CURSO: " MODELADO SIMULACION Y CONTROL DE EVAPORADORES-
REACTORES Y TORRES DE DESTILACION."

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INTRODUCCION AL MODELADO
DE
PROCESOS QUIMICOS.

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Introducción al Modelado de Procesos Químicos

Es de mi interés presentar en estas notas una introducción a los conceptos fundamentales con los cuales se pueda representar en forma matemática el comportamiento dinámico de los equipos básicos utilizados en procesos químicos.

El aspecto general de la presentación de los conceptos básicos, está basado en el planteamiento de ecuaciones algebraicas o ecuaciones diferenciales totales, sin embargo es importante mencionar que las ecuaciones diferenciales parciales de primera importancia en el modelo matemático de comportamiento de un proceso pueden ser aproximadas a una diferencial total con ciertas consideraciones, es por ello que en estas notas de introducción al modelado de procesos no se hace mención a las ecuaciones diferenciales parciales, quedando las mismas como un tema de interés para un curso posterior.

El modelado de procesos químicos está basado en las ecuaciones de masa, momento y energía, las cuales se aplican a todos los equipos en procesos como el caso de tanques, reactores, intercambiadores de calor, torres de destilación, tuberías, etc.

Una planta de proceso tiene dentro de sus operaciones unitarias que la constituyen el siguiente equipo básico:

Tanques de Alimentación

Son dispositivos de almacenamiento de líquidos, sólidos o gases, generalmente son los elementos de entrada al proceso.

Las Válvulas

Las válvulas tienen como función regular el gasto del fluido en las partes del proceso. Generalmen te son los elementos finales de control.

El Reactor

Es un recipiente con una chaqueta o camisa, en el interior del recipiente se coloca el reactante y en la chaqueta se alimenta ya se vapor para iniciar la reacción, o agua fría si la reacción es de tipo exotérmico.

El tiempo que debe permanecer el reactante para obtener el producto deseado depende de la reacción, la cual depende de el coeficiente de reacción, la temperatura y la presión.

Intercambiador de Calor

El intercambiador de calor tiene como función la transferencia de calor entre cuerpos calientes y fríos sin intercambio de masa, es decir solo existe transferencia de energía, dentro de este grupo tenemos los calentadores, los enfriadores, etc.

Evaporadores

El evaporador es un intercambiador de calor el cual tiene como finalidad la evaporación de un líquido para concentrar una solución determinada.

Torres de Destilación

La destilación es una separación de componentes que se encuentran en una solución líquida o mezcla, a partir de la cual se va a obtener uno o varios productos por medio de un proceso de ebullición basado en la diferencia de presiones y flujos en contracorriente en la Torre de Destilación

Leyes Fundamentales

Las leyes fundamentales en procesos están asociadas tanto al comportamiento físico como al químico del proceso en análisis siendo las ecuaciones de mayor importancia:

1. La ecuación de balance de masa
2. La ecuación de balance de componentes
3. La ecuación de balance de energía

Balance de Masa

El balance de masa se relaciona directamente con el principio de la conservación de la masa, la cual asociada a los procesos se entiende como:

Masa de entrada al sistema = Masa saliendo del sistema + cambio en la masa acumulada 1

Balance de Componente

El balance de componente se refiere al principio de la conservación de las componentes en el sistema en estudio, relacionadas en la siguiente forma.

Moles de entrada de la componente considerada + El cambio de las moles de la otra u otras componentes a la componente considerada = Moles de salida de la componente considerada + cambio de las moles de la componente considerada + cambio de moles de la componente considerada a otra componente debido a la reacción 2

Balance de Energía

El balance de energía se basa en el principio de la conservación de la energía, donde la energía es cinética, potencial, interna o suministrada en forma de calor por medio de un intercambiador. El balance está dado por:

Calor suministrado por conducción, radiación y reacción + Energía cinética, potencial e interna entrando al sistema por difusión o conducción = Energía cinética, potencial e interna saliendo del sistema por difusión o conducción + trabajo + cambio de energía cinética, potencial e interna 3

Consideraciones

a.- En muchos casos en procesos químicos el término correspondiente al trabajo mecanico es igual a cero.

b.- Si las velocidades del flujo en la entrada y salida del sistema son bajas la energía cinética es despreciable.

c.- Si la diferencia de alturas no es grande, la energía potencial es despreciable.

En algunos casos el balance de energía en términos de la entalpia, función de la presión y la temperatura. En general la entalpia la podemos expresar como:

$$Hoh = I + \frac{P\bar{V}}{J} \left(\frac{BTU}{lbm} \text{ ó } \frac{Kcal}{Kg} \right) \qquad 4$$

donde

Hoh = entalpia $\left(\frac{BTU}{lbm}\right)$ ó $\left(\frac{Kcal}{Kg}\right)$

I = Energía interna $\left(\frac{BTU}{lbm}\right)$ ó $\left(\frac{Kcal}{Kg}\right)$

P = Presión $\left(\frac{\overline{lb}^{*}}{ft^2}\right)$ ó $\frac{\overline{Kg}^{*}}{m^2}$

$\bar{V}$ = Volúmen específico $\left(\frac{ft^3}{lbm}\right)$

$J = 778 \frac{ft-\overline{lb}}{BTU}$ ó $427 \frac{m-\overline{kg}}{Kcal}$

* la flecha en la parte superior indica fuerza es decir: $\overline{Kg}$ = de Kilogramos fuerza

d.- La entalpia a su vez se puede relacionar con el calor especifico a presión constante, donde si consideramos una capacidad calorifica promedio constante tenemos

$$C_p = \frac{H}{T} = \frac{\text{Entalpia}}{\text{Temperatura}} \qquad 5$$

donde:

C_p = calor especifico a presión constante

e.- Si se cumple la condición d y además la densidad es constante

$$C_p = C_v \qquad 6$$

donde:

C_v = calor especifico a volumen constante

f.- Por último de la ecuación 4 la entalpia puede aproximarse a la energía interna ya que el término $\frac{PV}{J}$ es mucho menor que la energía interna o sea

$$H \doteq I$$

Otros conceptos importantes en el modelo de Procesos son:

1. Ecuación de Arrhenius

La ecuación de Arrhenius determina el coeficiente de reacción K de cada componente en la siguiente forma

$$K = \alpha e^{-E/RT}$$

donde:

K = coeficiente de reacción
α = factor preexponencial
E = energía de activación $\left(\frac{BTU}{mol}\right)$ ó $\left(\frac{Kcal}{mol}\right)$
R = constante de los Gases

$$\frac{BTU}{mol\,°R} \quad ó \quad \frac{Kcal}{mol\,°K}$$

T = temperatura absoluta (°R ó °K)

2. Ley de Raoult para líquidos ideales

$$P = \sum_{j=1}^{n} X_j P_{jo}$$

$$y_j = \frac{X_j P_{jo}}{P}$$

donde:

y_j = Jésima fracción de mol de vapor
P_{jo} = presión de vapor de la Jésima componente
X_j = Jésima fracción de líquido

donde:

$$P_{jo} = e^{a_1/T + a_2}$$

a_1, a_2 son constantes que dependen de la composición de la alimentación.
T = temperatura

3. Relación entre vapor y líquido de una componente:

$$y = \frac{\alpha x}{1+(\alpha-1)x}$$

donde:

y = componente de vapor
x = componente de líquido
α = coeficiente de volatilidad (coeficiente de relación de la componente más volatil entre la menos volátil)

4. Constante de equilibrio en vaporación

$$y_j = K_j X_j$$

donde:

K_j = coeficiente que depende de la temperatura
y_j = Jésima componente de vapor
X_j = Jésima componente de líquido

5. Ley de los Gases Ideales

$$PV = nRT$$

donde: P = presión $\overline{lb}/ft^2$ ó $\overline{Kg}/m^2$

V= volumen (ft^3 ó m^3)
n= número de moles
R= constante de los gases $= 154\ \frac{lb\text{-}ft}{mol\text{-}°R}$
T= temperatura absoluta (°R ó °K)

de donde se puede determinar la densidad:

$$\rho = \frac{nM}{V} = \frac{MP}{RT} \left(\frac{lbm}{ft^3} \text{ ó } \frac{kgm}{m^3} \right)$$

A continuación se procederá a plantear las ecuaciones de modelado para los siguientes elementos de proceso.

1.- Un tanque en el cual se van a plantear las ecuaciones de balance de masa, balance de componentes y balance de energía.
2. Un reactor con un líquido donde se va a plantear el balance de energía.
3. Un reactor de gases en donde se van a plantear las ecuaciones de continuidad y balance de componentes.
4 Un reactor con enfriamiento donde se planteará la ecuación de continuidad de balance de componentes y balance de energía.
5. Un evaporador donde se plantea la ecuación de continuidad y de balance de energía.
6. Un evaporador rápido donde se plantea la ecuación de continuidad y balance de energía.
7. Una torre de destilación donde se plantean las ecuaciones de continuidad, de componentes y energía.

Ejercicio 1

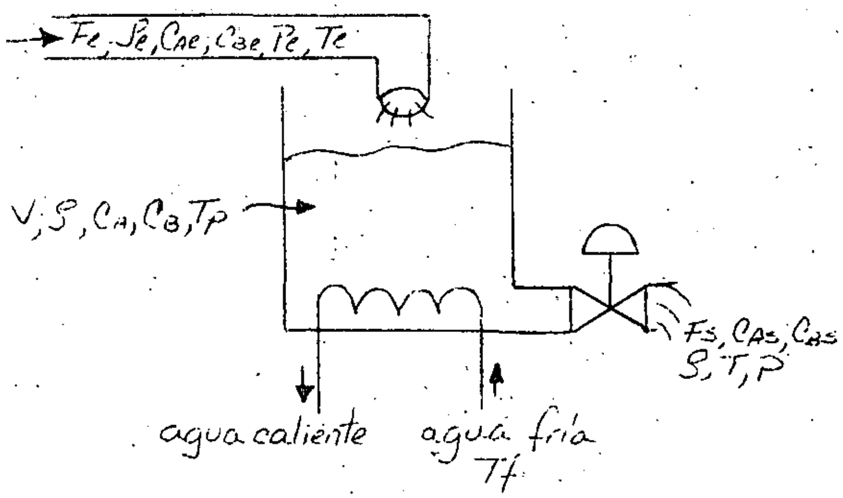
Para el tanque de la figura 1 considere un flujo de entrada como se muestra, un flujo de salida y un flujo almacenado donde se realiza una reacción.

Determine:

a) La ecuación de balance de masa considerando una densidad uniforme promedio.

b) Determine la ecuación de balance de componentes considerando en el depósito de la figura 1 una reacción irreversible, donde el flujo está perfectamente mezclado [4]. Determine la ecuación de balance de componentes si se tiene una doble reacción.

c) Plantear la ecuación de balance de energía, si se tiene un calor generado por la reacción, proporcional al volumen y concentración, así como un intercambiador de calor (enfriador) dentro del tanque para absorver el calor de la reacción.



F = flujo $\frac{m^3}{seg}$ ó $\frac{ft^3}{seg}$

ρ = densidad $\left(\frac{Kgm}{m^3}\right.$ ó $\left.\frac{lbm}{ft^3}\right)$

T = temperatura °R ó °K

V = volumen m^3 ó ft^3

C_A = concentración de A

C_B = concentración de B

P = presion $\frac{Kg}{m^2}$

Fig. 1 Tanque de Almacenamiento

Solución

a) De el balance de masa tenemos

$$F_e \rho_e = F_s \rho_s + \frac{d}{dt}(\rho V) \qquad 1.1$$

$$\rho \frac{dV}{dt} = F_e \rho_e - F_s \rho_s$$

análisis de unidades

$$\frac{\cancel{m^3}}{seg}\,\frac{Kg}{m^3} = \frac{\cancel{m^3}}{seg}\,\frac{Kg}{\cancel{m^3}} + \frac{Kg}{m^3}\,\frac{\cancel{m^3}}{seg}$$

b) De el balance de componentes tenemos $A \xrightarrow{K} B$

1. Para la componente A

$$F_e C_{Ae} = F_s C_A + \frac{d}{dt}(V C_A) + K_1 V C_A \qquad 1.2$$

Si $V = cte$

$$V \frac{d}{dt} C_A = F_e C_{Ae} - F_s C_A - K_1 V C_A$$

análisis de unidades

$$\frac{m^3}{seg}\,\frac{moles A}{m^3} = \frac{m^3}{seg}\,\frac{moles A}{m^3} + \frac{m^3}{seg}\,\frac{moles A}{m^3} + \frac{1}{seg}\, m^3\, \frac{moles A}{m^3}$$

2. Para la componente B

Si $V = cte$

$$V \frac{dC_B}{dt} = F_e C_{Be} - F_s C_B + V K_1 C_A \qquad 1.3$$

3. En el caso de tener una doble reacción $A \xrightarrow{K_1} B \xrightarrow{K_2} C$

Si $V = cte$ tenemos

$$\frac{dC_A}{dt} = F_e \frac{C_{Ae}}{V} - F_s \frac{C_A}{V} - K_1 C_A \qquad 1.4$$

$$\frac{dC_B}{dt} = F_e \frac{C_{Be}}{V} - F_s \frac{C_B}{V} + K_1 C_A - K_2 C_B \qquad 1.5$$

$$\frac{dC_C}{dt} = F_e \frac{C_{Ce}}{V} - F_s \frac{C_C}{V} + K_2 C_B \qquad 1.6$$

donde las concentraciones están relacionadas con la densidad de la siguiente manera:

$$\sum_{i=A}^{C} M_i C_i = \rho \qquad 1.7$$

donde:

M = Peso molecular
C = Concentración
ρ = Densidad

para la solución de este 3° caso pueden utilizarse dos de las ecuaciones obtenidas y la ecuación del primer inciso.

c) La reacción en el depósito de la figura 1 es exotérmica y la generación de calor es proporcional al volumen, a la concentración y al coeficiente de reacción de donde; del balance de energía tenemos:

$$F_e\rho_e(I_e+P_e+C_e)=F_s\rho(I+P+C)+Q_e+Q_r+WK_a^{*}+\frac{d}{dt}\left[\rho V(I+C+P)\right] \quad 1.8$$

donde: I = Energía interna $\left(\frac{BTU}{lbm}\right)$
P = Energía potencial $\left(\frac{BTU}{lbm}\right)$
C = Energía cinética $\left(\frac{BTU}{lbm}\right)$
W = $-$Trabajo mecánico + trabajo del fluido (W_f)
$W_f = F_sP - F_eP_e$

$K_a = \frac{1}{778}\ \frac{BTU}{ft-lb}$ ó $\frac{1}{427}\ \frac{Kcal}{Kg-m}$

Q_r = calor generado en la reacción
Q_e = calor extraído del sistema por el intercambiador

∴ Si se hacen las consideraciones de fluido a baja velocidad sin diferencia de nivel representativa, tenemos:

$$P_e = P = C_e = C = 0$$

y la ecuación anterior se reduce a:

$$\frac{d}{dt}(\rho V I_e) = F_e\rho_e I_e - F_s\rho I_e - Q_e - Q_r - F_s\rho\left(\frac{P}{\rho}\right)K_a + F_e\rho_e\left(\frac{P_e}{\rho_e}\right)(+K_a)$$

$$\frac{d}{dt}(\rho V I_e) = F_e\rho_e(I_e+P_eV_{ee}K_a) - F_s\rho(I_e+PV_eK_a) - Q_r - Q_e$$

donde:

V_{ee} = Volumen específico de entrada
V_e = Volumen específico de salida

* $\frac{1}{K_a}$ es conocida como J en termodinámica

Este resultado también se puede representar en función de la entalpía dada por h o $H = I + P\bar{V}$ Ka $\frac{BTU}{lbm}$ en la siguiente forma

$$\frac{d}{dt}(\rho V I) = F_e \rho_e H_e - F_s \rho H + Q_r + Q_e$$

o si $H = C_p T$ y la densidad y el volumen son constantes:

$$\rho C_p V \frac{d}{dt}(T_e) = \rho C_p (F_e T_e - F_s T) - Q_r - Q_e$$

donde

$Q_e = K_e (T - T_f)$

$Q_r = K_p K_1 V C_A$ $\frac{BTU}{seg}$ = calor de la reacción

K_p = coeficiente de calor de la reacción $\left(\frac{BTU}{\text{mol de A después de la reacción}}\right)$

K_e = constante que depende del material, área y longitud del intercambiador

Ejercicio 2

Se tiene un reactor como se muestra en la figura 2, el reactor tiene un flujo de alimentación F_e y dos flujos de salida, uno de vapor y otro de líquido como se puede observar en la figura 2, la presión en el reactor es P y las fases de vapor y líquido están en equilibrio, no existe trabajo y la energía cinética y potencial es despreciable.

Con las consideraciones mencionadas, plantear el balance de energía del reactor en función de la entalpía, del vapor y del líquido.

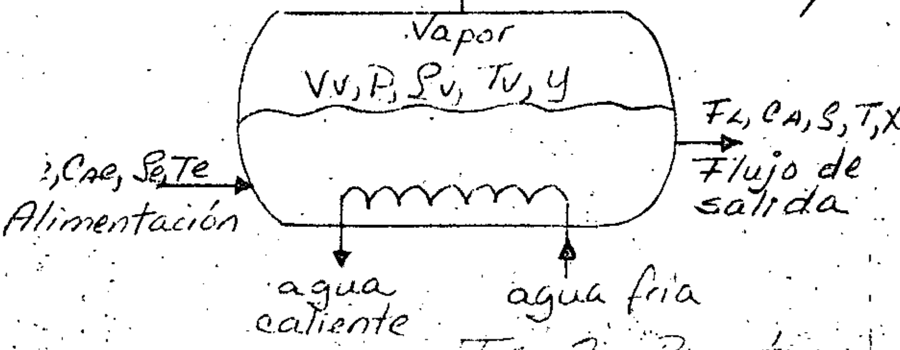


Fig. 2. Reactor

F = Flujo $\left(\frac{m^3}{seg}\right.$ ó $\left.\frac{ft^3}{seg}\right)$

T = Temperatura (°K ó °R)

P = Presión $\left(\frac{Kg}{m^2}\right.$ ó $\left.\frac{lb}{ft^2}\right)$

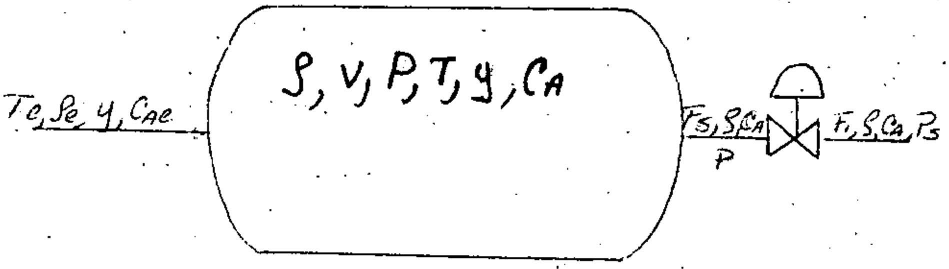
ρ = Densidad $\left(\frac{Kg}{m^3}\right.$ ó $\left.\frac{lbm}{ft^3}\right)$

y = Fracción de mol de vapor

Ejercicio 3

Se tiene una tubería donde fluye una mezcla de gases ideales entrando a un reactor como se puede observar en la figura 3. En el reactor se produce una reacción reversible de la forma $A \underset{K_2}{\overset{K_1}{\rightleftarrows}} B$ donde se genera calor proporcional al volumen del reactor y al cuadrado* la componente A; el volumen y temperatura son constantes.

El flujo de alimentación al reactor está regulado por una válvula de control y un control de nivel.
Considerando los datos mencionados plantear el modelo matemático del reactor.



P = presión
C_A = componente A
F = flujo
ρ = densidad
V = volumen
T = temperatura
y = fracción de mol de A en el reactor.

Fig. 3 Reactor de Gases

Solución

Es importante notar que el balance de energía no es necesario ya que el proceso es isotérmico.

Ecuación de continuidad o balance de masa

$$V\frac{d\rho}{dt} = F_e \rho_e - F_s \rho \qquad 3.1$$

Balance de Componentes

Para la componente A.

$$V\frac{dC_A}{dt} = F_e C_{Ae} - F_s C_A - K_1 V C_A^2 + K_2 V C_B \qquad 3.2$$

* También denominada reacción de 2° orden

X = Fracción de mol de líquido
V = Volumen (m^3 ó ft^3)
C_A = Composición de A $\left(\frac{\text{moles A}}{m^3} \text{ ó } \frac{\text{moles de A}}{ft^3}\right)$

Solución

Consideraciones

1. Si las fases de vapor líquido están en equilibrio térmico $T = T_v$
2. La energía interna es igual a la entalpía, o sea: $H = I$
3. Si no se realiza trabajo en el sistema, la entalpía del líquido y vapor se pueden representar como función de la temperatura* en la siguiente forma:

   $H = C_pT$ = Entalpía del líquido
   $h = C_pT + K_v$ = Entalpía del vapor
   K_v = calor promedio de vaporización de la mezcla
4. La variación de la energía interna es la suma de las energías en la fase de vapor y líquido.

