la concentración inicial de solutos, entre otros.

Las condiciones iniciales son los parámetros hidráulicos del acuífero y los procesos que ocurren en él. Estos incluyen, el coeficiente de almacenamiento (s), conductividad hidráulica (K), coeficiente de dispersión, porosidad (ϕ) y las constantes de atenuación y difusión. Estos valores son determinados en campo, en laboratorio o durante la calibración del modelo.

Los modelos de transporte son muy sensibles a la porosidad (ϕ) y a la conductividad hidráulica (K), dada su relación con la velocidad lineal (v) del medio. Por otra parte, se ha demostrado que la dispersión es un valor que depende de la escala de estudio. Por ello, valores de dispersión medidos en laboratorio son de varios ordenes de magnitud menores que los valores a escala regional.

Finalmente, en la formulación de un modelo para un problema practico, se sugiere mantener éste tan simple como sea posible; es decir, se recomienda aplicar soluciones básicas a problemas complejos.

III. Problema #1

Estimación del tiempo de arribo y concentración del lixiviado generado por un relleno sanitario, a través de un modelo de transporte.

Resumen Ejecutivo

El modelo de transporte MOCUSGS (Konikow, 1976), se utilizó para estimar el tiempo de arribo y la concentración de contaminante generada por un relleno sanitario en un río. Se estima que la pluma contaminante llegara al río después de 10 años de operación del relleno. Dado que la concentraciones de contaminantes se incrementa con el tiempo, la operación del relleno sanitario tendrá un efecto negativo en las aguas superficiales.

A fin de conocer la variación del modelo a los parámetros hidráulicos seleccionados, se realizó un análisis de sensibilidad con cada uno de ellos. El análisis mostró que la porosidad y conductividad hidráulica son los parámetros mas sensibles para el modelo de transporte.

El modelo de transporte permitió predecir la posición y tiempo de arribo de los contaminantes en el río. Sin embargo, la configuración de la pluma esta afectada por errores de estimación en los parámetros hidráulicos y la concentración inicial de los contaminantes en el relleno sanitario. Por ello, la concentración calculada se debe tomar como un indicador de la dirección y tiempo de tránsito de los solutos, y no como un dato exacto de dicha concentración.

3.1 Planteamiento del Problema

La figura No.(3) presenta a un río en contacto con un acuífero. Un relleno sanitario se propone construir en una zona aguas arriba del río. Debido a la preocupación por el impacto ambiental de esta obra, se requiere evaluar la posible contaminación que generaría los lixiviados del relleno en la calidad del agua del río. El sitio se localiza en un área con una precipitación de aproximadamente 20" (pulgadas) por año. La trasmisividad del acuífero se estima en 10,000 ft^2/día, conductividad hidráulica en 0.0023 ft/seg y la porosidad efectiva se calcula en 0.25.

El propósito de este reporte es determinar la evolución en el espacio y en el tiempo de la concentración

de contaminantes generada por la operación de un relleno sanitario y evaluar su posible impacto en un río cercano a este.

3.2. Metodología

a) Conceptualización del problema

La fig.(3) presenta un modelo esquemático de la infiltración de un lixiviado generado en relleno sanitario, al subsuelo.

b) Selección de las condiciones iniciales y de frontera

La malla y las condiciones iniciales del modelo se muestran en la fig.(4). Al río se le asigno una carga hidráulica constante y los limites restantes se asumieron como impermeables. Un valor fijo de concentración inicial del 100% fue seleccionado como porcentaje de un valor considerado. Las condiciones iniciales de la pluma contaminante fueron especificadas con concentración de +100 en los cinco nodos que representan la ubicación del relleno sanitario.

El valor de la recarga neta fue calculado como porcentaje de la precipitación inicial. Su valor original se ajustó en el modelo hasta obtener valores satisfactorios entre la carga hidráulica observada y la calculada. La mejor distribución de carga hidráulica correspondió a un 15%, alrededor de un 3", por año del valor de recarga original.

3.3. Aplicación del modelo MOCUSGS

1. Las condiciones iniciales y parámetros hidráulicos base se muestran en la Tabla No.1

Tabla No. 1 Parámetros Iniciales

Espesor del acuífero	50 ft
Conductividad hidráulica	0.116 ft/seg
Porosidad	0.25
Recarga neta (15% de la precipitación)	7.9E-09 ft/seg
Dispersión longitudinal	130 ft
LDT/LDL	0.1

2. Se calculó el mapa piezométrico y este se comparó con la distribución de carga hidráulica de campo hasta que ambos fueran lo mas cercanos.

3. Se utilizó la superficie potenciométrica simulada como base para calcular la distribución de la concentración de contaminantes en tiempo y espacio.

IV. Resultados

a) Distribución de la carga hidráulica

La figura No. 5, muestra el mapa piezométrico generado con parámetros base (tabla No. 1). La distribución de la carga hidráulica seleccionada fue aquella que mejor se ajusto con el mapa piezométrico de campo.

b) Distribución de los contaminantes

La figura No. 6, muestra la distribución de contaminantes para un período de 10 años. La distribución de la pluma contaminante muestra que, los contaminantes impactaran al río en diferentes porcentajes de acuerdo con la distancia del río al relleno sanitario.

c) Análisis de sensibilidad

Para conocer el efecto de la variación de los parámetros hidráulicos en la estimación de la concentración, se realizó un análisis de sensibilidad. Los perfiles de concentración a lo largo de la línea del relleno sanitario al río son presentados en la figura No. 7. En las gráficas un solo parámetro o condición en un tiempo fue permitido variar de su valor original.

V. Conclusiones

1. El modelo MOCGSUS permitió simular la distribución de los contaminantes generados por un relleno sanitario. De acuerdo con el modelo después de 10 años el lixiviado llegará al río. El punto mas cercano al relleno, tendría una concentración de 13% (de la concentración inicial) y el mas alejado de 1%. Las concentraciones se incrementaran en el tiempo creado un impacto negativo en el sistema ecológico .

2. El análisis de sensibilidad mostró que los parámetros hidráulicos que mayor influencia tienen en la distribución de la concentración fueron de la conductividad hidráulica y la porosidad..

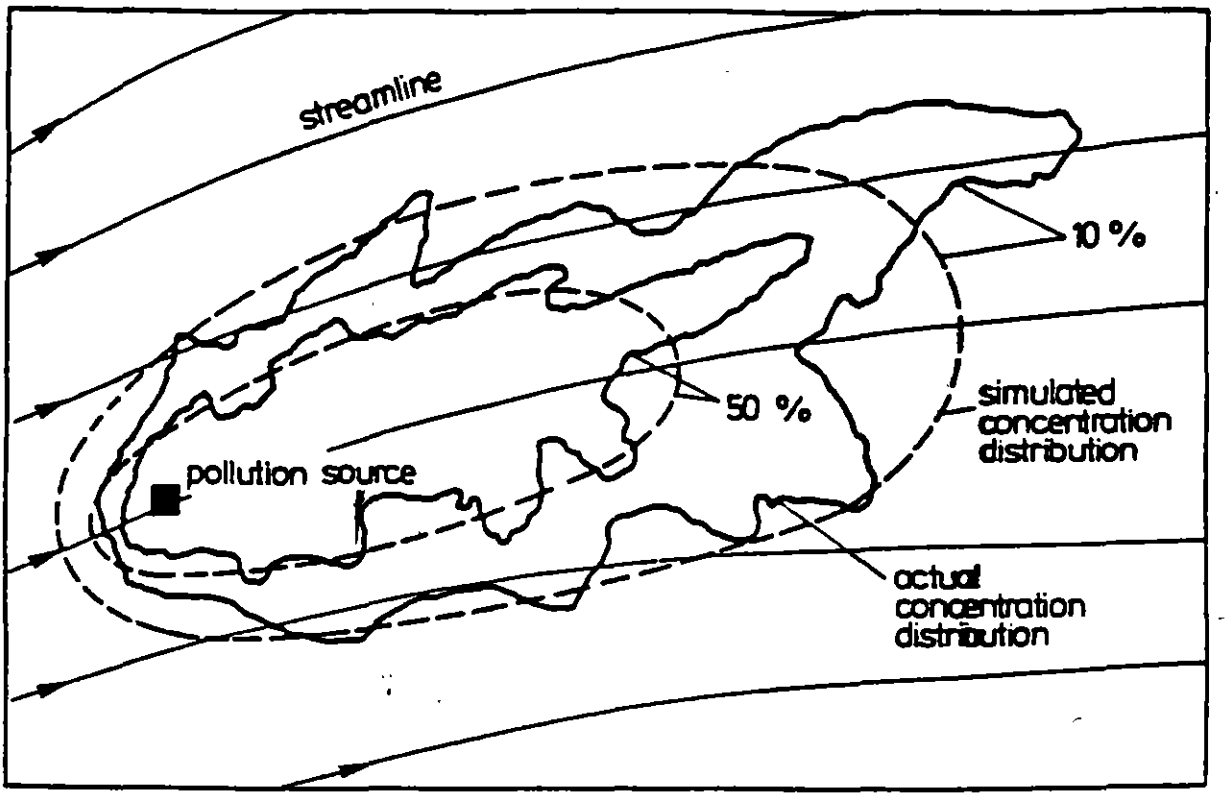


Fig. 1. Schematic representation of an actual concentration distribution and the concentration distribution that can be obtained from simulation

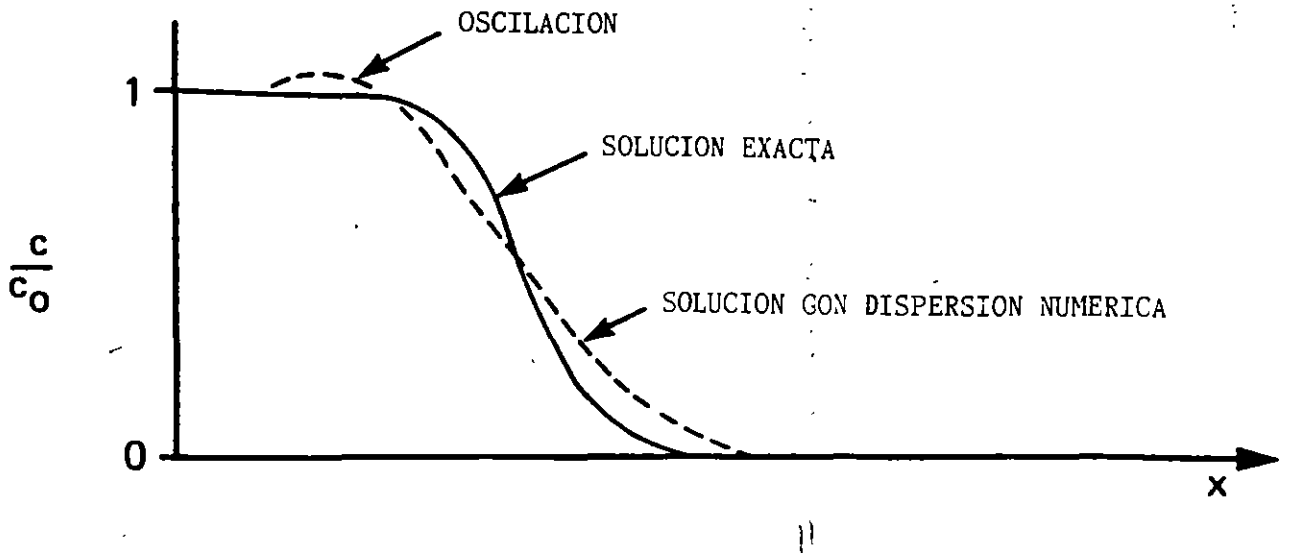


FIG. 2. DISPERSION NUMERICA Y OSCILACION

FIG. 3.

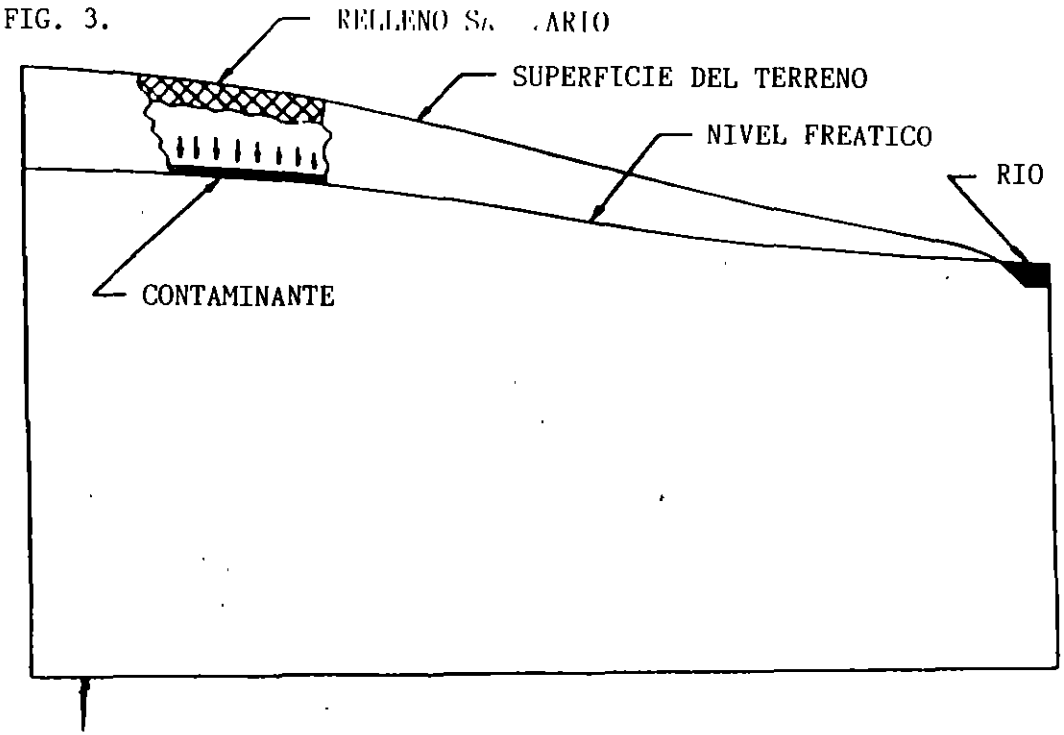


FIG. 4. MALLA NUMERICA Y CONDICIONES DE FRONTERA

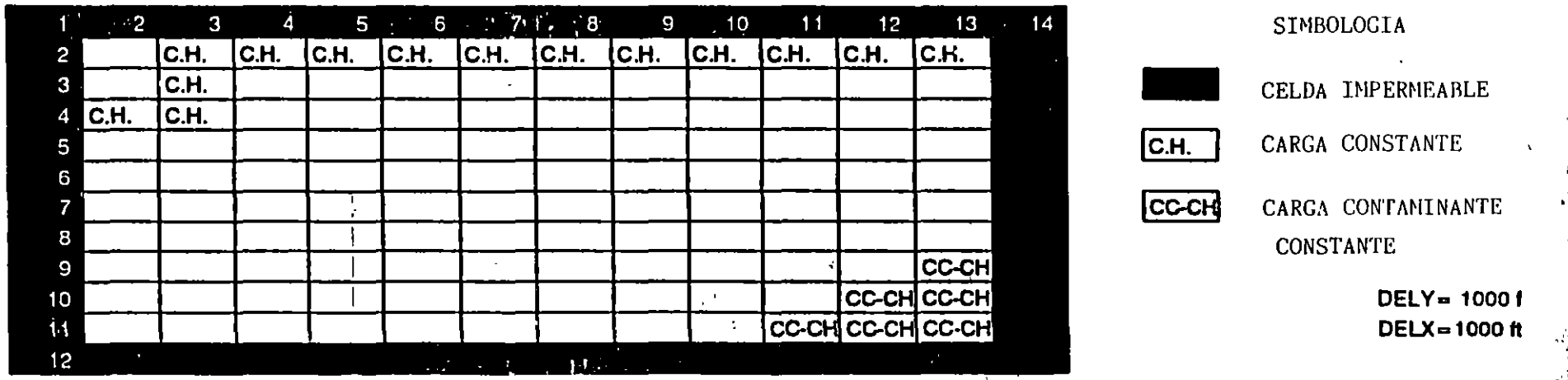


FIG. 5. MODELO NUMERICO

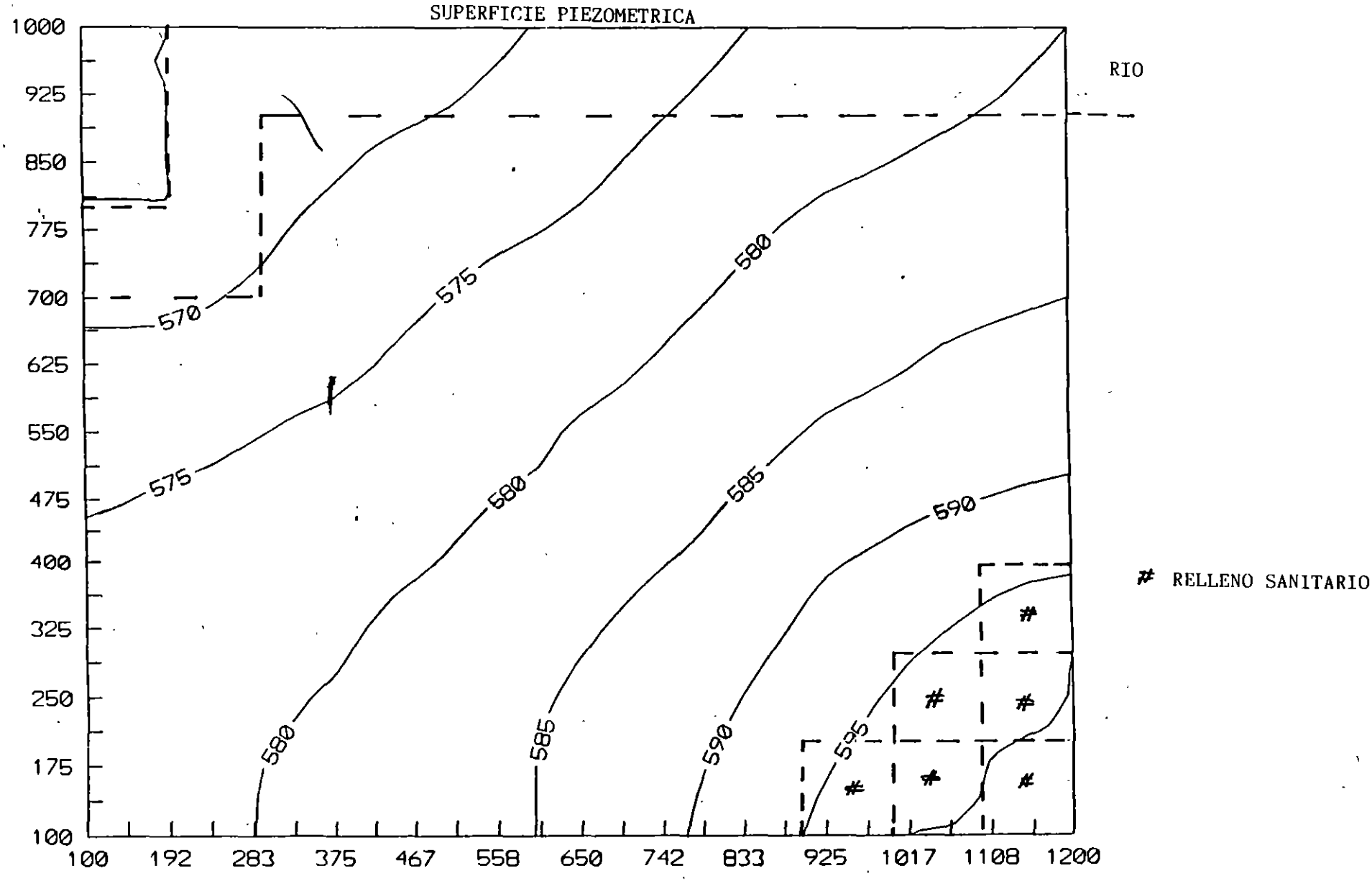


FIG. 6. DISTRIBUCION DE LA CONCENTRACION

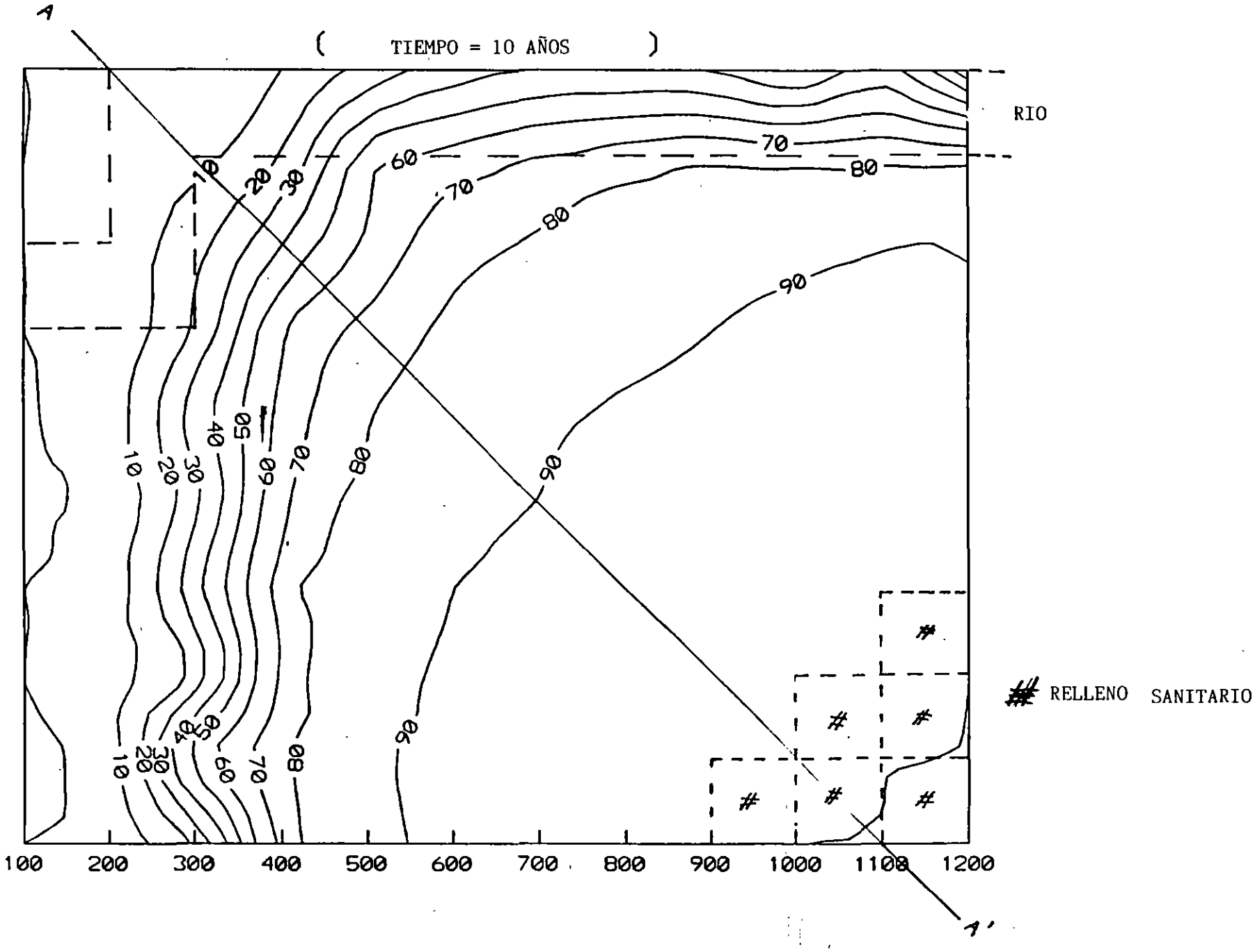
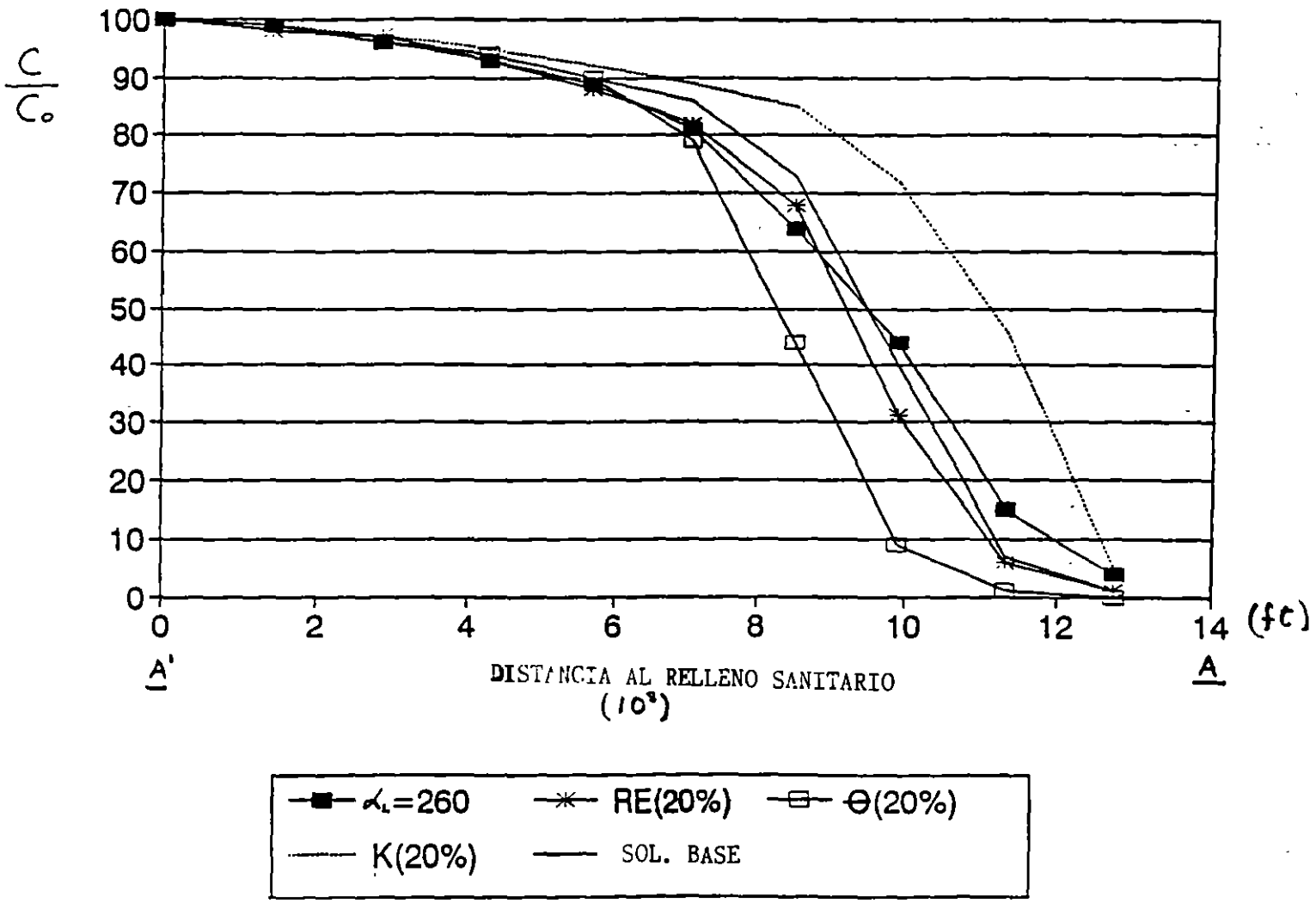


FIG. 7 ANALISIS DE SENSIBILIDAD



ANEXO 1

Techniques of Water-Resources Investigations
of the United States Geological Survey

Chapter C2

COMPUTER MODEL OF TWO-DIMENSIONAL SOLUTE TRANSPORT AND DISPERSION IN GROUND WATER

By L. F. Konikow and J. D. Bredehoeft

Book 7

AUTOMATED DATA PROCESSING AND COMPUTATIONS

PREFACE

The series of manuals on techniques describes procedures for planning and executing specialized work in water-resources investigations. The material is grouped under major headings called books and further subdivided into sections and chapters; section C of Book 7 is on computer programs.

This chapter presents a digital computer model for calculating changes in the concentration of a dissolved chemical species in flowing ground water. The computer program represents a basic and general model that may have to be modified by the user for efficient application to his specific field problem. Although this model will produce reliable calculations for a wide variety of field problems, the user is cautioned that in some cases the accuracy and efficiency of the model can be affected significantly by his selection of values for certain user-specified options.

COMPUTER MODEL OF TWO-DIMENSIONAL SOLUTE TRANSPORT AND DISPERSION IN GROUND WATER

By L. F. Konikow and J. D. Bredehoeft

Abstract

This report presents a model that simulates solute transport in flowing ground water. The model is both general and flexible in that it can be applied to a wide range of problem types. It is applicable to one- or two-dimensional problems involving steady-state or transient flow. The model computes changes in concentration over time caused by the processes of convective transport, hydrodynamic dispersion, and mixing (or dilution) from fluid sources. The model assumes that the solute is nonreactive and that gradients of fluid density, viscosity, and temperature do not affect the velocity distribution. However, the aquifer may be heterogeneous and (or) anisotropic.

The model couples the ground-water flow equation with the solute-transport equation. The digital computer program uses an alternating-direction implicit procedure to solve a finite-difference approximation to the ground-water flow equation, and it uses the method of characteristics to solve the solute-transport equation. The latter uses a particle-tracking procedure to represent convective transport and a two-step explicit procedure to solve a finite-difference equation that describes the effects of hydrodynamic dispersion, fluid sources and sinks, and divergence of velocity. This explicit procedure has several stability criteria, but the consequent time-step limitations are automatically determined by the program.

The report includes a listing of the computer program, which is written in FORTRAN IV and contains about 2,000 lines. The model is based on a rectangular, block-centered, finite-difference grid. It allows the specification of any number of injection or withdrawal wells and of spatially varying diffuse recharge or discharge, saturated thickness, transmissivity, boundary conditions, and initial heads and concentrations. The program also permits the designation of up to five nodes as observation points, for which a summary table of head and concentration versus time is printed at the end of the calculations. The data input formats for the model require three data cards and from seven to nine data sets to describe the aquifer properties, boundaries, and stresses.

The accuracy of the model was evaluated for two idealized problems for which analytical solutions could be obtained. In the case of one-dimensional flow the agreement was nearly exact, but in the case of plane radial flow a small amount of numerical dispersion occurred. An analysis of several test problems indicates that the error in the mass balance will be generally less than 10 percent. The test problems demonstrated that the accuracy and precision of the numerical solution is sensitive to the initial number of particles placed in each cell and to the size of the time increment, as determined by the stability criteria. Mass balance errors are commonly the greatest during the first several time increments, but tend to decrease and stabilize with time.

Introduction

This report describes and documents a computer model for calculating transient changes in the concentration of a nonreactive solute in flowing ground water. The computer program solves two simultaneous partial differential equations. One equation is the ground-water flow equation, which describes the head distribution in the aquifer. The second is the solute-transport equation, which describes the chemical concentration in the system. By coupling the flow equation with the solute-transport equation, the model can be applied to both steady-state and transient flow problems.

The purpose of the simulation model is to compute the concentration of a dissolved chemical species in an aquifer at any specified place and time. Changes in chemical concentration occur within a dynamic ground-water system primarily due to four

distinct processes: (1) convective transport, in which dissolved chemicals are moving with the flowing ground water; (2) hydrodynamic dispersion, in which molecular and ionic diffusion and small-scale variations in the velocity of flow through the porous media cause the paths of dissolved molecules and ions to diverge or spread from the average direction of ground-water flow; (3) fluid sources, where water of one composition is introduced into water of a different composition; and (4) reactions, in which some amount of a particular dissolved chemical species may be added to or removed from the ground water due to chemical and physical reactions in the water or between the water and the solid aquifer materials. The model presented in this report assumes (1) that no reactions occur that affect the concentration of the species of interest, and (2) that gradients of fluid density, viscosity, and temperature do not affect the velocity distribution.

This model can be applied to a wide variety of field problems. However, the user should first become aware of the assumptions and limitations inherent in the model, as described in this report. The computer program presented in this report is offered as a basic working tool that may have to be modified by the user for efficient application to specific field problems. The program is written in FORTRAN IV and is compatible with most high-speed computers. The data requirements, input format specifications, program options, and output formats are all structured in a general manner that should be readily adaptable to many field problems.

This report includes a detailed description of the numerical method used to solve the solute-transport equation. The reader is assumed to have (or can obtain elsewhere) a moderate familiarity with finite-difference methods and ground-water flow models.

Theoretical Background

Flow equation

By following the derivation of Pinder and Bredehoeft (1968), the equation describing the transient two-dimensional areal flow of a homogeneous compressible fluid through a nonhomogeneous anisotropic aquifer can be written in Cartesian tensor notation as

$$\frac{\partial}{\partial x_i}\left(T_{ij}\frac{\partial h}{\partial x_j}\right) = S\frac{\partial h}{\partial t} + W \qquad i,j = 1,2 \qquad (1)$$

where

T_{ij} is the transmissivity tensor, L^2/T;
h is the hydraulic head, L;
S is the storage coefficient, (dimensionless);
t is the time, T;
$W = W(x,y,t)$ is the volume flux per unit area (positive sign for outflow and negative for inflow), L/T; and
x_i and x_j are the Cartesian coordinates, L.

If we only consider fluxes of (1) direct withdrawal or recharge, such as well pumpage, well injection, or evapotranspiration, and (2) steady leakage into or out of the aquifer through a confining layer, streambed, or lakebed, then $W(x,y,t)$ may be expressed as

$$W(x,y,t) = Q(x,y,t) - \frac{K_s}{m}(H_s - h) \qquad (2)$$

where

Q is the rate of withdrawal (positive sign) or recharge (negative sign), L/T;
K_s is the vertical hydraulic conductivity of the confining layer, streambed, or lakebed, L/T;
m is the thickness of the confining layer, streambed, or lakebed, L; and
H_s is the hydraulic head in the source bed, stream, or lake, L.

Lohman (1972) shows that an expression for the average seepage velocity of ground water can be derived from Darcy's law. This expression can be written in Cartesian tensor notation as

$$V_i = -\frac{K_{ij}}{\epsilon}\frac{\partial h}{\partial x_j} \qquad (3)$$

where

V_i is the seepage velocity in the direction of x_i, L/T;
K_{ij} is the hydraulic conductivity tensor, L/T; and
ϵ is the effective porosity of the aquifer, (dimensionless).

Transport equation

The equation used to describe the two-dimensional areal transport and dispersion of a given nonreactive dissolved chemical species in flowing ground water was derived by Reddell and Sunada (1970), Bear (1972), Bredehoeft and Pinder (1973), and Konikow and Grove (1977). The equation may be written as

$$\frac{\partial(Cb)}{\partial t}=\frac{\partial}{\partial x_i}(bD_{ij}\frac{\partial C}{\partial x_j})-\frac{\partial}{\partial x_i}(bCV_i)-\frac{C'W}{\epsilon} \qquad i,j=1,2 \quad (4)$$

where

C is the concentration of the dissolved chemical species, M/L^3;
D_{ij} is the coefficient of hydrodynamic dispersion (a second-order tensor), L^2/T;
b is the saturated thickness of the aquifer, L; and
C' is the concentration of the dissolved chemical in a source or sink fluid, M/L^3.