∴ La ecuación general de balance de energía es:

$$F_e \rho_e H = F_v \rho_v h + F_L \rho H + Q + \frac{d}{dt}(\rho_v V_v h + \rho_L V_L H)$$

donde:

Q = Energía generada en la reacción + la energía removida por el intercambiador.

ó

$$\frac{d}{dt}(\rho_v V_v h + \rho_L V_L H) = F_e \rho_e H - F_v \rho_v h - F_L \rho H - Q$$

ó

$$\frac{d}{dt}\left[\rho_v V_v (C_pT + K_v) + \rho_L V_L C_p T\right] = F_e \rho_e C_p T_e - F_v \rho_v (C_pT + K_v) - F_L \rho C_p T - Q$$

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* El trabajo PV generalmente es un valor pequeño comparado con la energía interna.

Tres consideraciones con las cuales las ecuaciones 1 y 2 se pueden representar en otra forma son:

1. La regulación de flujo por la válvula [2] puede ser representado como

$$F_o = KA\sqrt{\frac{\Delta P}{\rho}}$$

donde

$KA = C_v =$ Coeficiente de capacidad de la válvula

2. La densidad para gases ideales es

$$\rho = \frac{MP}{RT} = \frac{P}{RT}\left[yM_A + (1-y)M_B\right]$$

donde:

$M =$ Peso molecular total
M_i ($i = A, B$) $=$ Peso molecular promedio de A o B
$R =$ Constante de los gases
$P =$ Presión

3. La fracción de mol de A (y) puede ser determinada en función de la componente A en la siguiente forma:

$$C_A = \frac{Py}{RT}\left(\frac{\text{mol de A}}{m^3} \text{ o } \frac{\text{mol de A}}{ft^3}\right)$$

de donde aplicando las 3 consideraciones a las ecuaciones 1 y 2 tenemos:

$$\frac{V}{RT}\frac{d}{dt}(Py) = F_e C_{Ae} - \frac{Py}{RT}(KA)\sqrt{\frac{\Delta P}{\rho}} - VK_1\left(\frac{Py}{RT}\right)^2 + \frac{VK_2P(1-y)}{RT}$$

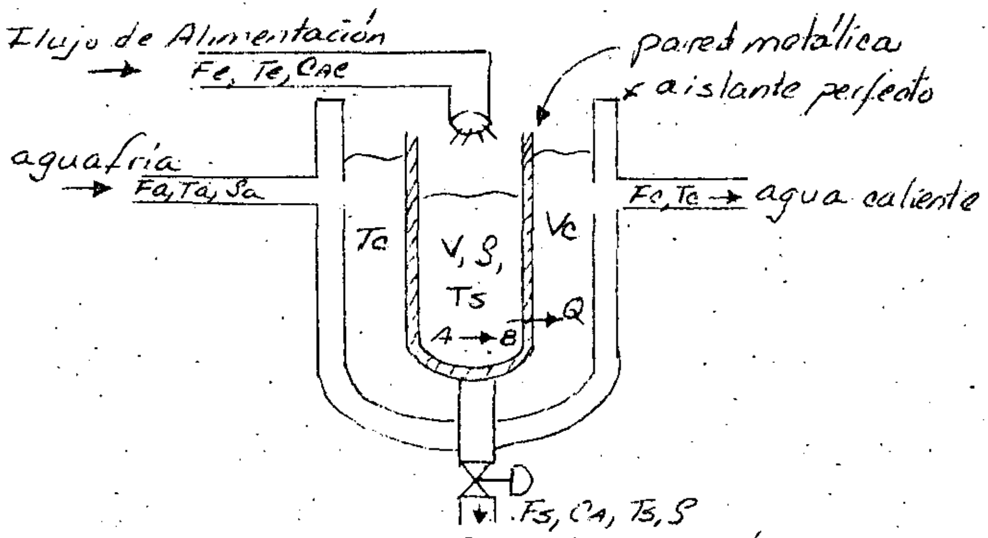
$$V\frac{d\rho}{dt} = F_e\rho_e - \rho KA\sqrt{\frac{\Delta P}{\rho}}$$

$$C_A = \frac{Py}{RT}$$

donde las incognitas son: ρ, P y y.

Ejercicio 4.

Se tiene un flujo de alimentación a un recipiente donde se realiza una reacción de orden n irreversible y exotérmica, donde para disminuir la temperatura en el reactor se tiene una chaqueta por donde circula agua fría como se puede observar en la figura 4.



V = volumen
T = temperatura
F = flujo
ρ = densidad
$C_A = \frac{\text{moles } A}{ft^3}$

Fig. 4 Reactor con enfriamiento forzado

Considerando despreciables las pérdidas de calor y las densidades constantes, determine las ecuaciones para balance de masa, balance de componentes y balance de energía.

Solución

Ecuaciones para el Reactor

Balance de Masa

$$\frac{dV\rho}{dt} = F_e\rho_e - F_s\rho \qquad 4.1$$

Balance de Componente

$$\frac{d}{dt}(VC_A) = F_eC_{Ae} - F_sC_A - VKC_A^n \qquad 4.2$$

Balance de Energía

$$\rho\frac{d}{dt}(VH) = \rho(F_eH_e - F_sH_s) - \lambda VK_1C_A^n - Q \qquad 4.3$$

donde:

Q = Calor transferido del recipiente al agua fría
λ = calor de vaporización

$$Q = AD(T_s - T_e) \qquad 4.4$$

siendo:

A = Area de la pared metálica en contacto con el fluido. (m^2 ó ft^2)

D = Coeficiente de transferencia de calor $\left(\frac{BTU}{seg\ ft^2\ °R}\right.$ ó $\left.\frac{Kcal}{seg\ m^2\ °K}\right)$

Ecuaciones para el encamizado

Balance de Masa

$$\rho \frac{d}{dt} V_a = F_a \rho_a - F_s \rho_a \qquad 4.5$$

Balance de Componentes

no se tiene

Balance de Energía

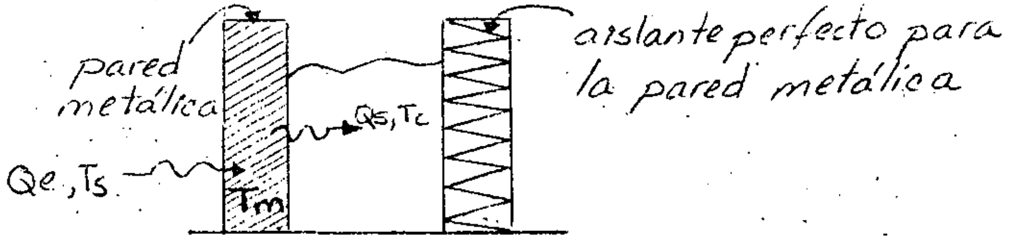
$$\rho_a V_c \frac{dH_a}{dt} = F_a \rho_a (H_{ae} - H_s) + AD(T_s - T_c) \qquad 4.6$$

donde

H_{ae} = entalpía de entrada

H_s = entalpía de salida

Para la pared metálica



$$\rho_m C_m V_m \frac{dT_m}{dt} = D_i A_i (T_s - T_m) - D_e A (T_m - T_c) \qquad 4.7$$

donde

El subíndice m indica las características de la pared metálica.

D = Coeficiente de Transferencia de calor

A = Area de Transferencia de calor

Siendo las variables desconocidas, V, F_s, C_A, T_s, T_m y T_c

Condiciones iniciales T_e, F_e, C_{Ae} y F_a

Parámetros conocidos $n, \alpha, \rho, C_p, I, A, \rho_a, V_a$ y T_a.

Como se tienen 6 incógnitas y 5 ecuaciones dadas por las ecuaciones (1, 2, 3, 6 y 7) podemos plantear otras más para el control de nivel o sea:

$$F_s = K(V - V_{ref})$$

K = cte. de proporcionalidad (control proporcional)
V_{ref} = volumen mínimo conocido o deseado

Consideraciones

1. Si las densidades son constantes la entalpía puede ser sustituida por C_pT.
2. Si se incluye el área de transferencia de calor como una variable se puede incluir otra ecuación, por ejemplo si se trata de un recipiente cilíndrico.

$$A = \frac{4}{D}V$$

siendo

A = área de transferencia de calor
D = diámetro del recipiente
V = volumen

3. Si la temperatura del agua no es uniforme se puede obtener una temperatura promedio más cercana a la realidad o sea

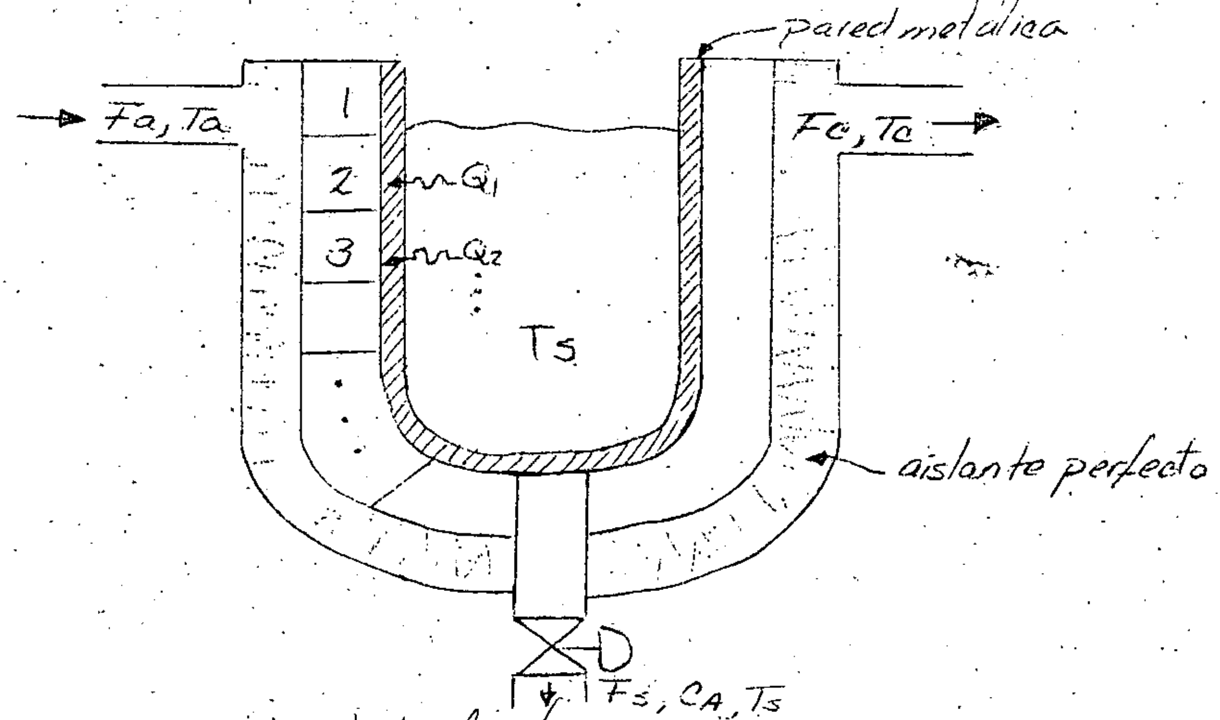
$$T_c = \frac{T_a + T_c}{2}$$

donde:

T_c = temperatura promedio en (°R o °K

4. Como en la transferencia de calor se tiene un modelo matemático expresado en ecuaciones diferenciales parciales, ya que la distribución de calor depende del tiempo y de la característica de los materiales puede plantearse un modelo para la Transferencia de calor donde se considere un número finito de compartimientos para determinar la variación de las temperaturas, como por ejemplo.

Si se divide la transferencia de calor en la chaqueta en n divisiones con iguales condiciones de volumen (V_i), calor específico (C_a), flujo (F_a), coeficiente de transferencia de calor (D) y área (A), como se muestra en la figura



tendremos ecuaciones de la forma

$$\frac{1}{n} V_a C_a S_a \frac{dT_i}{dt} = F_a C_a S_a (T_{i-1} - T_i) + \frac{1}{4} DA (T_s - T_i)$$

$i = 1, 2, \ldots n$

donde obtendremos la variación de temperatura del fluido en cualquier parte.

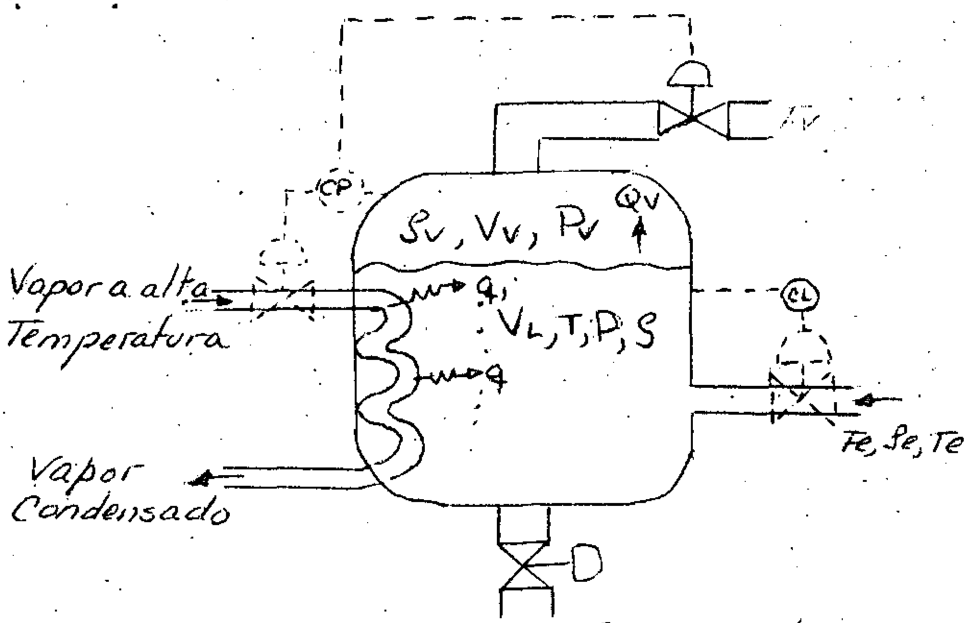
5. K_1 puede ser sustituido por la ecuación de Arrhenius o sea:

$$K_1 = \alpha e^{-E/RT} = \text{coeficiente de radiación}$$

Ejercicio 5

En una planta de proceso se tiene un flujo líquido de alimentación a un evaporador donde el líquido es calentado por un intercambiador de calor como se muestra en la figura 5. El líquido en el evaporador tiene densidad constante y se vaporiza a razón de $Q_v \left(\frac{kg}{seg} \text{ o } \frac{lbm}{seg}\right)$.

Considerando despreciable las pérdidas de calor, determine la ecuación de continuidad y balance de energía para el evaporador.



F = flujo
ρ = densidad
T = temperatura
V = volumen
Q_v = líquido vaporizado
P = presión
$Q = \sum_{i=1}^{n} q_i$
H = entalpía
Km = coeficiente de transformación de masa

Fig. 5 Evaporador

Solución

Ecuaciones para la fase líquida

Balance de materia

$$\rho \frac{dV_L}{dt} = F_e \rho_e - W_v \qquad 5.1$$

$$W_v = \rho_v F_v \quad \text{si} \quad P = P_v \qquad 5.2$$

$$W_v < \rho_v F_v \quad \text{si} \quad P > P_v \qquad 5.3$$

$$W_v = K(P - P_v) \quad \text{si} \quad P = P_v \quad K >> 1 \qquad 5.4$$

$$K_m = \left(\frac{kg}{seg - Kg/m^2} \ \text{o} \ \frac{lbm}{seg - lb/ft^2} \right) \qquad 5.5$$

cuando se tiene equilibrio entre vapor y líquido

$$P = e^{A_1/T + A_2} \qquad 5.6$$

Balance de energía

$$\rho \frac{d}{dt}(V_L T_L) = \rho_e F_e H_e - W_v H_L + Q \qquad 5.7$$

$$\rho_v = \frac{M P_v}{R T_v} \qquad 5.8$$

Ecuaciones para la fase de vapor

Balance de masa

$$\frac{d}{dt}(V_v \rho_v) = W_v - \rho_v F_v \qquad 5.9$$

Balance de energía

$$\frac{d}{dt}(V_v \rho_v I_v) = W_v H_L - \rho_v F_v H_v \qquad 5.10$$

como se tienen 10 incógnitas: $Q, F_e, V_L, W_v, T, V_v, \rho_v, T_v, P$ y P_v y sólo 7 ecuaciones: 5.1, 5.2 ó 5.4, 5.6, 5.7, 5.8, 5.9, 5.10 son necesarias 3 ecuaciones más

Del volumen total

$$V_v + V_L = V \qquad 5.11$$

Del control de presión

$$Q = f(P_v) \qquad 5.12$$

Del control de nivel

$$F_e = g(V_L) \qquad 5.13$$

∴ El sistema tiene solución.

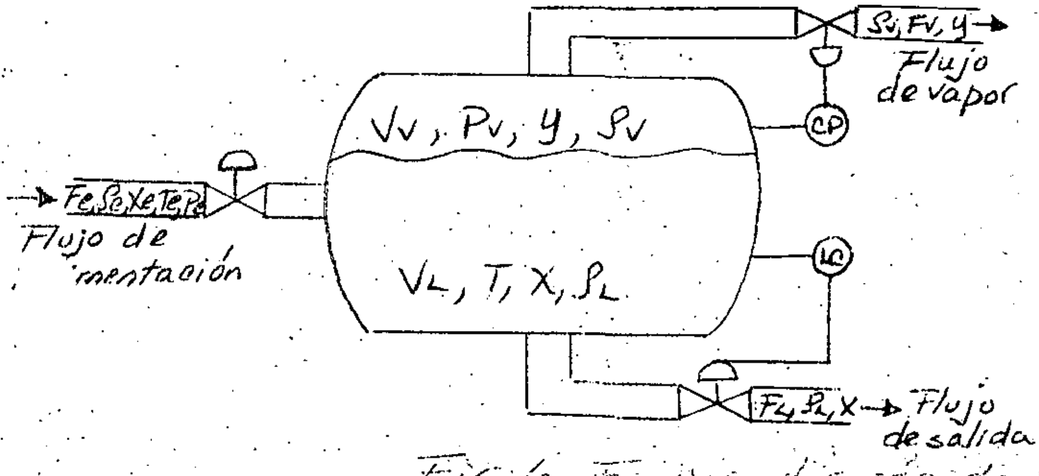
Por último es común tener un equilibrio térmico donde $T=T_v$ por lo que la ec. puede escribirse como:

$$\rho C_p \frac{d}{dt}(V_L T) = \rho_e F_e C_p T_e - W_v(C_p T + \lambda_v) + Q \qquad 5.14$$

y el balance de energía en la fase de vapor no es necesaria

Ejercicio 6

Se tiene un evaporador con un flujo a alta temperatura y alta presión alimentando a un tanque en el cual se tiene un sistema de control de presión nivel y temperatura como se muestra en la figura 6.



F = flujo
ρ = densidad
y = fracción de mol de vapor.
X = fracción de mol de líquido
P = presion
H = entalpia

Fig. 6 [illegible]

Determine a partir de los datos del evaporador la ecuación de balance de masa, la ecuación de balance de componentes entre la fase líquida y [illegible], así como la ecuación que representa el balance de energía.

Soluciones

1ª Solución

Las ecuaciones asociadas al comportamiento de el evaporador rápido son las mismas ecuaciones del ejercicio __ pero existen otras formas de representar en forma matemática su dinámica.

2ª Solución

Si el vapor esta en equilibrio con el líquido se pueden plantear las ecuaciones de equilibrio para la fase líquida.

Balance de masa

$$\frac{d}{dt}(V_L \rho_L) = \rho_e F_e - \rho_v F_v - \rho_L F_L \qquad 6.1$$

Balance de componentes

$$\frac{d}{dt}\left(\frac{V_L \rho_L x_i}{M_{Lp}}\right) = \frac{\rho_e F_e}{M_{ep}} x_{ei} - \frac{\rho_v F_v}{M_{vp}} y_i - \frac{\rho_L F_L}{M_{Lp}} x_i \qquad 6.2$$

donde:

M_{Lp}, M_{ep} y M_{vp} son pesos moleculares promedio calculados como:

$$M_p = \sum_{i=1}^{n} M_i (y_i \text{ o } x_i) \left(\frac{Kgm}{mol} \text{ o } \frac{lbm}{mol}\right) \qquad 6.3$$

El término i representa el número de componentes en la fase líquida o en la fase de vapor.

Los términos $\frac{x_i}{M_{Lp}}$, $\frac{x_{ei}}{M_{ep}}$, $\frac{y_i}{M_{vp}}$

Balance de energía

$$\frac{d}{dt}(V_L \rho_L H_L) = \rho_e F_e H_e - \rho_v F_v H_v - \rho_L F_L H_L \qquad 6.4$$

Si hasemos un análisis de el número de incógnitas veremos que son: 12+2N.

Es decir:

$P_V, T, \rho_L, F_V, \rho_V, V_L, M_{VP}, F_L, M_{LP}, H_L, H_V, H_e, y_1 \ldots y_n, x_1 \ldots x_n$

como tenemos 2N+12 incógnitas y solo n+4 ecuaciones dadas por el balance de masa (una ecuación), balance de componentes (n ecuaciones), peso molecular promedio (2 ecuaciones) y balance de energía (una ecuación).

Por lo tanto para que el sistema tenga solución son necesarias n+8 ecuaciones más, tales ecuaciones son:

1. Ecuaciones de equilibrio vapor-líquido

$$y_i = f(T, P_V, x_i) \qquad 6.5$$

2. Calculo de la densidad del vapor y el liquidido

$$\rho_L = f(x_i, T) \qquad 6.6$$

$$\rho_V = \frac{M_{VP} P}{RT} \qquad 6.7$$

3. Propiedad térmica

$$H_e = f_1(x_{ei}, T_e)$$
$$H_L = f_2(x_i, T)$$
$$H_V = f_3(y_i, T_L, P)$$

4 De los controles del sistema tenemos:

del control de nivel $C_L = f_3(V_L)$
del control de temp. $C_T = f_4(T)$
del control de presión $C_P = f(P_V)$

∴ El sistema ahora si se puede resolver.

Ejercicio 7

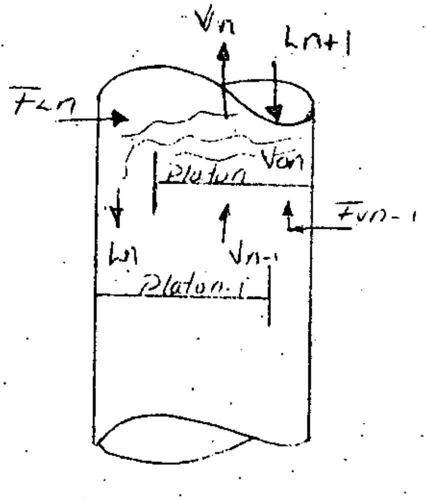
Se tiene una columna de destilación la cual es alimentada con una mezcla binaria. En la torre de destilación se desea separar las componentes que constituyen la mezcla

La torre de destilación está integrada de 3 partes: La primera es la columna constituida por dos secciones una de enriquecimiento y otra de empobrecimiento; la segunda parte es un condensador acoplado a la parte superior de la torre, donde se condensa la componente más volatil, se almacena teniendo dos flujos de salida regulados, uno para el producto destilado y el otro para el reflujo; la tercera parte es un recalentador localizado en la parte inferior de la torre de destilación el cual tiene como función calentar los productos de fondo para producir el vapor en contra corriente con el fluido como se observa en la figura

Considerando que no existe tiempo muerto en los flujos, que no hay almacenamiento de vapor y que la torre opera a presión constante determine las ecuaciones dinámicas del sistema

Solución

Antes de plantear las ecuaciones generales que describen la dinámica de la torre de destilación procederemos a plantear las ecuaciones de continuidad, equilibrio y energía en un solo plato de la torre de destilación como se muestra en la figura 7.1



F_{Ln} = flujo líquido de entrada
V_n = flujo de vapor saliendo
L_{n+1} = flujo líquido entrando
F_{vn-1} = flujo de vapor entrando
V_{n-1} = reflujo de vapor entrando
L_n = flujo de líquido saliendo
V_{on} = flujo almacenado en el nesimo plato
P_n = presión
T_n = temperatura

Fig. 7.1 Diagrama de un Plato en una Columna de Destilación

La ecuación de continuidad

$$\frac{dV_{on}}{dt} = L_{n+1} + F_{Ln} + F_{Vn-1} - V_n - L_n \qquad 7.1$$

Balance de componentes

$$\frac{d}{dt} V_{on} X_n = L_{n+1} X_{n+1} + F_{Ln} X_{Fn} + F_{Vn-1} Y_{Fn-1} + V_{n-1} Y_{n-1} - V_n Y_n - L_n X_n$$

Balance de energía

$$\frac{d}{dt}(V_{on} I_n) = L_{n+1} h_{n+1} + F_{Ln} h_{Fn} + F_{Vn-1} H_{Fn-1} + V_{n-1} H_{n-1} - V_n H_n - L_n h_n$$

Propiedades Térmicas:

$h_n = f_1(X_n, T_n)$ = Entalpia del vapor en el plato n
$H_n = f_2(Y, T_n, P_n)$ = Entalpia del líquido en el plato n
$H_{Fn} = f_3(Y_{Fn}, T_{Fn}, P_n)$ = Entalpia del flujo líquido de alimentación
$h_{Fn} = f_4(X_{Fn}, T_{Fn})$ = Entalpia del flujo del vapor de alimentación.

Equilibrio de fase

$Y_n = f(X_n, P_n, T_n)$ = composición de vapor en equilibrio con el líquido

Ecuaciones de movimiento

Para el líquido

$$L_n = f(V_{on}, V_n, X_n, T_n, P_n)$$

Para el vapor

$$V_n = f(P_n, P_{n-1}, Y_n, T_n)$$

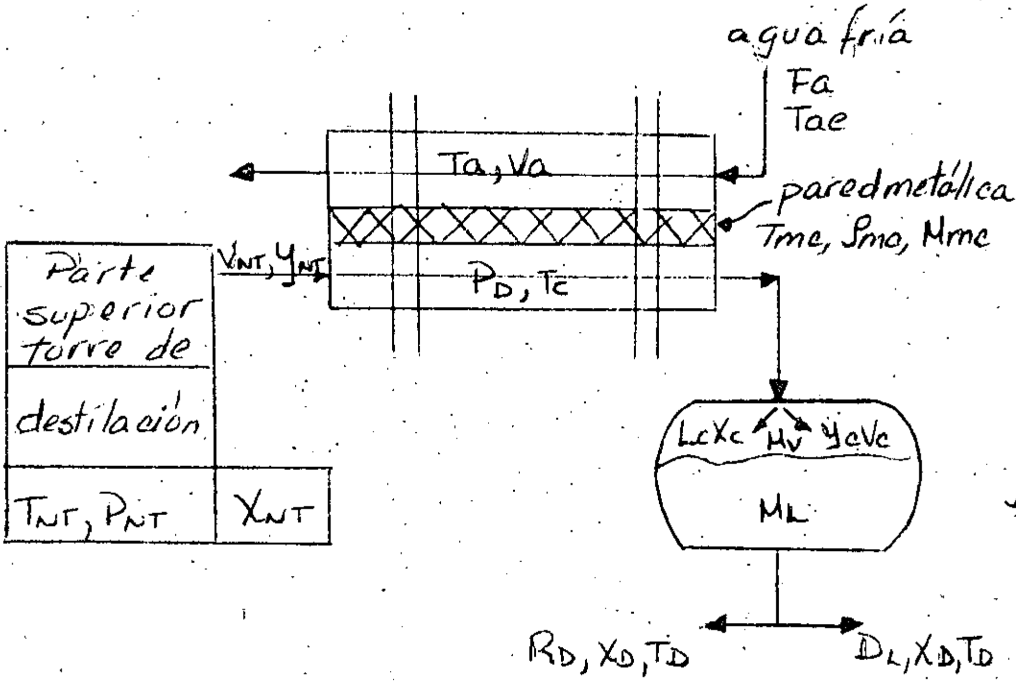
Las ecuaciones que representan una torre de destilación como se mencionó pueden ser desarrolladas en 3 partes, sin embargo en algunas secciones se considera que el recalentador y el condensador son dos platos más en la torre de destilación.

Partes para la representación de una torre de destilación:

1. Un condensador
2. La torre de destilación
3. Un recalentador.

El Condensador

El vapor que sale de la torre es parcial o totalmente condensado para despues pasar a un tanque de almacenamiento, el cual tiene dos salidas, una ver figura 7-2 destinada al reflujo y otra al producto destilado



M_V = moles de vapor
M_L = moles de liquido
L_C = moles de liquido entrando
V_C = moles de vapor entrando
X_C = fracción de mol liquida
y_C = fracción de mol de vapor
D_L = destilado de salida $\left(\frac{moles}{seg}\right)$
R_D = destilado en reflujo $\left(\frac{moles}{seg}\right)$

Fig. 7.2 Diagrama condensador tanque de almacenamiento

Ecuaciones del Condensador

$$V_{NT} = L_C + V_C$$

$$V_{NT} y_{NT} = L_C X_C + V_C y_C$$

$$P_D = P_{NT} - f(V_{NT}, y_{NT}, T_{NT})$$

$$Q_C = A_C (T_C - T_{MC})$$

$$H_{NT} V_{NT} = L_C h_C + V_C H_C + Q_C$$

$$y_C = f(X_C, P_D, T_C)$$

Suponiendo concentrado el efecto de la pared metálica

$$M_{MC} C_{MC} \frac{dT_{MC}}{dt} = V_C A_C (T_C - T_{MC}) - V_a A_a (T_{MC} - T_a)$$

Del lado del fluido frío

$$V_a S_a C_a \frac{dT_a}{dt} = S_a F_a C_a (T_{ae} - T_a) + V_a A_a (T_{MC} - T_a)$$

donde:

$$Fa = f_1(T_c)$$

Ecuaciones para el Tanque

Fase de vapor

$$\frac{d}{dt} M_V = V_c$$

$$\frac{d}{dt} M_V y_V = V_c y_c$$

$$M_V = \frac{V_V P_D}{R T_D}$$

Para la Fase líquida

$$\frac{d}{dt} M_L = L_c - D_L - R$$

$$\frac{d}{dt}(M_L X_D) = L_c X_c - (D_L + R) X_D$$

$$\frac{d}{dt}(M_L h_D) = h_c L_c - (D_L + R) h_D$$

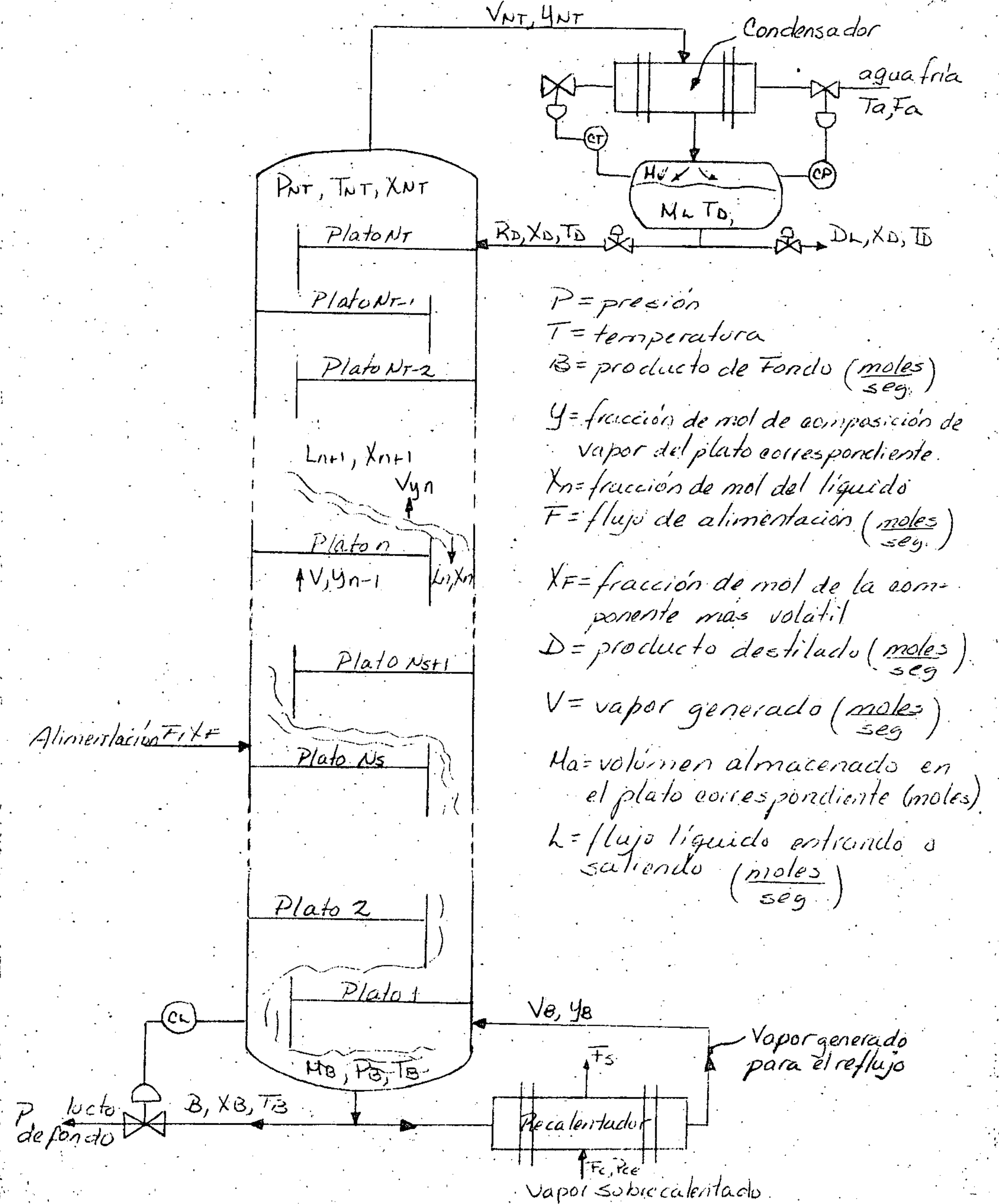
$$D_L = f(M_L)$$

Pueden plantearse dos ecuaciones más para el sistema de control en el tanque.

1. Control de nivel en el tanque para regular el flujo del producto destilado
2. Control de temperatura y presión para regular el gasto del fluido de enfriamiento

La Torre de Destilación

La columna consiste en una serie de platos colocados de tal forma que permitan que ascienda el vapor a través del líquido que desciende, donde en un plato intermedio se tiene un flujo de entrada con una composición X_F (fracción de mol de la componente más volátil) ver figura 7-3.



P = presión
T = temperatura
B = producto de Fondo $\left(\frac{moles}{seg}\right)$
Y = fracción de mol de composición de vapor del plato correspondiente.
X_n = fracción de mol del líquido
F = flujo de alimentación $\left(\frac{moles}{seg}\right)$
X_F = fracción de mol de la componente más volatil
D = producto destilado $\left(\frac{moles}{seg}\right)$
V = vapor generado $\left(\frac{moles}{seg}\right)$
M_a = volúmen almacenado en el plato correspondiente (moles)
L = flujo líquido entrando o saliendo $\left(\frac{moles}{seg}\right)$

Fig. 7.3 Torre de Destilación

Ecuaciones para la Torre de Destilación

Para el plato $n=N_T$

Ecuación de continuidad

$$\frac{d}{dt} M_{NT} = R-L_{NT}$$

Balance de Componentes

$$\frac{d}{dt}(M_{NT}-X_{nT}) = RX_D-L_{NT}X_{NT}-Vy_{NT-1}-Vy_{NT}$$

Para el plato N_{T-1}

Ecuación de continuidad

$$\frac{d}{dt} N_{NT-1} = L_{NT}-L_{NT-1}$$

Balance de Componentes

$$\frac{d}{dt}(M_{NT-1}, Y_{NT-1}) = L_{NT}X_{NT}-L_{NT-1}X_{NT-1}-Vy_{NT-2}-Vy_{NT-1}$$

Para el plato n

Ecuación de Continuidad

$$\frac{d}{dt}(M_n) = L_{n+1}-L_n$$

Balance de Componentes

$$\frac{d}{dt}(M_nX_n) = L_{n+1}X_{n+1}-L_nX_n-Vy_{n-1}--Vy_n$$

Para el plato de alimentación N_S

Ecuación de Continuidad

$$\frac{d}{dt}(M_{NS}) = L_{NS+1}-L_{NS}+F$$

Balance de Componentes

$$\frac{d}{dt}(M_{NS}X\ ) = L_{NS}X_{nS+1}-L_{nS}X_{nS}+Vy_{nS-1}+FX_F$$

Para el primer plato

Ecuación de Continuidad

$$\frac{d}{dt} M_1 = L_2 - L_1$$

Balance de Componentes

$$\frac{d}{dt}(M_1 X_1) = L_2 X_2 - L_1 X_1 + V y_B - V y_1$$

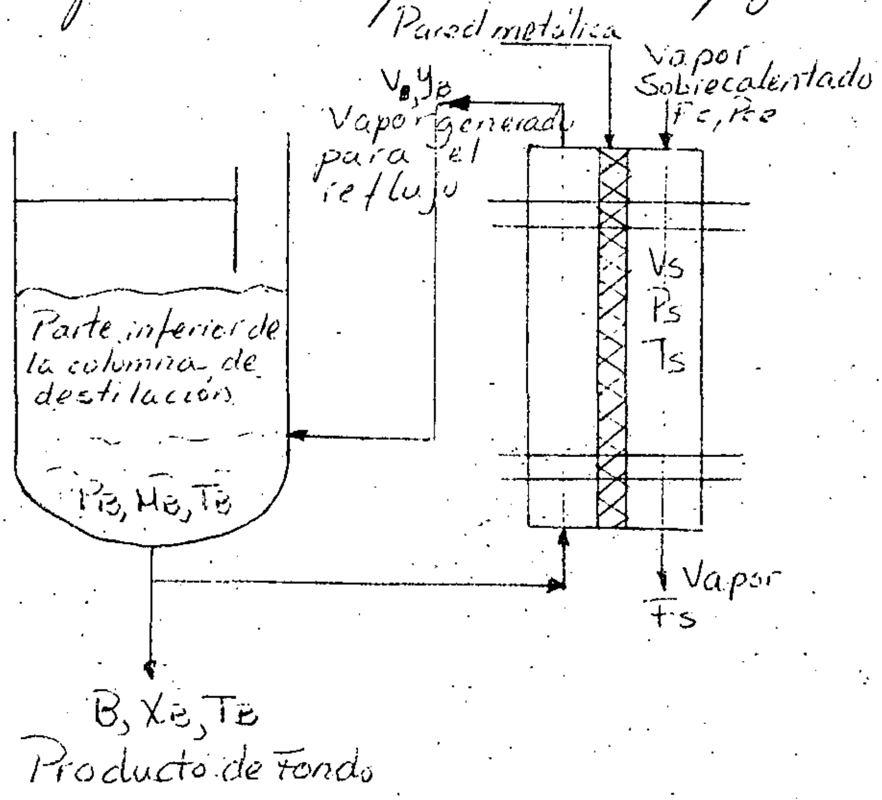
Se puede plantear otra ecuación a partir del control de nivel de la base de la columna de destilación.