The first term on the right side of equation 4 represents the change in concentration due to hydrodynamic dispersion. The second term describes the effects of convective transport, while the third term represents a fluid source or sink.

Dispersion coefficient

Bear (1972, p. 580–581) states that hydrodynamic dispersion is the macroscopic outcome of the actual movements of individual tracer particles through the pores and that it includes two processes. One process is mechanical dispersion, which depends upon both the flow of the fluid and the nature of the pore system through which the flow takes place. The second process is molecular and ionic diffusion, which because it depends on time, is more significant at low flow velocities. Bear (1972) further states that the separation between the two processes is artificial. In developing our model we assume for flowing ground-water systems that the definable contribution of molecular and ionic diffusion to hydrodynamic dispersion is negligible.

The dispersion coefficient may be related to the velocity of ground-water flow and to the nature of the aquifer using Scheidegger's (1961) equation:

$$D_{ij}=\alpha_{ijmn}\frac{V_mV_n}{|V|} \qquad (5)$$

where

α_{ijmn} is the dispersivity of the aquifer, L;
V_m and V_n are components of velocity in the m and n directions, respectively, L/T; and
$|V|$ is the magnitude of the velocity, L/T.

Scheidegger (1961) further shows that for an isotropic aquifer the dispersivity tensor can be defined in terms of two constants. These are the longitudinal and transverse dispersivities of the aquifer (α_L and α_T, respectively). These are related to the longitudinal and transverse dispersion coefficients by

$$D_L=\alpha_L|V| \qquad (6)$$

and

$$D_T=\alpha_T|V|. \qquad (7)$$

After expanding equation 5, substituting Scheidegger's identities, and eliminating terms with coefficients that equal zero, the components of the dispersion coefficient for two-dimensional flow in an isotropic aquifer may be stated explicitly as

$$D_{xx}=D_L\frac{(V_x)^2}{|V|^2}+D_T\frac{(V_y)^2}{|V|^2}; \qquad (8)$$

$$D_{yy}=D_T\frac{(V_x)^2}{|V|^2}+D_L\frac{(V_y)^2}{|V|^2}; \qquad (9)$$

$$D_{xy} = D_{yx} = (D_L - D_T)\frac{V_x V_y}{|V|^2}. \qquad (10)$$

Note that while D_{xx} and D_{yy} must have positive values, it is possible for the cross-product terms (eq 10) to have negative values if V_x and V_y have opposite signs.

Review of assumptions

A number of assumptions have been made in the development of the previous equations. Following is a list of the main assumptions that must be carefully evaluated before applying the model to a field problem.

1. Darcy's law is valid and hydraulic-head gradients are the only significant driving mechanism for fluid flow.
2. The porosity and hydraulic conductivity of the aquifer are constant with time, and porosity is uniform in space.
3. Gradients of fluid density, viscosity, and temperature do not affect the velocity distribution.
4. No chemical reactions occur that affect the concentration of the solute, the fluid properties, or the aquifer properties.
5. Ionic and molecular diffusion are negligible contributors to the total dispersive flux.
6. Vertical variations in head and concentration are negligible.
7. The aquifer is homogeneous and isotropic with respect to the coefficients of longitudinal and transverse dispersivity.

The nature of a specific field problem may be such that not all of these underlying assumptions are completely valid. The degree to which field conditions deviate from these assumptions will affect the applicability and reliability of the model for that problem. If the deviation from a particular assumption is significant, the governing equations will have to be modified to account for the appropriate processes or factors.

Numerical Methods

Because aquifers have variable properties and complex boundary conditions, exact analytical solutions to the partial differential equations of flow (eq 1) and solute transport (eq 4) cannot be obtained directly. Therefore, approximate numerical methods must be employed.

The numerical methods require that the area of interest be subdivided by a grid into a number of smaller subareas. The model developed here utilizes a rectangular, uniformly spaced, block-centered, finite-difference grid, in which nodes are defined at the centers of the rectangular cells.

Flow equation

Pinder and Bredehoeft (1968) show that if the coordinate axes are alined with the principal directions of the transmissivity tensor, equation 1 may be approximated by the following implicit finite-difference equation:

$$\begin{aligned} &T_{xx[i-\frac{1}{2},j]}\left[\frac{h_{i-1,j,k}-h_{i,j,k}}{(\Delta x)^2}\right] \\ &\quad + T_{xx[i+\frac{1}{2},j]}\left[\frac{h_{i+1,j,k}-h_{i,j,k}}{(\Delta x)^2}\right] \\ &\quad + T_{yy[j-\frac{1}{2}]}\left[\frac{h_{i,j-1,k}-h_{i,j,k}}{(\Delta y)^2}\right] \\ &\quad + T_{yy[j+\frac{1}{2}]}\left[\frac{h_{i,j+1,k}-h_{i,j,k}}{(\Delta y)^2}\right] \\ &= S\left[\frac{h_{i,j,k}-h_{i,j,k-1}}{\Delta t}\right] \\ &\quad + \frac{q_{w(i,j)}}{\Delta x \Delta y}\,\frac{K_z}{m}[H_{s(i,j)}-h_{i,j,k}] \end{aligned} \qquad (11)$$

where

i,j,k are indices in the x, y, and time dimensions, respectively;

$\Delta x, \Delta y, \Delta t$ are increments in the x, y, and time dimensions, respectively; and

q_w is the volumetric rate of withdrawal or recharge at the (i,j) node, L^3/T.

Note that k represents the new time level and $k-1$ represents the previous time level. To avoid confusion between tensor sub-

Attachment II
Definition of Selected Program Variables

AAQ	area of aquifer in model
ALNG	BETA
ANFCTR	anisotropy factor (ratio of T_{yy} to T_{xx})
AOPT	iteration parameters
AREA	area of one cell in finite-difference grid
BETA	longitudinal dispersivity of porous medium
CELDIS	maximum distance across one cell that a particle is permitted to move in one step (as fraction of width of cell)
CLKCN	concentration of leakage through confining layer or streambed
CMSIN	mass of solute recharged into aquifer
CMSOUT	mass of solute discharged from aquifer
CNCNC	change in concentration due to dispersion and sources
CNCPCT	change in concentration as percentage of concentration at node
CNOLD	concentration at node at end of previous time increment
CNREC	concentration of well withdrawal or injection
CNRECH	concentration in fluid source
CONC	concentration in aquifer at node
CONINT	concentration in aquifer at start of simulation
C1	CONC at node (IX,IY)
DALN	longitudinal dispersion coefficient
DDRW	drawdown
DELQ	volumetric rate of leakage across a confining layer or streambed
DELS	rate of change in ground-water storage
DERH	change in head with respect to time
DISP	dispersion equation coefficients
DISTX	distance particle moves in x-direction during time increment
DISTY	distance particle moves in y-direction during time increment
DLTRAT	ratio of transverse to longitudinal dispersivity
DTRN	transverse dispersion coefficient
FCTR	multiplication or conversion factor
FLMIN	solute mass entering modeled area during time step
FLMOT	solute mass leaving modeled area during time step
GRDX	hydraulic gradient in x-direction
GRDY	hydraulic gradient in y-direction
HC	head from column computation
HI	initial head in aquifer
HK	computed head at end of time step
HMIN	minimum iteration parameter
HR	head from row computation in subroutine ITERAT; elsewhere HR represents head from previous time step
IMOV	particle movement step number
INT	pumping period number
IPRNT	print control index for hydrographs
ITMAX	maximum permitted number of iterations
IXOBS	x-coordinate of observation point
IYOBS	y-coordinate of observation point
KOUNT	iteration number for ADIP
LIMBO	array for temporary storage of particles
N	time step number
NCA	number of aquifer nodes in model
NCODES	number of node identification codes
NITP	number of iteration parameters
NMOV	number of particle movements (or time increments) required to complete time step
NODEID	node identification code
NP	total number of active particles in grid
NPCELL	number of particles in a cell during time increment
NPMAX	maximum number of available particles
NPMP	number of pumping periods or simulation periods
NPNT	number of time steps between printouts
NPTPND	initial number of particles per node
NREC	number of pumping wells
NTIM	number of time steps
NUMOBS	number of observation wells
NX	number of nodes in x-direction
NY	number of nodes in y-direction
NZCRIT	maximum number of cells that can be void of particles
NZERO	number of cells that are void of particles at the end of a time increment
PARAM	iteration parameter for current iteration
PART	1. x-coordinate of particle; 2. y-coordinate of particle; 3. concentration of particle. Also note that the signs of coordinates are used as flags to store information on original location of particle.
PERM	hydraulic conductivity (in LT^{-1})
PINT	pumping period in years
POROS	effective porosity
PUMP	cumulative net pumpage
PYR	total duration of pumping period (in seconds)
QNET	net water flux (in L^3T^{-1})

Definition of selected program variables—Continued

QSTR	cumulative change in volume of water in storage
REC	point source or sink; negative for injection, positive for withdrawal (in L^3T^{-1})
RECH	diffuse recharge or discharge; negative for recharge, positive for discharge (in LT^{-1})
RN	range in concentration between regenerated particle and adjacent node having lower concentration
RP	range in concentration between regenerated particle and adjacent node having higher concentration
S	storage coefficient (or specific yield)
SLEAK	rate of leakage through confining layer or streambed
STORM	change in total solute mass in storage (by summation)
STORMI	initial mass of solute in storage
SUMC	summation of concentrations of all particles in a cell
SUMIO	change in total solute mass in storage (from inflows—outflows)
SUMT	total elapsed time (in seconds)
SUMTCH	cumulative elapsed time during particle moves (in seconds)
THCK	saturated thickness of aquifer
TIM	length of specific time step (in seconds)
TIMD	elapsed time in days
TIMY	elapsed time in years
TIMV	length of time increment for particle movement (in seconds)
TIMX	time step multiplier for transient flow problems
TINIT	size of initial time step for transient flow problems (in seconds)
TITLE	problem description
TMCN	computed concentrations at observation points
TMOBS	elapsed times for observation point records
TMRX	transmissivity coefficients (harmonic means on cell boundaries; forward values are stored)
TMWL	computed heads at observation points
TOL	convergence criteria (ADIP)
TOTLQ	cumulative net leakage through confining layer or streambed
TRAN	transverse dispersivity of porous medium
VMAX	maximum value of VX
VMAY	maximum value of VY
VMGE	magnitude of velocity vector
VMXBD	maximum value of VXBDY
VMYBD	maximum value of VYBDY
VPRM	initially used to read transmissivity values at nodes; then after line B2270, VPRM equals leakance factor for confining layer or streambed (vertical hydraulic conductivity/thickness). If VPRM≧0.09, then the program assumes that the node is a constant-head boundary and is flagged for subsequent special treatment in calculating convective transport.
VX	velocity in x-direction at a node
VXBDY	velocity in x-direction on a boundary between nodes
VY	velocity in y-direction at a node
VYBDY	velocity in y-direction on a boundary between nodes
WT	initial water-table or potentiometric elevation, or constant head in stream or source bed
XDEL	grid spacing in x-direction
XOLD	x-coordinate of particle at end of previous time increment
XVEL	velocity of particle in x-direction
YDEL	grid spacing in y-direction
YOLD	y-coordinate of particle at end of previous time increment
YVEL	velocity of particle in y-direction

Attachment III
Data Input Formats

Card	Column	Format	Variable	Definition
1	1–80	10A8	TITLE	Description of problem
2	1– 4	I4	NTIM	Maximum number of time steps in a pumping period (limit=100)*.
	5– 8	I4	NPMP	Number of pumping periods. Note that if NPMP>1, then data set 10 must be completed.
	9–12	I4	NX	Number of nodes in x direction (limit=20)*.
	13–16	I4	NY	Number of nodes in y direction (limit=20)*.
	17–20	I4	NPMAX	Maximum number of particles (limit=3200)*. (See eq 71.)
	21–24	I4	NPNT	Time-step interval for printing hydraulic and chemical output data.
	25–28	I4	NITP	Number of iteration parameters (usually $4 \leq NITP \leq 7$).
	29–32	I4	NUMOBS	Number of observation points to be specified in a following data set (limit=5)*.
	33–36	I4	ITMAX	Maximum allowable number of iterations in ADIP (usually $100 \leq ITMAX \leq 200$).
	37–40	I4	NREC	Number of pumping or injection wells to be specified in a following data set.
	41–44	I4	NPTPND	Initial number of particles per node (options=4, 5, 8, 9).
	45–48	I4	NCODES	Number of node identification codes to be specified in a following data set (limit=10)*.
	49–52	I4	NPNTMV	Particle movement interval (IMOV) for printing chemical output data. (Specify 0 to print only at end of time steps.)
	53–56	I4	NPNTVL	Option for printing computed velocities (0=do not print; 1=print for first time step; 2=print for all time steps).
	57–60	I4	NPNTD	Option for printing computed dispersion equation coefficients (option definition same as for NPNTVL).
	61–64	I4	NPDELC	Option for printing computed changes in concentration (0=do not print; 1=print).
	65–68	I4	NPNCHV	Option to punch velocity data (option definition same as for NPNTVL). When specified, program will punch on unit 7 the velocities at nodes.

See footnotes at end of table.

Data input formats—Continued

Card	Column	Format	Variable	Definition
3	1– 5	G5.0	PINT	Pumping period in years.
	6–10	G5.0	TOL	Convergence criteria in ADIP (usually TOL≤0.01).
	11–15	G5.0	POROS	Effective porosity.
	16–20	G5.0	BETA	Characteristic length, in feet (=longitudinal dispersivity).
	21–25	G5.0	S	Storage coefficient (set S=0 for steady flow problems).
	26–30	G5.0	TIMX	Time increment multiplier for transient flow problems. TIMX is disregarded if S=0 .
	31–35	G5.0	TINIT	Size of initial time step in seconds. TINIT is disregarded if S=0.
	36–40	G5.0	XDEL	Width of finite-difference cell in x direction, in feet.
	41–45	G5.0	YDEL	Width in finite-difference cell in y direction, in feet.
	46–50	G5.0	DLTRAT	Ratio of transverse to longitudinal dispersivity.
	51–55	G5.0	CELDIS	Maximum cell distance per particle move (value between 0 and 1.0).
	56–60	G5.0	ANFCTR	Ratio of T_{yy} to T_{xx}.

Data set	Number of cards	Format	Variable	Definition
1	Value of NUMOBS (limit=5)*	2I2	IXOBS, IYOBS	x and y coordinates of observation points. This data set is eliminated if NUMOBS is specified as =0.
2	Value of NREC	2I2, 2G8.2	IX, IY, REC, CNRECH	x and y coordinates of pumping (+) or injection (−) wells, rate in ft³/s, and if an injection well, the concentration of injected water. This data set is eliminated if NREC=0.
3	a. 1	I1, G10.0	INPUT, FCTR	Parameter card† for transmissivity.
	b. Value of NY (limit=20)*	20G4.1	VPRM	Array for temporary storage of transmissivity data, in ft²/s. For an anisotropic aquifer, read in values of T_{xx} and the program will adjust for anisotropy by multiplying T_{yy} by ANFCTR.
4	a. 1	I1, G10.0	INPUT, FCTR	Parameter card† for THCK.
	b. Value of NY (limit=20)*	20G3.0	THCK	Saturated thickness of aquifer, in feet.
5	a. 1	I1, G10.0	INPUT, FCTR	Parameter card† for RECH.
	b. Value of NY (limit=20)*	20G4.1	RECH	Diffuse recharge (−) or discharge (+), in ft/s.
6	a. 1	I1, G10.0	INPUT, FCTR	Parameter card† for NODEID.
	b. Value of NY (limit=20)*	20I1	NODEID	Node identification matrix (used to define constant-head nodes or other boundary conditions and stresses).

See footnotes at end of table.

Data input formats—Continued

Data set	Number of cards	Format	Variable	Definition
7	Value of NCODES (limit=10)*	I2, 3G10.2, I2	ICODE, FCTR1, FCTR2, FCTR3, OVERRD	Instructions for using NODEID array. When NODEID=ICODE, program sets leakance=FCTR1, CNRECH=FCTR2, and if OVERRD is nonzero, RECH =FCTR3. Set OVERRD=0 to preserve values of RECH specified in data set 5.
8	a. 1	I1, G10.0	INPUT, FCTR	Parameter card† for WT.
	b. Value of NY (limit=20)*	20G4.0	WT	Initial water-table or potentiometric elevation, or constant head in stream or source bed, in feet.
9	a. 1	I1, G10.0	INPUT, FCTR	Parameter card† for CONC.
	b. Value of NY (limit=20)*	20G4.0	CONC	Initial concentration in aquifer.
10				This data set allows time step parameters, print options, and pumpage data to be revised for each pumping period of the simulation. Data set 10 is only used if NPMP >1. The sequence of cards in data set 10 must be repeated (NPMP −1) times (that is, data set 10 is required for each pumping period after the first).
	a. 1	I1	ICHK	Parameter to check whether any revisions are desired. Set ICHK=1 if data are to be revised, and then complete data set 10b and c. Set ICHK=0 if data are not to be revised for the next pumping period, and skip rest of data set 10.
	b. 1	10I4,3G5.0	NTIM, NPNT, NITP, ITMAX, NREC, NPNTMV, NPNTVL, NPNTD, NPDELC, NPNCHV, PINT, TIMX, TINIT	Thirteen parameters to be revised for next pumping period; the parameters were previously defined in the description of data cards 2 and 3. Only include this card if ICHK=1 in previous part a.
	c. Value of NREC	2I2, 2G8.2	IX, IY, REC, CNRECH	Revision of previously defined data set 2. Include part c only if ICHK=1 in previous part a and if NREC>0 in previous part b.

* These limits can be modified if necessary by changing the corresponding array dimensions in the COMMON statements of the program.

† The parameter card must be the first card of the indicated data sets. It is used to specify whether the parameter is constant and uniform, and can be defined by one value, or whether it varies in space and must be defined at each node. If INPUT=0, the data set has a constant value, which is defined by FCTR. If INPUT=1, the data set is read from cards as described by part b. Then FCTR is a multiplication factor for the values read in the data set.

Attachment IV

Input Data for Test Problem 3

```
Card 1   TEST PROBLEM NO. 3 (STEADY FLOW, 1 WELL, CONSTANT-HEAD BOUNDARIES)
Card 2      1   1   9  10320U   1   7   2 100   1   9   2  10   1   0   0   0
Card 3    2.5.0001 0.30 100.  0.0  0.0  0.0 900. 900.  0.3 0.50  1.0
Data Set 1  5 4
            5 7
Data Set 2  4 7    1.0
Data Set 3  0  0.1
Data Set 4  0  20.0
Data Set 5  0  0.0
Data Set 6  1  1.0
            000000000
            022111220
            000000000
            000000000
            000000000
            000000000
            000000000
            000000000
            022222220
            000000000
Data Set 7  2    1.0         0.0         0.0       0
            1    1.0       100.0         0.0       0
Data Set 8  1  1.0

            0.0100.100.100.100.100.100.100. 0.0




            0.0 75. 75. 75. 75. 75. 75. 75. 0.0
Data Set 9  0  0.0
```

ANEXO 2

SOLUTION BASE

```
   5   1  14  126400   1   7   0 100   0   9   2 100   1   0   0   0   0
 10.0.0010  .25 100..0000  .00   0.1000.1000.  .1   .50 1.00
0  .116
0  50.0
0-7.9E-09
1  1.00
00000000000000
00111111111110
00100000000000
01100000000000
00000000000000
00000000000000
00000000000000
00000000000000
00000000000030
00000000000330
00000000003330
00000000000000
 1  1.00        0.        .000      0
 3  1.00      100.0       .000      0
1  1.00
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.565.566.567.568.570.572.574.576.578.579.580.   0.
   0.   0.565.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.565.565.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.600.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.600.600.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.600.600.600.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
     1.0
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.100.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.100.100.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.100.100.100.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
```

HEAD DISTRIBUTION - BASE SOLUTION
(15% OF RECHARGE)

```
NUMBER OF TIME STEPS =      1
      TIME(SECONDS)  =    .12623E+09
      TIME(DAYS)     =    .14610E+04
      TIME(YEARS)    =    .40000E+01
```

0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	565	565	566	567	568	570	572	574	576	578	579	580	0
0	0	565	565	567	569	570	572	574	576	578	579	580	581	0
0	0	565	565	569	571	573	574	576	578	580	581	582	583	0
0	0	569	569	571	573	575	577	578	580	582	583	584	585	0
0	0	572	572	574	575	577	579	580	582	584	585	587	587	0
0	0	574	575	576	577	579	580	582	584	586	588	589	590	0
0	0	576	577	578	579	580	582	584	586	589	591	593	594	0
0	0	578	578	579	580	582	584	586	588	591	594	597	600	0
0	0	579	579	580	581	583	585	587	590	593	597	600	600	0
0	0	579	580	580	582	583	585	588	591	595	600	600	600	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

CONCENTRATION DISTRIBUTION
(BASE SOLUTION)

```
NUMBER OF TIME STEPS =      5
      DELTA T        =    .63115E+08
      TIME(SECONDS)  =    .31558E+09
CHEM.TIME(SECONDS)   =    .31558E+09
CHEM.TIME(DAYS)      =    .36525E+04
      TIME(YEARS)    =    .10000E+02
CHEM.TIME(YEARS)     =    .10000E+02
NO. MOVES COMPLETED  =      7
```

0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	1	3	9	22	34	40	40	39	26	46	13	0
0	0	0	2	7	18	59	65	72	77	81	80	79	81	0
0	0	0	4	16	40	62	77	81	85	87	88	90	89	0
0	0	0	3	19	62	73	83	86	88	90	92	93	93	0
0	0	0	3	36	63	80	86	89	91	92	94	95	95	0
0	0	0	2	24	70	83	88	90	93	94	95	97	97	0
0	0	0	3	38	77	86	90	92	94	96	97	98	99	0
0	0	0	6	17	75	87	91	93	95	96	98	99	100	0
0	0	0	2	60	78	89	92	95	97	98	99	100	100	0
0	0	0	3	16	77	88	92	95	97	99	100	100	100	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

```
                   VARIABLE POROSITY
   5   1  14  126400   1   7   0 100   0   9   2 100   1   0   0   0   0
 10.0.0010  .30 100..0000  .00   0.1000.1000.  .1   .50 1.00
0  .116
0  50.0
0-7.9E-09
1  1.00
00000000000000
00111111111110
00100000000000
01100000000000
00000000000000
00000000000000
00000000000000
00000000000000
00000000000030
00000000000330
00000000003330
00000000000000
 1  1.00        0.       .000     0
 3  1.00      100.0     .000     0
1  1.00
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
  0.  0.565.566.567.568.570.572.574.576.578.579.580.  0.
  0.  0.565.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
  0.565.565.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.600.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.600.600.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.600.600.600.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
1   1.0
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.100.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.100.100.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.100.100.100.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
```

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CONCENTRATION DISTRIBUTION

(VARIABLE: POROSITY INC.20%)

NUMBER OF TIME STEPS = 5
DELTA T = .63115E+08
TIME(SECONDS) = .31558E+09
CHEM.TIME(SECONDS) = .31558E+09
CHEM.TIME(DAYS) = .36525E+04
TIME(YEARS) = .10000E+02
CHEM.TIME(YEARS) = .10000E+02
NO. MOVES COMPLETED = 6

0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	1	3	6	8	10	9	9	8	9	0
0	0	0	0	1	3	11	21	30	69	70	74	74	63	0
0	0	0	1	2	9	17	63	70	78	84	86	88	86	0
0	0	0	0	3	16	44	67	82	86	89	91	92	92	0
0	0	0	0	5	26	69	79	87	90	92	94	95	95	0
0	0	0	0	7	45	72	85	90	92	94	95	97	97	0
0	0	0	1	8	46	81	89	91	94	96	96	98	99	0
0	0	0	1	8	60	83	91	93	95	96	98	99	100	0
0	0	0	1	9	70	87	92	95	97	98	99	100	100	0
0	0	0	1	9	62	85	92	95	97	99	100	100	100	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

```
TITLE: TEST PROBLEM NO.1 (SPREADING OF A TRACER SLUG)
   1   1   9   93200   1   7   0 100   0   9   1 10   1   0   0   0
  2. .0001  0.3 100.   0.   0.   0. 900. 900.  0.3 0.49   1.
0 0.1
0 20.0
0 0.0
1 1.0
000000000
000001110
000000000
000000000
000000000
000000000
000000000
011100000
000000000
 1        1.0        0.0        0.0 0
1 1.0
  0.   0.   0.   0.   0.   0.   0.   0.   0.
  0.   0.   0.   0.  0.100.100.100.   0.
  0.   0.   0.   0.   0.   0.   0.   0.   0.
  0.   0.   0.   0.   0.   0.   0.   0.   0.
  0.   0.   0.   0.   0.   0.   0.   0.   0.
  0.   0.   0.   0.   0.   0.   0.   0.   0.
  0.   0.   0.   0.   0.   0.   0.   0.   0.
  0.  80.  80.  80.   0.   0.   0.   0.   0.
  0.   0.   0.   0.   0.   0.   0.   0.   0.
1 100.0
  0.   0.   0.   0.   0.   0.   0.   0.   0.
  0.   0.   0.   0.   0.   0.   0.   0.   0.
  0.   0.   0.   0.   1.   1.   1.   1.   0.
  0.   0.   0.   0.   0.   0.   0.   0.   0.
  0.   0.   0.   0.   0.   0.   0.   0.   0.
  0.   0.   0.   0.   0.   0.   0.   0.   0.
  0.   0.   0.   0.   0.   0.   0.   0.   0.
  0.   0.   0.   0.   0.   0.   0.   0.   0.
  0.   0.   0.   0.   0.   0.   0.   0.   0.
```

cte head

cte conc.

FACULTAD DE INGENIERIA U.N.A.M.
DIVISION DE EDUCACION CONTINUA

C U R S O S A B I E R T O S

VII CURSO INTERNACIONAL DE CONTAMINACION
DE ACUIFEROS.

MODULO III

TEMA: INTRODUCCION A LAS MICROCOMPUTADORAS

PONENTE:

ING. FEDERICO MEIXUEIRO TREJO.

CURSO INTERNACIONAL DE CONTAMINACION DE ACUIFEROS

Módulo III. Modelos en Geohidrología, Contaminación de Acuíferos.

Introducción a las Microcomputadoras.

Ponente: Ing. Federico Meixueiro T.

Contenido.

INTRODUCCION A LAS MICROCOMPUTADORAS.

1.- Introducción.

La finalidad del presente segmento del V Curso Internacional de Contaminación de Acuíferos es la de presentar los fundamentos necesarios y suficientes para la manipulación básica de un modelo matemático elaborado en Software para una computadora personal del tipo compatible con IBM.

Actualmente, la elaboración de modelos matemáticos que simulen la dispersión de elementos contaminantes en un acuífero no es concebible sin la utilización de una computadora. La gran cantidad de procesamiento de información y la gran velocidad de cálculo sólo es posible simultáneamente gracias a las computadoras.

De hecho, una gran cantidad de programas están hechos con tal finalidad o bien existen muchos más que pueden ser utilizados con tal fin, por lo que es indispensable familiarizarse con las técnicas básicas de manejo de microcomputadoras para poder realizar las tareas de procesamiento necesarias para la ejecución de un programa cualquiera.

Dentro de éste segmento, se realizará una descripción somera de un sistema operativo ampliamente difundido para computadores personales compatibles como lo es el Disk Operating System elaborado por Microsoft (MS-DOS), ofreciendo un panorama de su estructura y una referencia de los comandos más usuales.

Asimismo, se ofrecerán fundamentos de programación, aplicables a cualquier lenguaje de programación, pero enfocando el aspecto de compilación al Microsoft Fortran, de un gran uso en la Facultad y el Instituto de Ingeniería, así como en muchos otros centros de enseñanza e investigación de la Ingeniería en México.

Por último, se presentará un esbozo de un modelo matemático, presentando varias de las alternativas que existen en el mercado actual de software para su procesamiento.

2.- Sistema Operativo.

En una computadora, la información se proporciona a y se remueve de la unidad de procesamiento central (CPU) a través del uso de "archivos" grabados en disco flexible, disco duro, disco óptico, cinta, etc.

Un grupo de archivos administrativos, que se conocen colectivamente como el "sistema operativo", son necesarios para controlar la operación de la computadora y el manejo de los archivos generados por el usuario.

Visto de otra manera, el sistema operativo puede visualizarse como un intérprete entre el usuario y la computadora para poder administrar la memoria y los periféricos del ordenador por medio de órdenes fácilmente identificables con palabras (en inglés).

En computadoras personales compatibles con IBM es muy común emplear el sistema opertivo de Microsoft "Disk Operating System" o más conocido como MS-DOS, que será al que se haga referencia en éste segmento.

En un sistema de disco duro, el sistema operativo deberá estar residente en él, inicializándose cada vez que se enciende el interruptor de la computadora. En caso contrario, se deberá contar con una copia del sistema operativo en disco flexible para inicializar una computadora que no lo contenga.

2.1.- Programas y Archivos.

El sistema operativo permite el uso de la memoria a través de unidades variables en tamaño denominadas "archivos", tales archivos pueden contener instrucciones o datos y se hace referencia a él por un único nombre de archivo asignado por el programador. El nombre de archivo se utiliza para la identificación de un archivo para copiarlo, editarlo, renombrarlo, visualizarlo en la pantalla, imprimirlo, almacenarlo, etc. El nombre de archivo puede o no tener una extensión. La forma general del nombre de archivo con extensión es:

NOMBREDEARCHIVO.EXT

El nombre de archivo puede ser cualquier combinación de 1 a 8 letras, números u otros caracteres aceptables, asignados por el programador. La extensión podrá ser cualquier combinación de 1 a 3 letras, números u otros caracteres aceptables. El nombre de archivo y la extensión se separan por un punto. Los siguientes caracteres son aceptables en MS-DOS:

$ # $ @ ! ( ) - { } ' ` _ ; : |

Ni el nombre de archivo ni la extensión podrán contener blancos. El truncamiento del nombre del archivo y de la extensión ocurre en el primer blanco.

Los caracteres ? y * llamados caracteres globales de nombre de archivo o caracteres comodines pueden usarse en lugar de cualquier caracter de un nombre de archivo y extensión y significan cualquier caracter.

Los nombres de archivo y extensión que se elijan deberán ser descriptivos del contenido del archivo. Las siguientes extensiones reservadas tienen un significado especial para MS-DOS y deberán ser utilizadas con mucho cuidado:

BAT COM EXE SYS

Además, los siguientes nombres de archivo reservados también tienen un significado especial para DOS y no deberán asignarse por el programador en otros contextos:

Nombres de archivos para controlar dispositivos:

CON PRN NUL

LPT1 LPT2 LPT3

AUX COM1 COM2

Nombres de archivos asignados a comandos del sistema DOS:

DIR DEL DISKCOPY TYPE ERASE DISKCOMP RENAME

CLS CHKDSK COPY FORMAT EDLIN

2.2.- Manejo de Archivos.

Cambio de unidad de disco por omisión

Mientras no se indique algo distinto, ya sea por el programador desde el teclado o mediante una instrucción programada, la unidad de disco por omisión es la unidad A, es decir, al terminar de cargarse el sistema operativo aparece la petición A>. Toda la información se copia de o graba en el disco flexible en la unidad de disco A, la cual es la *unidad por omisión*.

La unidad de disco por omisión puede cambiarse de la unidad A a la B y regresar de nuevo a la A con:

```
A>_
A>B:_ ←┘
```

Para pasar la unidad de disco por omisión de la unidad A a la unidad B, escríbase B: y presiónese la tecla ←┘

```
B>_
B>A:_ ←┘
```

Para cambiar la unidad de disco por omisión de B a la unidad A, escríbase A: y oprímase la tecla ←┘

```
A>_
```

Los comandos del sistema DOS

El disco flexible de DOS contiene un procesador de comandos, archivado bajo el nombre y la extensión COMMAND.COM, que controla el hardware de la computadora y maneja el software. El archivo COMMAND.COM puede grabarse en un disco nuevo durante la operación de formateado, la cual se describirá más adelante en este apéndice. El archivo COMMAND.COM incluye los siguientes *comandos internos*, que son necesarios para el programador de FORTRAN:

DIR	TYPE	COPY
RENAME	DELETE	ERASE
CLS	VOL	FILENAME.BAT
AUTOEXEC.BAT	ECHO	

En adición a los comandos internos contiene el archivo COMMAND.COM, el disco de DOS contiene varios *comandos externos*, con extensión COM o EXE, indispensables para el programador FORTRAN:

FORMAT DISKCOPY DISKCOMP CHKDSK EDLIN SORT MORE

La función de los comandos externos e internos seleccionados se analiza en las Secciones C-6 a C-21 de este Apéndice.

La operación que se describe en las Secciones C-6 a C-21 requiere de un disco en la unidad A con el archivo procesador de comandos COMMAND.COM y el comando externo DOS específico. La ejecución de cada uno de los comandos del sistema se inicia cuando se presiona la tecla↵.

Preparación de un disco flexible para recibir información nueva

Para preparar un disco flexible nuevo para recibir información (*formateado*), úsese el comando externo FORMAT:

a) A>FORMAT B: ␣ ↵ — Borra todos los registros almacenados en el disco de la unidad B y establece la rejilla electrónica de pistas y sectores que se utilizan como "direcciones" para la nueva información.

b) A>FORMAT B:/S ␣ ↵ — /S después de FORMAT B: copia de manera automática el procesador de comandos de datos de DOS COMMAND.COM y ciertos "archivos ocultos" necesarios para cargar el sistema del disco de la unidad A al disco de la unidad B.

c) A>FORMAT B:/V ␣ ↵ — /V luego de FORMAT B: proporciona la etiqueta del disco (con 11 o menos caracteres) elegida por el programador. El punto de petición A> aparece después del formateado y de imprimir la etiqueta en el disco.

d) A>FORMAT B:/S/V ␣ ↵ — Si se quiere pueden emplearse los dos.

e) A>VOL B: ␣ ↵ — Visualiza la etiqueta que se asignó al disco en la unidad indicada, la unidad B en este ejemplo.

> ***Precaución:*** El comando FORMAT *borra todos los archivos* del disco flexible cuando se formatea. Cualquier archivo que deba salvarse *debe copiarse en otro disco* antes del formateo.

Presentación del directorio del contenido de un disco específico

Para exhibir un directorio del contenido de un disco flexible particular, úsese el comando DIR (interno):

a) A>DIR ␣ ↵ — Para cada archivo grabado en el disco de la unidad indicada, la unidad por omisión A en el caso *a*), la unidad B en el ejemplo *b*), lista el nombre del archivo, su extensión, el número de

o

bytes que se usaron y la fecha y la hora en la que se grabó. Si el directorio contiene más de 23 archivos, la lista se enrolla hasta que aparece la última línea del directorio, el espacio total disponible (bytes) en el disco.