Por último tenemos la ecuación de equilibrio hidráulico.

$$y_i = \frac{\alpha_i x_i}{1-(\alpha-1)x_i}$$

El Recalentador

En la base de la columna se tiene un volumen de líquido con el producto de fondo en el cual se tienen dos salidas, una para el recalentador el cual va a generar vapor en reflujo con el líquido y otra salida de productos de fondo. Ver figura 7.7



Ecuaciones del Recalentador

$$\frac{dM_B}{dt} = L_1 - V_B - B$$

$$\frac{d}{dt}(M_B X_B) = L_1 X_1 - V_B y_B - B X_B$$

$$\frac{d}{dt}(M_B h_B) = L_1 h_1 - V_B H_B - B h_B + A_B V_B \,(T_{MR} - T_B)$$

$$y_B = f(X_B, T_B, P_B)$$

$$B = f(M_B)$$

Para la pared metálica en el recalentador

$$M_{MR} C_{MR} \frac{d}{dt} T_{MR} = V_S A_S (T_S - T_{MR}) - V_B A_B (T_{MR} - T_B)$$

Para el lado del vapor

$$V_S \frac{d}{dt} S_S = F_C S_C - F_S S_S$$

aplicando un control de flujo proporcional

$$F_S = \frac{V_S A_S (T_S - T_{MR})}{K_V}$$

$$T_S = f_1(S_S)$$

$$P_S = f_2(S_S)$$

$$F_S = K_1 \sqrt{P_{CR} - P_S}$$

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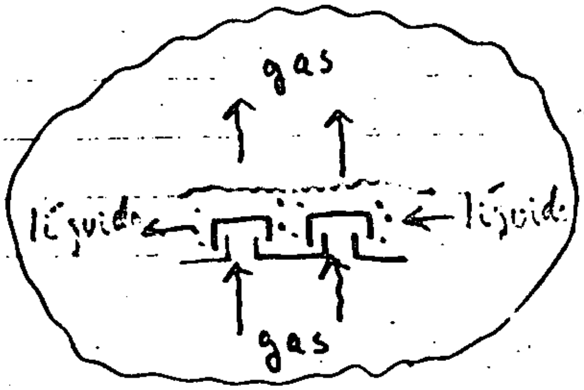
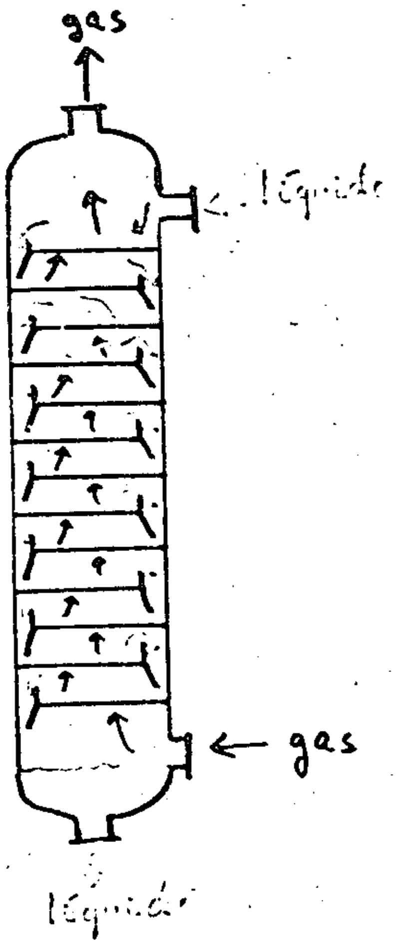

gas
liquid
liquid
gas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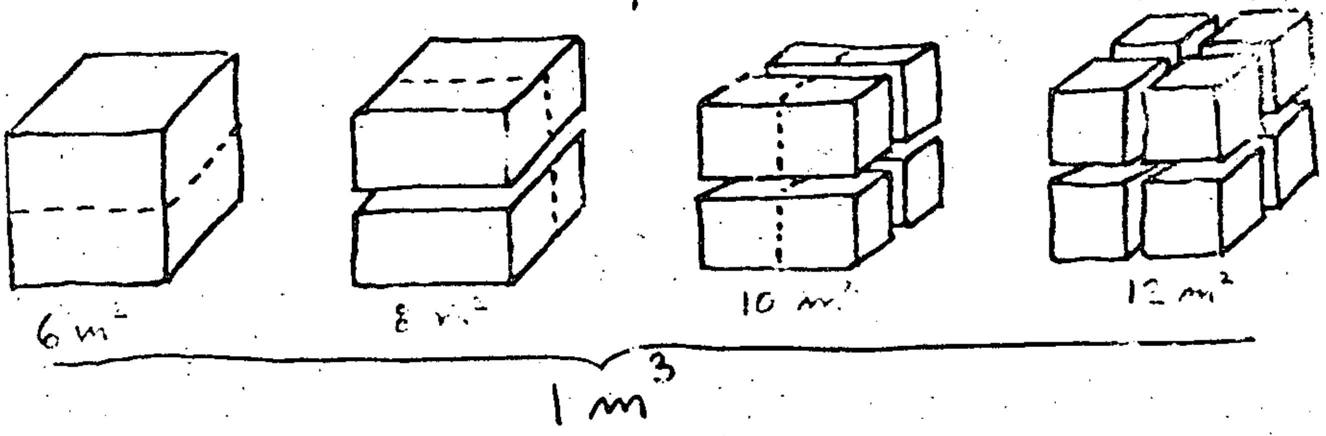

6 m²
8 m²
10 m²
12 m²
1 m³

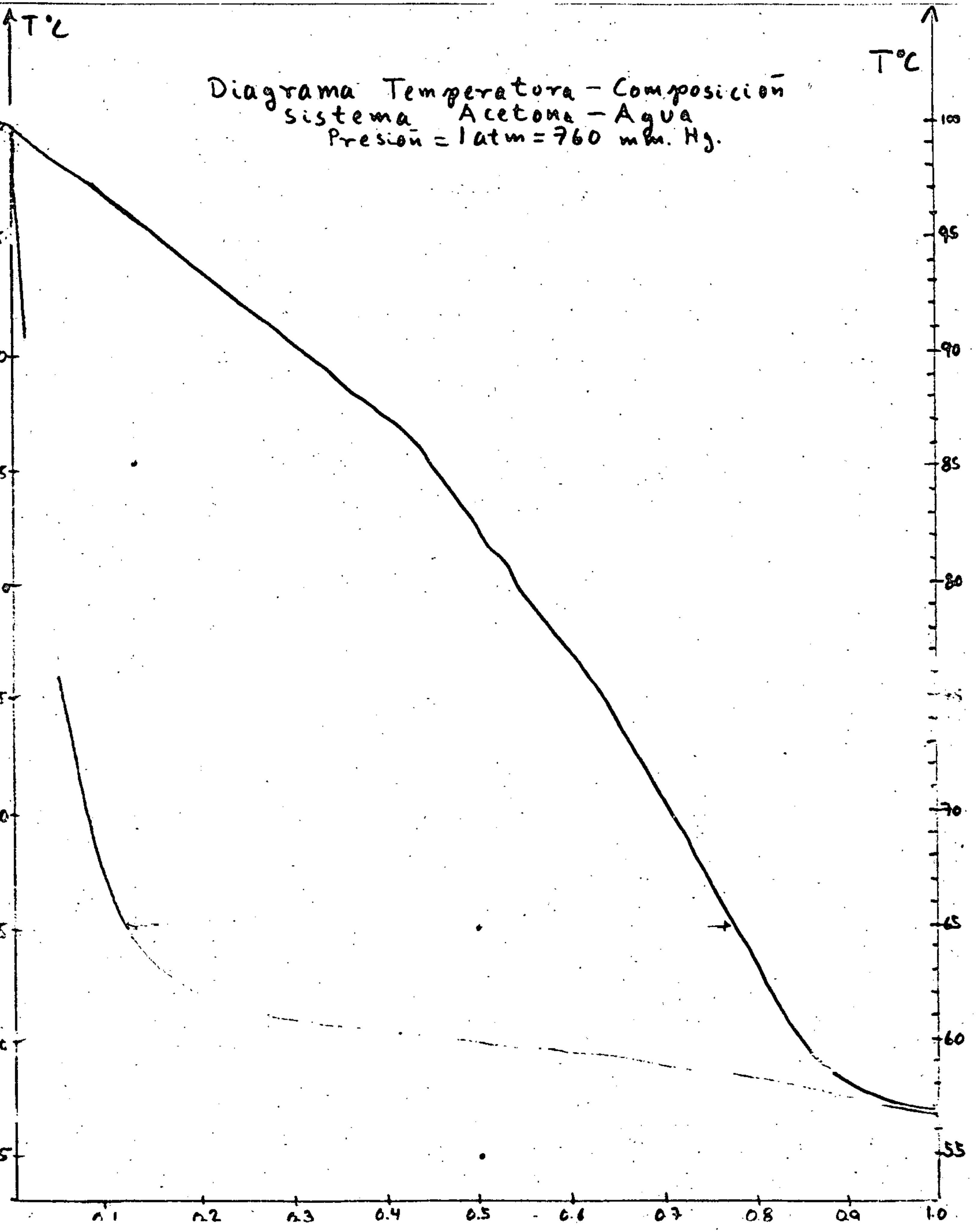
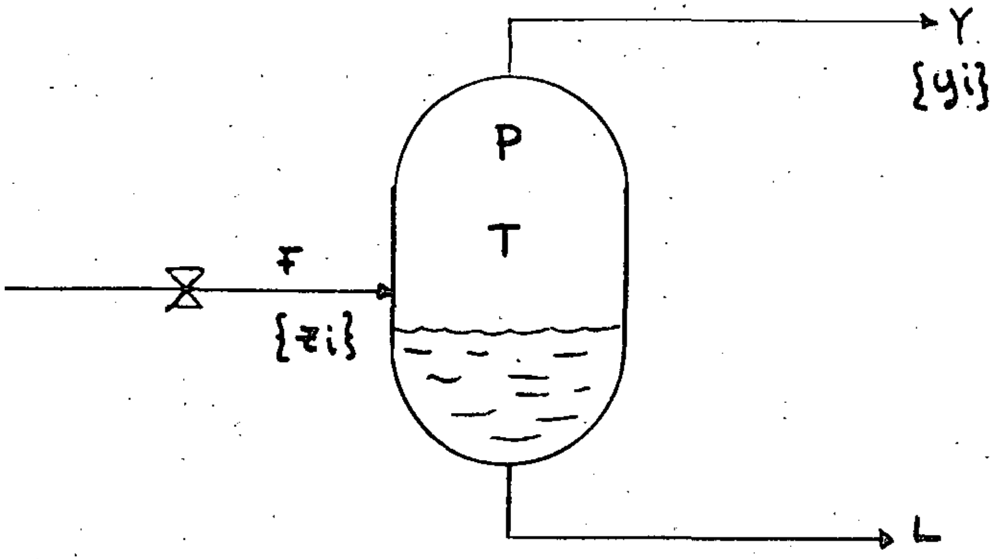


Diagrama Temperatura - Composición
sistema Acetona - Agua
Presión = 1atm = 760 mm. Hg.

Cálculo de temperaturas de burbuja y de rocío:



Relaciones de equilibrio:

$$y_i = K_i x_i \qquad i=1,c$$

$$\sum_{i=1}^{c} y_i = 1.0$$

$$\sum_{i=1}^{c} x_i = 1.0$$

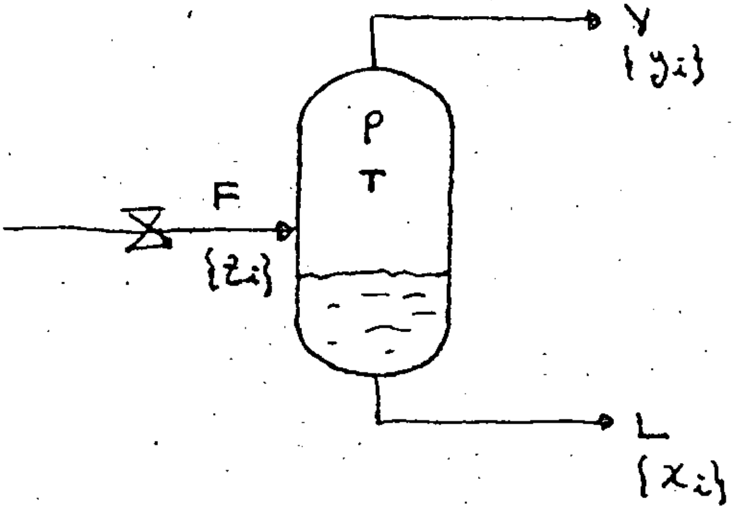
Constante de equilibrio:

$$K_i = \frac{p_i^\circ}{P}$$

Ecuación de Antoina:

$$p_i^\circ = \frac{e^{\left(A_i + \frac{B_i}{C_i+T}\right)}}{P}$$

Cálculo de Temperaturas de burbuja y de rocío



Relaciones de equilibrio

$$y_i = K_i x_i \qquad i=1,c$$

$$\sum_{i=1}^{c} y_i = 1.0$$

$$\sum_{i=1}^{c} x_i = 1.0$$

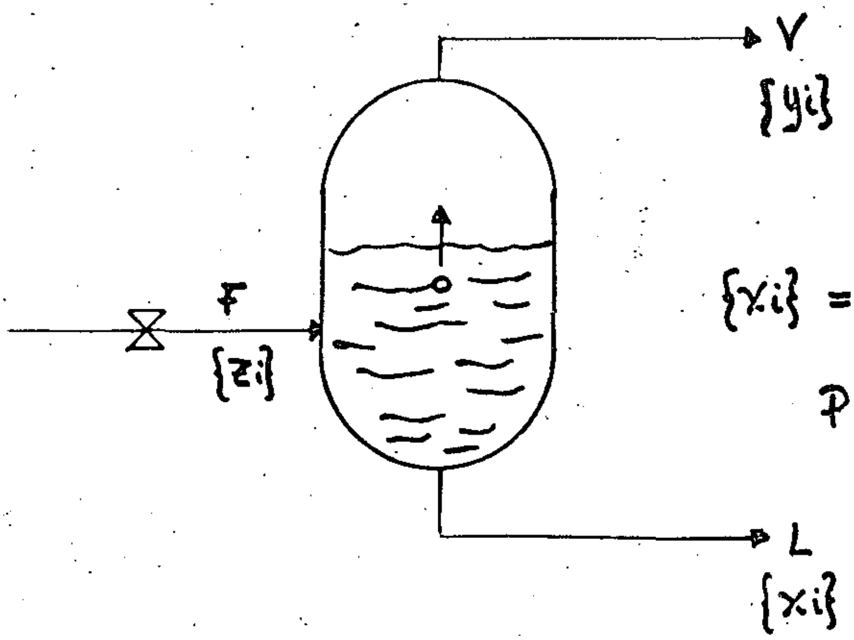
Constante de equilibrio

$$K_i = \frac{p_i^o}{P}$$

Ecuación de Antoine

$$p_i^o = \frac{e^{\left(A_i + \frac{B_i}{C_i + T}\right)}}{P}$$

Cálculo de la T_B:



$\{x_i\} = \{z_i\}$

$P = 585$ mm. Hg

$$\sum_{i=1}^{c} y_i = \sum_{i=1}^{c} K_i x_i = \sum_{i=1}^{c} \frac{\overset{o}{P_i}}{P} x_i = \sum_{i=1}^{c} \frac{e^{\left(A_i + \frac{B_i}{C_i+T}\right)}}{P} x_i = 1.0$$

Componente	z_i	A_i	B_i	C_i
1	1/3	15.904	-2,788.94	220.79
2	1/3	16.586	-3,448.10	235.88
3	1/3	16.142	-3,367.60	215.105

$$\sum_{i=1}^{3} \frac{e^{\left(A_i + \frac{B_i}{C_i \cdot T}\right)}}{P} x_i = \frac{e^{\left(15.904 + \frac{-2,788.94}{220.79+T}\right)}}{585} \times \frac{1}{3} + \frac{e^{\left(16.586 + \frac{-3448.1}{235.88+T}\right)}}{585} \times \frac{1}{3}$$

$$+ \frac{e^{\left(16.142 + \frac{-3,367.60}{215.105+T}\right)}}{585} \times \frac{1}{3} = 1.0$$

$$f(T) = \left[\sum_{i=1}^{3} \frac{e^{\left(A_i + \frac{B_i}{C_i+T}\right)}}{585} \times \frac{1}{3}\right] - 1.0 = 0$$

Cálculo de la T_B

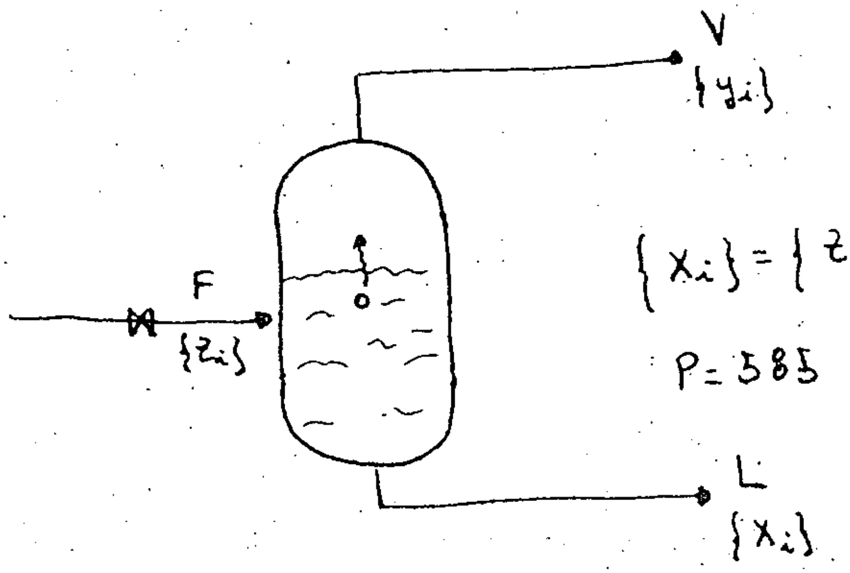
$$\sum_{i=1}^{c} y_i = \sum_{i=1}^{c} K_i X_i = \sum_{i=1}^{c} \frac{P_i^{\circ}}{P} x_i = \sum_{i=1}^{c} \frac{e^{\left(A_i + \frac{B_i}{C_i+T}\right)}}{P} x_i = 1.0$$

Componente	z_i	A_i	B_i	C_i
1	1/3	15.904	−2,788.94	220.79
2	1/3	16.586	−3,448.10	235.88
3	1/3	16.142	−3,367.60	215.105

$$\sum_{i=1}^{3} \frac{e^{\left(A_i + \frac{B_i}{C_i+T}\right)}}{P} x_i = \frac{e^{\left(15.904 + \frac{-2,788.94}{220.79+T}\right)}}{585} * \frac{1}{3} + \frac{e^{\left(16,586 + \frac{-3,448.10}{235.88+T}\right)}}{585} * \frac{1}{3}$$

$$+ \frac{e^{\left(16.142 + \frac{-3,367.60}{215.105+T}\right)}}{585} * \frac{1}{3} = 1.0$$

$$f(T) = \left[\sum_{i=1}^{3} \frac{e^{\left(A_i + \frac{B_i}{C_i+T}\right)}}{585} * \frac{1}{3}\right] - 1.0 = 0$$

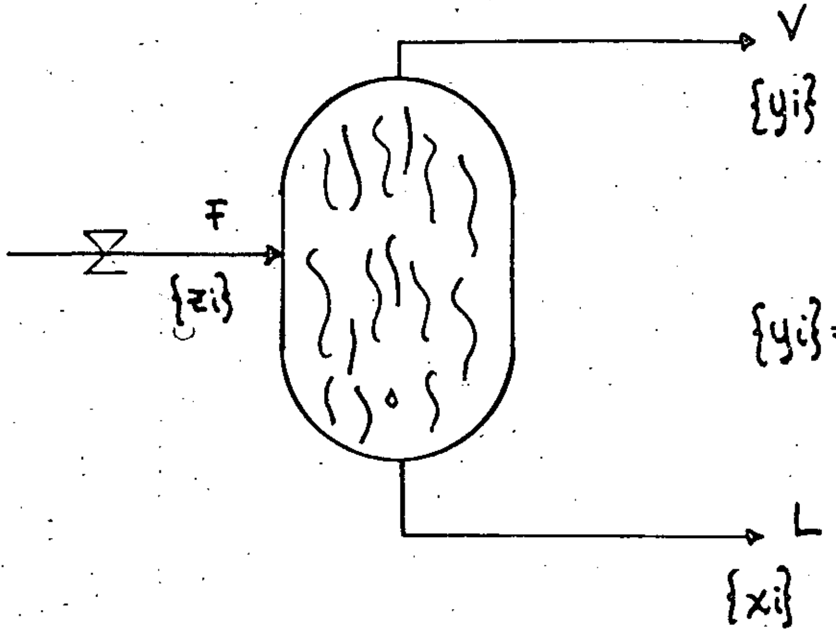


$\{X_i\} = \{z_i\}$

P = 585 mm. Hg

```
01♦LBL "PVAP"
02 RCL IND 05
03 RCL IND 06
04 RCL 17
05 +
06 /
07 RCL IND 04
08 +
09 E↑X
```

Cálculo de la Tv:



P = 585 mm. Hg

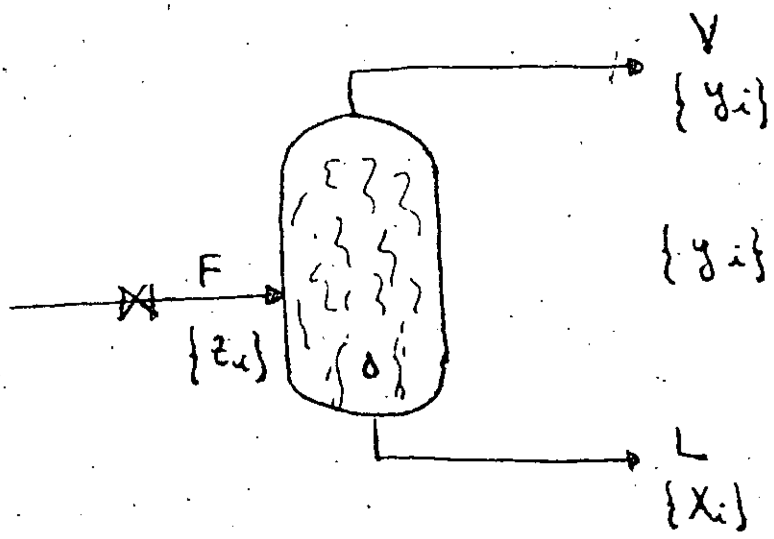
$\{y_i\} = \{z_i\}$

$$\sum_{i=1}^{c} x_i = \sum_{i=1}^{c} \frac{y_i}{K_i} = \sum_{i=1}^{c} \frac{y_i}{\overset{\circ}{P}_i} P = \sum_{i=1}^{c} \frac{y_i}{e^{\left(A_i + \frac{B_i}{C_i + T}\right)}} P = 1.0$$

Componente	zi	Ai	Bi	Ci
1	1/3	15.904	-2,788.94	220.79
2	1/3	16.586	-3,448.10	235.88
3	1/3	16.142	-3,367.60	215.105

$$f(T) = \left[\sum_{i=1}^{3} \frac{585}{e^{\left(A_i + \frac{B_i}{C_i + T}\right)}} \times \frac{1}{3} \right] - 1.0 = 0.0$$

Cálculo de la T_v



$P = 585$ mm. Hg.

$\{y_i\} = \{z_i\}$

$$\sum_{i=1}^{c} x_i = \sum_{i=1}^{c} \frac{y_i}{K_i} = \sum_{i=1}^{c} \frac{y_i}{p^\circ_i} P = \sum_{i=1}^{c} \frac{y_i}{e^{\left(A_i + \frac{B_i}{C_i+T}\right)}} P \doteq 1.0$$

Componente	z_i	A_i	B_i	C_i
1	1/3	15.904	−2,788.94	220.79
2	1/3	16.586	−3,448.10	235.88
3	1/3	16.142	−3,367.60	215.105

$$f(T) = \left[\sum_{i=1}^{3} \frac{585}{e^{\left(A_i + \frac{B_i}{C_i+T}\right)}} \cdot \frac{1}{3} \right] - 1.0 = 0.0$$

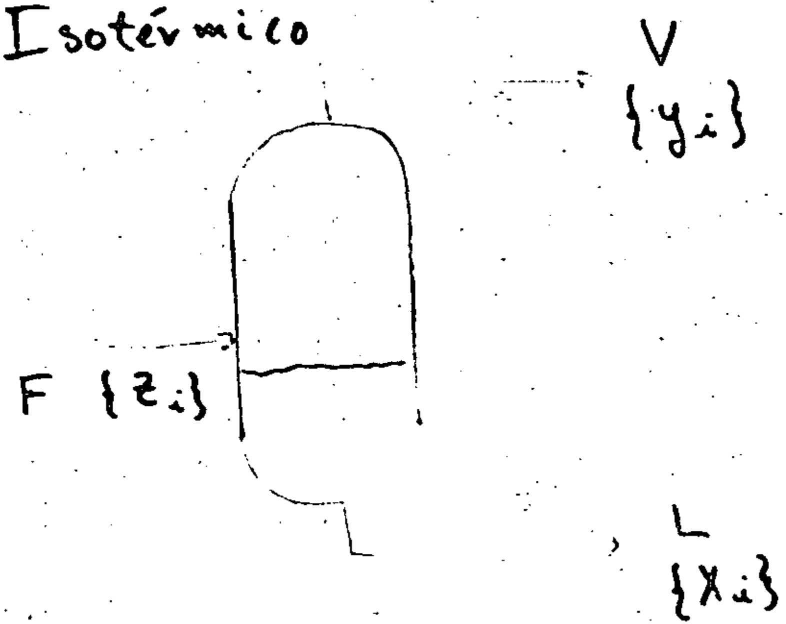
R_{20} → A

```
01•LBL "INI"
02 RCL 00
03 1000
04 /
05 1
06 +
07 STO 01
08 21
09 STO 04
10 RCL 00
11 +
12 STO 05
13 RCL 00
14 +
15 STO 06
16 RCL 00
17 +
18 STO 07
19 0
```

```
01•LBL "TER"
02 XEQ "INI"
03•LBL 01
04 "      YVAR"
05
06 R     D 07
07 *
08 ST+ 08
09 1
10 ST+ 04
11 ST+ 05
12 ST+ 06
13 ST+ 07
14 ISG 01
15 GTO 01
16 RCL 08
17 RCL 20
18 *
19 1
```

```
01•LBL "TEB"
02 XEQ "INI"
03•LBL 01
04 XEQ "YVAR"
05 RCL IND 07
06 *
07 ST+ 08
08 1
09 ST+ 04
10 ST+ 05
11 ST+ 06
12 ST+ 07
13 ISG 01
14 GTO 01
15 RCL 08
16 RCL 20
17 /
18 1
```

Flash Isotérmico



Relaciones de equilibrio
$$\begin{cases} y_i = K_i x_i & i=1,c \\ \sum_{i=1}^{c} y_i = 1 \\ \sum_{i=1}^{c} x_i = 1 \end{cases}$$

Balances de materia: $F z_i = V y_i + L x_i \quad i=1,c$

$$F z_i = V K_i x_i + L x_i = (V K_i + L) x_i$$

si $\phi = \frac{V}{F}$

$$x_i = \frac{F z_i}{V K_i + L} = \frac{z_i}{\frac{V}{F} K_i + \frac{L}{F}}$$

$$x_i = \frac{z_i}{\phi K_i + (1-\phi)}$$

$$f(\phi) = \left[\sum_{i=1}^{c} \frac{z_i}{\phi K_i + (1-\phi)}\right] - 1 = 0$$

```
01♦LBL "FIST1"
02 XEQ "INI"
03♦LBL 01
04 XEQ "PVAP1"
05 RCL 20
06 /
07 RCL 17
08 *
09 RCL 17
10 CHS
11 1
12 +
13 +
14 1/X
15 RCL IND 07
16 *
17 ST+ 08
18 1
19 ST+ 04
20 ST+ 05
21 ST+ 06
22 ST+ 07
23 ISG 01
24 GTO 01
25 RCL 08
26 1
27 -
28 END
```

```
01♦LBL "FIST2"
02 XEQ "INI"
03♦LBL 01
04 XEQ "PVAP"
05 RCL 20
06 /
07 RCL 02
08 *
09 RCL 02
10 CHS
11 1
12 +
13 +
14 1/X
15 RCL IND 07
16 *
17 ST+ 06
18 1
19 ST+ 04
20 ST+ 05
21 ST+ 06
22 ST+ 07
23 ISG 01
24 GTO 01
25 RCL 08
26 1
27 -
28 END
```

Temario para el curso propuesto:

Aplicaciones de los métodos numéricos a problemas de Ingeniería, con enfoque a computadoras manuales.

1.- Solución de ecuaciones.

- a) Cáculo del volumen de un reactor
- ✓ b) Flujo de fluidos en tuberías
- ✓ c) Pérdidas de calor en cámaras de combustión
- ✓ d) Cálculo de la temperatura de burbuja de una mezcla de multicomponentes.
- ✓ e) Cálculo de la temperatura de rocío de una mezcla de multicomponentes.
- f) Destilación Flash isotérmica

2.- Solución de Sistemas lineales

- a) Modelos económicos de Leontief
- b) Crecimiento de la población y las edades específicas.
- c) Explotación racional de poblaciones animales.

3.- Interpolación, Derivación e Integración numérica

- a) Destilación diferencial
- b) Diseño de un cambiador de tubo y coraza.
- c) Diseño de torres de absorción empacadas

4.- Solución numérica de ecuaciones en derivadas parciales

- a) Diseño de un reactor químico.
- b) Simulación del almacenamiento de gas natural en recintos subterraneos porosos.

Duración: 20 hr.

Expositor: Víctor Flores Zavala

1.- Reacción irreversible de 2° orden

$$k a_1^2 = \frac{v(a_0 - a_1)}{V} \qquad k a_2^2 = \frac{v(a_1 - a_2)}{V}$$

$$k a_2^2 = \frac{v a_1 - v a_2}{V} \qquad k a_2^2 V = v a_1 - v a_2$$

$$v a_1 = k a_2^2 V + v a_2 \qquad a_1 = \frac{k a_2^2 V + v a_2}{v}$$

$$k\left[\frac{k a_2^2 V - v a_2}{v}\right]^2 = \cancel{v a_1 - v a_2} \quad \frac{v\left[\frac{k a_2^2 V + v a_2}{v}\right] - v a_2}{V}$$

$$\left[\frac{k^3 a_2^2 V - k^2 v a_2}{v}\right]^2 = \frac{k a_2^2 V + \cancel{v a_2} - \cancel{v a_2}}{V}$$

$$\left[\frac{k^3 a_2 V}{v} - \frac{k^2 v a_2}{v}\right]^2 = k a_2^2$$

$$\left[\frac{k^3 a_2}{v} V - k^2 a_2\right]^2 = k a_2^2$$

$$A = \begin{bmatrix} 13+P_{11} & 4+P_{12} & 4+P_{13} \\ 4+P_{21} & 9+P_{22} & -3+P_{23} \\ 4+P_{31} & -3+P_{32} & 17+P_{33} \end{bmatrix} \begin{bmatrix} F_{21} \\ F_{11} \\ F_{31} \end{bmatrix}$$

76

```
11
STO 03

"FANCO=?"
AVIEW
STOP
STO 00
1000
/
1
+
STO 01
STO 02
STO 04
LBL 01
FIX 0
    CF 29
RCL 01
RCL 0[illegible]
"A("
ARCL X
",)"
ARCL Y
")=?"       SF 29
AVIEW       FIX 4
STOP        PRX
STO IND 03
1
STO + 03
ISG 01
GTO 01
RCL 04
STO 01
ISG 02
GTO 01
[illegible]
RCL 0[illegible]
STO 01
    [illegible] 02
FIX [illegible]
CF 29
[illegible]
"[illegible]
[illegible]
```

```
-99E99
STO 09

PRX
STO IND 03
1
STO + 03
ISG 01
GTO 02

LBL 03
RCL IND 01
RCL IND 02
*
STO + IND 03
1.5
STO + 01
STO + 02
ISG 06
GTO 03
RCL 0[illegible]
STO 02
1
STO + 03
RCL 04
STO 06
ISG 03
GTO 03
XEQ MX
1
STO + 02
ISG 01
GTO 04
RCL 08
STO 06
RCL 04
STO 01
LBL 0[illegible]
RCL IND 08
RCL 09
/
STO IND 02
1
STO + 04
ISG 01
GTO 0[illegible]
RCL 04
11
ACCHR [illegible]
RCL 0[illegible]
```

```
RCL 07
STO 01
RCL 0[illegible]
STO 02
LBL 0[illegible]
```

XEQ B

```
RCL 01
CF 29
FIX 0
"L("
ARCL X
",)="
ARCL Y
AVIEW
```

```
72 FIX 1
   RCL 11
   "ITERACION="
01 ARCL X
   AVIEW
```

```
11
STO 01
RCL 00
X↑2
+
STO 02
STO 05
1
1000
/
11
+
STO 01
```

```
11
STO 01
RCL 00
X↑2
+
STO 02
STO 07
RCL 04
STO 06
STO 07
RCL 03
STO 05

LBL MX
RCL 09
RCL IND 02
X>Y?
GTO 0
RTN
LBL
STO 09
RTN
```

```
RCL 0[illegible]
STO 06
STO 07
```

```
RCL 09
RCL 10
-
0.0001
X>Y?
[illegible]
RCL 09
STO 10
RTN
LBL 13
"RESULTADO"
AVIEW
ADV
RCL 0[illegible]
STO 06
RCL 09
STO 02
```

```
RCL 0[illegible]
RCL 0[illegible]
1000
/
+
RCL 0[illegible]
1E[illegible]
/
+
XEQ RECIBIE

RCL [illegible]
STO 0[illegible]
RCL 0[illegible]
STO 0[illegible]
LBL 0[illegible]
0
STO IND 02
1
STO + 0[illegible]
```

Mezcla 1 (T, P)

Pentano (1.9, 100) (18.5, 400), (36.5, 760)
(92.4, 5atm)
hexano (5.4, 60), (31.6, 200), (68.7, 760)
(131.7, 5atm)
heptano (9.5, 20), (58.7, 200), (98.4, 760)

Mezcla 2

Tolueno (18.4, 20), (51.9, 100), (110.6, 760)
ciclohexano (6.7, 40), (42.0, 200), (80.7, 760)
Benceno (7.6, 40), (42.2, 200), (80.1, 760)

Mezcla 3

Clorobenceno (22.2, 10) (70.7, 100), (132.[illegible], 760)
Benceno (7.6, 40), (42.2, 200), (80.1, 760)
bromobenceno (53.8, 40), (110.1, 200), (156.2, 760)

Mezcla 4

octano (8.3, 5) (53.8, 60) (125.6, 760)
~~[illegible] 40, 400) (27.8, 760)~~
hexano (5.7, 60), (31.6, 200) (68.7, 760)
heptano (9.5, 20) (58.7, 200) (98.4, 760)

```
70 "DESEA CORREGIR
ALGUN DATO?
72 PFA
STOP
X=4?
STO ERR
```

```
LBL ED
"I = ?"
AVIEW
STOP
"J = ?"    ( 1
AVIEW      RCL 00
STOP       * = X≤0?
+          STO
10
STO 02
"A(I, J) = ?"
AVIEW
STOP
```

XEQ A

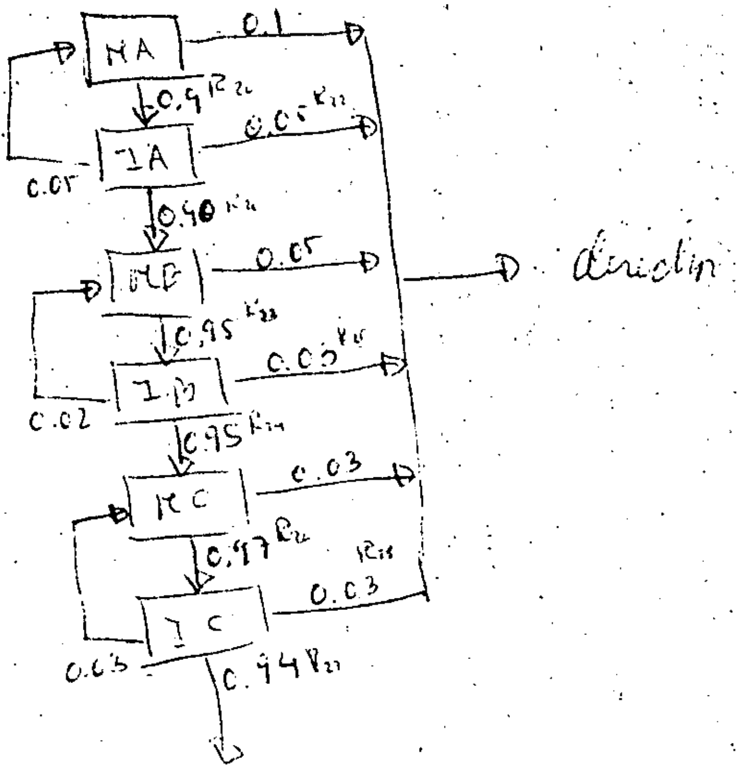
ARCL X

R10 → SUSC
R11 → EUF
R12 → RECOP

R14 → CURA
R19 → INF

```
01♦LBL "EFIDE"
02 RCL 10
03 RCL 11
04 -
05 RCL 12
06 -
07 STO 17
08♦LBL 01
09 RCL 11
10 RCL 16
11 /
12 STO 14
13 RCL 15
14 *
15 RCL 12
16 -
17 STO 12
18 RCL 10
19 RCL 17
[illegible]
21 STO 09
22 .3
23 [illegible]
24 [illegible]
25 STO 05
26 1
27 *
28 STO 15
29 GTO 06
30♦LBL 07
31 RCL 07
32 E
33
34 E
35 -
36 STO 1
[illegible]
40 RCL 11
[illegible]
```

```
45 +
46 RCL 10
47 +
48 STO 00
49 RCL 13
50 RCL 14
51 -
52 RCL 11
53 [illegible]
54 RCL 11
55 +
56 STO 11
57 RCL 12
58 ST+ 00
59 RCL 00
60 2
61 /
62 STO 01
63 INT
64 RCL 01
65 -
66 X=0?
67 GTO 03
68 GTO 01
69♦LBL 03
70 FIX 0
71 RCL 10
72 "SUSC="
73 XEQ 04
74 RCL 11
75 "EUF="
76 XEQ 04
77 RCL 12
78 "RECOP="
79 XEQ 04
80 FIX 2
81 RCL 14
82 "CURA="
83 XEQ 04
84 RCL 15
85 "INF="
86 XEQ 04
87 GTO 01
88♦LBL 04
89 ARCL X
90 AVIEW
91 STOP
92 RTN
93 END
```



LBL 01

```
LBL 01
XEG RNUM
RCL 20
X ≮ y?
GTO 07
XEQ RNUM
RCL 21
X>y?
GTO 02
RCL 00
RCL 22
X<y?
GTO 07
GTO 01
LBL 02
XEG RNUM
RCL 23
X<y?
GTO 07
XEG RNUM
RCL 24
X>y?
GTO 03
RCL 00
RCL 25
X<y?
[illegible]
```

```
LBL 07
"ARTICULO"
"RECHAZADO"
AVIEW
1
STO + 30
```

```
LBL 03
XEG RNUM
RCL 26
X<y?
GTO 07
XEG RNUM
RCL 27
X>y?
GTO 04
RCL 00
RCL 28
X<y?
GTO 07
GTO 03
LBL 04
"ARTICULO"
"EMPACAD."
[illegible]
1
STO + [illegible]
```

```
20 → STO 10
21 → STO 11
22 → STO 13
2 → STO 14
1 → STO 15
XEQ RNUM
RCL IND 10
X<y?
GTO 07
XEQ RNUM
RCL IND 11
X>y?
GTO IND 14
RCL 00
RCL IND 13
X<y?
GTO 07
GTO IND 15
```

XEQ A

CF_{11} → 1 comin
CF_{12} → 2 comin

Genim ål fir
øying flis

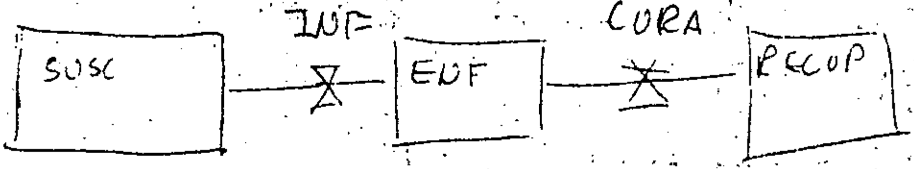
```
y RCL 27
x RCL 28
X≥y?
GTO 10
RCL 27
STO 28
```

~~LBL 10~~
~~SF 11?~~
~~LBL 11~~

```
RCL 28
RCL 27
-
STO 31
RCL 26
X≤y?
GTO 12
SF 11?
```

```
LBL 10
RCL 30
X≤0?
GTO 11
GTO 13
```

```
LBL 12
RCL 26
15
*
2.5
*
4.5 E6
STO + 40
```



$$SUSC|_{t+1} = SUSC|_{t} + \Delta t(-INF|_{t \to t+1})$$

$$SUSC|_{t=0} = 988$$

$$INF|_{t \to t+1} = ENF|_{t} * CONT|_{t} * FRC \quad (4)$$

$$FRC = 0.05$$

$$ENF|_{t+1} = ENF|_{t} + \Delta t(INF|_{t \to t+1} - CURA|_{t \to t+1}) \quad —(6)$$

$$ENF|_{t=0} = 2$$

CONT| = [illegible] — (1)

21.00

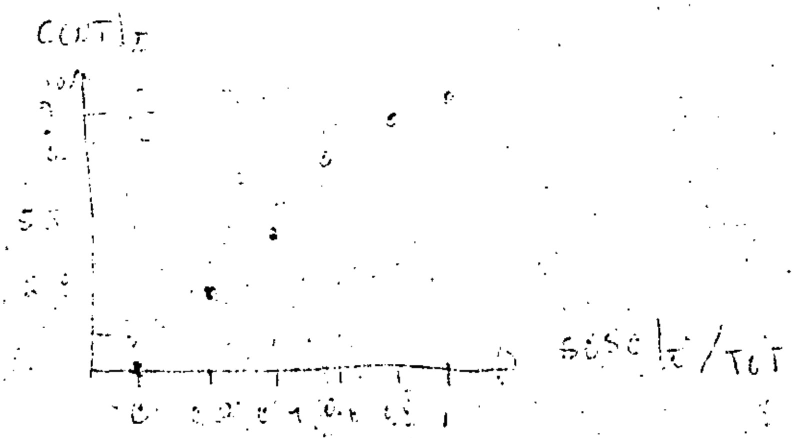
$CURA|_{t,t+1}$ —(1.)