A>DIR A: ↵

b) A>DIR B: ↵

c) A>DIR B:/P ↵ — /P detiene el enrollamiento de la lista cuando la pantalla está llena (23 líneas). Para visualizar los siguientes 23 renglones presiónese la tecla ↵

d) A>DIR B:/W ↵ — /W muestra sólo los nombres del archivo y la extensión (sin la fecha, la hora, y el tamaño) de todos los archivos grabados en el disco en la unidad especifica, en 5 columnas a lo ancho de la pantalla. Este comando exhibe en la pantalla al mismo tiempo la lista sin enrollar de todos los archivos del disco

e) A>DIR | MORE ↵ — El comando MORE visualiza a un tiempo 23 líneas (una pantalla completa). Al oprimir la tecla ↵ se exhiben los siguientes 23 renglones, etc. El archivo MORE.COM debe estar en el disco cuyo directorio se listará. Nótese el uso del caracter |

f) A>DIR | SORT ↵ — El comando SORT muestra el directorio en orden alfabetico por el nombre del archivo. El archivo SORT EXE debe estar en el disco cuyo directorio se listará. Obsérvese la utilización del simbolo |.

g) A>DIR *.FOR | SORT ↵ — Son posibles otras combinaciones del comando DIR. Por ejemplo, DIR *.FOR | SORT visualiza en orden alfabetico todos los archivos con extensión FOR

Los casos anteriores muestran como unidad por omisión la (A). Esta puede cambiarse por la unidad B como se indica en la Sección C-4.

Exhibición del texto de un archivo

Para visualizar el texto de un archivo especifico, utilícese el comando TYPE (interno):

a) A>TYPE NOMBREDEARCHIVO.EXT ↵
o
A>TYPE A:NOMBREDEARCHIVO.EXT ↵

b) A>TYPE B:NOMBREDEARCHIVO.EXT ↵

Exhibe el texto del archivo grabado en el disco bajo el nombre del archivo y la extensión que se especifican en la unidad de disco correspondiente. la unidad por omisión A en el ejemplo *a)* la unidad B en el caso *b)*

Cambio del nombre o extensión de un archivo

Para cambiar el nombre o la extensión de un archivo particular, utilícese el comando RENAME (interno):

a) A>RENAME NOMBREVIEJO.EXT NOMBRENUEVO.EXT ↵
o
A>RENAME A:NOMBREVIEJO.EXT NOMBRENUEVO.EXT ↵

b) A>RENAME B:NOMBREVIEJO.EXT NOMBRENUEVO.EXT ↵

RENAME cambia el nombre del archivo del primer nombre listado por el segundo de la unidad indicada, por ejemplo, NOMBREVIEJO.EXT a NOMBRENUEVO.EXT en la unidad A, en el caso *a)*, la unidad B en el ejemplo *b)*.

Borrar la pantalla

Empléese el comando CLS (interno) para borrar la pantalla.

A>CLS ↵

Borra la pantalla y después coloca el punto de petición A> y el cursor centelleando en la esquina superior izquierda de la pantalla.

Borrar en forma permanente un archivo de un disco

Para eliminar un archivo de un disco flexible, empléese alguno de los siguientes dos comandos, DEL o ERASE (internos). (Los dos ejecutan la misma función).

a) A>DEL NOMBREDEARCHIVO.EXT ↵
o
A>ERASE A:NOMBREDEARCHIVO.EXT ↵

Borra del disco en la unidad por omisión A el archivo específico. NOMBREDEARCHIVO.EXT.

b) A>DEL B:NOMBREDEARCHIVO.EXT ↵
o
A>ERASE B:NOMBREDEARCHIVO.EXT ↵

Elimina del disco en la unidad B el archivo indicado. NOMBREDEARCHIVO.EXT.

c) A>DEL B:PROGRAMA.??? ↵
o
A>ERASE B:PROGRAMA.* ↵

Usa el caracter "comodín" (?) para borrar todos los archivos cuyo nombre sea PROGRAMA (con cualquier extensión) del disco en la unidad B. El otro "comodín" (*) también puede emplearse, en ese caso sólo se necesita un asterisco.

d) A>DEL B:*.BAK ↵
o
A>DEL ????????.BAK ↵

Mediante el caracter "comodín" (*) se eliminan todos los archivos con la extensión BAK (cualquier nombre de archivo) del disco de la unidad B. El otro carácter "comodín' (?) también puede utilizarse; sin embargo, se requieren 8 signos de interrogación o 1 por cada símbolo del nombre del archivo.

Duplicación de un archivo específico y almacenamiento con otro nombre

Úsese el comando COPY (interno) para duplicar un archivo particular y almacenarlo con un nombre de archivo distinto, como en:

A>COPY ARCHIVOVIEJO.EXT ARCHIVONUEVO.EXT ↵

Este comando copia el texto de un archivo específico (ARCHIVOVIEJO.EXT) a un archivo nuevo (ARCHIVONUEVO.EXT). El nombre y el contenido del archivo viejo permanecen sin cambio.

NOTA: Si hay un archivo con el mismo nombre del archivo nuevo (ARCHIVONUEVO.EXT) en el disco, su contenido se reemplaza por la información del archivo viejo (ARCHIVOVIEJO.EXT).

Copiar un archivo de un disco flexible en la unidad A a un disco flexible en la unidad B

Utilícese el comando COPY (interno) para duplicar un archivo de un disco flexible en la unidad A a uno en la unidad de disco B, como:

a) **A>COPY NOMBREDEARCHIVO.EXT B:** ↵

Copia el texto de un archivo específico (NOMBREDEARCHIVO EXT) del disco fuente en la unidad A, al disco destino en la unidad B y asigna el mismo nombre de archivo NOMBREDEARCHIVO EXT a la copia

b) **A>COPY A:ARCHIVOVIEJO.EXT B:ARCHIVONUEVO.EXT** ↵

Copia el contenido del archivo indicado (ARCHIVOVIEJO EXT) del disco fuente en la unidad A, al disco destino. Asigna un nombre de archivo (ARCHIVONUEVO EXT) al nuevo archivo. El nombre del archivo y el texto en el disco fuente permanece sin cambio

Nota: En *a)* y *b)* si existe un archivo con el mismo nombre (ARCHIVONUEVO EXT) en el disco destino, su contenido se sustituye por la información del archivo del disco fuente

Copiar todos los archivos de un disco flexible en la unidad A a la unidad B

Para copiar todos los archivos de un disco flexible de la unidad de disco A al disco flexible de la unidad B, un archivo a la vez, úsese el comando COPY (interno) como sigue:

A>COPY *.* B: ↵

Copia el texto de cada archivo del disco fuente en la unidad A al disco destino en la unidad B. Los archivos se duplican uno a uno y se listan en la pantalla conforme se copian.

Introducir de manera directa un archivo desde la consola a un disco flexible

Para introducir de modo directo un archivo desde la consola (teclado) a un disco flexible, empléese el comando COPY (interno) como en:

A>COPY CON B:ARCHIVO.DAT ↵

123.456 ↵
987.654 ↵
1 0.123 ↵
2 1.875 ↵
3 2.375 ↵
^Z F6 ↵

texto del archivo

Copia de manera directa el contenido desde la consola (teclado) a el disco en la unidad B y asigna el nombre del archivo ARCHIVO DAT

Siguiendo la última línea del texto, presiónese F6 entonces oprímase la tecla ↵ (El presionar F6 causa la aparición de ^Z).

Imprimir el texto de un archivo

Úsese el comando COPY (interno) para imprimir el contenido de un archivo específico, como sigue:

```
A>COPY B:NOMBREDEARCHIVO.EXT PRN ↵
o
A>COPY B:NOMBREDEARCHIVO.EXT LPT1 ↵
```

Con la impresora activada, este comando hace que la impresora imprima el texto del archivo indicado (NOMBREDEARCHIVO.EXT) del disco en la unidad B).

Duplicar un disco flexible

Para duplicar un disco flexible, por ejemplo, copiar el contenido entero del disco flexible a otro disco flexible, utilícese el comando DISCKCOPY (externo). Iniciese con un disco flexible que contenga el archivo DISKCOPY.COM en la unidad A.

```
A>DISKCOPY A: B: ↵
```

Respóndase a la petición removiendo el disco DOS de la unidad A e insértese el disco fuente en la unidad A y el disco destino en la unidad B. Este comando formatea el disco de la unidad B y copia el contenido completo del disco en la unidad A (el disco fuente) al disco en la unidad B (el disco destino).

Precaución: En DOS 2.10, la ejecución del comando DISKCOPY formatea de manera autómatica el disco destino. ***Toda la información almacenada en el disco en la unidad B se borra.***

Comparar y verificar los contenidos de dos discos

Para comparar los contenidos de dos discos y verificar que son idénticos, úsese el comando DISKCOMP (externo). Empiécese con un disco que contenga el archivo DISKCOMP.COM en la unidad A.

```
A>DISKCOMP A: B: ↵
```

Respóndase a la petición retirando el disco DOS de la unidad A e insértese ahí mismo el disco original y la copia en la unidad B. Este comando compara los archivos del disco de la unidad B con los del disco de la unidad A y verifica que sean iguales.

Nota: El comando DISKCOMP puede emplearse después de duplicar un disco para asegurarse que los archivos en la copia son idénticos con los archivos del original.

Revisar el estado de un disco

Úsese el comando CHDSK (externo) para revisar el estado de un disco:

```
A>CHKDSK B: ↵
```

Proporciona un informe del estado en el disco en la unidad indicada. Revisa los sectores y pistas no utilizados; cuantifica el espacio usado (bytes) e indica el numero de bytes disponibles en el espacio restante del disco.

2.3.- Manejo de Directorios.

Un disco contiene grupos de archivos denominados directorios. Cuando un directorio contiene tanta información que ya no se puede encontrar fácilmente lo que se desea, se subdivide en subdirectorios.

Uso de directorios

Los directorios son muy importantes cuando se utiliza un disco duro. Si se utilizan sólo disquetes, los archivos se pueden mantener organizados colocándolos en disquetes distintos. Con un disco duro, que normalmente puede almacenar mucha más información que un disquete, se hace necesario organizar los archivos en categorías, de forma que se puedan encontrar fácilmente.

El árbol de directorios

Cada disco tiene por lo menos un directorio. Cuando se da formato a un disquete o al disco duro, MS-DOS crea un directorio en el que se almacenan el resto de los archivos y directorios. Este directorio se denomina *directorio raíz*. Se pueden crear subdirectorios del directorio raíz para organizar los archivos. Los directorios y subdirectorios forman una estructura denominada *árbol de directorios*. Se pueden crear subdirectorios dentro de estos subdirectorios para organizar incluso más archivos.

Puede seguir añadiendo directorios en cualquier nivel de la estructura, hasta 512 archivos y directorios en el directorio raíz del disco duro (un directorio raíz en un disquete tiene menos archivos y directorios). No obstante, MS-DOS se ejecuta más lentamente si hay más de 150 archivos y subdirectorios en el mismo directorio.

Hablando con propiedad, el resto de los directorios distintos del directorio raíz son subdirectorios. Sin embargo, es normal utilizar el término *directorio*. En el manual, el término *subdirectorio* se utiliza sólo para dar mayor énfasis a la relación entre dos directorios. Un subdirectorio a veces se denomina *directorio hijo*, y el directorio que lo contiene se denomina con frecuencia *directorio padre*.

Nombres para directorios

Con excepción del directorio raíz, que siempre se representa por una barra invertida (\), cada directorio tiene un nombre y algunas veces una extensión. Para dar nombre a los directorios se siguen estas reglas:

- El nombre tiene que contener entre 1 y 8 caracteres.
- La extensión puede tener un máximo de 3 caracteres, separados del nombre del directorio por un punto.
- El nombre y la extensión pueden tener cualquier letra desde la A a la Z, números desde el 0 al 9, y los siguientes caracteres especiales: subrayado (_), símbolo de intercalación (^), símbolo de dolar ($), tilde (~), signo de exclamación de cierre (!), símbolo de número (#), signo de porcentaje (%), símbolo de unión (&), guión (-), llaves ({ }), y paréntesis ( ). No se aceptan otros caracteres especiales.
- El nombre no puede contener espacios, barras invertidas (\), comas o puntos. El nombre puede contener caracteres extendidos.
- Dos subdirectorios que estén en el mismo directorio no pueden tener el mismo nombre. Sin embargo, subdirectorios de diferentes directorios pueden tener el mismo nombre.

El directorio actual se indica con su nombre o con un punto. Al directorio padre del directorio actual se le puede nombrar por su nombre o por un doble punto. Cuando se utiliza el comando **dir** para examinar los archivos y directorios de un directorio (diferentes del directorio raía), se pueden ver estos símbolos en pantalla, que representan los directorios padre e hijo.

Rutas de acceso

La *ruta de acceso* indica el emplazamiento de un archivo dentro del árbol de directorios. Es el camino que debe seguir MS-DOS, partiendo del directorio raíz, para llegar a un archivo de otro directorio. MS-DOS reconoce rutas de acceso de hasta 66 caracteres, (incluyendo la letra de la unidad y los dos puntos). Por ejemplo suponga que la unidad C tiene este árbol de directorios:

```
[C:\] tree
Lista de directorios en RUTA y estructura del Volumen CESAR
Número de serie del volumen es 1575-6935
C:.
├── DOS
└── ARTE
    ├── TRABAJO
    ├── PERSONAL
    └── ESTUDIO
```

Para llegar hasta los archivos del directorio PERSONAL, MS-DOS debe pasar por los siguientes directorios: raíz (\), ARTE y PERSONAL. Por lo tanto el nombre de la ruta de acceso sería: `\arte\personal`

La primera barra invertida representa el directorio raíz; la segunda separa el directorio PERSONAL del directorio padre, ARTE.

Para encontrar el directorio PERSONAL, debe escribir primero la ruta de acceso del directorio. Si desea especificar el archivo FIG1.MSP en el directorio \ARTE\PERSONAL, debe agregar a la ruta otra barra invertida y el nombre del archivo:

```
\arte\personal\fig1.msp
```

Puede haber otros archivos denominados FIG1.MSP en otros directorios y puede haber otros directorios denominados \ARTE\PERSONAL en otros discos. Para distinguir específicamente un archivo del resto de los archivos, se tiene que agregar una letra de unidad a la ruta de acceso y al nombre del archivo. Por ejemplo, la ruta de acceso completa del archivo FIG1.MSP del directorio ARTE\PERSONAL de la unidad C es:

```
c:\arte\personal\fig1.msp
```

La unidad actual

A menos que se indique lo contrario, MS-DOS supone que se quiere utilizar el árbol de directorios en la unidad actual. La letra de la unidad actual normalmente es parte del símbolo del sistema. Si actualmente se está utilizando el directorio raíz de la unidad A y se quiere suprimir el archivo A:\FIG1.MSP, se debe escribir el siguiente comando:

```
del fig1.msp
```

Sólo puede haber una unidad actual a la vez. Para trabajar con los archivos de la unidad que no es la actual, se debe escribir otra letra de unidad seguida por dos puntos y presionar la tecla ENTRAR.

El directorio actual

El directorio en el que se está trabajando es el directorio actual para esa unidad. MS-DOS puede presentar en pantalla la ruta de acceso del directorio actual como parte del símbolo del sistema. Si se desea realizar alguna operación en un archivo, y se está utilizando actualmente el directorio en el que está el archivo, no se necesita escribir la ruta de acceso del directorio actual. Si C es la unidad actual y \ARTE\PERSONAL es el directorio actual, se puede suprimir el archivo siguiente C:\ARTE\PERSONAL\FIG1.MSP escribiendo lo siguiente: `del fig1.msp`

Si se está trabajando con dos unidades, cada una de ellas tiene un directorio actual. Suponemos que C es la unidad actual y \ARTE\PERSONAL es el directorio actual. En su disco de la unidad A, suponga que el directorio \FIGS es el directorio actual. Se debe

escribir el siguiente comando para copiar el archivo FIG2.MSP desde A:\FIGS a C:\ARTE\PERSONAL: `copy a:fig2.msp c:`

A menos que se especifique una ruta de acceso diferente, se trabaja en el directorio actual en cada unidad. Cuando se inicia el sistema se está en los directorios raíces de las unidades del sistema. El directorio actual de una unidad de disquete cambia al directorio raíz si se cambian los discos.

Para trabajar con archivos en un directorio que no es el actual, hay dos opciones: se escribe la ruta de acceso del otro directorio o se hace actual el otro directorio utilizando el comando **cd** (cambio de directorio), que se describe posteriormente.

Si se está trabajando con archivos de programa que no están en el directorio actual, se puede incluir la ruta de acceso del otro directorio en el comando **path**. Vea el tema "Especificación de una ruta de búsqueda" en este capítulo.

Si se quiere escribir la ruta de acceso de otro directorio, se incluye la parte de la ruta de acceso que es diferente desde la ruta de acceso del directorio actual. Si el directorio actual es \ARTE, se puede suprimir el archivo \ARTE\PERSONAL\FIG1.MSP escribiendo el siguiente comando: `del personal\fig1.msp`

En este caso no es necesario escribir la ruta de acceso completa, ya que el archivo que se quiere escribir está en un subdirectorio del directorio actual.

Modificación del símbolo del sistema

Se puede utilizar el comando **prompt** para modificar la apariencia del símbolo del sistema. A menos que se indique lo contrario, MS-DOS visualiza la letra de la unidad actual seguida de un signo mayor que (>) como símbolo del sistema. Por ejemplo, el siguiente símbolo le indica que la unidad activa es la A: `A>`

Se pueden utilizar varios parámetros con el comando **prompt** para cambiar el símbolo del sistema.

Presentación del contenido de directorios

Este apartado describe cómo presentar la lista del contenido de directorios utilizando la línea de comandos.

Presentación de directorios completos.

Para ver el contenido de un directorio, se utiliza el comando dir. Para ver el contenido del directorio C:\TRABAJO se utiliza éste comando:

```
dir c:\trabajo
```

Presentación de grupos de nombres de archivos.

Para presentar la lista de un determinado grupo de nombres de archivos de un directorio, se incluyen comodines con el comando dir. El siguiente comando presenta una lista de todos los archivos del directorio actual que tengan la extensión .COM:

```
dir *.com
```

Presentación de todos los directorios de un disco.

Para presentar en la pantalla la estructura de un directorio y sus subdirectorios, se utiliza el comando tree (árbol). Por ejemplo, el siguiente comando presenta en pantalla la relación entre el directorio C:\TEMP y sus subdirectorios:

```
tree c:\temp
```

Creación de directorios.

Para crear un directorio, se utiliza el comando md (mkdir). Si el directorio C:\IMPUESTO\ANUAL es el directorio actual, rl siguiente comando crea un subdirectorio llamado MENSUAL:

```
md mensual
```

Cambio de directorio.

Para desplazarse a un directorio diferente en la unidad actual, se utiliza el comando cd (o en su forma ampliada chdir). El siguiente comando cambia el directorio actual al directorio C:\OFICINA\INFORMES:

```
cd oficina\informes
```

Eliminación de directorios.

Para eliminar un directorio se utiliza el comando rd (rmdir), como en el siguiente ejemplo:

```
rd c:\oficina\informes\finanzas
```

El sistema MS-DOS elimina el subdirectorio FINANZAS del directorio C:\OFICINA\INFORMES de la unidad actual. El directorio que elimina no puede contener ningún archivo o subdirectorio.

Copia de todos los archivos de un directorio.

Para copiar un solo directorio (sin subdirectorios), se utiliza el comando xcopy sin modificadores. Por ejemplo, para copiar todos los archivos del directorio C:\INFORMES\FINANZAS al directorio FINANZAS de la unidad A, se deberá escribir el siguiente comando:

```
xcopy c:\informes\finanzas a:\finanzas
```

2.4.- Manejo de Discos.

La información se guarda en discos y permanece intacta hasta que se eliminan. En contraste, la memoria RAM (memoria de acceso aleatorio), proporciona almacenamiento de información que se pierde cada vez que se apaga el ordenador.

Tipos de discos

Un disquete es un disco flexible y muy delgado que tiene una cubierta protectora de plástico. Un disco duro tiene uno o más discos rígidos apilados uno encima del otro dentro de una caja cerrada completamente. A los discos duros también se los denomina *discos fijos* porque permanecen dentro del sistema. Una vez que se ha instalado el disco duro, no se debe retirar a no ser que esté dañado o se desee sustituir por un disco de mayor capacidad.

La información de los discos se divide en pistas. Cada pista es un círculo concéntrico que puede contener una cierta cantidad de información. Cuantas más pistas tenga un disco, más información puede almacenar. Un disco duro puede almacenar más información que los disquetes porque tiene más caras y más pistas por cara.

Los disquetes varían en cuanto al tamaño y la cantidad de información que pueden contener. A continuación se presenta una lista con los principales tipos de disquetes con los que se puede trabajar en MS-DOS, y la cantidad de información que cada uno puede almacenar:

5 1/4 pulgadas una sola cara/doble densidad	160K
5 1/4 pulgadas una sola cara/doble densidad	180K
5 1/4 pulgadas dos caras/doble densidad	320K
5 1/4 pulgadas dos caras/doble densidad	360K
5 1/4 pulgadas dos caras/cuadruple densidad	1200K ó 1,2 MB
3 1/2 pulgadas dos caras/doble densidad	720K
3 1/2 pulgadas dos caras/cuadruple densidad	1440K ó 1,44 MB
3 1/2 pulgadas dos caras/alta densidad	2880K ó 2,88 MB

La mayor parte de los disquetes tienen etiquetas que indican de qué tipo son. También se puede utilizar el comando **dir** o **chkdsk** para ver la información sobre la capacidad de

almacenamiento de un disco que ya tiene formato.

Bytes, Kilobytes y Megabytes

El tamaño de los archivos se mide en *bytes*. Un byte es la cantidad de espacio que se necesita para almacenar un solo carácter. Un kilobytes equivale a 1024 bytes. En este manual el *kilobyte* se abrevia como KB. Un megabytes equivale a 1024 K (casi un millón de bytes). En este manual la palabra *megabytes* se abrevia como MB. Por ejemplo, si un disco puede almacenar casi 1,2 millones de bytes de información, es un disco de 1,2 MB.

Tipos de unidades de disco

No todos los tipos de disquetes son compatibles con todos los tipos de unidades de disco. En general, al disquete se le debe dar un formato con una capacidad menor o igual que la de la unidad en la que se utilice para que el disco y la unidad sean compatibles. Para comprobar si un disco funciona con una determinada unidad, el disco se inserta en la unidad y se utiliza el comando **dir**. Si el disco y la unidad son compatibles o el disco no tiene formato, MS–DOS presenta un mensaje de error que le comunica que hay un fallo general.

MS–DOS ajusta sus operaciones para trabajar con el tipo de unidad de disco que se está utilizando. Para algunos comandos, se incluye un modificador si la unidad de disco y el disquete no tienen la misma capacidad.

El formato de los discos

Antes de poder utilizar un disco, se debe preparar utilizando el comando **format**. El disco puede tener o no formato previo. Cuando se da formato a un disco, MS–DOS realiza un *formato de seguridad*. Con este formato de seguridad, se puede restaurar el disco a su condición anterior mediante el comando **unformat**, siempre que no se hayan guardado archivos en dicho disco.

Se puede incluir el modificador /u con el comando **format** para ejecutar un formato incondicional. Este formato destruye toda la información del disco. Si de forma errónea se da formato a un disco incondicionalmente, todavía se puede recuperar la información perdida siempre que se haya instalado el programa Mirror antes de utilizar el comando **format**. El programa Mirror se describe en la siguiente sección.

Cuando se da formato a un disquete o a un disco duro, MS-DOS reserva una pequeña parte del disco para su sistema de registro. El sistema de registro se compone de dos partes: *una tabla de asignación de archivos* (que determina el emplazamiento de cada archivo del disco) y el *directorio raíz* (que almacena el nombre, tamaño, fecha y hora de creación y los atributos de los archivos del disco).

Un *sector* es la unidad de almacenamiento básica de un disco. Cada sector de un disco puede almacenar medio kilobyte de información. Cuando MS-DOS da formato a un disco, MS-DOS verifica cada sector para detectar si tiene algún defecto, y marcarlo para que no pueda almacenar datos en ellos. Cuando MS-DOS almacena un archivo en un disco, utiliza grupos de sectores llamados ***unidades de asignación***. El número de sectores por unidad de asignación depende del tamaño del disco.

Si se utiliza un disco duro nuevo, se debe realizar una partición antes de poder darle formato. Mientras se ejecuta el programa de instalación de MS-DOS puede crear particiones y dar formato al disco duro.

Formato de un disco

En breve

Para dar formato a un disquete o a un disco duro, se utiliza el comando **format**. Se debe especificar la unidad que contiene el disco al que se quiere dar formato. Por ejemplo, el siguiente comando da formato a un disquete de la unidad A: `format a:`

MS-DOS realiza un formato de seguridad de forma predeterminada. Si se desea deshacer el formato de seguridad, se añade el modificador **/u** al comando **format** el modificador **/u** elimina todos los datos existentes en un disco. Cuando se utiliza el comando **format** con el modificador **/u** para dar formato al disco duro, aparece el siguiente mensaje:

```
Peligro, todos los datos del disquete de la unidad C: se perderán
¿Continuar con el formato (S/N)?
```

Escriba **s** para continuar, o **n** para cancelar el comando.

Utilizando el modificador **/q** con el comando **format**, se puede realizar un formato rápido en un disco con formato previo, lo cual reduce el tiempo que MS-DOS necesita para dar formato a un disco. Sólo se utiliza el modificador **/q** si no se han recibido errores de lectura/escritura en el disco al que se esté dando formato.

Mientras se da formato al disco, MS-DOS presenta un mensaje que indica el porcentaje del disco al que se da formato. Una vez terminado el proceso, se pregunta si se desea dar al disco una *etiqueta del volumen*. Se debe escribir el nombre que se desee dar al disco o presionar la tecla ENTRAR si no se desea una etiqueta.

MS-DOS presenta la siguiente información:

```
1213952 bytes de espacio total en disco
1213952 bytes disponibles en disco
    512 bytes en cada unidad de asignación
   2371 unidades de asignación disponibles en disco

Número de serie del volumen 382C-17F4
```

Bytes de espacio total en disco Indica la capacidad de almacenamiento del disco.

Bytes utilizados por el sistema Aparece si se han transferido al disco los archivos del sistema de MS-DOS e indica el espacio que ha sido ocupado por los tres archivos del sistema.

Bytes en sectores defectuosos Indica la cantidad de espacio que no es posible utilizar debido a sectores defectuosos. Si no hay sectores defectuosos, esta línea se omite. Si un disquete tiene sectores defectuosos, se debe considerar no almacenar archivos importantes o archivos de copia de seguridad en él. La mayor parte de los discos duros tienen un pequeño número de sectores defectuosos.

Bytes disponibles en disco Indica el espacio total del disco menos la cantidad de espacio utilizado por los archivos del sistema y los sectores defectuosos. Si el disco no contiene archivos del sistema y no hay sectores defectuosos, este número es igual al número de bytes del espacio total del disco.

Bytes en cada unidad de asignación y unidades de asignación disponibles en un disco Indican la forma en que MS-DOS ha dividido el disco para el almacenamiento de los archivos. Si se multiplican las dos cifras de estas líneas, el resultado debe coincidir con la cifra que corresponde al número de "Bytes disponibles en disco".

El número de serie del volumen Indica el número de serie asignado al disco. Este número no cambia a menos que se dé nuevamente formato al disco.

La siguiente línea es un símbolo del sistema para dar formato a otro disco. Se escribe **s** para dar formato a otro disco en la misma unidad con los mismos modificadores, o se escribe **n** para volver al símbolo del sistema.

Especificación de la capacidad de un disquete

A menos que se indique lo contrario, MS-DOS supone que el disco que se quiere dar formato tiene la capacidad máxima que corresponde a la unidad. Para dar formato a un disco de menor capacidad, se debe utilizar el modificador **/f:**. Por ejemplo, si la unidad A es de 1,2 MB, para discos de 5 1/4 pulgadas y se desea dar formato a un disco de 360 KB, se debe utilizar el siguiente comando:

format a: /f:360

Algunas de las unidades de disco modernas pueden detectar la capacidad del disquete. Si se dispone de este tipo de unidad, no se necesita especificar estos modificadores.

NOTA Existen diferencias de hardware entre unidades de disco, por lo que algunas unidades de 360 KB no pueden leer de manera fiable discos a los que se ha dado formato en una unidad de 1,2 MB con el modificador **/f:360**.

2.5.- Manejo de un Editor.

Con la finalidad de generar un código para un programa, para revisar listas de resultados, añadir texto a una presentación, etc., se precisa del manejo de un editor de texto.

Para ello, desde las tempranas versiones de MS-DOS, se ha incluído en los diskettes de programas, editores de texto, que aunque un tanto cándidos, son eficientes. Las últimas versiones de MS-DOS incluyen editores (EDIT), que son más refinados y permiten un procesamiento de texto más capaz.

Asimismo, para la edición de texto tipo ASCII (American Standard Code for Information Interchange), se pueden utilizar editores de texto comerciales (WordStar, WordPerfect, Norton Editor, etc).

Tales editores de texto deberán invocarse desde el sistema operativo y contienen reglas internas de operación que pueden consultarse en sus respectivos manuales de referencia o en sus subprogramas de ayuda.

3.- Fundamentos de Programación.

Para un entendimiento claro de las estructuras y funciones de un programa, es necesario conocer varios tópicos referentes a la programación, para tal efecto, se ha escogido para éste segmento, el lenguaje de programación Fortran, el cual es de uso muy extendido; sin embargo, se tratarán los temas de una manera muy general, de tal forma que puedan sin ninguna dificultad ser extendidos a lenguajes tales como Basic, Pascal y otros.

La comprensión completa del lenguaje técnico no es prerrequisito para la preparación inteligente de una secuencia lógica de instrucciones (un programa) que puedan usarse en la computadora para resolver algún problema. Sólo se necesita aceptar la premisa de que en un disco flexible o en alguna parte del disco duro existe un conjunto de instrucciones detalladas en lenguaje de máquina que habilitan a la computadora para ejecutar una serie de instrucciones simplificadas orientadas al usuario y

preparadas bajo las reglas del Fortran, Basic, Pascal, etc. Este juego de instrucciones en lenguaje de máquina se origina con un programa compilador.

3.1.- Constantes y Variables.

Un valor matemático se representa mediante una serie de dígitos numéricos con o sin punto decimal o signo algebráico. Las constantes que se empleen, podrán ser de tipo real, entero, exponencial, lógico, de caracter, de cadena de caracteres y en algunos casos, definidas por el usuario.

Una cantidad cuyo valor numérico se desconoce temporalmente o que pueda cambiar durante la ejecución de un programa, se llama variable y se expresa por un nombre de variable. El nombre de variable lo crea el programador y dependiendo del sistema de computadora que se utilice podrá consistir de una a varias letras o combinaciones de letras y numeros.

3.2.- Proposiciones y Asignaciones.

El lenguaje Fortran usa los caracteres alfabéticos, numéricos y especiales del idioma inglés y de la matemática; las 26 letras del alfabeto inglés, A a Z; los 10 dígitos decimales 0 a 9 y 10 caracteres especiales:

+ - * / = . , ' ( )

Aunque éstos son los más comunes, existen otros caracteres también disponibles.

Estos caracteres se combinan para formar palabras, números y expresiones que se utilizan para construir proposiciones. Una proposición puede ser una instrucción explícita para que la computadora ejecute una tarea sencilla, por ejemplo leer un valor introducido desde el teclado y asignarlo al nombre de una variable o realizar operaciones aritméticas y asignar el resultado a una variable, repetir una serie de tareas, o imprimir los resultados de un cálculo.

Además, una proposición puede proporcionar información para definir un arreglo, identificar una variable compleja o especificar un formato de salida.

Un programa consiste en una serie detallada de instrucciones y proposiciones organizadas en secuencia lógica para alcanzar resultados predecibles.

Una proposición de asignación es una proposición ejecutable que asigna los valores numéricos de una expresión aritmética a un nombre de variable en una dirección de memoria específica. El símbolo de asignación es el signo = o en ocasiones := (Pascal).

3.3.- Lectura y Escritura.

Existen proposiciones ejecutables que proporcionan medios sencillos y directos para suministrar valores de datos a los nombres de las variables que se usan en un programa.

Cuando es necesario que los valores por asignar a los nombres de las variables en la lista se deben leer desde un archivo de datos almacenado en un disco flexible o en disco duro, existen proposiciones específicas para ello.

Los valores en cada registro del archivo de datos deben concordar en número (cantidad), orden y tipo con los nombres de las variables en la lista de lectura. Si el conjunto de datos que se proporciona en un sólo registro excede al número de nombres de las variables en la lista, los valores de datos se asignarán, en el orden correspondiente, hasta que a cada nombre de variable de la lista se la haya asignado un valor. Cualquier dato adicional del registro se ignora.

Existen asimismo proposiciones ejecutables para la salida de datos a la pantalla, impresora o archivo.

3.4.- Iteraciones y Transferencias.

Para utilizar todo el potencial de la computadora es necesario saber cómo repetir una secuencia de tareas, tomar decisiones basadas en comparaciones sencillas y saltar a otra proposición específica en el programa. La iteración o repetición de cálculos se llama ciclo y es el resultado de la ejecución de varias transferencias mediante proposiciones de control.

Una proposición de transferencia es una proposición ejecutable que transfiere o ramifica a otra proposición identificada por una etiqueta de proposición única. Una proposición de transferencia puede ser condicional o incondicional. Las proposiciones de transferencia incondicional siempre transfiere a una sóla proposición, miestras que una proposición de transferencia condicional puede transferir a una de varias proposiciones específicas, dependiendo de las condiciones de los datos.

Una proposición de control puede repetir un conjunto particular de propposiciones un determinado número de veces.

Existen y son de gran trascendencia, las proposiciones de transferencia condicional de tipo lógico. Este tipo de proposición emplea expresiones lógicas con operadores relacionales y toma decisiones en función de la relación entre los valores de dos o más variables o expresiones aritméticas.

3.5.- Vectores.

Con frecuencia es necesario trabajar con cantidades numéricas que son elementos de un grupo llamado arreglo, y de acuerdo con su forma también se les puede llamar matrices o vectores. Un arreglo es una familia de elementos o cantidades, relacionados, todos asignados al mismo nombre de variable, cada elemento del arreglo se identifica con un subíndice diferente. Las variables que son elementos de un arreglo se conocen como variables con subíndices.

En la mayoría de los lenguajes, antes de que pueda usarse una variable con subíndice en un programa, primero es necesario

definir el arreglo del que forma parte con una proposición de dimensionamiento que establece el arreglo con nombre y número de subíndice (1, 2, n dimensiones), define el máximo valor numérico de cada subíndice y reserva las localidades de almacenamiento para acomodar cada elemento del arreglo.

3.6.- Subprogramas.

El motivo principal para usar la computadora en la solución de problemas es reducir el tiempo necesario para hacer cálculos repetitivos. Con frecuencia, planear y escribir un programa de computadora es una tarea laboriosa, consume tiempo y requiere atención cuidadosa para cada detalle de las proposiciones del programa. Cuantas más proposiciones tenga el programa, mayores posibilidades de error existen. Cualquier cosa que pueda hacerse para eliminar proposiciones innecesarias o evite escribir la misma proposición más de una vez, vale la pena.

Muchos programas contienen cálculos que necesitan proposiciones sencillas o que requieren de un segmento de programa con muchas proposiciones para repetirse en ése programa o en programas relacionados. Semejantes rutinas de repetición pueden suprimirse del programa principal y escribirse en forma separada com osubprogramas. Despúes, ésos subprogramas pueden llamarse de un modo individual mediante una proposición sencilla colocada de manera apropiada en el programa principal siempre que se le necesite. El subprograma desarrollado por el programador sirve al mismo propósito para aplicaciones limitadas como las funciones intrínsecas más generalmente aplicables y puede grabarse para usos subsecuentes en otros programas.