$$RECUP|_{t=0} = 10$$

$$\Delta t = 0.25$$

$$TOT|_{t=0} = SUSC|_{t=0} + ENF|_{t=0} + RECUP|_{t=0} \quad —(3)$$

$R_{10} \to SUSC$
$R_{11} \to ENF$
$R_{12} \to RECUP$
$R_{13} \to INF$
$R_{14} \to CURA$
$R_{15} \to FRC$
$R_{16} \to DUR$
$R_{17} \to TOT$
$R_{18} \to \Delta t$
$R_{19} \to CONT$



```
RCL 10
RCL 11
+
RCL 12
+
STO 17 →TOT LBL 01
RCL 11
RCL 16
/
STO 14 → CURA
RCL 18
*
RCL 12
+
STO 12 → RECUP
RCL 10
RCL 17
/
14
*
STO 19 → CONT
RCL 15
*
RCL 11
*
STO 13 → INF
RCL 18 - S
```

```
D=
RCL 10
+
STO 10 → SUSC
RCL 13
RCL 14
-
RCL 18
*
RCL 11
+
STO 11
GTO 01
```

```
SUS(2)
                      SUS(1)=988.        DUR=10
                      FRENF=0.05
                      ENF(1)=2.
                      TOTAL=SUS(1)+ENF(1)+REC(1)
                      [illegible]

      SUS(2)=SUS(1)+DT*(-INF(1))
      INF(2)=ENF(2)*CONT*FRENF
      ENF(2)=ENF(1)+DT*(INF(2)-CURA(2))
      FRCON=SUS(2)/TOTAL
      IF(FRCON.LE.0.6) GO TO 10
      CONT(2)=14.*FRCON
      CURA(2)=ENF(2)/DUR
      REC(2)=REC(1)+DT*CURA(2)
```

```
R01 → FRCON
R10 → SOS
R11 → ENF
R12 → REC
R13 → INF
R14 → CURA
R17 → TOTAL
R18 → DT
R19 → CONT
```

```
      CURA(2)=ENF(1)/DUR ✓
      INF(2)=ENF(1)*CONT*FRENF
      ENF(2)=ENF(1)+DT*(INF(2)-CURA(2))
      SUS(2)=SUS(1)+DT*(-INF(2))
      FRCON=SUS(2)/TOTAL
      IF(FRCON.LE.0.8) GO TO 10
      CONT(2)=14.*FRCON
      GO TO 20
10

      CURA    =ENF(1)/DUR
      REC(2)=REC(1)+DT*CURA
      FRCON=SUS(1)/TOTAL
      IF(FRCON.LE.0.8) GO TO 10
      CONT(2)=5.*FRCON+5

      INF    =ENF(1)*CONT(2)*FRENF
      SUS(2)=SOS(1)+DT*(-INF    )
      ENF(2)=ENF(1)+DT*(INF     -CURA    )
```

$$\frac{k\,(k a_2^2 V + v a_2)^2}{v^2} = \frac{v a_0 - k a_2^2 V - v a_2}{V}$$

$$\frac{k\left[(k a_2^2)^2 V^2 + 2(k a_2^2)(v a_2)V + (v a_2)^2\right]}{v^2} = \frac{v a_0 - k a_2^2 V - v a_2}{V}$$

$$\frac{k}{v^2}\left[k^2 a_2^4 V^2 + 2 k v a_2^3 V + v^2 a_2^2\right] = \frac{v a_0 - k a_2^2 V - v a_2}{V}$$

$$\frac{k}{v^2}\left[k^2 a_2^4 V^3 + 2 k v a_2^3 V^2 + v^2 a_2^2 V\right] = v a_0 - k a_2^2 V - v a_2$$

$$\frac{k^3 a_2^4}{v^2} V^3 + \frac{2 k^2 a_2^3}{v} V^2 + k a_2^2 V = v a_0 - k a_2^2 V - v a_2$$

$$\frac{k^3 a_2^4}{v^2} V^3 + \frac{2 k^2 a_2^3}{v} V^2 + 2 k a_2^2 V = v a_0 - v a_2$$

$$\frac{k^2 a_2^4}{v^2} V^3 + \frac{2 k a_2^3}{v} V^2 + 2 a_2^2 V = \frac{v}{k}(a_0 - a_2)$$

~~$6.5536 \times 10^{-0} V^3 + 1.6384 \times 10^{-4} V^2 +$~~

$$\frac{k^2 a_2^2}{v^2} V^3 + \frac{2 k a_2}{v} V^2 + 2V = \frac{v(a_0 - a_2)}{k a_2^2}$$

$$\left(\frac{k a_2}{v}\right)^2 V^3 + \frac{2 k a_2}{v} V^2 + 2V = \frac{v(a_0 - a_2)}{k a_2^2}$$

$$6.4 \times 10^{-7} V^3 + 0.0016 V^2 + 2V = 5000$$

CE REFRESHER: PROCESS DYNAMICS/1

Fundamentals of chemical process dynamics

The modeling of dynamic systems involves a thorough analysis of their physical relationships in order to develop, and subsequently solve, the mathematical equations. Here is how to apply the basics to a variety of dynamic conditions.

John L. Guy, Dynamod Enterprises

A new CE REFRESHER begins in this issue. The material in this series will deal with the dynamics of chemical processes and their control systems, and will cover. . . .

- Fundamentals
- Analog computer simulation
- Digital computer simulation
- Control and instrumentation
- Modeling, process optimization and control for chemical reactors, heat transfer, distillation
- Application to startup, shutdown and emergency procedures

☐ Following conventional practice, a distillation column was placed on standby service in order to perform maintenance on other parts of the process system. Under total reflux conditions, the overhead-product valve continuously leaked the more volatile components in the system. After eight hours, only the heavier components remained.

As the liquid level fell below the surface of the tubes in the reboiler, several polymerizations were initiated, with an accompanying increase in temperature and pressure. The resulting shock wave and generated heat caused some reboiler tubes to rupture, and decomposed one of the components in the vapor phase to produce a deflagration wave up the column. At one point in the column, the concentration of a key component was sufficiently high that, when coupled with the temperature wave, the liquid in the column detonated. This destroyed the column and released a large amount of hydrocarbons, which provided the fuel for a second ignition to occur [*1*].

The orderly analyses of possible causes of catastrophes can provide the means for designing emergency shutdown systems, and thus prevent disasters in any CPI (chemical process industries) plant. Basically, the problem is a "what would happen if" situation that must be analyzed—preferably before the plant is built. The various emergencies regularly faced in any plant are: (1) failures due to loss of inplant power, cooling-water supply, steam supply, firewater supply (at time of need), general utilities (air, inert gas, etc.), electrical power from power companies; (2) plant disruptions caused by fire or explosion, spills, etc.; and (3) runaway reactions [*2*].

This dramatic example is not the typical problem that chemical engineers encounter but does illustrate a situation for the study of process dynamics. Most problems encountered in chemical engineering involve less-drastic conditions, as exemplified in the next paragraph.

Design a batch distillation column to separate a certain chemical mixture. This involves the optimization of capital and operating costs to meet a yearly production rate. The process engineer must determine the size of the tower, tanks and auxiliary equipment (investment costs) in relation to energy, operating and maintenance costs.

Hence, we will learn that process dynamics involves the modeling of processing systems in order to optimize investment and operating costs, achieve automatic control, and provide for startup, shutdown and emergency procedures.

In this new CE REFRESHER, we will cover the types of problems in which dynamic analysis must be considered, procedures for analyzing process dynamics, and methods for solving problems. Examples will be included to illustrate the calculations.

The conservation equations

In solving any problem, the first step is definition. After being assigned a problem, we proceed to analyze the various factors that may cause difficulties. Such an analysis may significantly change the procedures for solving the problem, but this step can save considerable engineering time. Then, we can define the system that we are dealing with, and start the calculations.

After defining the problem, the next step for solving it is usually the application of conservation equations. These apply to mass, energy and momentum balances. Generally, this procedure is applied to steady-state or static problems. The general equations for mass, energy or momentum conservation for a system are given by:

$$\text{Flow in} - \text{Flow out} + \text{Reaction product} = \text{Accumulation} \qquad (1)$$

$$\text{Energy in} - \text{Energy out} + \text{Reaction energy} = \text{Accumulation of energy} \qquad (2)$$

$$\text{Sum of forces acting} = \text{Change of momentum} \qquad (3)$$

In Eq. (1), the flows and accumulation term can represent the amount of a particular component, or all (i.e., total) components of the system. In Eq. (3), the change of momentum represents the mass multiplied by its velocity. Eq. (3) is applicable to a specific direction—i.e., it is a vector equation.

Applications to physical systems

Chemical engineering systems can commonly be grouped in two major categories: systems that vary with time only, and those that vary with both time and position. Examples of the former are tank problems; and of the latter, pipe problems. Such systems can also be referred to as macroscopic and microscopic. Let us look at some examples of these systems, and the application of the conservation equations.

Mixing tank—Consider the mixing tank in Fig. 1. Here, we are mixing equal amounts of Components A and B. The flow of each stream (F_A, F_B) is 10 ft^3/h, and the flow from the tank, F_o, is 20 ft^3/h. At a certain instant in time (mathematically referred to as time equal to zero), flow F_A is increased to 15 ft^3/h, and F_B is maintained at 10 ft^3/h. The problem is to determine the change in composition of F_o as a function of time.

In analyzing this problem, let us first define the system that, in this case, is the tank, which is filled with 100 ft^3 of liquid. We will state that (1) the liquid is incompressible, (2) there is no change in volume upon mixing the two liquid streams, and (3) there is no temperature change either in the inlet streams or in the vessel itself via a chemical reaction. Now, we can apply the conservation-of-mass equation, Eq. (1), to the system in which $F_A = 15$ ft^3/h:

Input: $F_A + F_B = 15 + 10 = 25$ ft^3/h

Output: F_o ft^3/h

Reaction: None (zero)

Accumulation: $dV/d\theta$ ft^3/h

where V is the holdup in the system, and θ is time. Note that we have assured ourselves of consistency in units.

Because the tank is liquid-filled, there is no change in accumulation, and $dV/d\theta = 0$. Substituting the values into Eq. (1), we find that the total flow $F_o = 25$ ft^3/h. Hence, the instantaneous change in total output flow is 5 ft^3/h, after the increase in flow for stream F_A.

Let us now look at how the composition of the output stream is changing. First, we will define x_A and x_B as the volume fraction of Liquids A and B, and note that $x_A + x_B = 1$. By solving for one composition, we immediately know the other. Looking at our conservation equation, we proceed to solve for x_A as a function of time.

Input: $F_A x_{Ai} + F_B x_A = 15(1) + 10(0) = 15$ ft^3 of A/h

Output: $F_o x_A$ ft^3 of A/h

Reaction: None (zero)

Accumulation: $d(Vx_A)/d\theta$

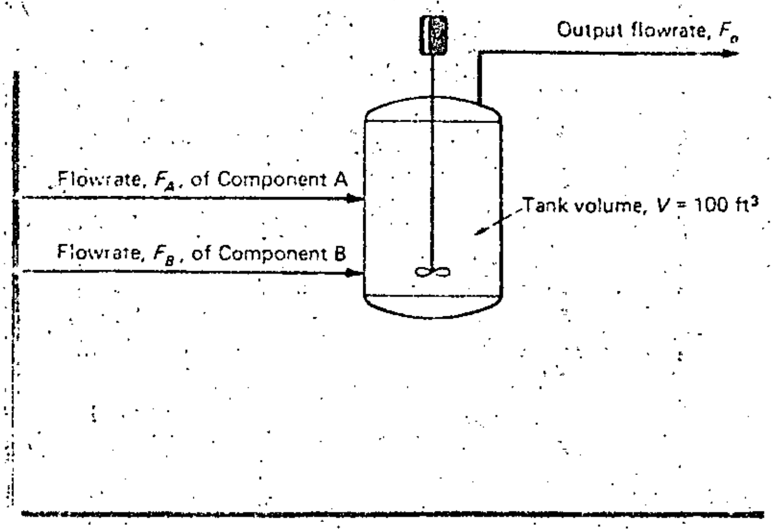
We immediately note that the composition of A in the tank and in the output stream, F_o, are the same. This is one characteristic that makes this a tank or macroscopic system.

Substituting the values into Eq. (1), we obtain:

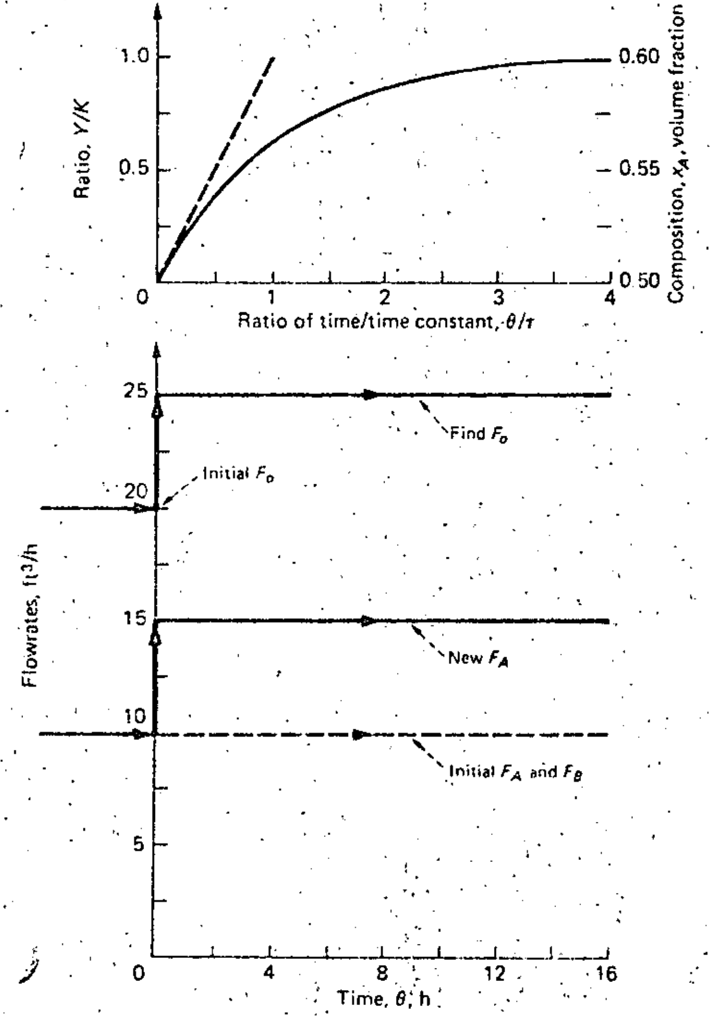
$$F_A x_{Ai} - F_o x_A = d(Vx_A)/d\theta \qquad (4)$$

Since the holdup is constant ($V = 100$), we can rewrite Eq. (4) as:

$$F_A - F_o x_A = V dx_A/d\theta \qquad (5)$$



Parameters for the example for a mixing tank **Fig. 1**



Responses of a first-order system **Fig. 2**

We can now separate the variables, x_A and θ, and provide the limits of integration to solve Eq. (5):

$$\int_{0.5}^{x_A} \frac{dx_A}{\left(\frac{F_A}{F_o} - x_A\right)} = \int_0^{\theta} \left(\frac{F_o}{V}\right) d\theta$$

Solving the integral equation yields the solution as:

$$x_A = \frac{F_A}{F_o} - \left[\frac{F_A - 0.5F_o}{F_o}\right] \exp(-F_o\theta/V) \qquad (6)$$

The results are shown graphically in Fig. 2.

General first-order systems

Eq. (5) is an example of a first-order system that can be transformed to the general equation:

$$X - Y = \tau(dY/d\theta) \qquad (7)$$

where X is a function of the independent variable θ; Y, a dependent variable; τ, a system time constant.

For a step change of X (say $X = K$, where K is a constant), the solution to Eq. (7) is:

$$Y = K(1 - e^{-\theta/\tau}) \qquad (8)$$

To convert Eq. (5) to the general equation for a first-order system, we convert the variables, F_A and x_A, to

Nomenclature

A	Area, ft²
C	Valve (or orifice-restriction) coefficient, defined by Eq. (18)
C_p	Heat capacity, Btu/(lb)(°F)
d	Tube dia., in.
F	Volumetric flowrate, ft³/h
H	Height, ft
h	Heat-transfer coefficient, Btu/(h)(ft²)(°F)
L	Liquid holdup, moles
T	Temperature of shellside fluid, °F
t	Temperature of tubeside fluid, °F
T_w	Tube-wall temperature, °F
V	Holdup volume, ft³
V_R	Vapor rate, moles/h
v	Velocity, ft/h
W	Flowrate, lb/h
x	Volume-, mole-, or weight-fraction in liquid phase
y	Mole fraction in vapor phase
α	Relative volatility
ρ	Density, lb/ft³
θ	Time, h or min
τ	Time constant, h^{-1}

Subscripts

A,B	Component identification
i	Inside or tubeside fluid properties, etc., or inlet conditions
o	Outside or shellside fluid, property, etc., or outlet conditions
w	Wall property
0	Initial condition
ss	Steady-state value

new variables. The new variables are differences of the variable and the initial steady-state values. To solve for the time constant, we divide Eq. (5) by F_o:

$$\frac{F_A}{F_o} - x_A = \frac{V dx_A}{F_o d\theta} \qquad (9)$$

Expressing Y and X as the new variables, and setting these into Eq. (5), yields: perturbaciones o [illegible]

$$Y = x_A - x_{A_0} = x_A - 0.5 \qquad (10)$$

$$X = \frac{F_A}{F_o} - \frac{F_{A_0}}{F_{o_0}} = \frac{15}{25} - \frac{10}{20} = 0.1 \qquad (11)$$

Therefore, $K = 0.1$ in Eq. (8). Substituting these numbers into Eq. (8) produces

$$Y = x_A - 0.5 = 0.1(1 - e^{-\theta/\tau}) \qquad (12)$$

where $\tau = V/F_o = 100/25 = 4$. We can rearrange Eq. (12) and see that it is the same as Eq. (6).

Fig. 2 also shows a plot of Y/K vs. θ/τ. From Fig. 2, we see that the system responds to 63.2% of the new steady-state value when time, θ, equals the time constant, τ. The system has essentially responded to the upset when time, θ, equals 4τ (98.5%).

If the system responded linearly with the initial rate of response, the new steady-state value would be reached after $\theta = \tau$.

Heat-exchanger tube

Let us consider the heat-exchanger tube shown in Fig. 3. We are heating a fluid (no phase change) inside a tube, with steam on the outside as the heating medium. We are looking at the flow of one tube, and assume that each tube in the bundle operates identically.