3.7.- Almacenamiento y Compilación.

Algunos lenguajes, tal como el Fortran, son lenguajes compiladores, es decir, el programa fuente escrito por el programador debe traducirse (compilarse) a un código simbólico o lenguaje de máquina que sea comprensible para la computadora personal. Se requiere de un programa intermedio llamado compilador para hacer ésta operación. Hay diversos compiladores disponnibles. El compilador que se usó para la traducción (compilación) del programa ejemplo de éste segmento es el Compilador Microsoft Fortran.

El compilador MS-Fortran consiste en un conjunto de discos flexibles, guía del usuario y un manual de referencia que proporcionan información detallada de los archivos de los discos y la forma en que pueden aplicarse. En ésta sección se muestra de manera somera cómo se realiza la escritura, edición, compilación y ejecución de un programa fuente Fortran de ejemplo (consúltense la gúia y el manual del usuario para obtener un conocimiento más completo del compilador Fortran).

4.- Modelos Matemáticos.

4.1.- Qué es un Modelo Matemático.

Los modelos matemáticos en geohidrología son una importante herramienta que ayuda a conocer el funcionamiento de los acuíferos. Los modelos pueden utilizarse para simular el funcionamiento de un acuífero, inclusive cuando éste es complejo, incluyendo efectos producidos por barreras, la existencia de límites irregulares, la presencia de heterogeneidades en el subsuelo, etc. Se puede definir tanto el flujo del agua, como el transporte de contaminantes, así como el análisis de la deformación del terreno, como es su hundimiento.

Los modelos matemáticos son un valioso auxiliar en la planeación del manejo de acuíferos, al simular su comportamiento bajo diferentes políticas de operación.

Para la elaboración del modelo matemático de un acuífero, primeramente hay que conceptualizar su funcionamiento; el siguiente paso consiste en transcribir los procesos físicos a términos matemáticos, mediante el desarrollo de las ecuaciones que gobiernan el flujo de agua subterránea; son necesarios también la recopilación y depuración de datos del acuífero, su preparación o procesamiento, la calibración y la simulación.

Es indispensable tener una clara idea del funcionamiento del acuífero lo cual incluye, por una parte, las causas modificadoras del acuífero que corresponden a los medios de recarga y descarga. La recarga puede corresponder a la infiltración y la descarga a salidas por flujo subterráneo y a la extracción por bombeo. Las variaciones en la recarga y descarga dan fluctuaciones de la superficie piezométrica.

Ya conocido el funcionamiento del acuífero se transcriben los procesos físicos que rigen el funcionamiento de este a términos matemáticos mediante el desarrollo de ecuaciones que simulan el comportamiento del flujo de agua subterránea. El entendimiento de estas ecuaciones y sus limitaciones son condiciones necesarias para el buen desarrollo del modelo.

Otro punto por desarrollar en la formación de un modelo matemático es la obtención de las características del acuífero, tales como transmisividad, coeficiente de almacenamiento, espesor del acuífero, límites, gastos de extracción por pozos, etc. Estos datos deben de ser procesados y adaptados a los requerimientos del modelo. La calidad de este tipo de datos está en relación directa a la exactitud de los resultados que se obtengan.

El acuífero por estudiar se discretiza o se divide en pequeñas áreas denominadas elementos, las cuales pueden tener formas regulares o irregulares.

La malla regular, o de diferencias finitas, tiene la ventaja de que su construcción es simple, pudiendo consistir ésta de rectángulos. Las mallas pueden también ser irregulares (método de elementos finitos) y su diferencia fundamental respecto a la malla regular, es que al permitir el diseño de elementos irregulares llegan a representar los límites del acuífero con mayor exactitud. El trazo de la malla irregular es más complejo y las ecuaciones aplicables presentan limitantes. Para cada elemento discretizado, se aplican las ecuaciones de flujos, obteniéndose un sistema de ecuaciones simultáneas cuya incógnita es la carga hidráulica en un tiempo determinado.

La calibración consiste en efectuar corridas del programa matemático alimentado con los datos del acuífero, comparando los resultados con datos observados. En los sitios donde existen variaciones entre valores calculados y observados, se revisan los datos de entrada y se realizan ajustes para efectuar nuevas corridas, hasta lograr la mejor aproximación posible.

La primera corrida se conoce como "análisis de sensibilidad", en el cual se observan, en forma general, los resultados obtenidos. Posteriormente, se hace un "ajuste mayor" que consíste en efectuar los cambios necesarios en forma global dentro del modelo. Posteriormente se hacen "ajustes puntuales" a fin de llegar a la calibración del modelo.

Es importante que los ajustes que se realizen tengan justificación; ya que de otra manera se estará forzando al modelo a conclusiones y procedimientos erróneos.

4.2.- Herramientas Computacionales.

En el procesamiento de la evolución de los niveles piezométricos, o en los datos obtenidos de hidrógrafos y cualquier comportamiento que registre tendencia, se pueden realizar procedimientos de aproximación, por medio de métodos numéricos, con el auxilio que la computadora representa. A continuación se referirán distintas formas:

4.3.- Paquetes de Análisis.

Como se observa en una de las figuras anexas, es posible realizar análisis de aproximación por diferentes técnicas a través de programas tales como Harvard Graphics, Lotus 123, Excel, etc.

Además, se encuentran programas tales como Curfit, Mathematica, etc., que realizan análisis a funciones en general (se observa un ejemplo anexo).

4.4.- Lenguajes.

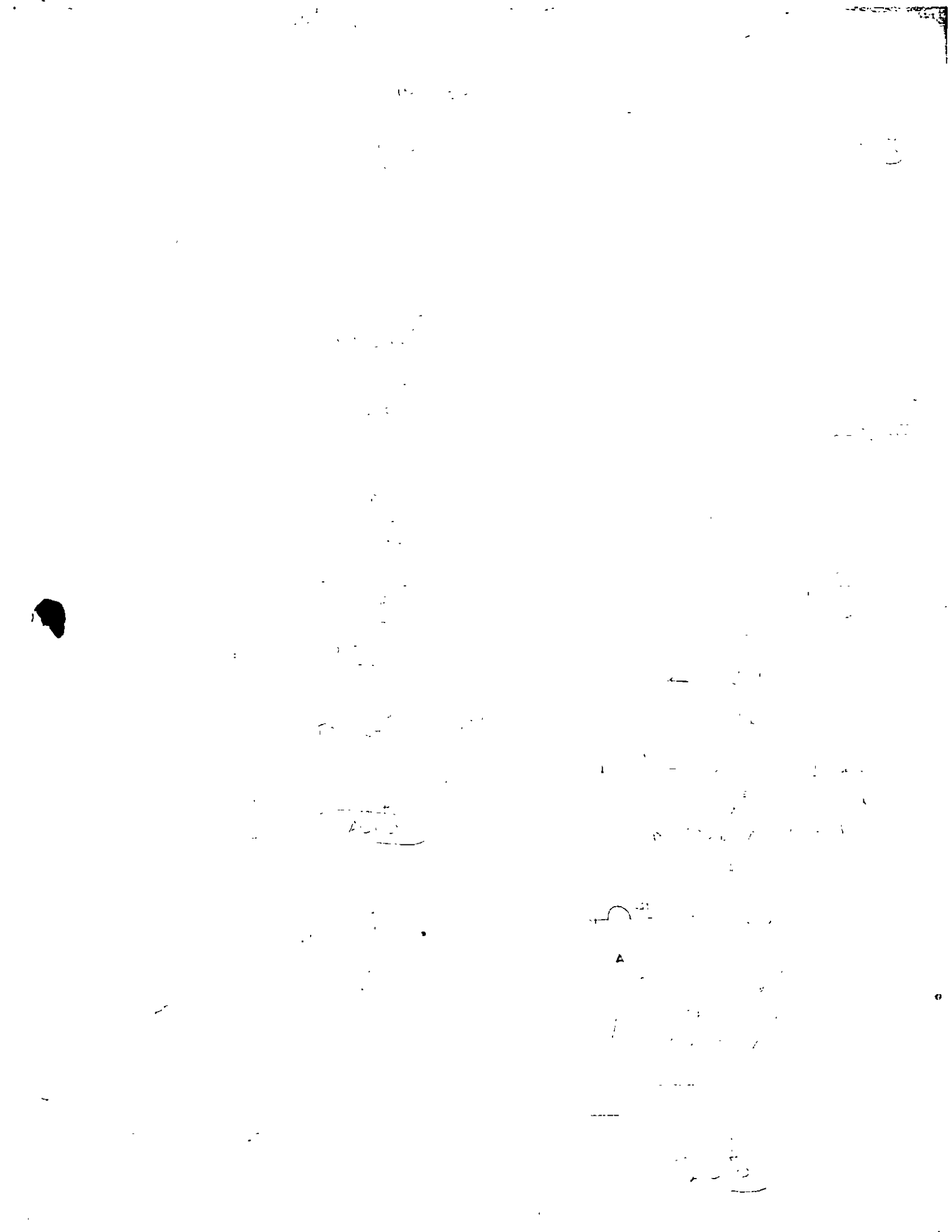
De manera similar, un ingeniero puede realizar programas de modelado en cualquiera de los lenguajes mencionados u otros.

En los Estados Unidos existen empresas que se dedican a la ingeniería de software especializado en geohidrología y contaminación de acuíferos, que trabajan con una alta calidad y resolución. En México, el Instituto de Ingeniería de la UNAM y otras instituciones de educación superior así como dependencias gubernamentales trabajan con gran éxito del modelado matemático de fenómenos de dispersión de contaminantes.

Elaboró: Ing. F. Meixueiro.

Figuras.

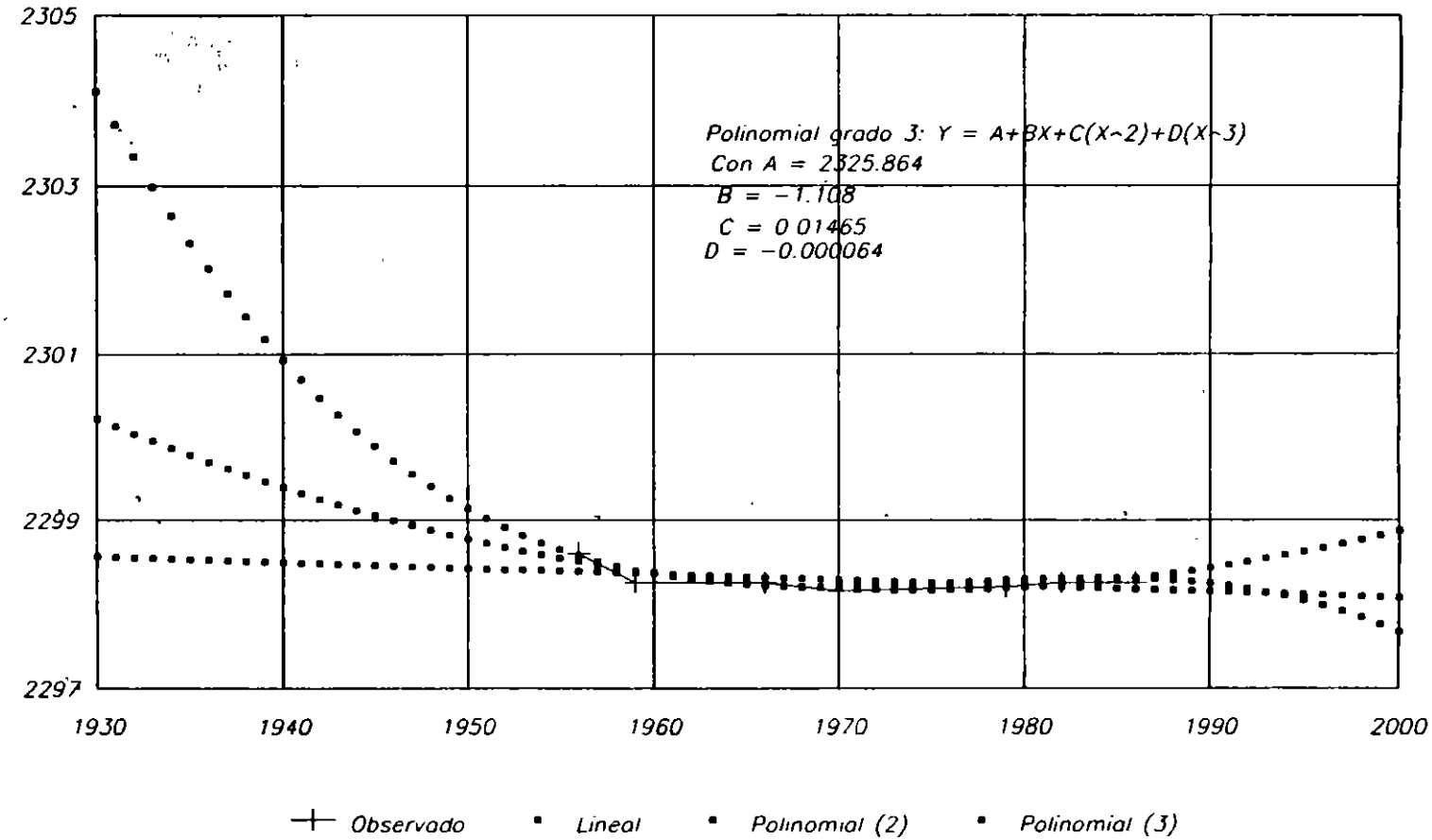
```
C     Programa de Demostración del Bubble Sort
C     Microsoft FORTRAN77
C     Agosto 29, 1993
C
C     La rutina principal lee de la terminal un vector
C     de diez números reales en formato F8.0 e invoca a
C     la subroutina BUBBLE para sortearlos.
C
      REAL R(10)
      INTEGER I
      WRITE (*,001)
  001 FORMAT(1X,'Programa de Demostración del Bubble Sort.')
  100 DO 103 I=1,10
      WRITE (*,101) I
  101 FORMAT(1X,'Anote el número real No. ',I2)
      READ (*,102) R(I)
  102 FORMAT(F8.0)
  103 CONTINUE
      CALL BUBBLE(R,10)
      WRITE (*,002)
  002 FORMAT(/1X,'Ya sorteados de menor a mayor quedan así:')
      WRITE (*,003) (R(I),I = 1,10)
  003 FORMAT(2(1x,5F13.3/))
      STOP
      END
C
C     Subroutina BUBBLE lleva a cabo un sorteo tipo bubble sobre un vector
C     unidimensional de longitud arbitraria.  Sortea al vector
C     en orden ascendente.
      SUBROUTINE BUBBLE(X,J)
      INTEGER J,A1,A2
      REAL X(J),TEMP
  100 IF (J .LE. 1) GOTO 101
  200 DO 201 A1 = 1,J-1
  300 DO 301 A2 = A1 + 1,J
  400 IF (X(A1) .LE. X(A2)) GOTO 401
      TEMP = X(A1)
      X(A1) = X(A2)
      X(A2) = TEMP
  401 CONTINUE
  301 CONTINUE
  201 CONTINUE
  101 CONTINUE
      RETURN
      END
```



Análisis de Optimización.

Hundimiento del Terreno.

Elemento 23



Manual de Hundimientos.
D.G.C.O.H.
Elaboró: F. Meixueiro.

Polinomial grado 2: Y = A+B•X+C•(X~2)
con A= 2303.974
B = −0.157
C = 0 00106

Lineal: Y = A + B•X
Con A = 2298 772
B = −0 00693

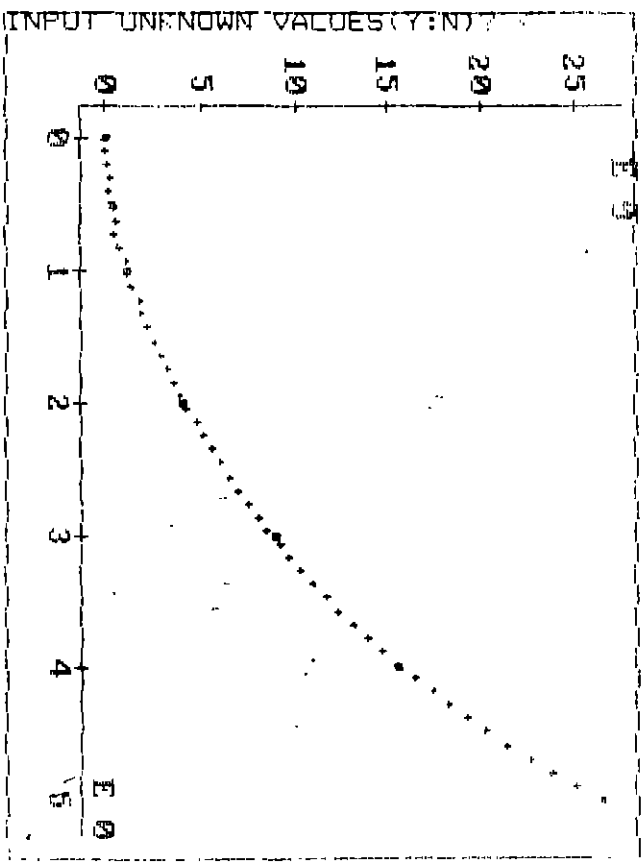
54

0 DEGREE COEFFICIENT= 1.828251174120139D-02
1 DEGREE COEFFICIENT=-.2780627554617205
2 DEGREE COEFFICIENT= 1.549968468439403
3 DEGREE COEFFICIENT=-.2807522906759306
4 DEGREE COEFFICIENT= 3.840469402319421D-02

FITTED EQUATION IS
Y = A + B*X + C*(X^2) + D*(X^3) + E*(X^4)

#	X VALUE	Y VALUE	Y CALC	%DEV
1	0	0	1.828251E-02	[illegible]
2	.5	.25	.2340495	-6.82
3	1	1.1	1.047841	-4.78
4	2	3.9	4.030488	+3.34
5	3	8.8	8.664279	-1.52
6	4	15.5	15.56898	+0.44
7	5	26.3	26.28608	-0.05

COEFFICIENT OF DETERMINATION = .9999247
COEFFICIENT OF CORRELATION = .9999623
STANDARD ERROR OF ESTIMATE = .1478324890398677
SATISFACTORY(Y:N)? Y
INPUT UNKNOWN VALUES(Y:N)?



FACULTAD DE INGENIERIA U.N.A.M.
DIVISION DE EDUCACION CONTINUA

C U R S O S A B I E R T O S .

VII CURSO INTERNACIONAL DE CONTAMINACION DE ACUIFEROS

MODULO III: MODELOS EN GEOHIDROLOGIA Y CONTAMINACION DE ACUIFEROS.

TEMA: S U R F E R .

EXPOSITOR: ING. FEDERICO MAIXUEIRO TREJO.

VII CURSO INTERACIONAL DE CONTAMINACION DE ACUIFEROS
MODULO III: Modelos Matemáticos en Geohidrología.

Tema: **SURFER.**

1.- Introducción.

El programa SURFER, versión 3.0, generado por Golden Software, Inc. se presenta en éste módulo como una herramienta indispensable para la ingeniería, por su capacidad de convertir una matriz de vectores de posición tridimensional, en un mapa de contorno o en una representacion de superficie tridimensional, para su almacenamiento en disco, para su presentación o para una impresión en dispositivo externo.

El programa SURFER viene equipado con una serie de herramientas, accesorios, tipos de letra, utilerías y un programa de acceso a los 5 programas que conforman el núcleo principal del SURFER.

Tales programas son:

a) Utilerías:

ALTERSYM.EXE	Programa de modificación de los juegos de símbolos (Symbol Set).
CONVERT.EXE	Convierte archivos .PLT de versiones anteriores a la 2.0
GRAFIT.EXE	Generador de gráficos por medio de una hoja electrónica de gran simplicidad para salida en formato .PLT.
GRIDCONV.EXE	Convierte mallas (grids) del Microsoft Basic al formato IEEE.
INSTALL.EXE	Programa de configuración de dispositivos externos.
SLICE.EXE	Programa que genera, una vez proporcionada una superficie producida por el programa GRID y una linea de frontera (formato .BLN), las elevaciones en las intersecciones de la malla (grid) con la línea de frontera (boundary line).
VOLUME.EXE	Programa que evalúa volúmenes por medio de dos procedimientos de cálculo integral (regla del trapezoide y regla de Simpson).

b) Programas-Núcleo:

SURFER.EXE	Sistema de acceso por medio de menús para accesar los múltiples programas y utilerías del SURFER.
GRID.EXE	Crea una malla regularmente espaciada a partir de datos irregularmente espaciados o por medio de una función definida por el usuario.
TOPO.EXE	Crea mapas de contorno a partir de archivos de malla generados por GRID.
SURF.EXE	Crea trazos de superficie tridimensional a partir de un archivo de malla generado por GRID.
VIEW.EXE	Muestra un archivo de impresión (plot) generado a partir de TOPO o SURF. El diagrama puede ser modificado dimensionalmente (pan y zoom).
PLOT.EXE	Programa que manda a impresión un archivo generado por TOPO o SURF. También puede configurarse para mandar la impresión a un archivo.

2.- Programa GRID.

2.1.- Generalidades.

Como ya se mencionó anteriormente, el programa GRID genera archivos (en formato binario o ascii) para ser leídos por porciones de código subsecuentes, con otras funciones colaterales.

El programa contiene opciones relativa a la creación de una malla a partir de una matriz de vectores de posición (asociados a un sistema rectangular de coordenadas), generada de manera irregular o a través de una función matemática.

Por ejemplo, el programa GRID podrá procesar ternas de valores reales o enteros y asociarlos internamente con un vector de posición en un sistema coordenado rectangular XYZ. De igual manera, podrá hacer uso de un sencillo editor de ecuaciones de dos variables para generar las ternas de posición; así que podrá definir una función continua $z = f(x,y)$.

Usualmente el primer paso consiste en incorporar ternas al programa GRID. La opción Input aceptará datos tanto del teclado como de diferentes tipos de archivos de datos. Después de aceptados los datos, las otras opciones del menú consisten en controlar el proceso de generación de malla regularmente espaciada.

2.2.- Métodos de Generación de la Malla.

El programa proporciona dos métodos diferentes de generación de una malla regularmente espaciada, el método del inverso de la distancia y el método Kriging. El método del inverso de la distancia es más rápido pero no representa los datos originales tan precisamente como el Kriging.

El método del inverso de la distancia utiliza una técnica de promedio ponderado para interpolar los nodos de la malla a partir de los vectores de posición. Las influencias son inversamente proporcionales a las distancias a los nodos. Además, las influencias pueden elevarse a una potencia para incrementar el efecto de la función ponderadora. El inverso de la distancia al cuadrado es el método más común.

El método del Kriging utiliza técnicas geoestadísticas para calcular la autocorrelación entre puntos y producir una mínima e imparcial variancia estimada. En teoría ningún otro método de generación de mallas puede producir estimados más precisos. En práctica, la efectividad del método del Kriging depende de la correcta selección de varios parámetros. Tales parámetros son estimados por el GRID y pueden no ser exactos. Aún así, el Kriging produce mapas más precisos que los generados a través del método del inverso de la distancia.

2.3.- Métodos de Normalización de la Malla.

El programa proporciona dos métodos de normalización o uniformización de las mallas generadas, el método matricial y el método de ajuste.

El método de normalización matricial evalúa una matriz de normalización sobre la malla existente para promediar aquellos puntos de la malla más cercanos a cada punto de la malla que va a normalizarse. La matriz se especifica por el número de columnas y de renglones a cada lado del punto de la malla a normalizarse, así como la influencia al punto central de la matriz.

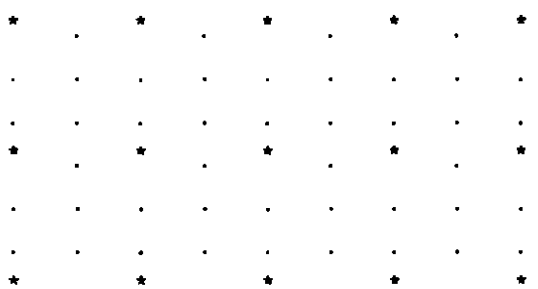
	1	2	3	4	5	6	7
1	+	+	+	+	+	+	+
2	+	x	x	x	x	x	+
3	+	x	x	o	x	x	+
4	+	x	x	x	x	x	+
5	+	+	+	+	+	+	+

En el ejemplo anterior, los signos + representan los nodos de la malla, mientras que las x y las o representan a la matriz de normalización. La malla es de 5 renglones por 7 columnas, mientras que la matriz de normalización es de 3 renglones por 5 columnas. El nodo de la malla que está siendo normalizado está en el renglón 3 y la columna 4.

Cada nodo de la malla bajo una x será ponderado por el valor de la matriz de normalización y promediado para obtener un nuevo valor para el nodo central de la malla. La matriz cambiará por ello y el proceso se repetirá hasta que la malla entera se normalice. Nótese que las orilla de la malla no están definidas y quedarán sin cambio.

Para una normalización ponderada no por la distancia, los nodos x tendrán una influencia de 1.0 y el nodo o se le asignará como el punto central de la influencia. En la normalización basada en la distancia, se le asignarán influencias a cada x basadas en el inverso de la distancia al centro, elevadas a la correspondiente potencia.

En el método de ajuste, la normalización se basa en el ajuste a través de un polinomio de grado cúbico para interpolar nuevos valores entre nodos existentes de la malla. Esto incrementa la densidad de la malla permitiendo contornos y superficies más suaves. Los factores de expansión en X y en Y se refieren al número de puntos a insertar entre los nodos existentes en las direcciones X y Y respectivamente. Este tipo de normalización podría incrementar las bajas y altas de la malla original.



En el ejemplo anterior, los asteriscos representan la malla original de 3 por 5. Los nodos representados por los puntos fueron interpolados usando una normalización por medio de un ajuste a una curva polinomial cúbica. 1 puntos fué calculado entre cada nodo en la dirección X y 2 puntos fueron calculados entre cada nodo en la dirección Y, para arrojar una malla final de 7 renglones por 9 columnas.

3.- Programa TOPO.

El programa TOPO es un generador de contornos que funciona por medio de menús. El trazo del contorno puede observarse en el monitor de la computadora, mandarse a impresión o mandarse a un archivo. Los parámetros de generación del mapa de contorno y de impresión pueden controlarse en su totalidad por el usuario.

Los datos de la malla deberán estar en el formato utilizado por el programa GRID, el cual está en formato ascii o en binario. El acceso al programa TOPO podrá ser desde la línea de comandos del DOS o desde el menú del SURFER.

4.- Programa SURF.

Este programa es un programa interactivo, controlado por menús que produce representaciones de superficies tridimensionales para su salida a la pantalla, impresora, plotter o archivo. La entrada para éste programa está conformada por los archivos de extensión .GRD generados por el GRID en base a datos proporcionados por el usuario.

A semejanza del TOPO, el SURF contiene una gran cantidad de opciones alternas, como ejes, colores, títulos, complementación con otros gráficos, opciones de control de generado de superficies y muchas otras opciones.

5.- Programa VIEW.

El programa VIEW es un subprograma que le permite observar detalles del gráfico generado (mediante sencillos comandos de "zoom" y "pan"), así como permitir la generación por pasos. Esto és, observar mediante control del usuario, la generación de las líneas que componen el trazo.

Este programa acepta archivos de extensión .PLT y no genera nada.

5.- Programa PLOT.

Este subprograma genera salidas a impresora, plotter o archivo previo procedimiento de "optimización", convirtiendo el archivo de salida .PLT generado por TOPO o SURF en un archivo .OPT, preparado para la impresora o dispositivo especificado en la configuración del programa PLOT.

Dentro del programa PLOT se pueden controlar varios parámetros, tales como factores de escala, posición del gráfico dentro de la página, el formato del archivo, el número de dígitos de exactitud del trazado, etc.

APENDICES.

Apéndice 1.- Tipos de Archivos que Maneja el SURFER.

El SURFER trabaja con una serie de archivos, formateados para una función específica; tales archivos son diferenciados internamente mediante una extensión característica. En la tabla siguiente se muestran tales extensiones con una breve descripción de los archivos, así como su génesis y utilización.

Extensión	Uso
.PLT	Archivos de trazo (plot) de cualquier índole, bien generados por TOPO como por SURF. Son leídos por PLOT o dentro de las utilerías de impresión de TOPO o de SURF (que no son sino llamadas a PLOT), para ser procesados.
.OPT	Archivos de optimización para impresión. Son procesados por PLOT y listos para su envío a los dispositivos generadores de impresión.
.SYM	Archivo que contiene un juego de caracteres en un determinado tipo de letra. Pueden crearse y editarse mediante utilerías.
.BLN	Archivo que contiene las denominadas "líneas de frontera", que pueden ser en código ascii y que representan un polígono bidimensional que se implanta en un mapa de contorno o en la generación de una superficie. Puede generarse externamente al SURFER.
.DAT	Archivo que contiene datos (vectores de posición, localización de puntos, datos para un contorno o vértices de un polígono); puede estar en ascii o en binario. Este tipo de archivos son leídos por GRID, SURF y TOPO.
.GRD	Archivos que contienen (en ascii o en binario) la malla regularmente espaciada que será leída por TOPO o por SURF y que es generada únicamente por el GRID.

Apéndice 2.- Menús de Ayuda.

Todos los programas del SURFER (programas-núcleo) contienen un menú de ayuda (tecleando F1), así como una ayuda sensitiva al contexto.

A pesar de que el programa se encuentra en una versión bastante primitiva, las ayudas se presentan medianamente inteligibles, para el usuario latinoamericano con conocimiento regular del inglés técnico.

Apéndice 3.- Requerimientos para el SURFER.

El SURFER puede copiarse íntegramente en un disco de 3.5 pulg. de alta densidad (1.44 Mb) y ejecutarse en la unidad de disco flexible de cualquier computadora serie 286 y posterior sin ninguna dificultad. Tal computadora de preferencia deberá contar con 1.0 Mb o más de memoria RAM.

Probablemente no tendrá usted problemas para desplegar sus diagramas en el monitor, puesto que entre las versiones de configuración que el SURFER presenta, se contempla un driver automático de detección de modo de video, así como los drivers típicos para los modos CGA, EGA y VGA, así como para los modos Hércules y Olivetti.

Esta versión no soporta (que lástima), mouses ni tabletas digitalizadoras.

De igual manera, en el programa INSTALL de esta versión, se contemplan 84 impresoras y plotters de las más variadas marcas, incluyendo las impresoras Epson, Okidata, Star, Hewlett Packard, tanto de matriz como láser, aunque de manera bastante general. Así mismo, se presentan opciones para puertos de salida, serial o paralelo, la velocidad de transmisión para el puerto serial y la elección de plumas para los plotters.

SURFER

[Main Menu] GRID TOPO SURF VIEW PLOT Quit
Run the TOPO program to create a contour map from a grid file

The SURFER Access system provides an easy, menu-driven way to access the SURFER programs and utilities. Options may be selected by moving the highlighted pointer with the arrow keys to the selection you want and then pressing the Enter key. Options may also be selected by typing the first letter of the option name. Here is a summary of the current options:

GRID	Creates a regularly spaced grid of data from irregularly spaced data or a user specified function.
TOPO	Creates contour maps from a grid created with GRID.
SURF	Creates surface plots from a grid created with GRID.
VIEW	Views a plot created with TOPO or SURF on the screen. Plots may be panned and zoomed.
PLOT	Sends a plot created with TOPO or SURF to a hardcopy device. To install a new device enter /I at the filespec prompt.

To obtain more help select the desired option, and then use the F1 key. This access system requires approximately 10K of memory. If insufficient memory messages occur, the above options may be run directly from DOS to save the 10K.
Press any key to continue...

F1=Help Esc=Backup Arrows keys move pointer

GRID

[Help System] Help Keys Menus Equations CmdLine GridIO Format Prev Next
How to use the HELP system

Random Menu

The Random menu contains all options related to creating a grid from random or irregularly spaced XYZ data. Each data point consists of 3 values: an X,Y, and Z coordinate. See the GRID manual for examples of randomly spaced data.

Usually the first step is to get the XYZ data into GRID. The Input option will accept data from the keyboard or from several different types of data files. After the data is entered, the other options in the Random menu are used to control the gridding process.

Output assigns a name to the output grid file. Duplicate tells GRID how to handle points with identical XY coordinates. GridSize specifies the size or density of the final grid. In general, the denser the grid, the smoother and more detailed the final plots will be. Method allows the user to specify the gridding method to use. See the GRID manual for a discussion of the merits of the various gridding techniques. Search will set the parameters used to search for data points during the gridding process. Limits specifies the coordinates of the edge of the grid. Begin is used to begin creating the grid after all the above parameters have been set to their desired values.

Method Menu

There are currently two different gridding methods available; Inverse distance and Kriging. Inverse distance is faster but does not represent the original data as accurately as Kriging.

Inverse distance uses a weighted averaging technique to interpolate grid nodes from the XYZ data. The weights are inversely proportional to the distance to the grid node. Data points further away from a given grid node will have less influence. In addition, the weights may be raised to a power to increase the effect of the weighting function. Inverse distance squared is the most common weighting power.

Kriging uses geostatistical techniques to calculate the autocorrelation between data points and produce a minimum variance unbiased estimate. In theory, no other gridding method can produce more accurate estimates. In practice, the effectiveness of kriging depends upon proper selection of various parameters. These parameters are estimated by GRID and may not be exact. Even so, Kriging produces much more accurate maps than Inverse Distance. See the GRID manual for more information about these methods.

Matrix Smoothing

Matrix smoothing passes a smoothing matrix over an existing grid to average those grid points nearest each grid point to be smoothed. The matrix is specified by the number of columns and rows on either side of the grid point to be smoothed, and the weight of the center point of the matrix.

```
  1 2 3 4 5 6 7
1 + + + + + + +
2 + x x x x x +
3 + x x o x x +
4 + x x x x x +
5 + + + + + + +
```

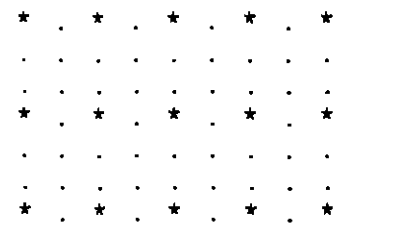
In the example at left, + signs represent grid nodes, while x's and the o represent the smoothing matrix. The grid is 5 rows by 7 columns, the smoothing matrix is 3 rows by 5 columns. The grid node currently being smoothed is row 3 column 4. Each grid node under an x will be weighted by the value of the smoothing matrix and averaged in to obtain a new value for the center grid node. The matrix will then be shifted and the process repeated until the entire grid is smoothed. Notice that the edges of the grid are undefined and will be blanked.

For non-distance weighted smoothing, the x nodes will have a weight of 1.0 and the o node will be assigned the center point weight. Distance weighted smoothing will assign weights to each x based on the inverse of the distance to the center raised to a specified power.

Spline Smoothing

Spline smoothing fits a cubic spline to an existing grid to interpolate new values between existing grid nodes. This increases the density of the grid allowing smoother contours and surfaces. The X and Y expansion factors refer to

the number of points to insert between existing grid nodes in the X and Y directions respectively. Spline smoothing may increase the highs and lows of the original grid.



In the example at right, the asterisks represent the original 3 by 5 grid. The nodes represented by the dots were interpolated using cubic spline smoothing. 1 point was calculated between each node in the X direction, and 2 points were calculated between each node in the Y direction to give a final grid of 7 rows by 9 columns.

TOPO

[Help System] Help Keys Menus Symbols CmdLine Viewing Format Prev Next
How to use the HELP system

TOPO Menu

TOPO is a menu-driven contouring program. The contour plot may be viewed on the screen, output to a plot file, and/or sent to a hardcopy device. Contour and plot parameters may be default values or fully specified by the user.

Gridded data, in the format used by the GRID program, is input from a data file in either ASCII or binary format. The fastest way to view a contour map on a graphics screen from DOS is to type the command

TOPO filename

and press function key F2. filename is any grid file produced by the GRID program, and may include an optional drive and path. If the extension is omitted, .GRD will be used. The contour plot will appear on the screen using default values for the contour and plot parameters. To modify the default values press Esc to return to the TOPO Menu.

Level

The values of the contour lines may be changed by specifying the minimum, maximum, and interval values, or by specifying a data file containing the contour levels desired. The default values are chosen to give between 11 and 21 contours.

Minimum contour	The lowest contour level to apper on the map.
Maximum contour	The highest contour level to appear on the map.
Contour interval	The interval or stepsize to use between the minimum and maximum contour levels. The total number of levels plotted will be int((Maximum - Minimum) / Interval). To omit all contour lines specify minimum and maximum contour levels that will exclude all Z values of the grid.
Level file	The level file must be a valid DOS filespec consisting of an optional drive, optional path, filename, and optional extension. If the extension is omitted, .DAT is used. The level file is an ASCII data file with one contour level per line. There is a maximum of 200 levels if a level file is used. The levels do not need to be in any order, and do not need to be evenly spaced.

SURF

[Help System] Help Keys Menus Symbols CmdLine Viewing Format Prev Next
How to use the HELP system

SURF Menu

SURF is an interactive, menu-driven graphics program that produces three dimensional surface representations for output to the screen, printer, or plotter. Gridded data, in the format used by the GRID program, is input from a data file in either ASCII or binary format. The fastest way to view a plot on a graphics screen from DOS is to type the command

SURF filename

and press function key F2. filename is any grid file produced by the GRID program, and may include an optional drive and path. If the extension is omitted, .GRD will be used. The surface plot will appear on the screen using default values for the contour and plot parameters. To modify the default values press Esc to return to the Main Menu.

View (Page 1 of 2)

Projection Orthographic projection is better when measurements are to be taken off the surface. Parallel lines will remain parallel. The perspective projection creates a visual effect similar to that of the human eye. Parallel lines appear to converge at a distance similar to railroad tracks at the horizon.

Rotation This is the number of degrees from the positive X axis. The surface appears to rotate clockwise, or equivalently, the viewer's eye appears to rotate counter-clockwise. 0=looking west, 90=south, 180=east, 270=north.

Tilt Tilt specifies the angle, above or below the X-Y plane, from which the surface is to be viewed. The default of 30 degrees puts the viewer's eye 30 degrees above the plane.

<Select Next for more help on View>

PLOT

Output

Create a plot file of the current surface plot. Optionally, send output to a printer or plotter via the PLOT program.

Name of plot file	Specify the optional drive, optional path, filename, and optional extension of the plot file to create.
Scale factor	Scale factor for the entire plot. For example, 2.0 will make the plot twice as big.
Page position	Position of the entire plot in inches, from the bottom left corner. May be used to offset multiple plots when appending.
Plot file format	ASCII may be read by any text editor. Binary is efficient.
File write mode	Overwrite will cause the plot to be written over any old information in the file (hence destroying it). Append will write the current plot at the end of the specified plot file. If the plot file does not exist, a new one will be created.
Number of decimal digits in file	Accuracy in decimal digits of values in the plot file. This value should reflect the resolution of the output device.
Send plot to installed device	Answer Yes to call program PLOT from within SURF. PLOT immediately begins plotting on the installed printer or plotter. Be sure to install PLOT first.

Symbol sets

The following Symbol sets are available. The sets may be altered using the ALTERSYM program.

DEFAULT.SYM	Built in to TOPO	SET10.SYM	Triplex Roman
SET1.SYM	Same as default	SET11.SYM	Triplex Italics
SET2.SYM	Simplex Greek	SET12.SYM	Old German
SET3.SYM	Script	SET13.SYM	Olde English
SET4.SYM	Simplex Roman	SET14.SYM	Old Italian
SET5.SYM	Duplex Greek	SET15.SYM	Special Symbols
SET6.SYM	Simplex Italics	SET16.SYM	Special Symbols
SET7.SYM	Duplex Hershey	CENTERED.SYM	Centered Symbols
SET8.SYM	Duplex Script		
SET9.SYM	Cyrillic		

For math symbols, use SET15 and SET16. The DEFAULT symbol set contains both centered symbols, and a complete character set. Since this is built in to TOPO, it does not need to be loaded and will plot faster. If a plot file is to be created, CENTERED.SYM will be substituted for DEFAULT.SYM for the posting centered symbol set.

SLICE Documentation:

SCRIPTION

Given a surface (represented by a .GRD file produced by the GRID program) and a "boundary line", such as may be found in a .BLN boundary file used by GRID, TOPO or SURF, SLICE will produce the elevation at each grid-line crossing by the boundary line. If the line extends outside of the grid area, it may be clipped.

The user may select output files in two formats:

1.) BOUNDARY (.BLN) FILE OUTPUT

The .BLN file produced by SLICE is similar to the .BLN format used by GRID, TOPO and SURF. The .BLN file is used by SURF to plot, for example, a highway on a surface plot. When SLICE generates a .BLN file, the first two columns have the X and Y's where the 'slice' intersected a grid line. A third column has the Z elevation at each of the XY coordinates. The third column is not intended for a specific purpose.

2.) DATA (.DAT) FILE OUTPUT

The .DAT file produced by SLICE is used by GRAPHER to plot the Z elevation of the boundary line on an XY type graph. The .DAT file's first three columns are the same as the .BLN file. A fourth column is the (accumulated) distance measured (horizontally) from the beginning of the boundary line. It does not take elevation change into account. This distance is accumulated even if the line leaves the grid region and is clipped. The distance starts over at zero for each new input boundary line. Use the fourth column in plotting elevation against traversed distance. A fifth column is the number of the input boundary, starting at 1. Use the fifth column to identify the start of a new boundary. Alternatively, at the start of each new boundary line after the first, the user is given the choice of specifying a new .DAT file.

Two clip options are allowed:

1.) The first option asks:

Insert clipping value whenever boundary line exits region?

Answer Yes to allow GRAPHER to leave gaps in the XY graph whenever the boundary line leaves the edge of the grid. When the boundary line leaves the grid, a value is inserted into the third column of the .DAT file which is less than the minimum Z value for the entire grid. If GRAPHER's data is clipped, then the plot will show gaps whenever the boundary line leaves the grid.

2.) The second option asks:

Use clipping value over blanked areas?

Answer Yes to allow GRAPHER to leave gaps in the XY graph line whenever the boundary line enters a grid area that has been blanked. If No is answered, then those values will be omitted from the .DAT file.

Tópicos Relacionados con la Evaluación de Volúmenes.

1.- Cálculo de integrales.

Aunque la existencia de la integral de una función continua se asegura fácilmente por medio de la aplicación de los teoremas fundamentales del cálculo, la evaluación o "cuadratura" de dicha integral no puede realizarse mediante funciones elementales, salvo en casoso relativamente raros. Deberán desarrollarse, por consiguiente, métodos de integración numérica y también de estimación de la exactitud de tales aproximaciones numéricas.

Para calcular en forma aproximada la integral

$$J = \int_a^b f(x)\ dx$$

con $a < b$, se subdivide el intervalo $a \leq x \leq b$ en n partes iguales, cada una de longitud $h = (b-a)/n$, mediante los $n+1$ puntos

$$x_v = a + vh, \quad nh = b - a, \quad v = 0, 1, \ldots\ldots\ldots\ldots\ldots, n.$$

Entonces,

$$J = \sum_{v=1}^{n} J_v$$

donde

$$J_v = \int_{x_{v-1}}^{x_v} f(x)\ dx$$

El problema de calcular la integral J queda reducido al de obtener buenas aproximaciones para las áreas J_v de anchura h en las cuales se ha dividido el área total representada por J.

1.1.- Aproximación mediante rectángulos

La aproximación más directa, sugerida por la definición original de la integral, conduce a la relación

$$J = \sum_{v=1}^{n} J_v \approx h(f_1 + f_2 + \ldots\ldots\ldots + f_n)$$

donde por brevedad, se ha hecho

$$f_v = f(x_v)$$

1.2.- Aproximaciones refinadas - Regla de Simpson.

Una mejor aproximación se obtiene casi sin esfuerzo adicional si las áreas J_v se aproximan, no mediante franjas rectangulares, sino mediante trapezoides angostos. La fórmula de aproximación (fórmula del trapezoide) es entonces

$$J \approx \frac{1}{2}h(f_0+f_1) + \frac{1}{2}h(f_1+f_2) + \ldots\ldots\ldots + \frac{1}{2}h(f_{n-1}+f_n)$$

$$= h\,(f_1+f_2+\ldots\ldots+f_{n-1}) + \frac{h}{2}\,(f_0+f_n)$$

pues cada valor de la función, excepto el primero y el último, aparece dos veces.

Finalmente, se menciona la famosa aproximación de Simpson, la cual, con poco mayor trabajo conduce a una aproximación mucho más precisa si la cuarta derivada de f existe y es uniformemente acotada en el intervalo dado.

La fórmula de Simpson para n = 2m es

$$J \approx \frac{4h}{3}\,(f_1+f_3+f_5+\ldots+f_{2m-1}) + \frac{2h}{3}\,(f_2+f_4+f_6+\ldots+f_{2m-2}) + \frac{h}{3}\,(f_0+f_{2m})$$

Tomado de:

R. Courant y F. John.
"Introducción al Cálculo y al Análisis Matemático", Vol. I.
Cap. 6, Métodos Numéricos. pp. 501-505.
Ed. Limusa, México, 1971, 1ª Ed.

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VII CURSO INTERNACIONAL DE CONTAMINACION DE ACUIFEROS

MODULO III: MODELOS EN GEOHIDROLOGIA Y CONTAMINACION DE ACUIFEROS

A N E X O

ING. FERNANDO LOSA

DEPARTMENT OF THE INTERIOR

WILLIAM P. CLARK, Secretary

U.S. GEOLOGICAL SURVEY

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scripts and nodal indices, the latter are separated by commas.

The finite-difference equation (eq 11) is solved numerically for each node in the grid using an iterative alternating-direction implicit (ADI) procedure. The derivation and solution of the finite-difference equation and the use of the iterative ADI procedure have been previously discussed in detail in the literature. Some of the more relevant references include Pinder and Bredehoeft (1968), Prickett and Lonnquist (1971), and Trescott, Pinder, and Larson (1976).

After the head distribution has been computed for a given time step, the velocity of ground-water flow is computed at each node using an explicit finite-difference form of equation 3. For example, the velocity in the x direction at node (i,j) would be computed as

$$V_{x(i,j)} = \frac{K_{xx(i,j)}}{\epsilon} \frac{(h_{i-1,j,k} - h_{i+1,j,k})}{2\Delta x}. \quad (12)$$

The velocity in the x direction can also be computed on the boundary between node (i,j) and node $(i+1,j)$ using the following equation:

$$V_{x(i+\frac{1}{2},j)} = \frac{K_{xx(i+\frac{1}{2},j)}}{\epsilon} \frac{(h_{i,j,k} - h_{i+1,j,k})}{\Delta x} \quad (13)$$

where the hydraulic conductivity on the boundary is computed as the harmonic mean of the hydraulic conductivities at the two adjacent nodes.

Expressions similar to equations 12 and 13 are used to compute the velocities in the y direction at (i,j) and $(i,j+\frac{1}{2})$ respectively. Note that equation 13, which computes the head difference over a distance Δx, is more accurate than equation 12, which computes the head difference over $2\Delta x$.

Transport equation

Method of characteristics

The method of characteristics is used in this model to solve the solute-transport equation. This method was developed to solve hyperbolic differential equations. If solute transport is dominated by convective transport, as is common in many field problems, then equation 4 may closely approximate a hyperbolic partial differential equation and be highly compatible with the method of characteristics. Although it is difficult to present a rigorous mathematical proof for this numerical scheme, it has been successfully applied to a variety of field problems. The development of this technique for problems of flow through porous media has been presented by Garder, Peaceman, and Pozzi (1964), Pinder and Cooper (1970), Reddell and Sunada (1970), and Bredehoeft and Pinder (1973). Garder, Peaceman, and Pozzi (1964) state that this technique does not introduce numerical dispersion (artificial dispersion resulting from the numerical calculation process). They and Reddell and Sunada (1970) also compared solutions obtained using the method of characteristics with those derived by analytical methods and found good agreement for the cases investigated. Applications of the method to field problems have been documented by Bredehoeft and Pinder (1973), Konikow and Bredehoeft (1974), Robertson (1974), Robson (1974), and Konikow (1977).

The approach taken by the method of characteristics is not to solve equation 4 directly, but rather to solve an equivalent system of ordinary differential equations. Konikow and Grove (1977, eq 61) show that by considering saturated thickness as a variable and by expanding the convective transport term, equation 4 may be rewritten as

$$\frac{\partial C}{\partial t} = \frac{1}{b}\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right) - V_i\frac{\partial C}{\partial x_i} + \frac{C\left(S\frac{\partial h}{\partial t} + W - \epsilon\frac{\partial b}{\partial t}\right) - C'W}{\epsilon b}. \quad (14)$$

Equation 14 is the form of the solute-transport equation that is solved in the computer program presented in this report. For convenience we may also write equation 14 as

$$\frac{\partial C}{\partial t} = \frac{1}{b}\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right) - V_x\frac{\partial C}{\partial x} - V_y\frac{\partial C}{\partial y} + F \quad (15)$$

where

$$F=\frac{C(S\frac{\partial h}{\partial t}+W-\epsilon\frac{\partial b}{\partial t})-C'W}{\epsilon b}. \quad (16)$$

Next consider representative fluid particles that are convected with flowing ground water. Note that changes with time in properties of the fluid, such as concentration, may be described either for fixed points within a stationary coordinate system as successive fluid particles pass the reference points, or for reference fluid particles as they move along their respective paths past fixed points in space. Aris (1962, p. 78) states that "associated with these two descriptions are two derivatives with respect to time." Thus $\partial C/\partial t$ is the rate of change of concentration as observed from a fixed point, whereas dC/dt is the rate of change as observed when moving with the fluid particle. Aris (1962) calls the latter the *material derivative*.

The material derivative of concentration may be defined as

$$\frac{dC}{dt}=\frac{\partial C}{\partial t}+\frac{\partial C}{\partial x}\frac{dx}{dt}+\frac{\partial C}{\partial y}\frac{dy}{dt}. \quad (17)$$

Note the correspondence of the second and third terms on the right side of equation 15 with the second and third terms on the right side of equation 17. The latter includes the material derivatives of position, which are defined by velocity. Thus for the x and y components, respectively, of position and velocity we have

$$\frac{dx}{dt}=V_x \quad (18)$$

and

$$\frac{dy}{dt}=V_y. \quad (19)$$

If we next substitute the right sides of equations 15, 18, and 19 for the corresponding terms in equation 17, we obtain

$$\frac{dC}{dt}=\frac{1}{b}\frac{\partial}{\partial x_i}(bD_{ij}\frac{\partial C}{\partial x_j})+F. \quad (20)$$

The solutions of the system of equations comprising equations 18–20 may be given as

$$x=x(t)\,;\ y=y(t)\,;\ \text{and}\ C=C(t) \quad (21)$$

and are called the characteristic curves of equation 15.

Given solutions to equations 18–20, a solution to the partial differential equation (eq 15) may be obtained by following the characteristic curves. This is accomplished numerically by introducing a set of moving points (or reference particles) that can be traced within the stationary coordinates of the finite-difference grid. Garder, Peaceman, and Pozzi (1964, p. 27) state, "Each point corresponds to one characteristic curve, and values of x, y, and C are obtained as functions of t for each characteristic." Each point has a concentration and position associated with it and is moved through the flow field in proportion to the flow velocity at its location. Intuitively, the method may be visualized as tracing a number of fluid particles through a flow field and observing changes in chemical concentration in the fluid particles as they move.

Particle tracking

The first step in the method of characteristics involves placing a number of traceable particles or points in each cell of the finite-difference grid to form a set of points that are distributed in a geometrically uniform pattern throughout the area of interest. It was found that placing from four to nine points per cell provided satisfactory results for most two-dimensional problems. The location or position of each particle is specified by its x- and y- coordinates in the finite-difference grid. The initial concentration assigned to each point is the initial concentration associated with the node of the cell containing the point.

For each time step every point is moved a distance proportional to the length of the time increment and the velocity at the location of the point. (See fig. 1.) The new position of a point is thus computed with the following finite-difference forms of equations 18 and 19:

$$x_{p,k}=x_{p,k-1}+\delta x_p=x_{p,k-1}+\Delta t V_{x[x_{(p,k)},y_{(p,k)}]} \quad (22)$$

and

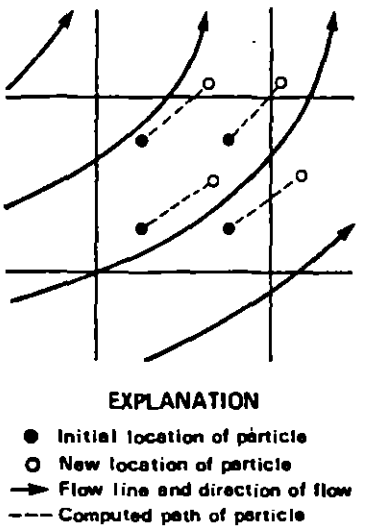

Figure 1.—Part of hypothetical finite-difference grid showing relation of flow field to movement of points.

$$y_{p,k} = y_{p,k-1} + \delta y_p = y_{p,k-1} + \Delta t V_{y[x_{(p,k)}, y_{(p,k)}]} \quad (23)$$

where

p is the index number for point identification; and

δx_p and δy_p are the distances moved in the x and y directions, respectively.

The x and y velocities at the position of any particular point p, indicated as $V_{i[x_{(p,k)}, y_{(p,k)}]}$, for time k are calculated through bilinear interpolation over the area of half of a cell using the x and y velocities computed at adjacent nodes and cell boundaries. For example, figure 2 illustrates that the velocity in the x direction of point p, located in the southeast quadrant of cell (i,j), would be computed using bilinear interpolation between the x velocities computed with equations 12 and 13 at (i,j), $(i,j+1)$, $(i+\frac{1}{2},j)$, and $(i+\frac{1}{2},j+1)$. Similarly, the velocity in the y direction of point p would be based on the y velocities computed at (i,j), $(i+1,j)$, $(i,j+\frac{1}{2})$ and $(i+1,j+\frac{1}{2})$.

After all points have been moved, the concentration at each node is temporarily assigned the average of the concentrations of all points then located within the area of that cell; this average concentration is denoted as $C_{i,j,k}^*$. The time index is distinguished with an asterisk here because this temporarily assigned average concentration represents the new time level only with respect to convective transport. The moving points simulate convective transport because the concentration at each node of the grid will change with each time step as different points having different concentrations enter and leave the area of that cell.

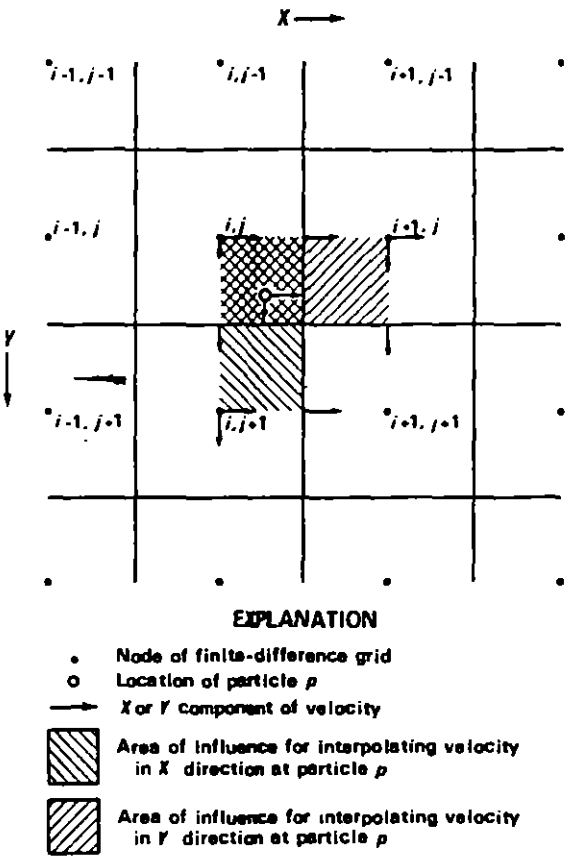

Figure 2.—Part of hypothetical finite-difference grid showing areas over which bilinear interpolation is used to compute the velocity at a point. Note that each area of influence is equal to one-half of the area of a cell.

Finite-difference approximations

The total change in concentration in an aquifer may be computed by solving equations 18–20. Equations 18 and 19, which are related to changes in concentration caused

by convective transport alone, are solved by the movement of points as described previously. The changes in concentration caused by hydrodynamic dispersion, fluid sources, divergence of velocity, and changes in saturated thickness are calculated using an explicit finite-difference approximation to equation 20, which can be expressed as

$$\Delta C_{i,j,k} = \Delta t\left[\frac{1}{b}\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right) + F\right]. \quad (24)$$

Note that a solution to equation 20 requires the computation of the change in concentration at the tracer particles. However, primarily because of the difficulty in computing the concentration gradient at a large number of moving points, the change in concentration represented by equation 20 is solved at each node of the grid rather than directly at the location of each point. The material derivative of concentration on any characteristic curve (or for any tracer particle) is then related to the change in concentration for a node during one time step, which was computed with the solution to equation 24.

The right side of equation 24 can be considered as the sum of two separate terms, as follows:

$$\Delta C_{i,j,k} = (\Delta C_{i,j,k})_{\mathrm{I}} + (\Delta C_{i,j,k})_{\mathrm{II}} \quad (25)$$

where

$(\Delta C_{i,j,k})_{\mathrm{I}}$ is the change in concentration caused by hydrodynamic dispersion, and is defined as

$$(\Delta C_{i,j,k})_{\mathrm{I}} = \frac{\Delta t}{b}\left[\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right)\right] \quad (26)$$

and

$(\Delta C_{i,j,k})_{\mathrm{II}}$ is the change in concentration resulting from an external fluid source and changes in saturated thickness, and from equation 16 is defined as

$$(\Delta C_{i,j,k})_{\mathrm{II}} = \Delta t\, F = \Delta t\left[\frac{C\left(S\frac{\partial h}{\partial t} + W - \epsilon\frac{\partial b}{\partial t}\right) - C'W}{\epsilon b}\right]. \quad (27)$$

First we will examine the change in concentration due to dispersion, partly following the development of Reddell and Sunada (1970). The right side of equation 26 can be expanded according to the summation convention of tensor notation to obtain

$$(\Delta C_{i,j,k})_{\mathrm{I}} = \frac{\Delta t}{b}\left[\frac{\partial}{\partial x}\left(bD_{xx}\frac{\partial C}{\partial x} + bD_{xy}\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial y}\left(bD_{yy}\frac{\partial C}{\partial y} + bD_{yx}\frac{\partial C}{\partial x}\right)\right]. \quad (28)$$

A finite-difference approximation for the derivative in the x direction at (i,j) may be written as

$$\frac{\partial}{\partial x}\left(bD_{xx}\frac{\partial C}{\partial x} + bD_{xy}\frac{\partial C}{\partial y}\right) = \frac{\partial}{\partial x}\left(bD_{xx}\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial x}\left(bD_{xy}\frac{\partial C}{\partial y}\right) = \frac{\left(bD_{xx}\frac{\partial C}{\partial x}\right)_{i+\frac{1}{2},j} - \left(bD_{xx}\frac{\partial C}{\partial x}\right)_{i-\frac{1}{2},j}}{\Delta x} + \frac{\left(bD_{xy}\frac{\partial C}{\partial y}\right)_{i+\frac{1}{2},j} - \left(bD_{xy}\frac{\partial C}{\partial y}\right)_{i-\frac{1}{2},j}}{\Delta x}. \quad (29)$$

In the following expansion of equation 29 it is implied that concentrations (C) are known from the previous (k–1) time level; hence, equation 29 is an explicit finite-difference equation. The spatial derivatives of concentration at $(i+\frac{1}{2},j)$ may be approximated by

$$\left(\frac{\partial C}{\partial x}\right)_{i+\frac{1}{2},j} = \frac{C_{i+1,j} - C_{i,j}}{\Delta x} \quad (30)$$

and

$$\left(\frac{\partial C}{\partial y}\right)_{i+\frac{1}{2},j} = \frac{C_{i+\frac{1}{2},j+1} - C_{i+\frac{1}{2},j-1}}{2\Delta y}. \quad (31)$$

Because concentrations are defined only at nodes, we must express the right side of equation 31 in terms of concentrations at nodes. Assuming that the concentration at a

cell boundary is approximately equal to the average (arithmetic mean) of the concentrations at adjacent nodes, we have

$$C_{i+\frac{1}{2},j+1} = \frac{C_{i,j+1} + C_{i+1,j+1}}{2} \tag{32}$$

and

$$C_{i+\frac{1}{2},j-1} = \frac{C_{i,j-1} + C_{i+1,j-1}}{2}. \tag{33}$$

Substitution of equations 32 and 33 into equation 31 results in:

$$\left(\frac{\partial C}{\partial y}\right)_{i+\frac{1}{2},j} = \frac{C_{i,j+1} + C_{i+1,j+1} - C_{i,j-1} - C_{i+1,j-1}}{4\Delta y}. \tag{34}$$

Similarly, the spatial derivatives of concentration at $(i-\frac{1}{2},j)$ are

$$\left(\frac{\partial C}{\partial x}\right)_{i-\frac{1}{2},j} = \frac{C_{ij} - C_{i-1}}{\Delta x} \tag{35}$$

and

$$\left(\frac{\partial C}{\partial y}\right)_{i-\frac{1}{2},j} = \frac{C_{i-1,j+1} + C_{i,j+1} - C_{i-1,j-1} - C_{i,j-1}}{4\Delta y}. \tag{36}$$

After substituting equations 30, 34, 35, and 36 into equation 29, we have

$$\begin{aligned}\frac{\partial}{\partial x}\left(bD_{xx}\frac{\partial C}{\partial x} + bD_{xy}\frac{\partial C}{\partial y}\right) &= \frac{bD_{xx[i+\frac{1}{2},j]}(C_{i+1,j} - C_{ij})}{(\Delta x)^2} - \frac{bD_{xx[i-\frac{1}{2},j]}(C_{ij} - C_{i-1,j})}{(\Delta x)^2} \\ &+ \frac{bD_{xy[i+\frac{1}{2},j]}(C_{ij+1} + C_{i+1,j+1} - C_{ij-1} - C_{i+1,j-1})}{4\Delta x\Delta y} \\ &- \frac{bD_{xy[i-\frac{1}{2},j]}(C_{i-1,j+1} + C_{ij+1} - C_{i-1,j-1} - C_{ij-1})}{4\Delta x\Delta y}.\end{aligned} \tag{37}$$

A finite-difference approximation for the derivative in the y direction in equation 28 may be developed for node (i,j) in an analogous manner to equation 37 to produce

$$\begin{aligned}\frac{\partial}{\partial y}\left(bD_{yy}\frac{\partial C}{\partial y} + bD_{yx}\frac{\partial C}{\partial x}\right) &= \frac{\left(bD_{yy}\frac{\partial C}{\partial y}\right)_{ij+\frac{1}{2}} - \left(bD_{yy}\frac{\partial C}{\partial y}\right)_{ij-\frac{1}{2}}}{\Delta y} + \frac{\left(bD_{yx}\frac{\partial C}{\partial x}\right)_{ij+\frac{1}{2}} - \left(bD_{yx}\frac{\partial C}{\partial x}\right)_{ij-\frac{1}{2}}}{\Delta y} \\ &= \frac{bD_{yy[i,j+\frac{1}{2}]}(C_{ij+1} - C_{ij})}{(\Delta y)^2} - \frac{bD_{yy[i,j-\frac{1}{2}]}(C_{ij} - C_{ij-1})}{(\Delta y)^2} \\ &+ \frac{bD_{yx[i,j+\frac{1}{2}]}(C_{i+1,j} + C_{i+1,j+1} - C_{i-1,j} - C_{i-1,j+1})}{4\Delta x\Delta y} \\ &- \frac{bD_{yx[i,j-\frac{1}{2}]}(C_{i+1,j-1} + C_{i+1,j} - C_{i-1,j-1} - C_{i-1,j})}{4\Delta x\Delta y}.\end{aligned} \tag{38}$$

Equation 28 may then be solved explicitly by substituting the relationships expressed by equations 37 and 38 for the terms within brackets on the right side of equation 28.

Next we will examine the change in concentration denoted by equation 27. Substituting explicit finite-difference approximations for the terms in equation 27, we have

$$(\Delta C_{i,j,k})_{II} = \frac{\Delta t}{\epsilon b_{i,j,k}}\left[C_{i,j,k-1}\left(S\left[\frac{h_{i,j,k}-h_{i,j,k-1}}{\Delta t}\right] + W_{i,j,k}-\epsilon\left[\frac{b_{i,j,k}-b_{i,j,k-1}}{\Delta t}\right]\right) - C'_{i,j,k}W_{i,j,k}\right]. \quad (39)$$

Equations 28, 37, 38, and 39 together provide a solution to equation 24, which in turn allows us to solve equation 20 and complete the definition of the characteristic curves of equation 15.

Because the processes of convective transport, hydrodynamic dispersion, and mixing are occurring continuously and simultaneously, equations 18, 19, and 20 should be solved simultaneously. However, equations 18 and 19 are solved by particle movement based on implicitly computed heads while equation 20 is solved explicitly with respect to concentrations. Because the change in concentration at a source node due to mixing is proportional to the difference in concentration between the node and the source fluid (see eq 27), the accuracy of estimating the concentration at the node during a time increment will clearly affect the computed change. Similarly, because the change in concentration due to dispersion is proportional to the concentration gradient at a point, the accuracy of estimating the concentration gradient will clearly affect the accuracy of the numerical results. As the position of a front or breakthrough curve advances with time, say from the $k-1$ to k time level, the concentration gradient at any fixed reference point and the concentration differences at sources are continuosly changing. The consequent limitations imposed by estimating nodal concentrations in a strict explicit manner can be minimized by using a two-step explicit procedure in which equation 24 is solved at each node by giving equal weight to concentration gradients computed from the concentrations at the previous time level $(k-1)$ and to concentration gradients computed from concentrations at time level (k^*), which represents the convected position of the front at the new time level (k) prior to adjustments of concentration for dispersion and mixing. Figure 3 illustrates the sequence of calculations to solve equations 18–20 over a given time increment. First the concentration gradients at the previous time level $(k-1)$ are determined at each node. Then the front is convected to a new position for time level k^* based on the velocity of flow and length of the time increment. Next the concentration gradients at each node are recomputed for the new position of the front. The concentration distribution for the new frontal position is then adjusted at each node in two steps: first based on concentration gradients at $k-1$ and second based on concentration gradients at k^*.

The finite-difference approximation to equation 24 may thus be expressed as

$$\Delta C_{i,j,k} = \frac{0.5\,\Delta t}{b}\left[\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C_{(k-1)}}{\partial x_j}\right) + \frac{C_{(k-1)}\left(S\frac{\partial h}{\partial t}+W-\epsilon\frac{\partial b}{\partial t}\right)-C'W}{\epsilon}\right] + \frac{0.5\,\Delta t}{b}\left[\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C_{(k^*)}}{\partial x_j}\right) + \frac{C_{(k^*)}\left(S\frac{\partial h}{\partial t}+W-\epsilon\frac{\partial b}{\partial t}\right)-C'W}{\epsilon}\right] \quad (40)$$

in which the appropriate finite-difference approximations for the terms within brackets are indicated by equations 37, 38, and 39.

The new nodal concentrations at the end of time increment k are computed as

$$C_{i,j,k} = C_{i,j,k^*} + \Delta C_{i,j,k} \quad (41)$$

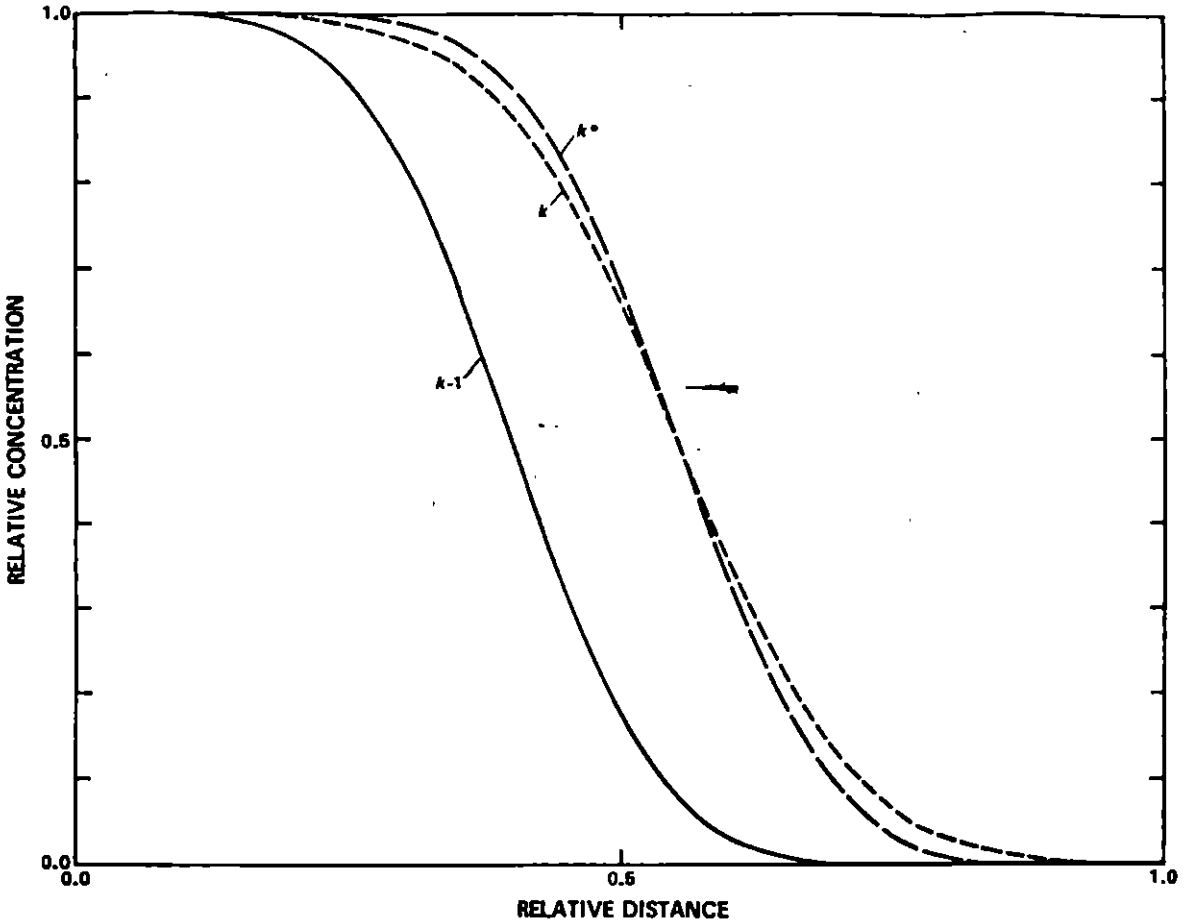

Figure 3.—Representative change in breakthrough curve from time level $k-1$ to k. Note that concentration changes are exaggerated to help illustrate the sequence of calculations.

where C_{i,j,k^*} is the average of the concentrations of all points in cell (i,j) after equations 22 and 23 were solved for all points for time step k, and $\Delta C_{i,j,k}$ is the change in concentration caused by hydrodynamic dispersion, sources, and sinks, as calculated in equation 40.