In analyzing the heat transfer, we assume that:

- ✓ Temperature of the condensing steam can vary with time but not with position in the exchanger.
- ✓ Temperature gradients vary in the Y-direction along the tube, but radial temperature gradients are negligible.
- ✓ Inside and outside heat-transfer coefficients are constant with position in the exchanger but not with time; and the effects of fouling are either negligible or are included in the calculated coefficients.
- ✓ Fluid inside the tube is incompressible.
- ✓ Tubeside fluid properties are constant. Fluido dentro tubo

Applying Eq. (2) to the tubeside fluid in the differential length, ΔY, we find that the input, output and accumulation terms are:

$$W_i C_{P_i} t + \left[h_i\left(\frac{\pi d_i}{12}\right)\Delta Y\right](T_w - t)$$

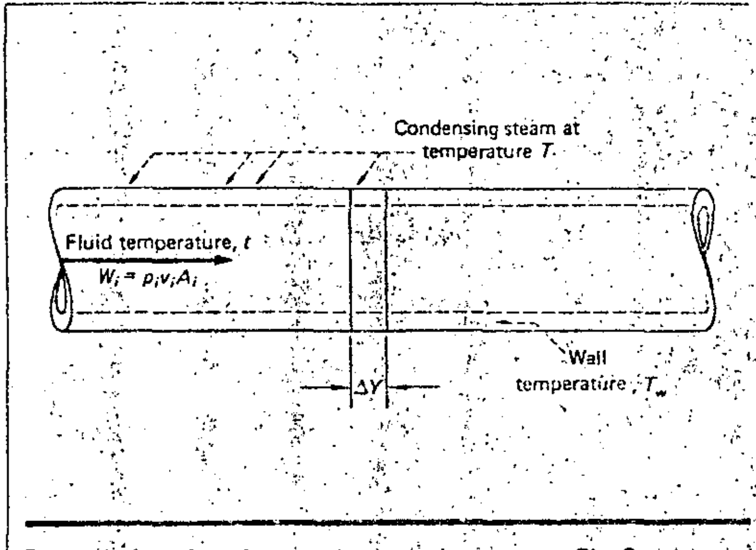
$$\frac{\text{lb}}{\text{h}} \cdot \frac{\text{Btu}}{\text{lb} \cdot {}^\circ\text{F}} \cdot {}^\circ\text{F} + \frac{\text{Btu}}{\text{h} \cdot \text{ft}^2 \cdot {}^\circ\text{F}} \cdot \text{ft}^2 \cdot {}^\circ\text{F} = \frac{\text{Btu}}{\text{h}}$$

$$W_i C_{P_i}\left[t + \frac{\partial t}{\partial Y}\Delta Y\right]$$

$$\frac{\text{lb}}{\text{h}} \cdot \frac{\text{Btu} \cdot {}^\circ\text{F}}{\text{lb} \cdot {}^\circ\text{F}} = \frac{\text{Btu}}{\text{h}}$$

$$\frac{\partial}{\partial \theta}\left[\rho_i\left(\frac{\pi d_i^2}{144}\right)\Delta Y C_p t\right]$$

$$\frac{1}{\text{h}} \cdot \frac{\text{lb}}{\text{ft}^3} \cdot \text{ft}^2 \cdot \text{ft} \cdot \frac{\text{Btu}}{\text{lb} \cdot {}^\circ\text{F}} \cdot {}^\circ\text{F} = \frac{\text{Btu}}{\text{h}}$$



Flow relations for a heat-exchanger tube **Fig. 3**

Substituting these terms into Eq. (2), we obtain:

$$W_i C_{P_i} t - W_i C_{P_i}\left(t + \frac{\partial t}{\partial Y}\Delta Y\right) + h_i\left[\pi\left(\frac{d_i}{12}\right)\Delta Y\right](T_w - t) = \frac{\partial}{\partial \theta}\left[\rho_i\left(\frac{\pi d_i^2}{144}\right)\Delta Y C_p t\right] \qquad (13)$$

We simplify the various quantities by allowing ΔY to approach a differential length, dY:

$$-W_i C_{P_i}\frac{\partial t}{\partial Y} + h_i\left[\left(\frac{\pi d_i}{12}\right)(T_w - t)\right] = \frac{\partial}{\partial \theta}\left[\frac{\rho_i \pi d_i^2}{144} C_p t\right] \qquad (14)$$

$$\left(\frac{\pi \rho_i d_i^2}{144}\right) C_P \frac{\partial t}{\partial \theta} = h_i \pi \frac{d_i}{12}(T_w - t) - \rho_i v_i \frac{\pi d_i^2}{144} C_P \frac{\partial t}{\partial Y} \qquad (15)$$

$$\frac{\partial t}{\partial \theta} = \frac{12 h_i}{\rho_i d_i C_P}(T_w - t) - v_i \frac{\partial t}{\partial Y} \qquad (16)$$

Next, we will apply Eq. (2) to the tube wall. We will neglect the thermal resistance but take into account the thermal capacity of the wall. Input, output and accumulation terms become:

$$h_o\left(\frac{\pi d_o}{12}\right)\Delta Y(T - T_w)$$

$$h_i\left[\left(\frac{\pi d_i}{12}\right)\Delta Y\right](T_w - t)$$

$$\rho_w\left[\frac{\pi(d_o^2 - d_i^2)}{144}\right]\Delta Y C_{P_w}\left(\frac{\partial T_w}{\partial \theta}\right)$$

Substituting into Eq. (2), allowing ΔY to approach dY and rearranging, we obtain:

$$\frac{\partial T_w}{\partial \theta} = \left(\frac{12 h_o d_o}{\rho_w(d_o^2 - d_i^2)C_{P_w}}\right)(T - T_w) - \left(\frac{12 h_i d_i}{\rho_w(d_o^2 - d_i^2)C_{P_w}}\right)(T_w - t) \qquad (17)$$

We now have more than one equation and are deal-

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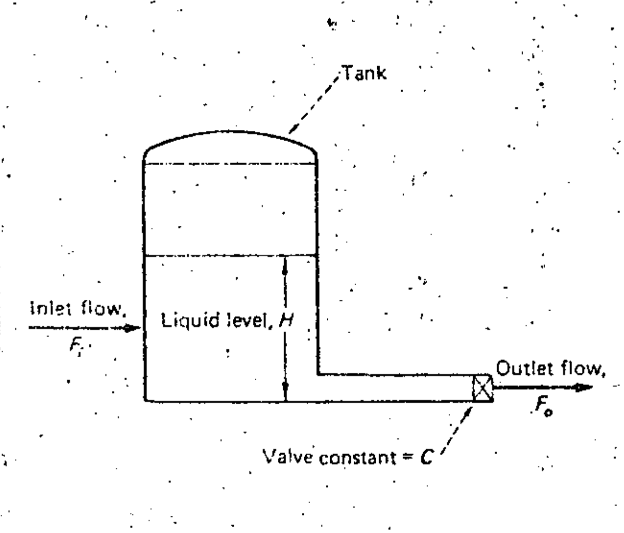
ing with partial differential equations. We have increased the mathematical difficulty and computational effort. We will return to the solution of this problem in a future article. For the moment, we simply note the method of setting up the mathematical equations.



Surge tank for the variable-holdup example **Fig. 4**

Surge tank

Let us next consider a variable-holdup problem, shown in Fig. 4. The inlet flow, F_i ft^3/h, is initially at steady state and equals the outlet flow, F_o. The restriction in the outlet line causes the outlet flow to vary with the liquid level, H, in the tank, according to the following relationship:

$$F_o = C\sqrt{H} \tag{18}$$

where C is a constant for the valve resistance.

The conservation-of-mass equation is set up as:

Input: F_i, ft^3/min
Output: F_o, ft^3/min
Accumulation: $dV/d\theta$, ft^3/min

where V is the tank volume equal to AH. Substituting these quantities into Eq. (1):

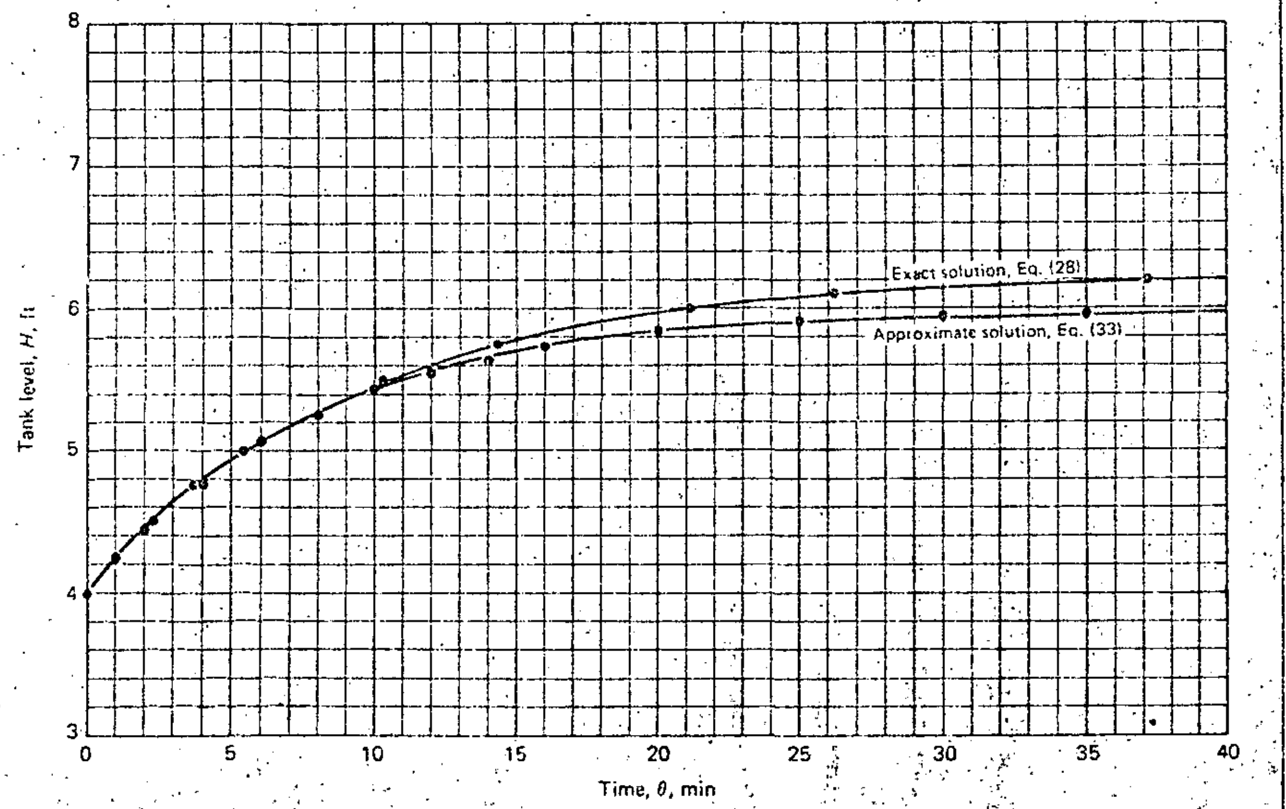
$$F_i - F_o = \frac{dV}{dt} = \frac{dAH}{dt} = \frac{AdH}{d\theta} \tag{19}$$

Substituting $C\sqrt{H}$ for F_o in Eq. (19):

$$F_i - C\sqrt{H} = AdH/d\theta \tag{20}$$

To solve Eq. (20) exactly, we make the following substitutions [3]:

$$u = \sqrt{H} \tag{21}$$



Comparison of results for exact and approximate solutions for surge-tank example **Fig. 5**

$$dH = 2u\,du \tag{22}$$

$$2Au(du/d\theta) = F_i - Cu \tag{23}$$

Separating the variables of Eq. (23):

$$2A\left(\frac{u\,du}{F_i - Cu}\right) = d\theta \tag{24}$$

Now, we set numerical values for the several variables: $C = 10$ ft^3/min; $A = 20$ ft^2; $F_i = 20$ ft^3/min before $\theta = 0$, and 25 ft^3/min after $\theta = 0$; $F_o = 20$ ft^3/min before $\theta = 0$; $H = (F_o/C)^2 = (20/10)^2 = 4$ ft initially; and $u = \sqrt{H} = \sqrt{4} = 2$ initially.

We solve Eq. (24) by integration. Substituting the appropriate numerical values and setting limits of integration, we find that:

$$40\int_{u=2}^{u=u} \frac{u\,du}{F_i - 10u} = \int_0^{\theta/d\theta} d\theta \tag{25}$$

$$\frac{40}{100}[F_i - 10u - F_i \ln(F_i - 10u)]_{u=2}^{u=u} = \theta \tag{26}$$

$$0.4\left[-10(u - 2) - F_i \ln\left(\frac{F_i - 10u}{F_i - 20}\right)\right] = \theta \tag{27}$$

$$\ln\left[\frac{F_i - 10\sqrt{H}}{F_i - 20}\right] = \frac{-2.5\theta}{F_i} - \frac{10}{F_i}\left[\sqrt{H} - 2\right] \tag{28}$$

The response of the tank level and the output flowrate is shown in Fig. 5. When dealing with nonlinear equations such as Eq. (20), and the substitution of Eq. (21) cannot be found, we can linearize them to obtain an analytical solution, by using a Taylor-series expansion around the steady-state operating conditions. The Taylor-series expansion for one variable is:

$$G(z) = G(z_{ss}) + \left.\frac{\partial G}{\partial z}\right|_{z_{ss}}(z - z_{ss}) + \left.\frac{\partial^2 G}{\partial H^2}\right|_{z_{ss}}\frac{(z - z_{ss})^2}{2} + \cdots \tag{29}$$

where G is a given function, z is a dependent variable, and z_{ss} is the steady-state term.

Neglecting all but the first differential term, and applying:

$$\left.\begin{aligned} h &= \sqrt{H} \\ h &\approx \sqrt{H_{ss}} + \left(\frac{1}{2\sqrt{H_{ss}}}\right)(H - H_{ss}) \\ h &= C_1 + C_2 H \end{aligned}\right\} \tag{30}$$

We can then linearize the relationships of Eq. (30) because $H_{ss} = 4$. Therefore:

$$\sqrt{H} = 1 + 0.25H \tag{31}$$

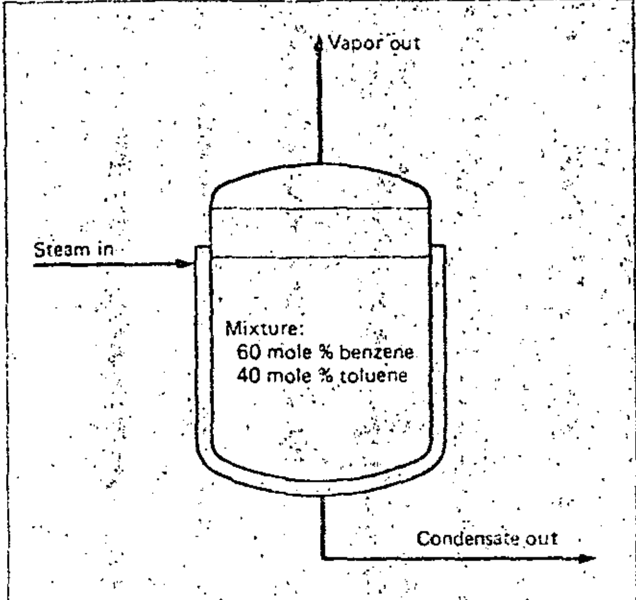
Substituting the linearized variable of Eq. (31) into Eq. (20), we obtain:

$$F_i - C(1 + 0.25H) = A(dH/d\theta) \tag{32}$$

Solving Eq. (32) produces the expression for the height of liquid, H, in the surge tank for this example:

$$H = 6 - 2e^{-0.125\theta} \tag{33}$$

This linearized solution, Eq. (33), is also shown graphically in Fig. 5. Eventually, the exact solution, Eq. (28), reaches a new steady-state value at 6.25—while the approximate solution, Eq. (33), predicts a new steady-state value of 6.00.



Conditions for the example for a Rayleigh distillation **Fig. 6**

This example illustrates that approximate results can be obtained for nonlinear differential equations by using the Taylor-series expansion. It also demonstrates why an analysis around the steady-state values can lead to errors in analysis if we impose large upsets into the physical system.

Rayleigh distillation

Let us conclude our discussion of setting up dynamic problems by considering the batch distillation shown in Fig. 6. The problem is taken from King [4]. To allow for continuity in our analysis, we will change the problem slightly. The initial contents of the vessel are 100 moles of a mixture containing 60 mole% benzene and 40 mole% toluene. The vessel will operate at a total pressure of 1.2 atm.

We will solve for the composition of the liquid in the vessel, the vapor leaving the vessel, and the composition in the product tank after the vapor is condensed—all as functions of time.

Setting up the problem via Eq. (1) for the total mass balance, we find:

Input: 0 lb-moles/h
Output: V_R lb-moles/h
Accumulation: $dL/d\theta$ lb-moles/h

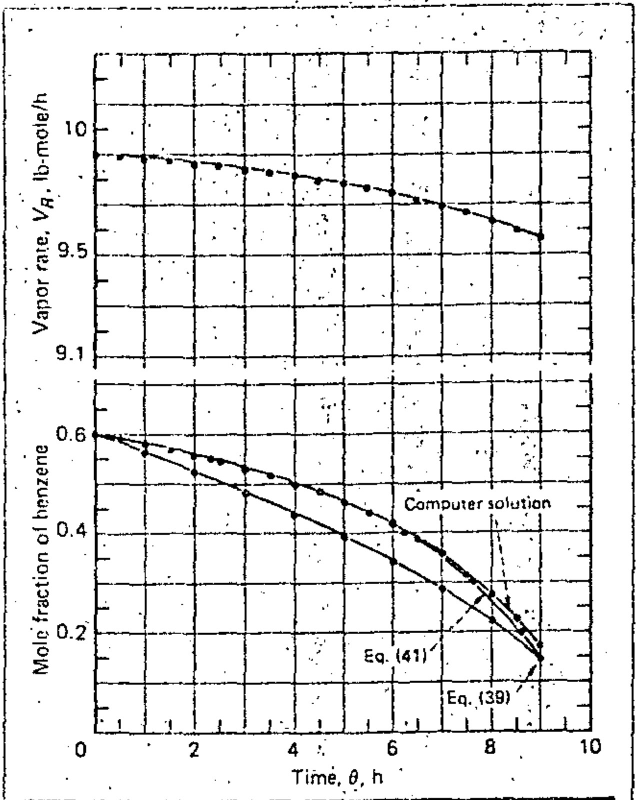
Similarly, for the benzene (or toluene) component:

Input: 0
Output: $V_R y$
Accumulation: $d(Lx)/d\theta$

Substituting these expressions into Eq. (1), we obtain:

$$-V_R = dL/d\theta \tag{34}$$

$$-V_R y = \frac{d(Lx)}{d\theta} = L\left(\frac{dx}{d\theta}\right) + x\left(\frac{dL}{d\theta}\right) \tag{35}$$



Compositions and rates for Rayleigh distillation example **Fig. 7**

Combining Eq. (34) and (35), we get the equation for the rate of change for the component:

$$\frac{dx}{d\theta} = \frac{-V_R(y - x)}{L} \qquad (36)$$

King [4] provides two assumptions that are commonly used to simplify the solution of this example:

1. If we assume that the equilibrium constant, $k, = y/x$, and that V_R is constant, then:

$$L = L_o - V_R\theta \qquad (37)$$

$$\int_{x=0.6}^{x} \frac{dx}{kx - x} = \int_0^{\theta} \frac{-V_R d\theta}{L_o - V_R\theta} \qquad (38)$$

Eq. (38) can be directly solved to give:

$$\left(\frac{1}{k-1}\right)\ln\frac{x}{0.6} = \ln\frac{(L_o - V_R\theta)}{L_o} \qquad (39)$$

2. If we assume constant relative volatility, α, which is defined by:

$$y = \frac{\alpha x}{1 + (\alpha - 1)x} \qquad (40)$$

then, by substituting Eq. (40) into Eq. (36) and integrating, we obtain:

$$-\ln\frac{(L_o - V_R\theta)}{L_o} = \frac{1}{(\alpha - 1)}\ln\left[\frac{x(1 - 0.6)}{0.6(1 - x)}\right] + \ln\left[\frac{1 - 0.6}{1 - x}\right] \qquad (41)$$

We can use either Eq. (39) or Eq. (41) with the assumed constant vapor rate to produce the results shown in Fig. 7. Assuming a constant vapor may be reasonable for this system—especially for preliminary studies.

To design the unit for a constant vapor rate requires a control system that introduces its own dynamics; because a simple feedback-control system will adjust the heat input to the vessel only after sensing an error in the setpoint. Controlling the pressure (especially after vaporization begins) could introduce additional dynamics into the system. A more serious variable that we have ignored is the reduction in the heat-transfer surface as the distillation proceeds.

Although these additional effects may not be critical for the Rayleigh distillation of this example, let us consider the effects on large distillation towers (either batch or continuous) having interactive- and dynamic-control systems.

✓Finally, let us examine the assumptions in our analysis. Both the equilibrium constant and the relative volatility change with temperature, and the temperature changes as the distillation proceeds. The assumption of constant heat input (usually adhered to in practice) can produce changes in vapor rates because of the heat capacity of the liquid and the nonlinear change occurring in temperature.

A computer program taking these effects into account produces the results shown in Fig. 7 for a constant heat-input to the vessel. Because of the closeness of latent heat, we only have a 4% change in the vapor rate. Since the relative volatility varies only from 2.46 to 2.35, the computer results are very close to those obtained from Eq. (41). However, the results can change with the materials being distilled.

In summary

Analysis of the physical system is the most important step in any problem. But it is the step usually skipped when time constraints and work pressures are imposed.

The second article in this CE REFRESHER series will appear in the issue of Aug. 24, and will deal with process control loops.

Steven Danatos, Editor

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The author

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Process control loops

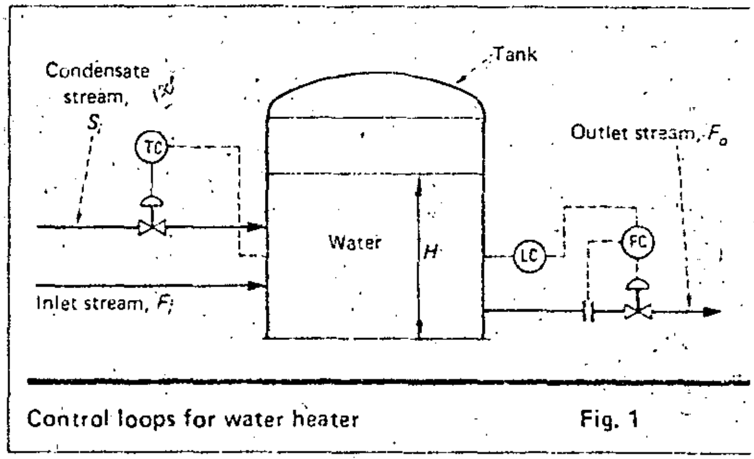
How to develop mathematical models that simulate the dynamic operation of process control loops.