Because the concentrations of points in a cell vary about the concentration of the node, the change in concentration computed at a node using equation 40 cannot be applied directly in all cases to the concentrations of the points. If the change in concentration at the node ($\Delta C_{i,j,k}$) is positive, the increase is simply added to the point concentrations. But if the concentration change is negative, it is applied to points in that cell as a percentage decrease in concentration at each point that is equal to the percentage decrease at the node. This technique preserves a mass balance within each cell, but when a decrease in concentration is computed for a node, it will also prevent a possible but erroneous computation of negative concentrations at those points that had a concentration less than that at the node.

Stability criteria

The explicit numerical solution of the solute-transport equation has a number of stability criteria associated with it. These may require that the time step used to solve the flow equation be subdivided into a number of smaller time increments to accurately solve the solute-transport equation.

First, Reddell and Sunada (1970, p. 62) show that for an explicit finite-difference solution of equation 26 to be stable,

$$\frac{D_{xx}\,\Delta t}{(\Delta x)^2}+\frac{D_{yy}\,\Delta t}{(\Delta y)^2}\leq\frac{1}{2}. \quad (42)$$

Solving equation 42 for Δt, we see that

$$\Delta t\leq \underset{\text{(over grid)}}{\text{Min}}\left[\frac{0.5}{\frac{D_{xx}}{(\Delta x)^2}+\frac{D_{yy}}{(\Delta y)^2}}\right]. \quad (43)$$

Because the solution to equation 26 is actually written as a set of N equations for N nodes, the maximum permissible time increment is the smallest Δt computed for any individual node in the entire grid. The smallest Δt will then occur at the node having the largest value of

$$\frac{D_{xx}}{(\Delta x)^2}+\frac{D_{yy}}{(\Delta y)^2}.$$

Next consider the effects of mixing ground water of one concentration with injected or recharged water of a different concentration, as represented by the source terms in equation 39. The change in concentration in a source node cannot exceed the difference between the source concentration ($C'_{i,j}$) and the concentration in the aquifer ($C_{i,j}$), and the maximum possible change occurs when a source completely flushes out the volume of water in an aquifer cell at the start of a time step. Therefore

$$\Delta C_{i,j,k}\leq C_{i,j,k-1}-C'_{i,j,k}. \quad (44)$$

After rearranging terms in equation 44, we have

$$\frac{\Delta C_{i,j,k}}{(C_{i,j,k-1}-C'_{i,j,k})}\leq 1.0. \quad (45)$$

We may isolate the effects of mixing represented in equation 39 by assuming steady-state flow in which $\partial h/\partial t=0$ and $\partial b/\partial t=0$. Then we can rewrite equation 39 as

$$(\Delta C_{i,j,k})_{II}=\frac{\Delta t\,W_{i,j,k}\,(C_{i,j,k-1}-C'_{i,j,k})}{\epsilon b_{i,j,k}}. \quad (46)$$

After rearranging terms in equation 46, we have

$$\frac{(\Delta C_{i,j,k})_{II}}{(C_{i,j,k-1}-C'_{i,j,k})}=\frac{\Delta t\,W_{i,j,k}}{\epsilon b_{i,j,k}}. \quad (47)$$

Substituting equation 47 into equation 45 results in

$$\frac{\Delta t\,W_{i,j,k}}{\epsilon b_{i,j,k}}\leq 1.0. \quad (48)$$

Solving equation 48 for Δt at all nodes yields the following criterion:

$$\Delta t\leq \underset{\text{(over grid)}}{\text{Min}}\left[\frac{\epsilon b_{i,j,k}}{W_{i,j,k}}\right]. \quad (49)$$

A third type of stability check involves the movement of points computed by equations 22 and 23 to simulate convective transport. The distance a particle moves is defined as

$$\delta x=\Delta t\,V_{x[x_{(p,h)},y_{(p,h)}]} \quad (50)$$

and

$$\delta y=\Delta t\,V_{y[x_{(p,h)},y_{(p,h)}]}. \quad (51)$$

In effect, this constitutes a linear spatial extrapolation of the position of a particle from one time step to the next. Where streamlines are curvilinear, the extrapolated position of a particle will deviate from the streamline on which it was previously located. This deviation introduces an error into the numerical solution that is proportional to Δt. Thus, it is thought that an accurate computation of concentration changes caused by convective transport requires the maintenance of a relatively uniformly spaced field of marker particles that are moving along relatively smooth and continuous pathlines. Also, if δx is greater than Δx, or δy is greater than Δy, it might be possible for particles to move beyond the boundaries of the grid during one time increment. Thus, for a given velocity field and grid, some restriction must be placed on the size of the time increment to assure that neither δx nor δy exceed some critical distances, called δx^* and δy^*. Therefore

$$\delta x\leq\delta x^* \quad (52)$$

and

$$\delta y\leq\delta y^*. \quad (53)$$

These critical distances can be related to the dimensions of the finite-difference grid by

$$\delta x^*=\gamma\Delta x \quad (54)$$

and

$$\delta y^* = \gamma \Delta y \qquad (55)$$

where γ is the fraction of the grid dimensions that particles will be allowed to move ($0 < \gamma \leq 1$).

If we replace the terms in equations 52 and 53 with the corresponding terms from equations 50, 51, 54, and 55, we have

$$\Delta t\, V_{x[x_{(p,q)}, y_{(p,q)}]} \leq \gamma \Delta x \qquad (56)$$

and

$$\Delta t\, V_{y[x_{(p,q)}, y_{(p,q)}]} \leq \gamma \Delta y. \qquad (57)$$

Because these criteria are governed by the maximum velocities in the system, and since the computed velocity of a tracer particle will always be less than or equal to the maximum velocity computed at a node or cell boundary, we have to check only the latter. Substituting the grid velocities and solving equations 56 and 57 for Δt results in

$$\Delta t \leq \frac{\gamma \Delta x}{(V_x)_{max}} \qquad (58)$$

and

$$\Delta t \leq \frac{\gamma \Delta y}{(V_y)_{max}}. \qquad (59)$$

If the time step used to solve the flow equation exceeds the smallest of the time limits determined by equations 43, 49, 58, or 59, then the time step will be subdivided into the appropriate number of smaller time increments required for solving the solute-transport equation.

Boundary and Initial Conditions

Obtaining a solution to the equations that describe ground-water flow and solute transport requires the specification of boundary and initial conditions for the domain of the problem. Specifications for solving the flow equation must be compatible with the solution of the solute-transport equation. Several different types of boundary conditions can be incorporated into the solute-transport model. Two general types are incorporated in this model; these are constant-flux and constant-head conditions. These can be used to represent the real boundaries of an aquifer as well as to represent artificial boundaries for the model. The use of the latter can help to minimize data requirements and the areal extent of the modeled part of the aquifer.

A constant-flux boundary can be used to represent aquifer underflow, well withdrawals, or well injection. A finite flux is designated by specifying the flux rate as a well discharge or injection rate for the appropriate nodes. A no-flow boundary is a special case of a constant-flux boundary. The numerical procedure used in this model requires that the area of interest be surrounded by a no-flow boundary. Thus the model will automatically specify the outer rows and columns of the finite-difference grid as no-flow boundaries. No-flow boundaries can also be located elsewhere in the grid to simulate natural limits or barriers to ground-water flow. No-flow boundaries are designated by setting the transmissivity equal to zero at appropriate nodes, thereby precluding the flow of water or dissolved chemicals across the boundaries of the cell containing that node.

A constant-head boundary in the model can represent parts of the aquifer where the head will not change with time, such as recharge boundaries or areas beyond the influence of hydraulic stresses. In this model constant-head boundaries are simulated by adjusting the leakage term (the last term on the right side of equation 11) at the appropriate nodes. This is accomplished by setting the leakance coefficient (K_z/m) to a sufficiently high value (such as 1.0 s^{-1}) to allow the head in the aquifer at a node to be implicitly computed as a value that is essentially equal to the value of H_s, which in this case would be specified as the desired constant-head altitude. The resulting rate of leakage into or out of the designated constant-head cell would equal the flux required to maintain the head in the aquifer at the specified constant-head altitude.

If a constant-flux or constant-head boundary represents a fluid source, then the chemical concentration in the source fluid (C') must also be specified. If the boundary represents a fluid sink, then the concentration of the produced fluid will equal the concen-

tration in the aquifer at the location of the sink.

Because solute transport directly depends upon hydraulic and concentration gradients, the head and concentration in the aquifer at the start of the simulation period must be specified. The initial conditions can be determined from field data and (or) from previous simulations. It is important to note that the simulation results may be sensitive to variations or errors in the initial conditions. In discussing computed heads, Trescott, Pinder, and Larson (1976, p. 30) state:

> If initial conditions are specified so that transient flow is occurring in the system at the start of the simulation, it should be recognized that water levels will change during the simulation, not only in response to the new pumping stress, but also due to the initial conditions. This may or may not be the intent of the user.

Mass balance

Mass balance calculations are performed after specified time increments to help check the numerical accuracy and precision of the solution. The principle of conservation of mass requires that the cumulative sums of mass inflows and outflows (or net flux) must equal the accumulation of mass (or change in mass stored). The difference between the net flux and the mass accumulation is the mass residual (R_m) and is one measure of the numerical accuracy of the solution. Although a small residual does not prove that the numerical solution is accurate, a large error in the mass balance is undesirable and may indicate the presence of a significant error in the numerical solution.

The model uses two methods to estimate the error in the mass balance. Both are based on the magnitude of the mass residual, R_m, which is computed from

$$R_m = \Delta M_s - M_f \qquad (60)$$

where

ΔM_s is the change in mass stored in the aquifer, M; and

M_f is the net mass flux, M.

The two mass terms, ΔM_s and M_f, are evaluated using the following equations:

$$\Delta M_s = \sum_i \sum_j b_{i,j,e} \Delta x \Delta y (C_{i,j,k} - C_{i,j,o}) \qquad (61a)$$

where $C_{i,j,o}$ is the initial concentration at node (i,j), M/L^3; and

$$M_f = \sum_i \sum_j \sum_k W_{i,j,k} \Delta x \Delta y \Delta t_k C'_{i,j,k}. \qquad (61b)$$

The percent error (E) in the mass balance is computed first by comparing the residual with the average of the net flux and net accumulation, as

$$E_1 = \frac{100.0(M_f - \Delta M_s)}{0.5(M_f + \Delta M_s)}. \qquad (62)$$

This is a good measure of the accuracy of the numerical solution when the flux and the change in mass stored are relatively large. However, equation 62 does not account for the initial mass of solute in the aquifer. If total fluxes are very small compared to the initial mass of solute in the aquifer, then equation 62 might indicate a relatively large error when the numerical solution is actually quite accurate. Therefore, the error may also be computed a second way by comparing the residual with the initial mass of solute (M_o) present in the aquifer, as

$$E_2 = \frac{100.0(M_f - \Delta M_s)}{M_o}. \qquad (63)$$

Equation 63 provides a good measure of the accuracy of the numerical solution when fluxes are zero or relatively small. But when M_o is zero or very small in comparison to ΔM_s, then E_2 becomes meaningless. This problem can be overcome by correcting M_o in the denominator of equation 63 for the net mass flux, resulting in

$$E_3 = \frac{100.0(M_f - \Delta M_s)}{M_o - M_f}. \qquad (64)$$

Note that as M_f becomes very small, equation 64 approaches equation 63, and as M_o becomes very small, E_3 becomes just a comparison of the residual with the net flux. In the latter case E_3 is a mass balance indicator similar to E_1 in equation 62. Thus, E_3 is considered a more reliable and versatile indicator of numerical accuracy than is E_2. Either one or both of E_1 and E_3 are computed by the model, as appropriate.

Special problems

There are a number of special problems associated with the use of the method of characteristics to solve the solute-transport equation. Some of these problems are associated with the movement and tracking of particles, while other problems are related to the computational transition between the concentrations of particles within a cell and the average concentration at that node. We will next describe the more significant problems and the procedures used to minimize errors that might result from them.

One possible problem is related to no-flow boundaries. Neither water nor dissolved chemicals can be allowed to cross a no-flow boundary. However, under certain conditions it might be possible for the interpolated velocity at the location of a particle near a no-flow boundary to be such that the particle will be convected across the boundary during one time increment. Figure 4 illustrates such a possible situation, which arises from the deviation between the curvilinear flow line and the linearly projected particle path. If a particle is convected across a no-flow boundary, then it is relocated within the aquifer by reflection across the boundary, as also shown in figure 4. This correction thus will tend to relocate the particle closer to the true flow line.

Fluid sources and sinks also require special treatment. Because they tend to represent singularities in the velocity field, the use of a central difference formulation (eq 12) to compute the velocity at a node may indicate zero or very small velocities at the nodes. Therefore, the velocity components at a source or sink node cannot be used for interpolation of the velocity at a point within or adjacent to that cell. To help maintain radial flow to or from a sink or source, respectively, the velocities computed on the boundaries of source or sink cells are assigned to that node. The appropriate boundary velocities are determined on the basis of the quadrant of interest. This can be illustrated by referring again to figure 2. If a point is located in the southeast quadrant of cell (i,j), the x velocity at node (i,j) would

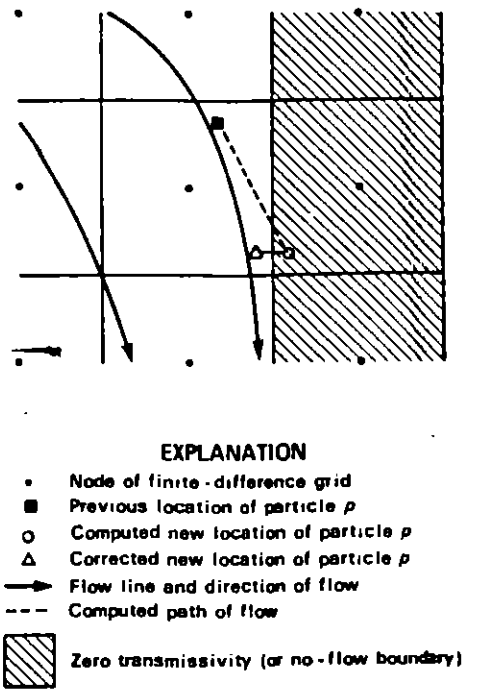

Figure 4.—Possible movement of particles near an impermeable (no-flow) boundary.

be set equal to $V_{x(i+\frac{1}{2},j)}$ and the y velocity to $V_{y(i,j+\frac{1}{2})}$. Corresponding adjustments are made for points in other quadrants, so that the magnitude and direction of velocity at the node are not fixed for a given time increment, but depend on the relative location of the point of interest within the cell. A similar approximation is made when a point of interest is located in a cell adjacent to a source or sink. Thus, if the same point, p, in figure 2 were located in an unstressed cell but the adjacent cell $(i+1,j)$ represented a source or sink, then the y velocity at node $(i+1,j)$ would be approximated by $V_{y(i+1,j+\frac{1}{2})}$ in order to estimate the y velocity at point p. A corresponding approximation for the x velocity at node $(i,j+1)$ would be made using $V_{x(i+\frac{1}{2},j+1)}$ if a source or sink were located at $(i,j+1)$.

The maintenance of a reasonably uniform and continuous spacing of points requires special treatment in areas where sources and sinks dominate the flow field. Points will continually move out of a cell that represents a source, but few or none will move in to re-

place them and thereby maintain a continuous stream of points. Thus, whenever a point that originated in a source cell moves out of that source cell, a new point is introduced into the source cell to replace it. Placement of new points in a source cell is compatible with and analogous to the generation of fluid and solute mass at the source.

The procedure used to replace points in source cells that are adjacent to no-flow boundaries is illustrated in figure 5. Here a steady, uniformly spaced stream of points is maintained by generating a new point at the same relative position in the source cell as the new position in the adjacent cell of the point that left the source cell. As an example, point 7 was convected from cell $(i-1,j)$ to cell (i,j). So the replacement point (22) was placed at a location within cell $(i-1,j)$ that is identical to the new location of point 7 within cell (i,j).

The procedure used to replace points in source cells that lie within the aquifer and not adjacent to a no-flow boundary is illustrated in figure 6. Here a steady, uniformly spaced stream of particles is maintained by generating a new point in the source cell at the original location of the point that left the source cell. When a relatively strong source is imposed on a relatively weak regional flow field, as illustrated in figure 6a, then radial flow will be maintained in the area of the source, and all initial and replacement points will move symmetrically away from node (i,j). For example, after point 7 moves from cell (i,j) to $(i+1, j-1)$, the replacement point (18) is positioned at time k in cell (i,j) at the same location as the initial position of point 7. Although the replacement procedure illustrated earlier by figure 5 would work just as well for the case illustrated in figure 6a, it would not be satisfactory for the situation presented in figure 6b, which illustrates the imposition of a relatively weak source in a relatively strong regional flow field. In this case the velocity distribution within the source cell does not possess radial symmetry, and the velocity within the upgradient part of the source cell is much lower than the velocity within the downgradient part of the source cell. Replacement of points at original locations in source cells, as illustrated in figure 6b, will maintain a steady stream of points leaving the source cell in proportion to the velocity field. However, the use of the procedure illustrated in figure 5 for the case presented in figure 6b would result in the accumulation of

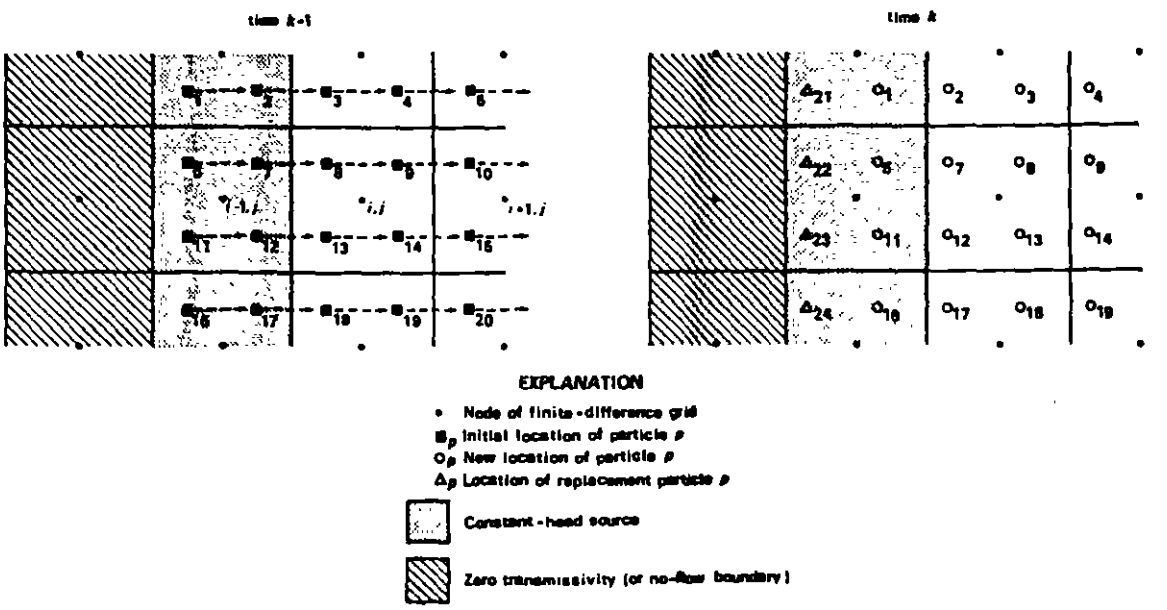

Figure 5.—Replacement of points in source cells adjacent to a no-flow boundary.

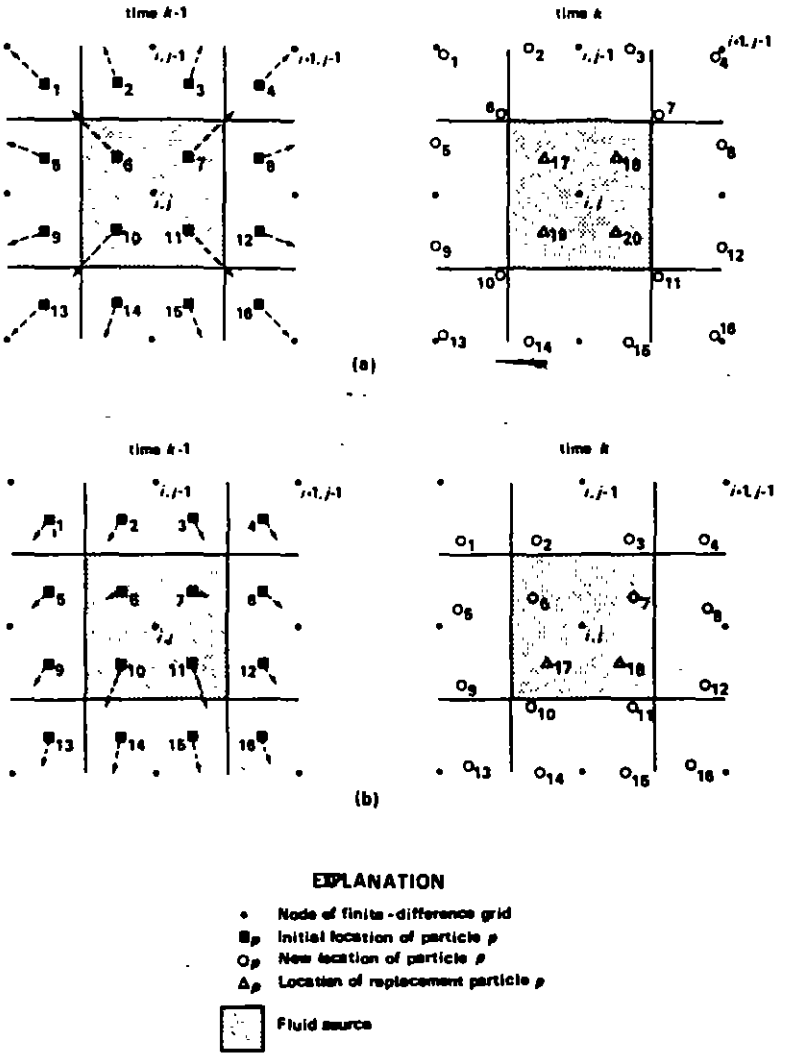

Figure 6.—Replacement of points in source cells not adjacent to a no-flow boundary for negligible regional flow (a) and for relatively strong regional flow (b).

points in the low-velocity area of the source cell (i,j), with few points being replaced into the high-velocity area, where convective transport is the greatest.

Although we normally expect points to be convected out of source cells, figure 6b also demonstrates the possibility that points may sometimes enter a source cell. This can also occur when two or more source cells of different strengths are adjacent to each other. An erroneous multiplication of points might then result if points that did not originate in a particular source cell are replaced when they in turn are convected out of that source cell. Therefore, points leaving a source cell are replaced only if they had originated in that source cell.

Hydraulic sinks also require some special treatment. Points will continually move into a cell representing a strong sink, but few or none will move out. To avoid the resultant crowding and stagnation of tracer points, any point moving into a sink cell is removed from the flow field after the calculations for that time increment have been completed. The numerical removal of points which enter

sink cells is analogous to the withdrawal of fluid and solute mass through the hydraulic sink. The combination of creating new points at sources and destroying old points at sinks will tend to maintain the total number of points in the flow field at a nearly constant value.

Both the flow model and the transport model assume that sources and sinks act over the entire cell area surrounding a source or sink node. Thus, in effect, heads and concentrations computed at source or sink nodes represent average values over the area of the cell. Part of the total concentration change computed at a source node represents mixing between the source water at one concentration and the ground water at a different concentration (eq 39). It can be shown from the relationship between the source concentration ($C'_{i,j,k}$) and the aquifer concentration ($C_{i,j,k-1}$), as indicated by equation 44, that the following constraints generally must be met in a source cell:

$$C_{i,j,k} \leq C'_{i,j,k} \quad \text{for} \quad C'_{i,j,k} > C_{i,j,k-1} \qquad (65a)$$

and

$$C_{i,j,k} \geq C'_{i,j,k} \quad \text{for} \quad C'_{i,j,k} < C_{i,j,k-1}. \qquad (65b)$$

If it is assumed that the sources act over the area of the source cell and that there is complete vertical mixing, then these same constraints should also apply to all points within the cell. Because of the possible deviation of the concentrations of individual points within a source cell from the average concentration, the change in concentration computed at a source node ($\Delta C_{i,j,k}$) should not be applied directly to each of the points in the cell. Rather, at the end of each time increment the concentration of each point in a source cell is updated by setting it equal to the final nodal concentration. Although this may introduce a small amount of numerical dispersion by eliminating possible concentration variations within the area of a source cell, it prevents the adjustment of the concentration at any point in the source cell to a value that would violate the constraints indicated by equation 65.

In areas of divergent flow there may be a problem because some cells can become void of points where pathlines become spaced widely apart. This would result in a calculation of zero change in concentration at a node due to convective transport, although the nodal concentration would still be adjusted for changes caused by hydrodynamic dispersion (eq 28). Also, some numerical dispersion is generated at nodes in and adjacent to the cells into which the convective transport of solute was underestimated because of the resulting error in the concentration gradient. This might not cause a serious problem if only a few cells in a large grid became void or if the voiding were transitory (that is, if upgradient points were convected into void cells during later or subsequent time increments). Figure 6a illustrates radial flow, which represents the most severe case of divergent flow. Here it can be seen that when four points per cell are used to simulate convective transport, then in the numerical procedure four of the eight surrounding cells would erroneously not receive any solute by convection from the adjacent source. If eight points per cell were used initially, then at a distance of two rows or columns from the source only 8 of 16 cells would be on pathlines originating in the source cell. So, while increasing the initial number of points per cell would help, it is obvious that for purely radial flow, an impractically large initial number of points per cell would be required to be certain that at least one particle pathline passes from the source through every cell in the grid.

The problem of cells becoming void of particles can be minimized by limiting the number of void cells to a small percentage of the total number of cells that represent the aquifer. If the limit is exceeded, the numerical solution to the solute-transport equation is terminated at the end of that time increment and the "final" concentrations at that time are saved. Next the problem is reinitialized at the time of termination by regenerating the initial particle distribution throughout the grid and assigning the "final" concentrations at the time of termination as new "initial" concentrations for nodes and particles. The solution to the solute-transport

equation is then simply continued in time from this new set of "initial" conditions until the total simulation period has elapsed. This procedure preserves the mass balance within each cell but also introduces a small amount of numerical dispersion by eliminating variations in concentration within individual cells.

To help minimize the amount of numerical dispersion resulting from the regeneration of points, the program also includes an optimization routine that attempts to maintain an approximation of the previous concentration gradient within a cell. The optimization routine aims to meet the following constraints:

$$\frac{\sum_{n=1}^{N_p} C_n^*}{N_p} = C_{i,j} \qquad (66a)$$

$$C_{i,j} \leq C_n^* \leq C_{l,m} \quad \text{for} \quad C_{i,j} \leq C_{l,m} \qquad (66b)$$

and

$$C_{l,m} \leq C_n^* \leq C_{i,j} \quad \text{for} \quad C_{i,j} \geq C_{l,m} \qquad (66c)$$

where

C_n^* is the concentration of the nth point in cell (i,j), M/L^3;

N_p is the total number of points initially placed in a cell; and

$C_{l,m}$ is the concentration at node (l,m), which represents a cell adjacent to (i,j) and on a line that starts at (i,j) and extends through the coordinates of the point (n) of interest, as illustrated in figure 7, M/L^3.

Note that equation 66a simply indicates that a mass balance must be preserved in a cell regardless of the range in variation of point concentrations within the cell. Equations 66b and c indicate that the concentration of any point must lie between $C_{i,j}$ and the concentration at the node adjacent to particle n. The coordinates of the adjacent node would take on values of $l=i$ or $l=i\pm1$ and $m=j$ or $m=j\pm1$. For example, figure 7 shows that for point 2, the coordinates (l,m) would equal $(i,j-1)$, while for point 3, (l,m) would equal $(i+1,j-1)$. The optimization routine is written so that if equations 66a–c cannot be satisfied simultaneously for node (i,j) within two iterations, then to avoid further computational delay all C_n^* are simply set equal to $C_{i,j}$.

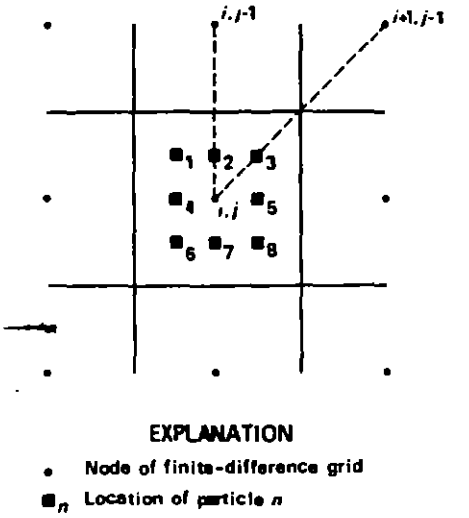

Figure 7.—Relation between possible initial locations of points and indices of adjacent nodes.

Computer Program

The computer program serves as a means of translating the numerical algorithm into machine executable instructions. The purpose of this chapter is to describe the overall structure of the program and to present a detailed description of its key elements, thereby providing a link between the numerical methods and the computer code. We hope that this link will make it easier for the model user to understand and, if necessary, modify the program. The FORTRAN IV source program developed for this model is listed in attachment I and includes almost 2,000 lines. For reference purposes columns 73–80 of each line contain a label that is numbered sequentially within each subroutine. The definition of selected variables used in the program is presented in attachment II; this glossary therefore also serves as a key for relating the program variables

to their corresponding mathematical terms. The computer program is compatible with many scientific computers; it has been successfully run on Honeywell, IBM, DEC, and CDC computers.

General program features

The program is segmented into a main routine and eight subroutines. The name and primary purpose of each segment are listed in Table 1. Each program segment will be described in more detail in later sections of this chapter.

Table 1.—List of subroutines for solute-transport model

Name	Purpose
MAIN	Control execution.
PARLOD	Data input and initialization.
ITERAT	Compute head distribution.
GENPT	Generate or reposition particles.
VELO	Compute hydraulic gradients, velocities, dispersion equation coefficients, and time increment for stable solution to transport equation.
MOVE	Move particles.
CNCON	Compute change in chemical concentrations and compute mass balance for transport model.
OUTPT	Print head distribution and compute mass balance for flow model.
CHMOT	Print concentrations, chemical mass balance, and observation well data.

The major steps in the calculation procedures are summarized in figure 8, which presents a simplified flow chart of the overall structure of the computer program. The flow chart illustrates that the tracer particles may have to be moved more than once to complete a given time step. In other words, the time step used to implicitly solve the flow equation may have to be subdivided into a number of smaller time increments for the explicit solution of the solute-transport equation. The maximum time increments allowable for the explicit calculations are computed automatically by the model. Thus, the model user cannot specify an erroneously large increment or an inefficiently small increment for solving the solute-transport equation. For transient flow problems, some discretion is still required in the specification of the initial time step and of the time-step multiplier, as discussed by Trescott, Pinder, and Larson (1976, p. 38–40).

The general program presented here is written to allow a grid having up to 20 rows and 20 columns. Because the numerical procedure requires that the outer rows and columns represent no-flow boundaries, the aquifer itself is then limited to maximum dimensions of 18 rows and 18 columns. If a problem requires a larger grid, then the appropriate arrays must be redimensioned accordingly. These arrays are contained in COMMON statements PRMK, HEDA, HEDB, CHMA, CHMC, and DIFUS, and in DIMENSION statements on lines C170, G200, H140, and I160.

The program allows the specification of one pumping well per node. The wells can represent injection (recharge) or withdrawal (discharge). If more than one well exists within the area of a cell, then the flux specified for that node should represent the net rate of injection or withdrawal of all wells in that cell. The model assumes that stresses are constant with time during each pumping period (NPMP). But the total number of wells, as well as their locations, flux rates, and source concentrations, may be changed for successive pumping periods. The program also allows the specification of observation wells at as many as five nodes in the grid. For nodes that are designated as observation wells, at the end of the simulation period or after every 50 time increments the model will print a summary table of the head and concentration at the previous time increments.

The program also includes a node identification array (NODEID), which allows certain nodes or zones to be identified by a unique code number. This feature can save much time in the preparation of input data by easily equating each code number with a desired boundary condition, flux, or source concentration.

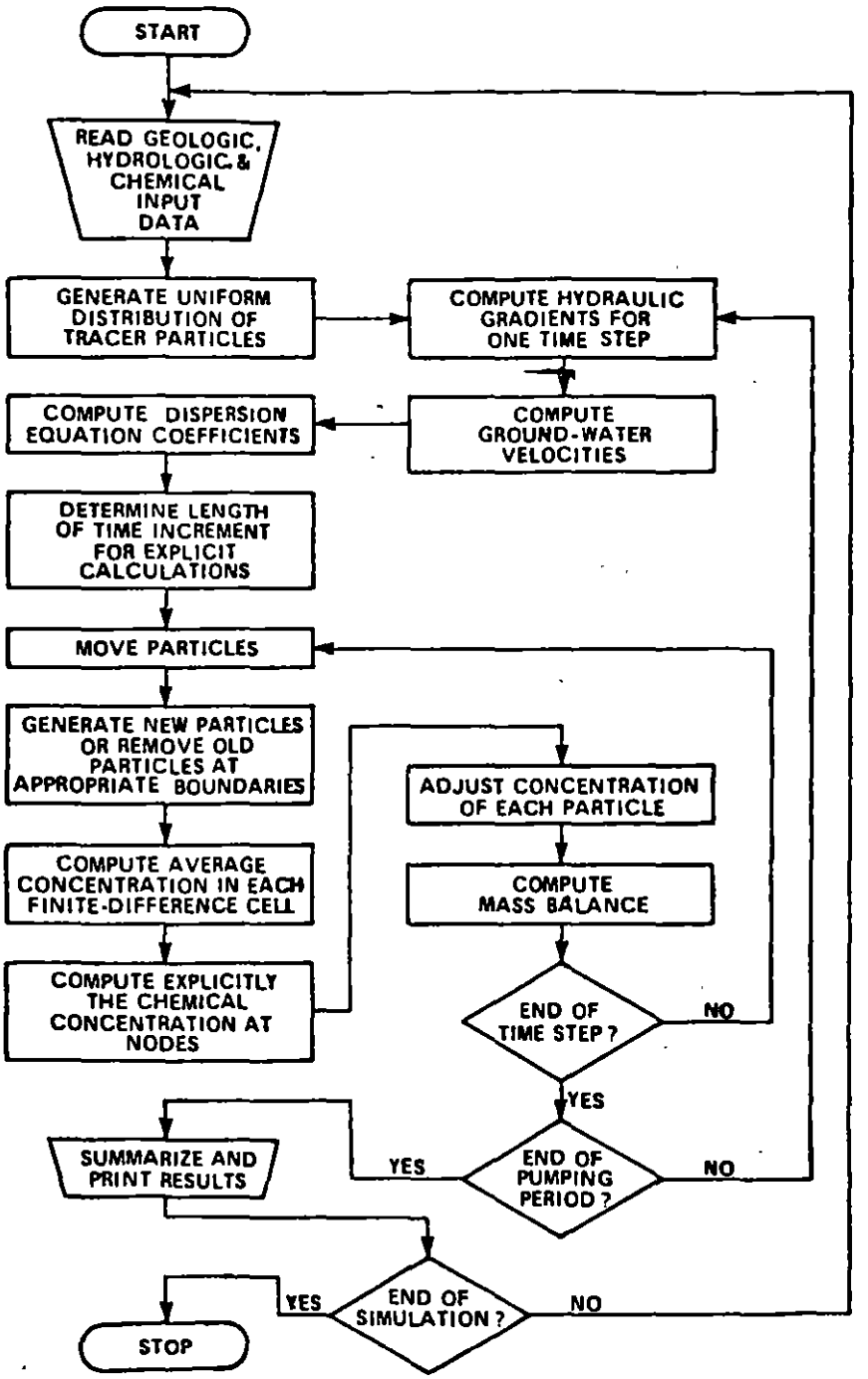

Figure 8.—Simplified flow chart illustrating the major steps in the calculation procedure.

Program segments

MAIN

The primary purpose of the MAIN routine is to control the overall execution sequence of the program. Subroutines for input, execution, and output are called from MAIN and the elapsed time simulated is compared with the desired total simulation period. Also, lines A500–A580 serve to store (or

record) observation well data for transient flow problems.

Subroutine PARLOD

All input data are read through subroutine PARLOD. These data define the properties, boundaries, initial conditions, and stresses for the aquifer, as well as spatial grid and time-step factors. The values of many variables are also initialized here. After the data are read, some preliminary calculations are made, such as (1) determining time increments for the flow model (lines B780–B890), (2) computing the harmonic mean transmissivities in the x and y directions (B1670–B1800), (3) adjusting transmissivity for anisotropy (B1810–B1820), (4) computing iteration parameters (B1840–B1910 and B2880–B2980), and (5) checking for possible inconsistencies among the input data (B3140–B3290). A printout is also provided of all input data so that the data may be rechecked and each run identified.

Subroutine ITERAT

This subroutine solves a finite-difference approximation of the flow equation (eq 11) using an iterative ADI procedure. The matrix generated by the finite-difference approximation is solved using the Thomas algorithm, as described by von Rosenberg (1964, p. 113). Row calculations are made in lines C270–C610, and column calculations are made in lines C630–C970. The calculations are assumed to have converged on a solution if the maximum difference at all nodes between heads computed along rows and heads computed along columns is less than the specified tolerance. Convergence is checked on lines C940–C950. Note that here (for example, lines C380, C700, C930, and C1150) and in other subroutines the thickness array (THCK) is used to check whether a node is in the aquifer.

It should also be noted here that the flow model, as written, assumes that the transmissivity of the aquifer is independent of the head (or saturated thickness) and remains constant with time. If this assumption is not appropriate to the particular aquifer system being modeled, then the solution algorithm presented in this subroutine should be modified accordingly. For example, flow models published by Prickett and Lonnquist (1971, p. 43–45) and Trescott, Pinder, and Larson (1976) include such a modification.

All parameters involved in the calculation of heads are defined as double precision variables and all calculations involving these parameters are performed in double precision. The number of double precision variables and operations can be reduced significantly if the program is to be executed on a high-precision scientific computer, thereby improving the efficiency of the model by reducing computer storage requirements and execution time.

The iterative ADI procedure used to solve the finite-difference equations is not necessarily the best possible solution technique for all problems. For example, it may be difficult to obtain a solution using the iterative ADI procedure for cases of steady-state flow when internal nodes in the grid have zero transmissivity and for cases in which the transmissivity is highly anisotropic. In such cases, a strongly implicit procedure, such as the one documented by Trescott, Pinder, and Larson (1976), should be substituted for the solution algorithm contained in subroutine ITERAT.

Subroutine GENPT

The primary purpose of subroutine GENPT is to generate a uniform initial distribution of tracer particles throughout the finite-difference grid. This is done either at the start of a simulation period or at an intermediate time when too many cells have become void of particles. In the latter case, the program attempts to preserve an approximation of the previous concentration gradient within each cell (lines D1420–D2040).

The placement of particles is accomplished in lines D510–D1410. The program allows the placement of either four, five, eight, or nine particles per cell. Of course each option will result in a slightly different geometry

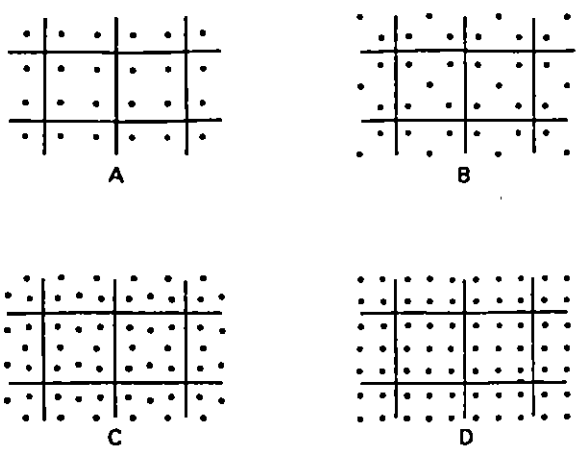

Figure 9.—Parts of finite-difference grids showing the initial geometry of particle distribution for the specification of four (*A*), five (*B*), eight (*C*), and nine (*D*) particles per cell.

and density of points, as illustrated by figure 9. The most regular or uniform patterns are produced when four or nine particles per cell are specified. If a different number of particles per cell or a different placement geometry are desired, this subroutine could be modified accordingly.

As particles are moved or convected through the grid during the calculation procedure, there is a need to remove particles at fluid sinks and create particles at fluid sources. A buffer array (called LIMBO) is created on lines D430–D480 that contains particles that can be added later to the grid at sources and that also contains space to store particles removed at sinks or discharge boundaries.

Subroutine VELO

Subroutine VELO accomplishes three objectives. First, it computes the flow velocities at nodes and on cell boundaries by solving equations having the form of equations 12 and 13. The velocities are computed on lines E420–E680. Second, the dispersion equation coefficients are calculated. These coefficients represent terms factored out of equations 37 and 38, as follows:

$$\mathrm{DISP(IX,IY,1)} = (bD_{xx})_{[i+\frac{1}{2},j]}/(\Delta x)^2 \quad (67a)$$

$$\mathrm{DISP(IX,IY,2)} = (bD_{yy})_{[i,j+\frac{1}{2}]}/(\Delta y)^2 \quad (67b)$$

$$\mathrm{DISP(IX,IY,3)} = (bD_{xy})_{[i+\frac{1}{2},j]}/4\Delta x\Delta y \quad (67c)$$

$$\mathrm{DISP(IX,IY,4)} = (bD_{yx})_{[i,j+\frac{1}{2}]}/4\Delta x\Delta y. \quad (67d)$$

Note that each dispersion coefficient (D_{xx}, D_{yy}, D_{xy}, D_{yx}) is computed on cell boundaries using the relationships expressed in equations 8–10. Therefore, the equation coefficients computed by equation 67 are stored as forward values from the indicated node in the DISP array. Third, this subroutine computes (on lines E1050–E1240 and E1800–E1930) the minimum number of particle moves (NMOV) required to solve the transport equation for the given time step so that the maximum time increment for the transport equation solution will not exceed any of the criteria indicated by equations 43, 49, 58, and 59.

Subroutine MOVE

Although this subroutine has only one main function, which is to move the tracer particles in accordance with equations 22 and 23, it is the longest and perhaps the most complex segment of the program. The complexities are mainly introduced by the treatment of particles at the various types of boundary conditions. To help illustrate the calculation procedure followed within subroutine MOVE, a flow chart is presented in figure 10. The numbers in the flow chart indicate the corresponding lines in subroutine MOVE where the indicated operation is executed.

If a node represents a fluid source or sink, then particles must be respectively created or destroyed in these cells. If the value of pumpage (REC) at a node does not equal zero, then the node is assumed to represent either a fluid source (for REC<0) or a fluid sink (for REC>0). Recharge or discharge can also be represented by the RECH array. But it is assumed that this type of flux is sufficiently diffuse so that it does not induce areas or points of strongly divergent or convergent flow and therefore particles need not be created or destroyed at these nodes. Note that here and in other subroutines the presence of a constant-head boundary is tested by checking the value of leakance (VPRM)

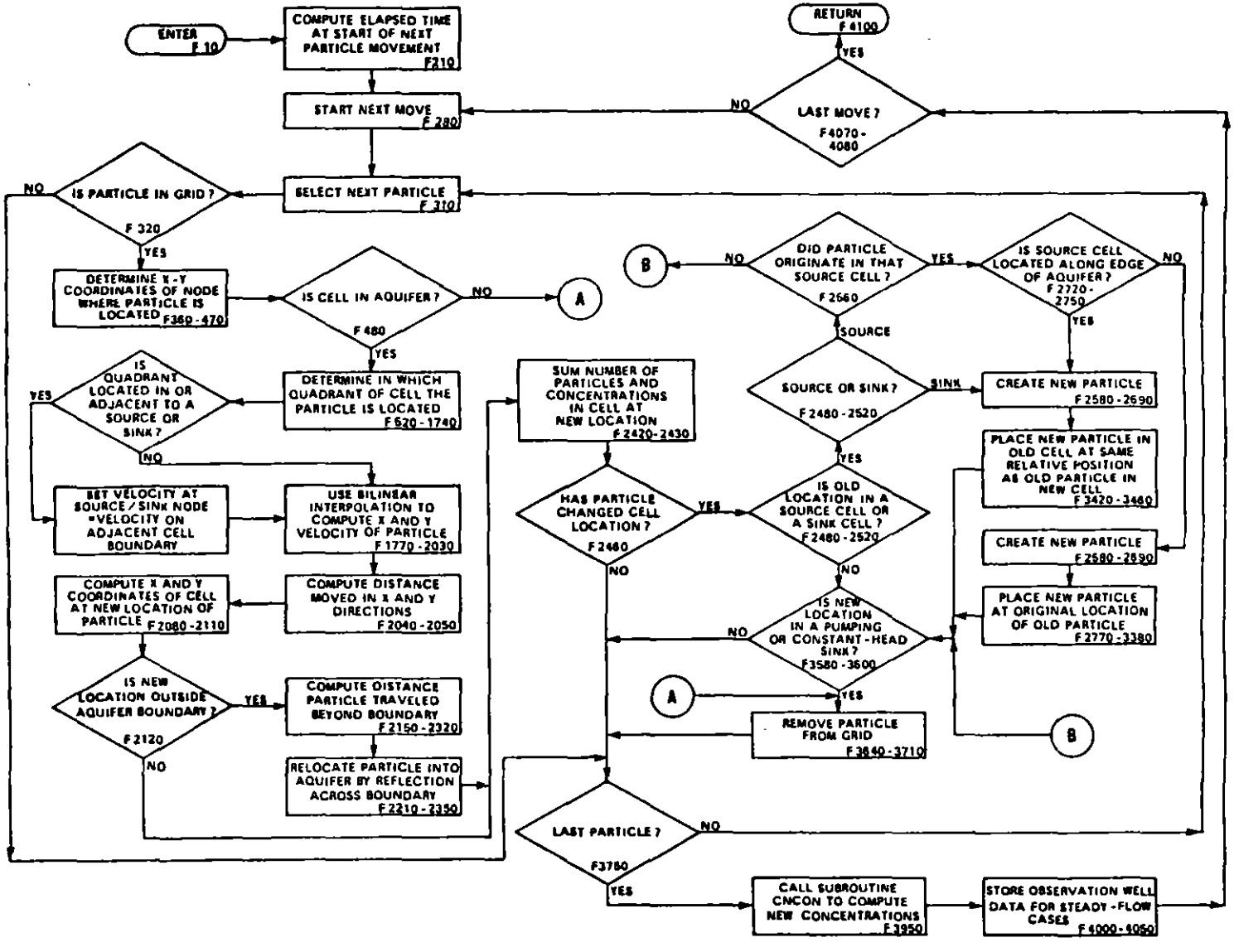

Figure 10.—Generalized flow chart of subroutine MOVE. Numbers indicate line numbers where the operation is executed.

at each node. If VPRM exceeds 0.09, it is assumed that the node represents a constant-head boundary condition and is treated as a fluid source or sink accordingly. At a constant-head node the difference in head between the aquifer and the source bed is used to determine whether the node represents a fluid source or sink (for example, lines F2500–F2520).

Subroutine CNCON

This subroutine computes the change in concentration at each node and at each particle for the given time increment. Equation 39, which denotes the change in concentration resulting from sources, divergence of velocity, and changes in saturated thickness, is solved on lines G350–G610. On the G520 the value of the storage coefficient is checked to determine whether the aquifer is confined or unconfined. It assumes that if $S<0.005$, then the aquifer is confined and $\partial b/\partial t=0$. If $S\geq 0.005$, the model assumes that $\partial b/\partial t = \partial h/\partial t$. If this criterion is not appropriate to a particular aquifer system, then line G520 should be modified accordingly. The change in concentration caused by hydrodynamic dispersion is computed on lines G640–G770 as indicated by equations 37 and 38.

The nodal changes in concentration caused by convective transport are computed on lines G850–G940. The number of cells that are void of particles at the new time level are also counted in this set of statements on lines G880–G910, and then compared with the critical number of void cells (NZCRIT) to determine if particles should be regenerated at initial positions before the next time level is started (lines G960–G1020).

The new (time level k) concentrations at nodes are computed on the basis of the previous concentration at time $k-1$ and the change during $k-1$ to k. The adjustment at nodes is accomplished on lines G1060–G1180, while the concentration of particles is adjusted on lines G1210–G1360.

A mass balance for the solute is next computed (lines G1400–G1730) at the end of each time increment. In computing the mass of solute withdrawn or leaking out of the aquifer at fluid sinks, the concentration at the sink node is assumed to equal the nodal concentration computed at time level $k-1$.

Subroutine OUTPT

This subroutine prints the results of the flow model calculations. When invoked, the subroutine prints (1) the new hydraulic head matrix (lines H190–H260), (2) a numeric map of head values (H300–H390), and (3) a drawdown map (H510–H710). This subroutine also computes a mass balance for the flow model and estimates its accuracy (H420–H820). A mass balance is performed both for cumulative volumes since the initial time and for flow rates during the present time step. The mass balance results are printed on lines H840–H930.

Subroutine CHMOT

This subroutine prints (1) maps of concentration (lines I250–I380), (2) change in concentration from initial conditions (I440–I580), and (3) the results of the cumulative mass balance for the solute (I670–I860). The accuracy of the chemical mass balance is estimated on lines I610–I660 using equations 62 and 64. The former is not computed if there was no change in the total mass of solute stored in the aquifer. The latter is not computed if the initial concentrations were zero everywhere. Lines I890–I1140 serve to print the head and concentration data recorded at observation wells. These data are recorded after each time step for a transient flow problem and after each particle movement for a steady-state flow problem. The data are printed after every 50 time increments and at the end of the simulation period.

Evaluation of Model

Comparison with analytical solutions

The accuracy of the numerical solution to the solute-transport equation can be evalu-

ated in part by analyzing relatively simple problems for which analytical solutions are available and then comparing the numerical calculations with the analytical solution. Figure 11 presents such a comparison for a problem of one-dimensional steady-state flow through a homogeneous isotropic porous medium. The analytical solution is obtained with the following equation presented by Bear (1972, p. 627):

$$\frac{C(x,t)-C_0}{C_1-C_0}=\frac{1}{2}\text{erfc}\left\{-\frac{x-qt/\epsilon}{\sqrt{4D_L t}}\right\} \quad (68)$$

where

erfc is the complimentary error function, and

$q=\epsilon V$ is the specific discharge, LT^{-1}.

Bear (1972, p. 627) shows that equation 68 is subject to the following initial conditions:

$$t\leq 0,\quad -\infty<x<0,\quad C=C_0$$
$$0\leq x<+\infty,\quad C=C_1$$

and to the following boundary conditions:

$$t>0,\quad x=\pm\infty,\quad \partial C/\partial x=0$$
$$x=+\infty,\quad C=C_1$$
$$x=-\infty,\quad C=C_0.$$

The general computer program presented in this report was modified in three simple ways for application to a problem equivalent to the one for which the analytical solution was derived. First, the program's arrays were redimensioned to 3 by 50 rather than 20 by 20. The aquifer (or column of porous medium) was thus represented by a 1-by-48 array of nodes. A grid spacing of 10 ft (3.05 m) was used. Second, the flow velocity was specified as a constant value, rather than being computed implicitly on the basis of hydraulic gradients and hydraulic conductivity. Third, the first (upstream) node of the aquifer was specified as a constant-concentration boundary, so that the concentration at node (2,2) was always equal to C_0 of

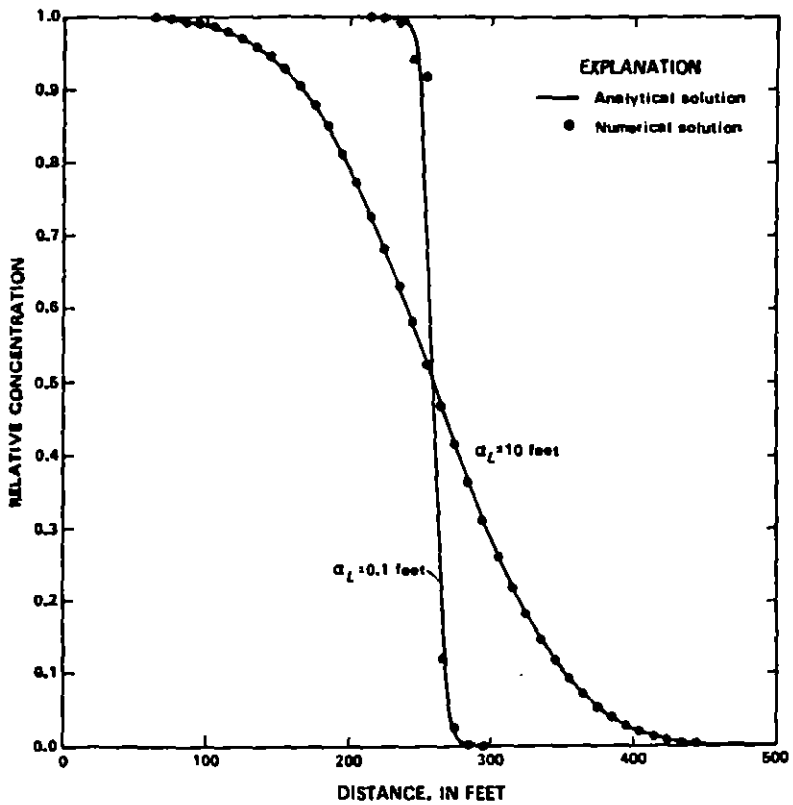

Figure 11.—Comparison between analytical and numerical solutions for dispersion in one-dimensional, steady-state flow.

equation 68. In the analysis of one-dimensional test problems, it was assumed that porosity equals 0.35, velocity equals 3.0×10^{-4} ft/s (9.1×10^{-5} m/s), and time equals 10.0 days.

As shown in figure 11, comparisons between the analytical and numerical solutions were made for two different values of dispersivity. For the higher dispersion there was essentially an exact agreement between the two curves. In the case of low dispersion, there is a very small difference at some nodes between the concentrations computed analytically and those computed numerically. This difference is caused primarily by the error in computing the concentration at a node as the arithmetic average of the concentrations of all particles located in that cell. This is not considered to be a serious problem since this error is not cumulative. Also note in the case of low dispersion that the grid spacing (10 ft or 3.05 m) was coarse relative to the width of the breakthrough curve between concentrations of 0.05 and 0.95. Nevertheless, the numerical model still accurately computed the shape and position of the front.

In computing the numerical solutions shown in figure 11 the program was executed using nine particles per cell and with CELDIS = 0.50 (γ in equations 54–55). The 10-day simulation required 52 time increments and used about 40 seconds of cpu on a Honeywell 60/68 computer.

An analytical solution is also available for the problem of plane radial flow in which a well continuously injects a tracer at constant rate q_w and constant concentration C_o. Bear (1972, p. 638) indicates that the following equation is appropriate for this problem (although there are some limitations discussed by Bear):

$$\frac{C}{C_o}=\frac{1}{2}\operatorname{erfc}\left\{\frac{r^2/2-Gt}{\sqrt{4/3a_L\bar{r}^3}}\right\} \qquad (69)$$

where

$G = \dfrac{q_w}{2\pi\epsilon b} = Vr$;

r is the radial distance from the center of the well, L; and

$\bar{r}=(2Gt)^{1/2}$ is the average radius of the body of injected water, L.

Again, the general computer program had to be somewhat modified to permit a suitable comparison to be made between the analytical solution and the numerical model. One change involved the direct calculation of velocity at any point based on its distance from the well using the following equation:

$$V=\frac{q_w}{2\pi r\epsilon b}. \qquad (70)$$

The other significant change was made in subroutine GENPT to allow the initial placement of 16 particles per cell, rather than the present maximum of 9. In the analysis of test problems for radial flow, it was assumed that porosity equals 0.35, the injection rate (q_w) equals 1.0 ft^3/s (0.028 m^3/s), saturated thickness equals 10.0 ft (3.05 m), and longitudinal dispersivity equals 10.0 ft (3.05 m).

The application of the method of characteristics, which was written for two-dimensional Cartesian coordinates, to a problem involving radially symmetric divergent flow represents a severe test of the model. Nevertheless, it can be seen in figure 12 that there is good agreement between the analytical and numerical solutions after both relatively short and long times. However, the presence of some numerical dispersion is evident, particularly for the longer time. The numerical dispersion is introduced in part during the regeneration of particles after the number of cells void of particles has exceeded the critical number. The geometry of initial particle placement minimized this problem in cells that lay in the same row or column of the grid as the injection well. The circles in figure 12, which indicate concentration values computed at these nodes, agree closely with the analytical solution. The greatest errors occur at nodes on radii from the injection well that are neither parallel to nor 45° from the main axes of the grid. These results indicate that this Cartesian coordinate model is not best suited for application to purely radial flow problems. However, if radially divergent flow is limited to areas of several

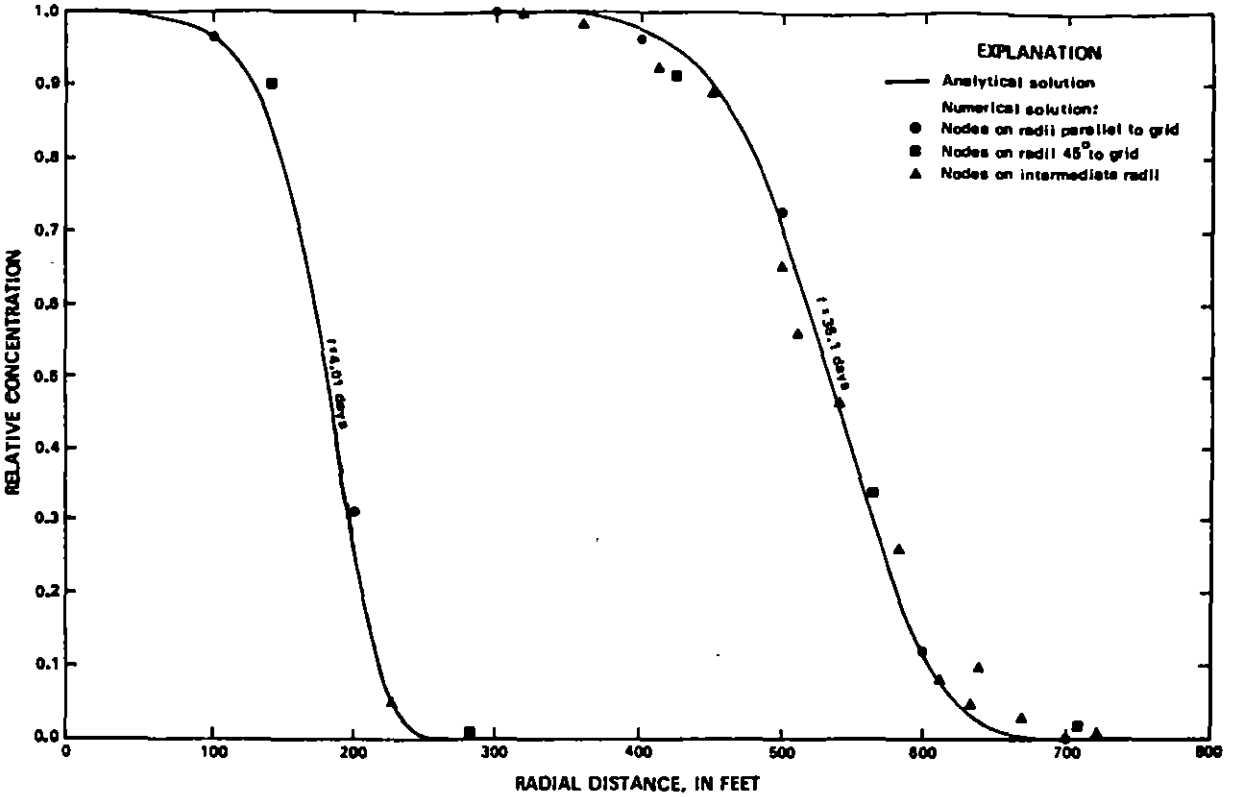

Figure 12.—Comparison between analytical and numerical solutions for dispersion in plane radial steady-state flow.

rows and columns within a more uniform regional flow field, the model will accurately compute concentration distributions. To apply the method of characteristics to a problem of plane radial flow, it would be best to rewrite the program in a system of radial coordinates, which should improve the accuracy for those problems to the same order shown in figure 11 for the analysis of one-dimensional flow.

Mass balance tests

The accuracy and precision of the numerical solution can also be partly evaluated by computing the magnitude of the error in the mass balance. The mass balance error will depend on the nature of the problem and will vary from one time step to the next. During the development of the program, the model was applied to a variety of hypothetical solute-transport problems to assure its flexibility, transferability, and accuracy under a wide range of conditions. To illustrate the range in mass balance errors that might be expected and some of the factors that affect it, several of these problems are presented here.

Test problem 1—spreading of a tracer slug

The first test described here was designed to evaluate the accuracy of simulating the processes of convective transport and dispersion independent of the effects of chemical sources. Thus, a slug of tracer was initially placed in four cells of a grid whose boundary conditions generated a steady-state flow field that was moderately divergent in some places and moderately convergent in other places, as illustrated in figure 13. The aquifer was assumed to be homogeneous and isotropic. Because flow was assumed to be in steady state, the storage coefficient was set equal to 0.0. The parameters used to define problem

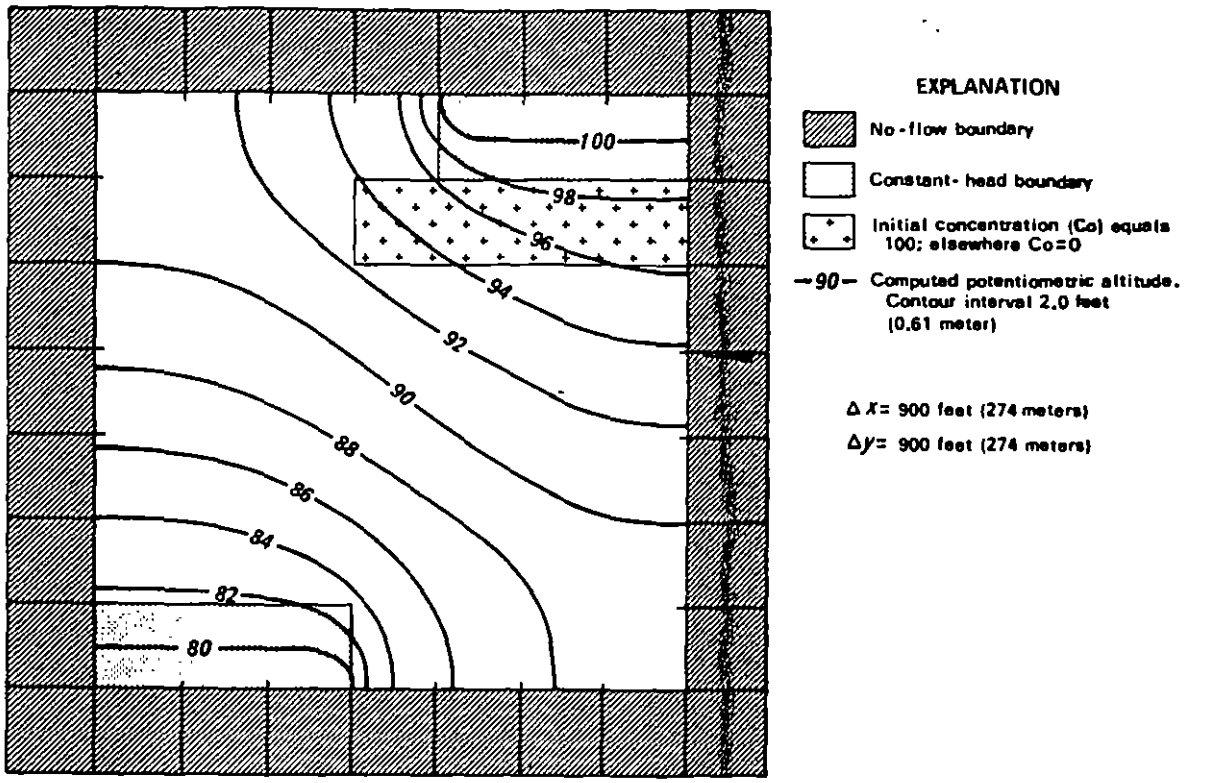

Figure 13.—Grid, boundary conditions, and flow field for test problem 1.

1 are listed in table 2. The slug of known mass was then allowed to spread downgradient for a period of 2.0 years.

Table 2.—Model parameters for test problem 1

Aquifer properties	Numerical parameters
K=0.005 ft/s (1.5×10^{-3} m/s)	Δx=900 ft (274 m)
b=20.0 ft (6.1 m)	Δy=900 ft (274 m)
S=0.0	CELDIS=0.49
ϵ=0.30	NPTPND=9
α_T/α_L=0.30	

The model first computed a steady-state head distribution, shown in figure 13, and velocity field. The model required 12 time increments (or particle movements) to simulate a 2.0-year period. The model was run to simulate conditions of no dispersion (α_L=0.0 ft) as well as moderate dispersion (α_L=100 ft or 30.5 m). The mass balance error computed using equation 64 is shown in figure 14 for both conditions. In these tests the error averages 1.9 percent and is always within a range of ±8 percent. Much of the error is related to the calculation of nodal concentrations based on the arithmetic mean of particle concentrations in each cell. When a particle moves across a cell boundary, its area of influence shifts entirely from the first node to the second. Thus, depending on the local density of points and local concentration gradients, the use of an arithmetic mean to compute nodal concentrations may give too much weight to some particles and too little weight to others. The use of a weighted mean, in which the weighting factor is a function of the distance between a node and a particle, reduced the error to some degree. But the improvement in precision was small compared with the increase in computational requirements, so this algorithm was not included in the general program. Because the error caused by using an arithmetic mean is not cumulative, it is not considered a serious

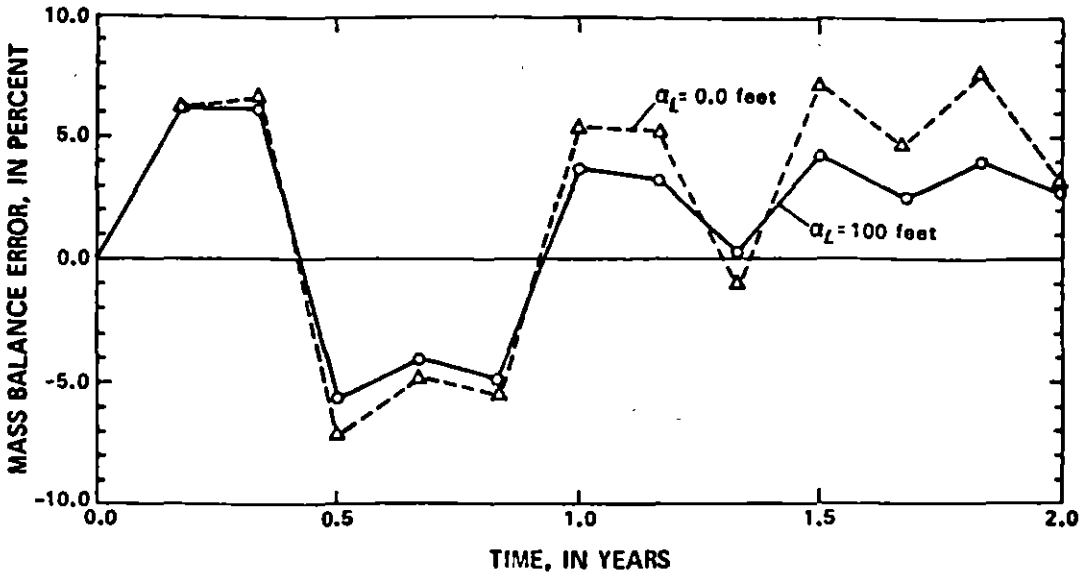

Figure 14.—Mass balance errors for test problem 1.

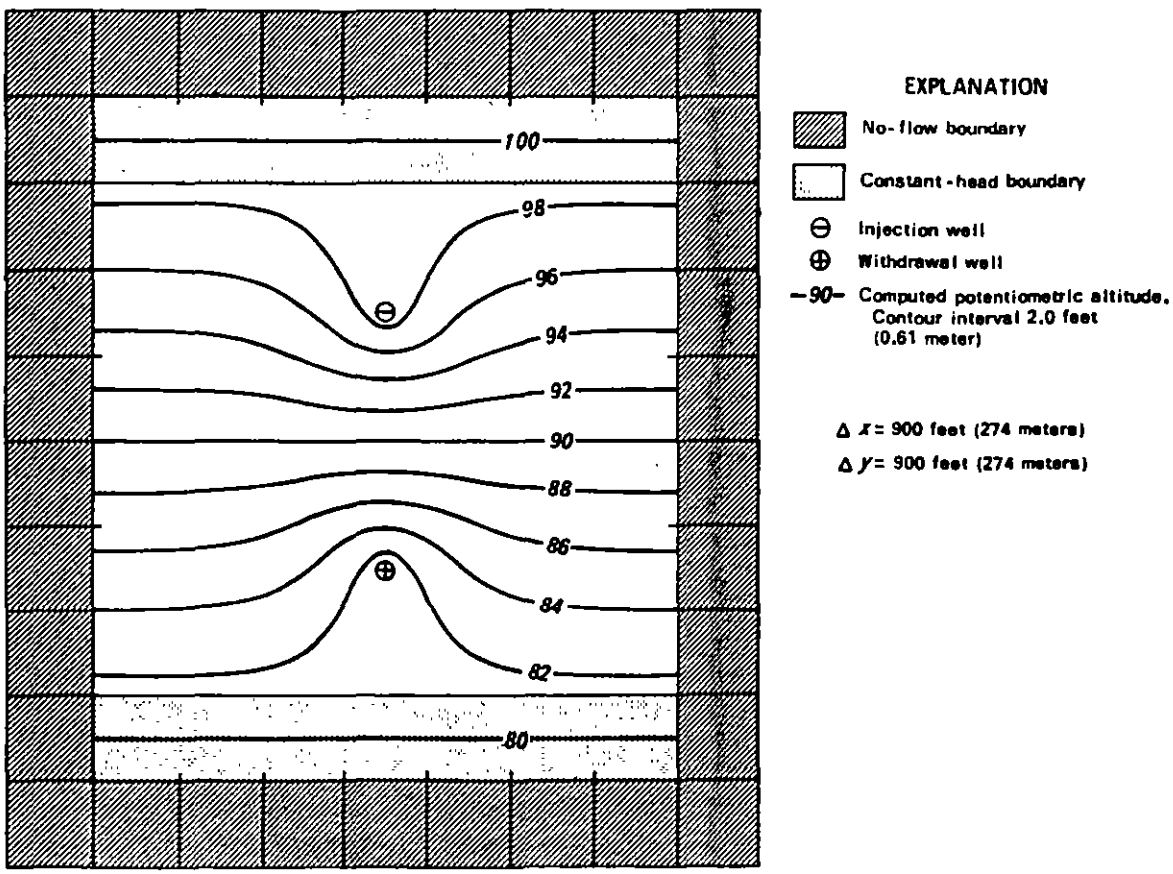

Figure 15.—Grid, boundary conditions, and flow field for test problem 2.

problem. Furthermore, figure 14 shows that the error decreases for a higher dispersivity because dispersion smooths out sharp fronts and minimizes strong concentration gradients.

Test problem 2—effects of wells

The second problem was designed to evaluate the application of the model to problems in which the flow field is strongly influenced by wells. The grid and boundary conditions used to define this problem are illustrated in figure 15. The problem consists of one injection well and one withdrawal well, whose effects are superimposed on a regional flow field controlled by two constant-head boundaries. The parameters for problem 2 are defined in table 3. The aquifer was also assumed to be homogeneous and isotropic. The model simulated a period of 2.4 years and assumed steady-state flow.

The model required 18 time increments (or particle movements) to simulate a 2.4-year period of solute transport. Problem 2 was also evaluated for conditions of no dispersion ($\alpha_L = 0.0$ ft) as well as moderate dispersion ($\alpha_L = 100$ ft or 30.5 m). The mass balance error was computed using equation 62 and is shown in figure 16 for both conditions. The average of the 36 values shown in figure 16 is −0.06 percent; the error always falls within the range of ±8 percent. It can be seen that in this case the errors are essentially coincident for almost 1 year, after which the error appears to be dependent on the magnitude of dispersion. However, the model output showed that when $\alpha_L = 100$ ft (30.5 m), the leading edge of the breakthrough curve (or chemical front) reaches the constant-head sink just prior to 1.0 year. When $\alpha_L = 0.0$ ft, the leading edge of the breakthrough curve still had not entered the constant-head sink after 2.4 years. Because the two curves in figure 16 are essentially coincident prior to 1.0 year, it thus appears that the divergence of the two curves is not caused directly by the difference in dispersivity. Rather, it is related to the difference in arrival times at the hydraulic sinks and is a direct effect of the manner in which con-

Table 3.—Model parameters for test problems 2 and 3

Aquifer properties and stresses	Numerical parameters
$K = 0.005$ ft/s (1.5×10^{-3} m/s)	$\Delta x = 900$ ft (274 m)
$b = 20.0$ ft (6.1 m)	$\Delta y = 900$ ft (274 m)
$S = 0.0$	CELDIS = 0.50
$\epsilon = 0.30$	NPTPND = 9
$\alpha_T/\alpha_L = 0.30$	
$C' = 100.0$	
$C_o = 0.0$	
$q_w = 1.0$ ft²/s (0.028 m²/s)	

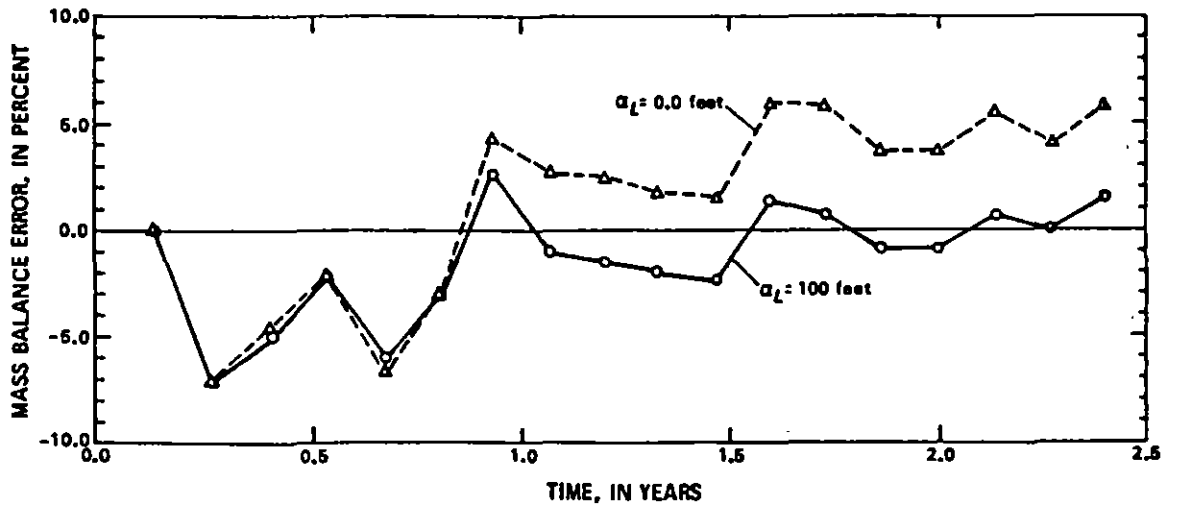

Figure 16.—Mass balance errors for test problem 2.

centrations are computed at sink nodes and (or) the method of estimating the mass of solute removed from the aquifer at sink nodes during each time increment.

Test problem 3—effects of user options

In addition to the input options that control the form or frequency of the output, there are two execution parameters that must be specified by the user and influence the accuracy, precision, and efficiency (or computational cost) of the solution to a particular problem. These execution parameters are the initial number of particles per node (NPTPND) and the maximum fraction of the grid dimensions that particles are allowed to move (γ in equations 54–55 or CELDIS in the program). The third test problem was designed to allow an evaluation of both of these parameters. As illustrated in figure 17, this problem consists of one withdrawal well located in a regional flow field that is controlled by two constant-head boundaries. The contamination sources are three central nodes along the upgradient constant-head boundary. The model parameters for test problem 3 are the same as for test problem 2, as listed in table 3. However, for test problem 3 solutions were obtained using a range in values for CELDIS and NPTPND.

The solution to this problem was found to be sensitive to the density of tracer particles used in the simulation. Figure 18 shows how the error in the mass balance varied with time for cases of NPTPND equal to 4, 5, 8, and 9. Table 4 lists the execution time and the mean and standard deviation of the mass balance error for each case. These data clearly indicate that the accuracy and precision

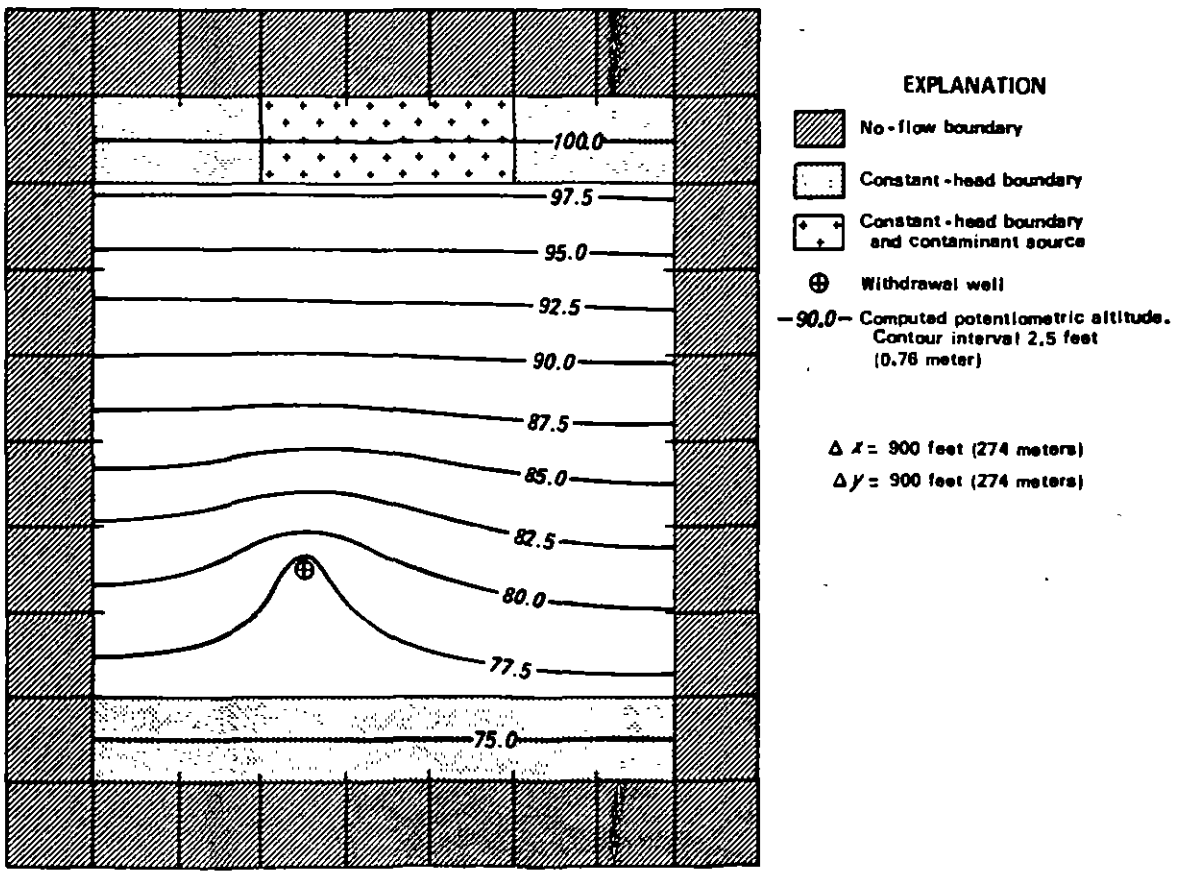

Figure 17.—Grid, boundary conditions, and flow field for test problem 3.

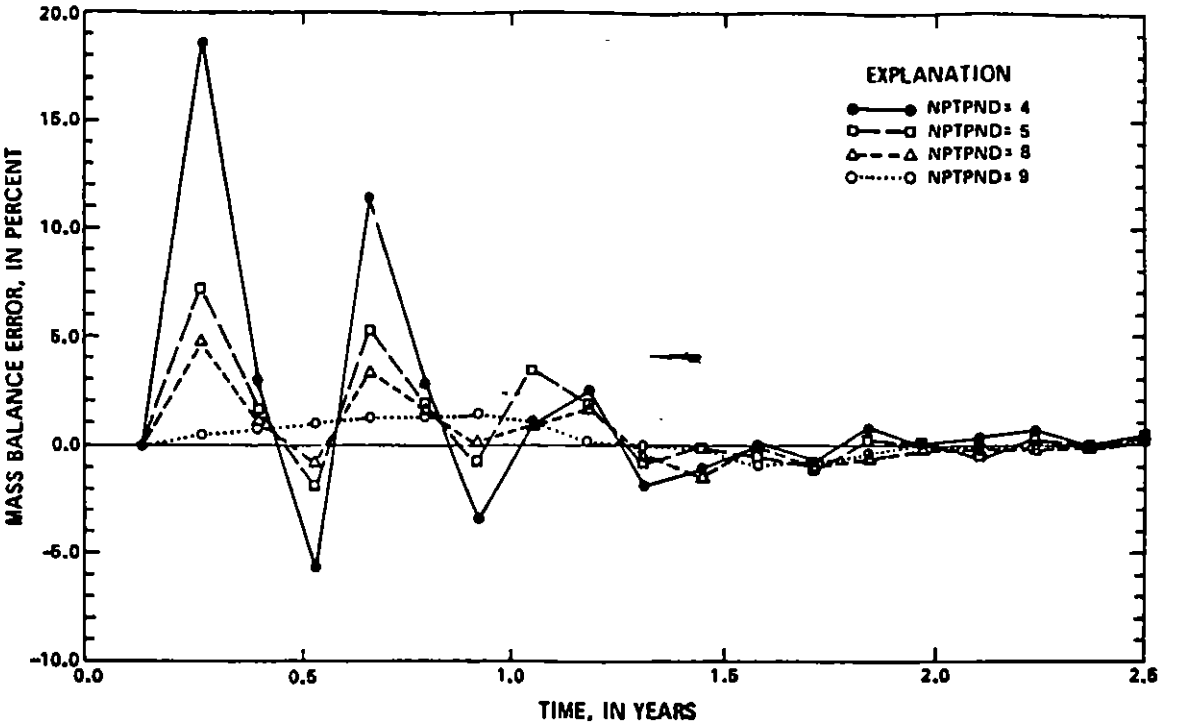

Figure 18.—Effect of NPTPND on mass balance error for test problem 3; CELDIS=0.50 in all cases.

Table 4.—Effect of NPTPND on accuracy, precision, and efficiency of solution to test problem 3

NPTPND	cpu-seconds[1]	Mass balance error (percent) Mean	Mass balance error (percent) Standard deviation
4	12.8	1.49	5.33
5	14.0	.90	2.29
8	17.9	.48	1.53
9	19.2	.26	.69

[1] The program was executed on a Honeywell 60/68 computer; CELDIS=0.50.

of the solution are directly proportional to particle density, while the efficiency of the solution is inversely related to NPTPND. In other words, a better solution will cost more. It is important to note that the oscillations or scatter shown in figure 18 decrease with time and that there is essentially no difference among the solutions and among the mass balance errors for times greater than about 1.5 years.

Next the effect of CELDIS (or γ) was evaluated for test problem 3 by setting NPTPND=9 and running the model with several possible values of CELDIS. Figure 19 shows how the error in the mass balance varied with time for cases of CELDIS equal to 0.25, 0.50, 0.75, and 1.00. Table 5 lists the execution time and the mean and standard deviation of the mass balance error for each case. These data indicate that the relationship between CELDIS and the mass balance error is not as simple and straightforward as for NPTPND. It is apparent that the results for 0.50, 0.75, and 1.00 are similar, and of these, the results for CELDIS=0.50 ap-

Table 5.—Effect of CELDIS on accuracy, precision, and efficiency of solution to test problem 3

CELDIS	cpu-seconds[1]	Mass balance error (percent) Mean	Mass balance error (percent) Standard deviation
0.25	34.6	1.50	2.99
.50	19.2	.26	.69
.75	14.4	.56	.69
1.00	12.1	.25	1.48

[1] The program was executed on a Honeywell 60/68 computer; NPTPND=9.

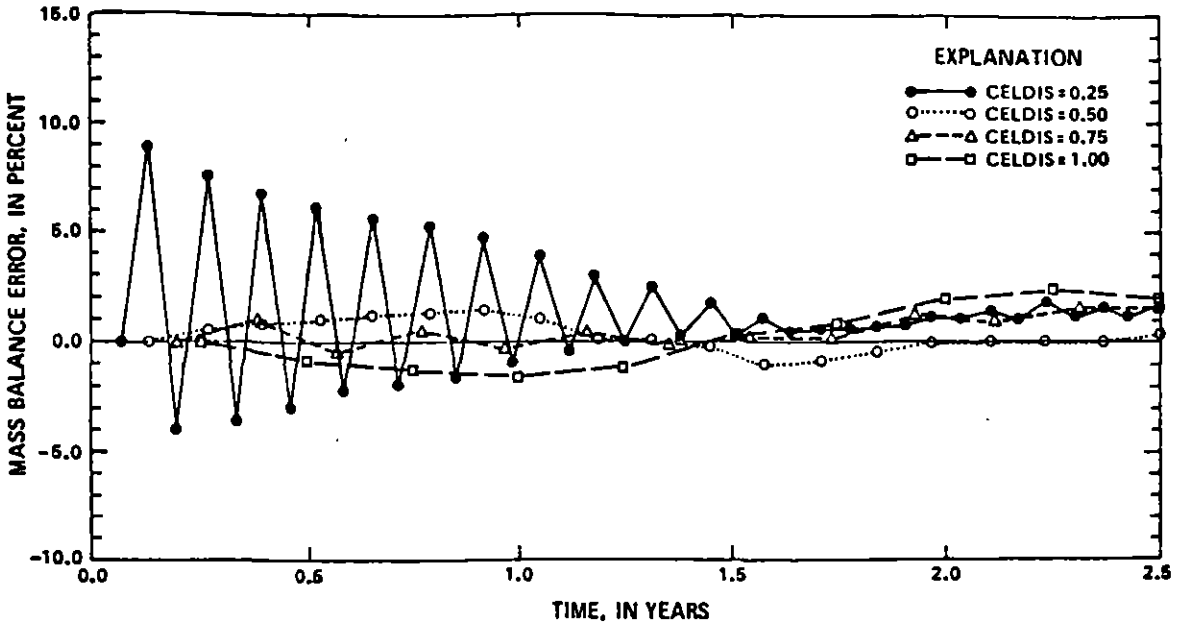

Figure 19.—Effect of CELDIS on mass balance error for test problem 3; NPTPND=9 in all cases.

pear to be the best. However, when CELDIS was reduced to 0.25, the error oscillated strongly for about 1.5 years before apparently converging to a small error within the range of the other curves. This oscillation occurred because the maximum distance a particle could move (25 percent of the grid dimensions) was less than the spacing between particles (33 percent of the grid dimensions for NPTPND=9). Thus, convective transport across the boundaries of cells could not be adequately represented for any single time step in those parts of the grid where the concentration was changing significantly with time. But over two successive time increments the error would average out to a minimum. As the contaminated area increases in size over time, the error in computed concentrations at cells near the front (that is, in areas of steep concentration gradient) becomes an increasingly smaller percentage of the total mass of solute present in the aquifer. Hence, the mass balance error generally tends to approach a minimal range with time for these types of problems.

The effects of NPTPND and CELDIS on the mass balance error are problem dependent. In problems for which CELDIS is not the limiting stability criterion, varying CELDIS will have no effect on the solution. Because of the possible tradeoff between accuracy and efficiency, it is recommended in general that the model user specify NPTPND as 4 or 5 and CELDIS as 0.75 to 1.0 for runs made during the early stages of model calibration when frequent runs are made and maximum efficiency is desired. For final runs when maximum accuracy is desired, set NPTPND equal to 9 and CELDIS equal to 0.50.

Possible program modifications

The program presented here represents a basic and general solute-transport model. Some program modifications may be desirable or even necessary to allow the model to be applied efficiently to a particular field problem. Some changes might require only minor adjustments, while others might involve major rewriting of the program. The purpose of this section is to discuss some of the modifications that might commonly be considered, and that might be incorporated into the present basic model, rather than using an entirely different solution technique.

Coordinate system and boundary conditions

After the finite-difference grid is designed, the first program modification that should be made is to modify the array dimensions for the specific grid used. This will permit the most efficient use of computer storage. The array sizes should be set equal to NX, NY, and NPMAX, which are specified on Input Card 2. The maximum number of particles, NPMAX, may be computed from the following equation:

$$NPMAX \cong (NX-2)(NY-2)(NPTPND) + (N_s)(NPTPND) + 250 \quad (71)$$

where

N_s is the number of nodes that represent fluid sources, either at wells or at constant-head cells.

The values of NX and NY should be substituted for the 20-by-20 arrays contained in COMMON statements PRMK, HEDA, HEDB, CHMA, CHMC, and DIFUS, and in DIMENSION statements on lines C170, G200, H140, and I160. The value of NPMAX should replace 3200 in the PART array in all the CHMA COMMON statements.

Although this program is designed for application to two-dimensional areal flow problems, it can be applied directly to two-dimensional cross sections. In this case the z-coordinate would replace the y-coordinate. Then the user would have to assume and specify unit width (THCK array) for Δy and substitute hydraulic conductivity for transmissivity in data set 3 of attachment III. If the problem involves transient flow, then specific storage (S_s) should be substituted for the storage coefficient. Also, if recharge or discharge is to be specified through the RECH array (data set 5), values should be divided by the thickness of the layer (Δz) to reduce the dimensionality of the stress rate to (T^{-1}) rather than (LT^{-1}) as indicated in the documentation. In applying the cross-sectional model to a field problem it is important that conditions meet the inherent assumption that there exist no significant components of flow into or out of the plane of the section. Because this assumption would probably be impossible to meet in the vicinity of a pumping well, the use of the REC array (data set 2) should usually be limited to representing special or known-flux boundary conditions.

The program can also be applied directly and simply to one-dimensional problems. In this case one of the dimensions (NX or NY) should be reduced to a value of 3, of which the outer two are used to represent the no-flow boundaries around the one-dimensional row or column.

The most complex type of change would involve rewriting the program for application to other than a two-dimensional rectangular grid. One possibility includes problems of flow to or from wells in which radial symmetry can be assumed. This would allow variables to be expressed in terms of r-z coordinates. Another possibility is to simulate three-dimensional flow in x-y-z coordinates. A three-dimensional finite-difference flow model is available (Trescott, 1975) and would be compatible with the method-of-characteristics solution to the solute-transport equation.

It is sometimes convenient to separately associate certain parts of the grid or certain boundary conditions with corresponding field conditions or hydrologic units. The analysis of flow patterns and water-quality changes may then be aided by performing separate mass balances (or budgets) for each characteristic type of node. The nodal types or zones can be conveniently identified through the NODEID array. Then the mass balance routines in subroutines CNCON and (or) OUTPT would have to be modified to tally fluxes separately for each NODEID; for an example, see Konikow (1977). Similarly, if a coupled stream-aquifer system is being considered, a separate subroutine may be added to route streamflow downstream and progressively account for ground-water gains and losses and for tributary inflow or diversions. An example of such a modification is discussed by Konikow and Bredehoeft (1974).

For certain types of problems it may be desirable to be able to specify a constant-concentration boundary condition. The pro-

gram could be modified to allow this by using a predetermined value or range in values of NODEID to identify this type of boundary. Then a statement could be added between lines G1090 and G1100 to reset the concentration at the node equal to the constant concentration where this condition is specified. The value of the constant concentration can be stored in the CNRECH array. Note that the mass balance calculation as presently written will not account for the mass of solute added or removed at a constant-concentration boundary.

Basic equations

The basic equations that are solved by this model were derived under a number of limiting assumptions. Some of these assumptions can be overcome through modifications of the basic equations and corresponding changes in the program.

The program assumes that molecular diffusion is negligible. But if it is necessary to consider the process of molecular diffusion in a particular problem, the coefficient of hydrodynamic dispersion (D_{ij}) can be redefined as the sum of the coefficient of mechanical dispersion, which is defined by the right side of equation 5, and a coefficient of molecular diffusion. The consequent program modification would have to be made only in subroutine VELO (lines E1280–E1680).

The solute-transport equation can also be modified to include the effects of first-order chemical reactions, as was done by Robertson (1974). The reaction term could be included in the right side of equation 39. The corresponding program modification would be required in subroutine CNCON.

In certain problems the range in concentrations may be so great that the dependence of fluid properties, such as density and viscosity, on the concentration may have to be considered because of the dependence of fluid flow on variations in fluid properties. In this case the flow equation (eq 1) would have to be rewritten in terms of fluid pressure, rather than hydraulic head, such as equation 15 of Bredehoeft and Pinder (1973, p. 197). Then the program can be modified to iterate between the solutions to the flow and solute-transport equations if the change in fluid properties at any node exceeds some criterion during one time increment.

The flow equation can also be modified for application to unconfined aquifers in which the saturated thickness is a direct function of water-table elevation. This would require the inclusion of steps in subroutine ITERAT to correct the transmissivity for changes in saturated thickness. Such a feature is included in the two-dimensional flow model documented by Trescott, Pinder, and Larson (1976).

Input and output

The input and output formats have been designed for flexibility of use and general compatibility with the analysis of a variety of types of flow problems. If any of the formats are not suitable for use with a particular problem, they should be modified accordingly. All input formats are described in attachment III and contained in subroutine PARLOD in the program.

It has been assumed that several aquifer parameters are constant and uniform in space, such as storage coefficient, effective porosity, and dispersivity. If any of these are known to vary in space, they should be redefined as two-dimensional arrays. Then statements to allow these arrays to be read into the program should be added to subroutine PARLOD. Similarly, values of leakance and source concentrations (CNRECH) are only read in data set 7, where values can be associated only with a limited number of unique node identification codes. If the variations of these parameters are known on a more detailed scale, then they too can be read as additional data sets by adding appropriate statements to subroutine PARLOD. For example, a typical sequence of statements for reading one data set is represented by lines B2650–B2750, where the initial water-table elevations (data set 8) are read. This sequence of statements can then be replicated for reading in a different data set and inserted into subroutine PARLOD.

A labeled listing of the input data deck for test problem 3 is provided in attachment IV. This example illustrates the use of the data input formats specified in attachment III and shows that only a few data cards are required by the model to simulate a relatively simple problem. This example will also allow the user to verify that his program deck and computer yield essentially the same results as obtained by the documented program. Thus, selected parts of the output for test problem 3 are included in attachment V. Not all of the printed output from test problem 3 has been duplicated in attachment III. Instead, it contains only a sufficient selection to illustrate the type and form of output provided by the model, as well as to allow the user to compare his calculated values of critical parameters, such as head, velocity, and concentration, with the values computed by the documented model.

Conclusions

The model presented in this report can simulate the two-dimensional transport and dispersion of a nonreactive solute in either steady-state or transient ground-water flow. The program is general and flexible in that it can be readily and directly applied to a wide range of types of problems, as defined by aquifer properties, boundary conditions, and stresses. However, some program modifications may be required for application to specialized problems or conditions not included in the general model.

The accuracy of the numerical results can be evaluated by comparison with analytical solutions only for relatively simple and idealized problems; in these cases there was good agreement between the numerical and analytical results. Mass balance tests also help to evaluate the accuracy and precision of the model results. The error in the mass balance is generally less than 10 percent. The range in mass balance errors is commonly the greatest during the first few time increments, but tends to decrease and stabilize with time. For some problems the accuracy and precision of the numerical results may be sensitive to the initial number of particles placed in each cell and to the size of the time increments, as determined by the stability criteria for the solute-transport equation. The results of several numerical experiments suggest that the accuracy and precision of the results are essentially independent of the magnitude of the dispersion coefficient, and comparable accuracies are attained for high, low, or zero dispersivities.

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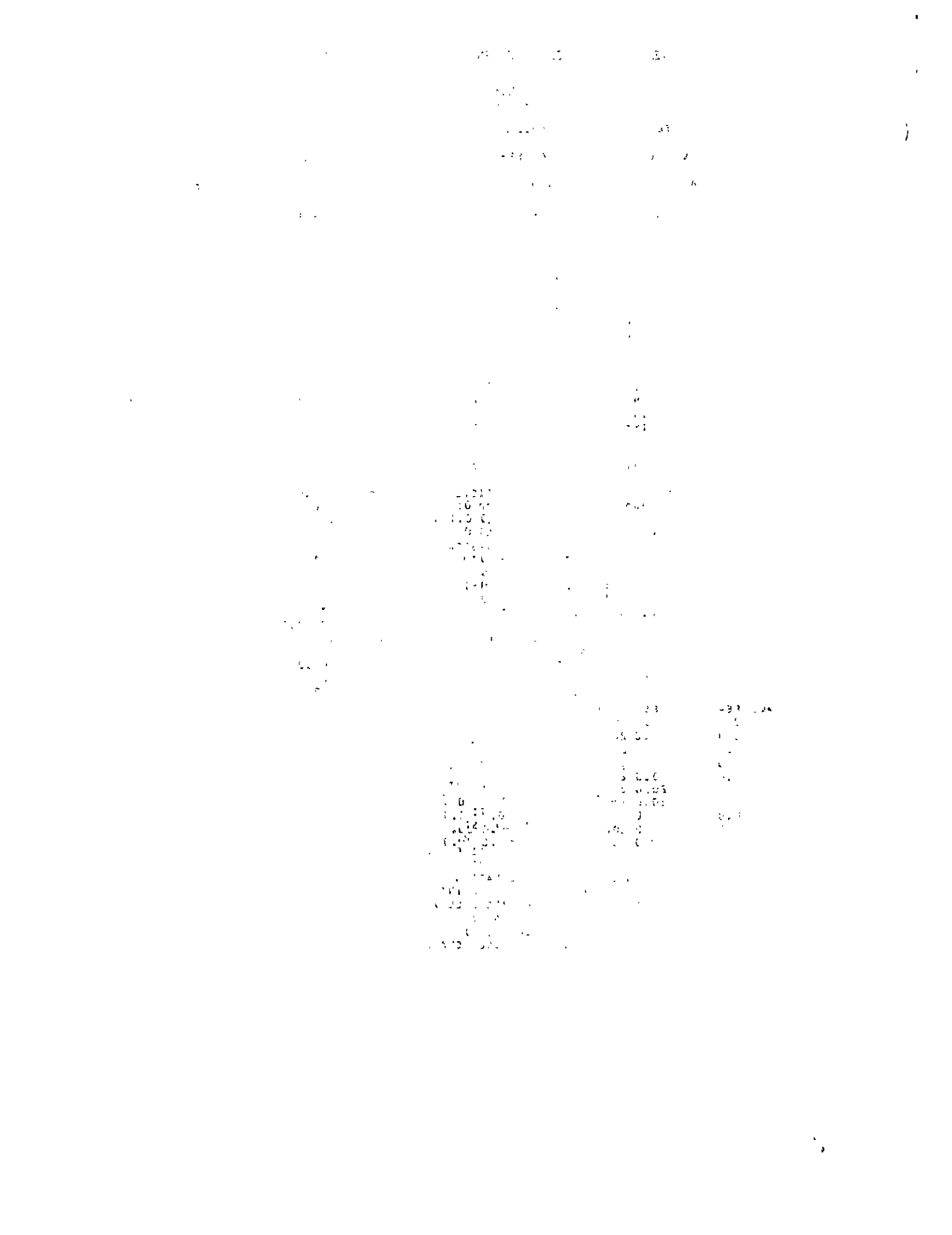
Attachment V
Selected Output for Test Problem 3

```
U.S.G.S. METHOD-OF-CHARACTERISTICS MODEL FOR SOLUTE TRANSPORT IN GROUND WATER

TEST PROBLEM NO. 3 (STEADY FLOW, 1 WELL, CONSTANT-HEAD BOUNDARIES)

                    I N P U T     D A T A

                      GRID DESCRIPTORS

NX     (NUMBER OF COLUMNS)  =      9
NY     (NUMBER OF ROWS)     =     10
XDEL   (X-DISTANCE IN FEET) =  900.0
YDEL   (Y-DISTANCE IN FEET) =  900.0

                      TIME  PARAMETERS

NTIM   (MAX. NO. OF TIME STEPS)        =       1
NPMP   (NO. OF PUMPING PERIODS)        =       1
PINT   (PUMPING PERIOD IN YEARS)       =    2.50
TIMX   (TIME INCREMENT MULTIPLIER)     =    0.00
TINIT  (INITIAL TIME STEP IN SEC.)     =      0.

  HYDROLOGIC AND CHEMICAL PARAMETERS

S       (STORAGE COEFFICIENT)          =    0.000000
POROS   (EFFECTIVE POROSITY)           =    0.30
BETA    (CHARACTERISTIC LENGTH)        =  100.0
DLTRAT  (RATIO OF TRANSVERSE TO
        LONGITUDINAL DISPERSIVITY)     =    0.30
ANFCTR  (RATIO OF T-YY TO T-XX)        =    1.000000

                    EXECUTION PARAMETERS

NITP   (NO. OF ITERATION PARAMETERS) =    7
TOL    (CONVERGENCE CRITERIA - ADIP) =    0.0001
ITMAX  (MAX.NO.OF ITERATIONS - ADIP) =  100
CELDIS (MAX.CELL DISTANCE PER MOVE
          OF PARTICLES - M.O.C.)     =    0.500
NPMAX  (MAX. NO. OF PARTICLES)       = 3200
NPTPND (NO. PARTICLES PER NODE)      =    9

                      PROGRAM OPTIONS

NPNT   (TIME STEP INTERVAL FOR
        COMPLETE PRINTOUT)           =    1
NPNTKV (MOVE INTERVAL FOR CHEM.
        CONCENTRATION PRINTOUT)      =   10
NPNTVL (PRINT OPTION-VELOCITY
        0=NO; 1=FIRST TIME STEP;
        2=ALL TIME STEPS)            =    1
NPNTD  (PRINT OPTION-DISP.COEF.
        0=NO; 1=FIRST TIME STEP;
        2=ALL TIME STEPS)            =    0
NUMOBS (NO. OF OBSERVATION WELLS
        FOR HYDROGRAPH PRINTOUT)     =    2
NREC   (NO. OF PUMPING WELLS)        =    1
NCODES (FOR NODE IDENT.)             =    2
NPNCHV (PUNCH VELOCITIES)            =    0
NPDELC (PRINT OPT.-CONC. CHANGE)     =    0
```



Selected output for test problem 3—Continued

```
          STEADY-STATE FLOW

TIME INTERVAL (IN SEC) FOR SOLUTE-TRANSPORT SIMULATION =  0.78894d+08

      LOCATION OF OBSERVATION WELLS

            NO.      X     Y

             1       5     4
             2       5     7

      LOCATION  OF  PUMPING  WELLS

      X   Y   RATE(IN CFS)   CONC.

      4   7       1.00        0.0

      AREA OF ONE CELL =   0.8100d+06

      X-Y SPACING:
          900.00
          900.00




TRANSMISSIVITY MAP (FT*FT/SEC)
   0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
   0.00 0.10 0.10 0.10 0.10 0.10 0.10 0.10 0.00
   0.00 0.10 0.10 0.10 0.10 0.10 0.10 0.10 0.00
   0.00 0.10 0.10 0.10 0.10 0.10 0.10 0.10 0.00
   0.00 0.10 0.10 0.10 0.10 0.10 0.10 0.10 0.00
   0.00 0.10 0.10 0.10 0.10 0.10 0.10 0.10 0.00
   0.00 0.10 0.10 0.10 0.10 0.10 0.10 0.10 0.00
   0.00 0.10 0.10 0.10 0.10 0.10 0.10 0.10 0.00
   0.00 0.10 0.10 0.10 0.10 0.10 0.10 0.10 0.00
   0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00




AQUIFER THICKNESS (FT)
    0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
    0.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0  0.0
    0.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0  0.0
    0.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0  0.0
    0.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0  0.0
    0.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0  0.0
    0.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0  0.0
    0.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0  0.0
    0.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0  0.0
    0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
```