*John L. Guy, Dynamod Enterprises**

☐ Simulation of process control loops includes models for the:

- Sensing devices that measure the process variables of the system.
- Controllers.
- Control valves.

Here, we will show how to analyze the various components of the control loop (i.e., the "hardware"). In a later article, we will show how to use the resulting equations for the process equipment (see Part 1, *Chem. Eng.*, ne 29, p. 74) and the control loops, in order to simulate the complete system.



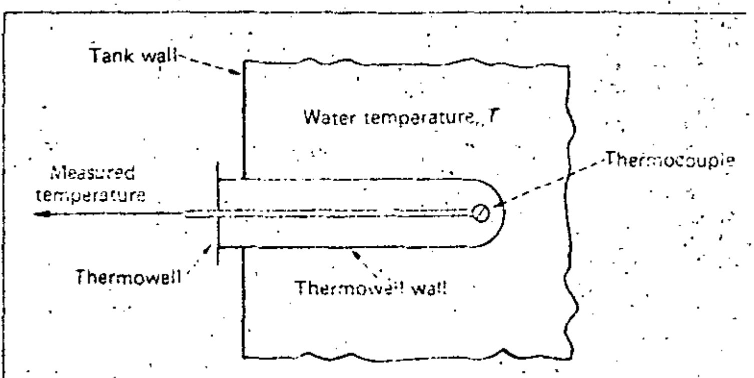
Control loops for water heater **Fig. 1**

Typical process control

Let us consider the hot-water heater shown in Fig. 1. In this process, we are heating water by adding steam condensate to produce an output stream of water at the desired temperature. The temperature-control loop measures the temperature in the tank, and increases the flow of steam condensate when the desired outlet temperature drops below the temperature of the tank or of the outlet stream, F_o. The desired outlet temperature is called the setpoint of the temperature controller.

The outlet flow, F_o, will control the liquid level, H, in the tank. In this system, we have specified cascade control of the liquid level so as to adjust a flow controller that produces less of a variation in flow, or a more-constant outlet flow. In this system, a change in liquid level produces an error in the setpoint of the level controller, LC. The level controller changes the setpoint of the flow controller, FC, and, therefore, produces an error signal that causes the control valve in the outlet line to adjust F_o.

Let us now look at the elements (sensing devices, controllers, and final control elements: usually control valves) for which we must develop dynamic equations.



Temperature-sensing element in a thermowell **Fig. 2**

Sensors: temperature

A temperature-sensing element inside a thermowell is shown in Fig. 2. For this analysis, we will assume that the major and only resistance to heat transfer is located on the outside of the thermowell casing, and that the temperature inside the thermowell is the same as the temperature sensed by the thermocouple.

The elements for this analysis are shown in Fig. 3a. We note that a higher temperature exists inside the tank than in the thermocouple and the surrounding liquid. This analysis also corresponds to a thermocouple that is directly exposed to the tank liquid.

We will analyze this system by the same procedures that were outlined in Part 1—namely, as was done for

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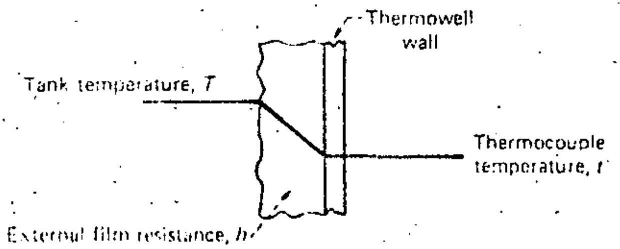
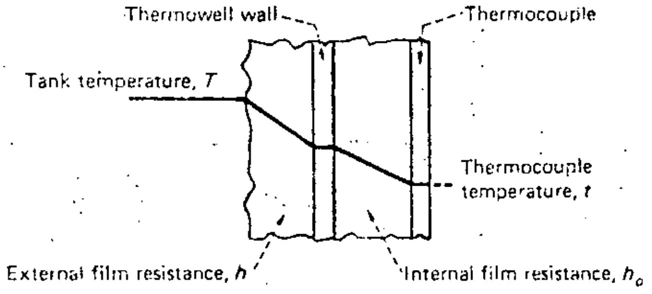
*To meet the author, see *Chem. Eng.*, June 29, p. 80



a. Negligible resistance to heat transfer [given by Eq. (1)]



b. Considerable resistance to heat transfer [given by Eq. (3)]

Temperature profiles for temperature-sensing elements **Fig. 3**

an energy balance for the system defined as the thermocouple itself. Initially, the temperature of the thermocouple will be equal to the liquid temperature, T. When the liquid temperature changes, energy will be transferred to the thermocouple (for a rising temperature in the tank), and the energy balance can be set up as:

Input: $hA(T - t)$
Output: 0
Accumulation: $d(M_t C_{pt} t)/d\theta$

where A = area of thermocouple or thermowell, C_{pt} = heat capacity for thermocouple and thermowell, h = heat-transfer coefficient, M_t = mass of thermocouple and thermowell, and θ = time.

If we assume that the heat-transfer coefficient, h, and the heat capacity are constant, then:

$$M_t C_{pt}\left(\frac{dt}{d\theta}\right) = hA(T - t) \tag{1}$$

After setting the time constant, τ, equal to $M_t C_{pt}/hA$, Eq. (1) becomes the general equation for a first-order system. We developed the solution for a step change in a first-order system in Part 1 (*Chem. Eng.*, June 29, p. 76). Applying this result to a step change in tank temperature will yield:

$$t = T - e^{-\theta/\tau} \tag{2}$$

This is the resulting equation for first-order sensing elements, and we must calculate or estimate the system time constant, τ.

Murrill [*1*] set up the equation for the system shown in Fig. 3b, where film resistances inside and outside the thermowell introduce resistance to heat transfer. In this analysis, he assumed negligible heat-transfer resistance in the wall of the thermowell and the thermowell itself.

After evaluating the appropriate energy balances around the thermowell wall and the conducting fluids, we obtain a second-order differential equation:

$$\left[\frac{M_t C_{pt} M_w C_{pw}}{h_o A_o h A}\right]\frac{d^2 t}{d\theta^2} + \left[\frac{M_t C_{pt}}{h_o A_o} + \frac{M_t C_{pt}}{hA} + \frac{M_w C_{pw}}{hA}\right]\frac{dt}{d\theta} + t = T \tag{3}$$ ✓

where the subscript w refers to the thermowell's wall properties. The area A_o refers to the area corresponding to the second series resistance.

The net effect of adding the second resistance is to slow down the response of the system. Fig. 4 shows the response for a bare bulb or a thermowell having negligible inside resistance compared with systems that include the analysis for the thermowell fluid resistance.

Sensors: pressure actuated

The liquid level, H, in the tank of Fig. 1 can be converted to a pressure signal in a sensing element such as the one shown in Fig. 5.

Sensing elements for measuring liquid level, pressure and flow are examples of systems that use pressure differential to infer the value for the variable. All result in the same analysis.

In Fig. 5, for example, the head pressure of the liquid is transferred through an isolating diaphragm and fill liquid in a sealed-capillary-system differential-pressure sensing element. Here, the pressure is transmitted through a second isolating diaphragm and fill liquid, to a sensing diaphragm in the differential-pressure cell. Atmospheric or reference pressure will balance the sensing diaphragm and fill liquid on the other side of this diaphragm. The displacement of the sensing diaphragm (maximum motion for this device is 0.004 in.) is proportional to the pressure across it.

The position of the sensing diaphragm is detected by capacitor plates on both sides of the diaphragm. The differential capacitance between the sensing diaphragm and the capacitor plates is converted electronically into a direct-current signal of 4 to 20 mA or 10 to 50 mA.

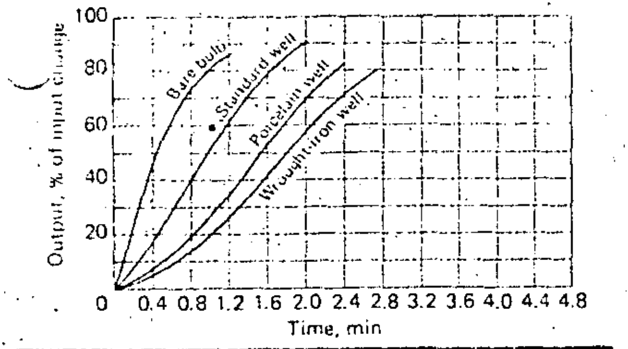
A change in pressure P_1 in the process (such as change in liquid level, H, in the tank) will cause the pressure P_2 at the end of the capillary tube to change, but not instantaneously. A force-balance or conservation-of-momentum equation around the capillary will yield:

$$P_1 A_c - P_2 A_c = \left(\frac{A_c L_c \rho_c}{g_c}\right)\frac{d^2 Z}{d\theta^2} \tag{4}$$

where A_c = area of the capillary tube, L_c = length of the capillary tube, ρ_c = density of fluid in the capillary tube, Z = fluid displacement in the capillary tube, and g_c = gravitational constant.

The increase or decrease in pressure causes a force to be applied to the compensating diaphragm. The mechanical resistance of the diaphragm will act like a spring having a resistance K. The force acting on the diaphragm, $P_2 A_c$, will balance the force, KZ, and the capacitance, C, in the diaphragm. Mathematically:

$$P_2 A_c = KZ + C\left(\frac{dZ}{d\theta}\right) \tag{5}$$



Effect of thermowell on temperature-bulb response Fig. 4

Combining Eq. (4) and (5), we get:

$$\left(\frac{A_c L_c \rho_c}{g_c K}\right)\frac{d^2Z}{d\theta^2} + \frac{CdZ}{Kd\theta} + Z = P_1 A_c K \qquad (6)$$

We can convert Eq. (6) to a general second-order transfer-function equation:

$$\tau^2\left(\frac{d^2Z}{d\theta^2}\right) + 2\zeta\tau\left(\frac{dZ}{d\theta}\right) + Z = GH \qquad (7)$$

where G = system gain, τ = time constant, and ζ = damping ratio.

If a unit-step forcing function is applied to Eq. (7), its [illegible]tion is as is shown in Fig. 6. Here, Z represents the ratio of the output signal from the sensing element to a given input function—say, H.

For values of the damping ratio less than 1, the system is said to be underdamped. The system reacts with an oscillatory response, but this decreases with time.

For a damping ratio equal to 1, the system is said to be critically damped. This value of ζ allows the most rapid response of the system without oscillation.

For values of the damping ratio greater than 1, the system produces an overdamped response. This response is not oscillatory and becomes slower as ζ becomes larger.

Sensors: process analyzers

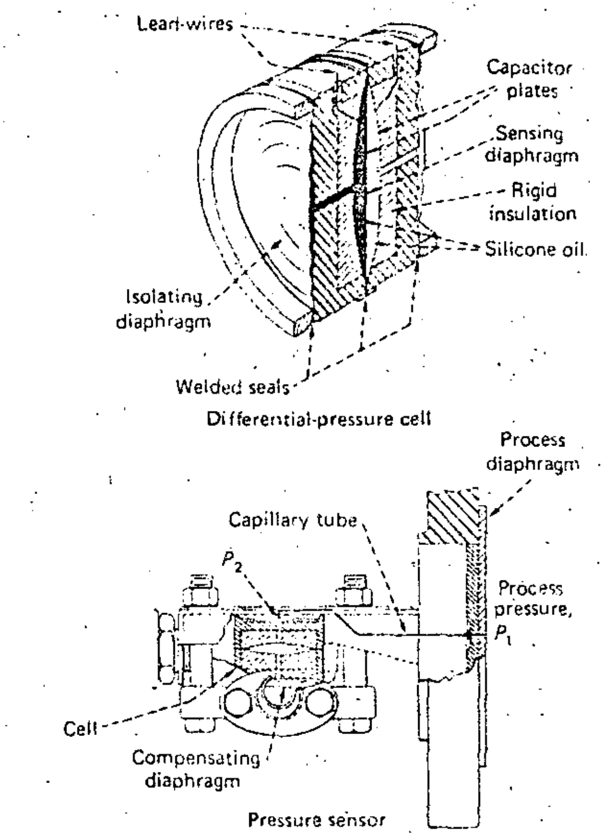
Process analyzers are devices that measure the composition of liquids and gases. Depending on the application, we can measure all of the components present in the process stream, or just one or two key components. A block diagram for a process gas chromatograph is shown in Fig. 7.

The major problem in applying the data from process analyzers is the delay in response time. Chromatographic and spectroscopic methods show similar problems when incorporated into a process control scheme.

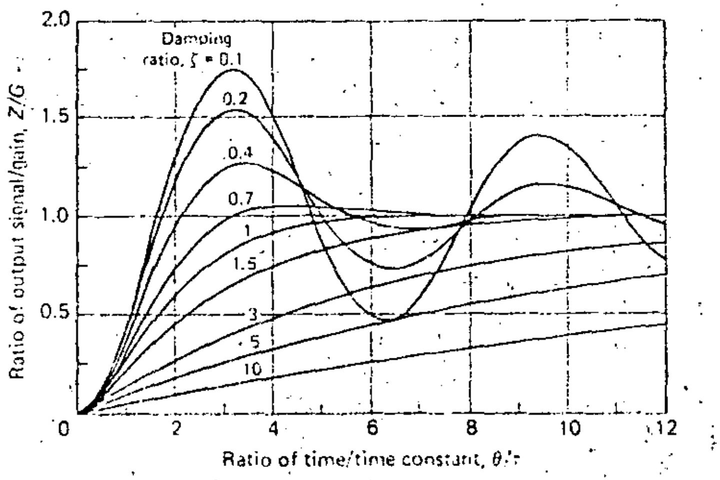
In gas chromatography, time delay occurs from several sources:

The first delay is the time for the sample to travel from the process stream to the chromatography column. This can be a major delay for analyzers that are located far from the sampling device.

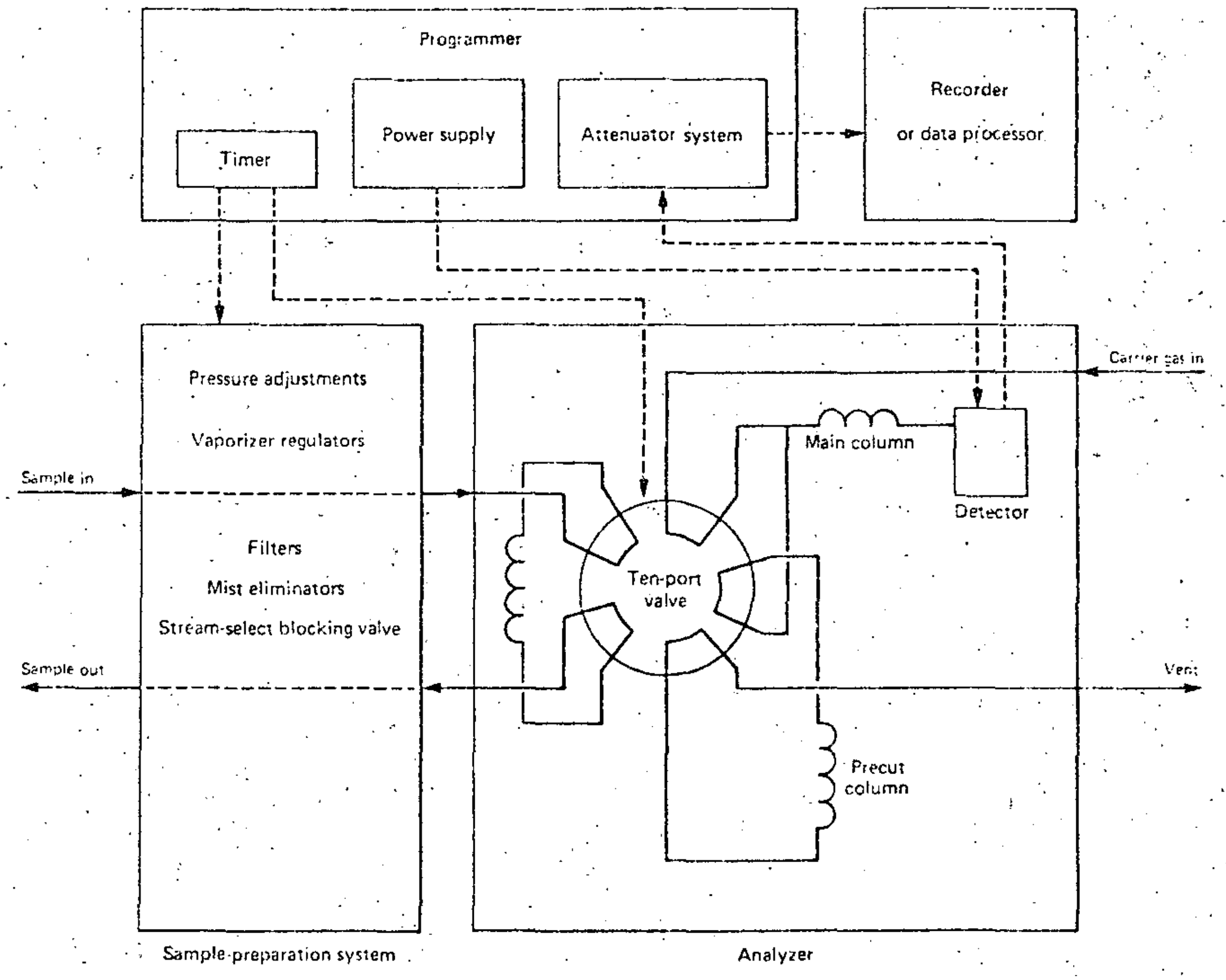
—The second delay is due to (a) the time required for travel through the column (i.e., to pass over the theoretical plates) and (b) the velocity of the carrier gas. Temperature programming can be used to reduce this time delay, and to hasten the exit of the less-volatile components from the system when detection of the more-volatile gases is also desired.



Pressure transmitter for liquid level Fig. 5



Response of a second-order system to a unit-step input Fig. 6



Sampling and recording systems are major components of process gas chromatographs **Fig. 7**

The third delay is due to the time required for detector response. Once the component of interest reaches the detector, a finite time is needed for the detector to sense the component and to relay the information through the electronics of the system to the recording device, readout, or integrating computer. This delay can be analyzed by developing an appropriate transfer function, as was done in the preceding sections.

All of these factors contribute to time delay. This means that the composition of the process stream at the sampling location, and the composition of the sample being analyzed by the instrument, can be different. These factors must be considered when analyzing the process dynamics.

Liquid chromatography, not as widely used, must include the same type of analysis as gas chromatography for a process-dynamics evaluation.

Similar time delays exist in spectroscopy but are not as severe as in chromatography.

Many spectroscopic analyzers read directly from the process by shining a beam of radiation (of an appropriate wavelength) through the process stream. This eliminates the delay from a separate sample loop. In most cases, the detector response is nearly instantaneous. A limiting factor in this procedure is the need to relay the signal from the detector to the recorder or readout device. However, the analyzer readings are still not instantaneous representations of stream composition, and time delay must be considered in our analysis.

Typical curves for process analyzers are shown in Fig. 8. These include the process composition as the input, and the response signal from the analyzers as the output.

Process controllers

On-off controllers—The simplest controller provides on-off control. The most familiar example of this type is the home thermostat. The thermostat is set to a desired temperature. When the temperature of the surroundings, as sensed by the thermostat, falls below a certain setpoint, the thermostat closes a circuit to start the heater. When the room reaches the desired temperature, the thermostat opens the circuit and the device shuts off the heater.

Proportional controller—A proportional controller receives data about a measured process variable, compares the data to the given setpoint, calculates the error (i.e., the difference between the setpoint and the measured value), and outputs a signal as a fixed multiple of the measured error. Such controllers are commonly described with a proportional-band variable, PB, or a controller-gain constant, K_c. The relationship between proportional band and controller gain is:

$$PB = 100/K_c \tag{8}$$

We can express the output, ϕ, of a proportional controller to an input signal, I, by:

$$\phi = K_c e + R = K_c(I - SP) + R \tag{9}$$

where ϕ = output signal, e = error, R = manual reset, SP = setpoint, and I = input signal.

The disadvantages of a proportional controller include offset. To correct this, a proportional-plus-reset (PI) controller is used.

Proportional-plus-reset controller—The relationship for a proportional-plus-reset controller is given by:

$$\phi = K_c e + \frac{K_c}{T_i}\int e\,d\theta \tag{10}$$

where T_i = reset time (another tuning constant).

The controller output, ϕ, consists of a response that is proportional to the error signal, and a second response that is due to controller action and is the integral of the error. Thus, the controller has both proportional plus integral control (or, proportional plus reset action, as it is usually called).

The reset action causes the controller output to change as long as an error exists. Even for small errors, the controller can cause the error in the process to disappear and can eliminate the offset error.

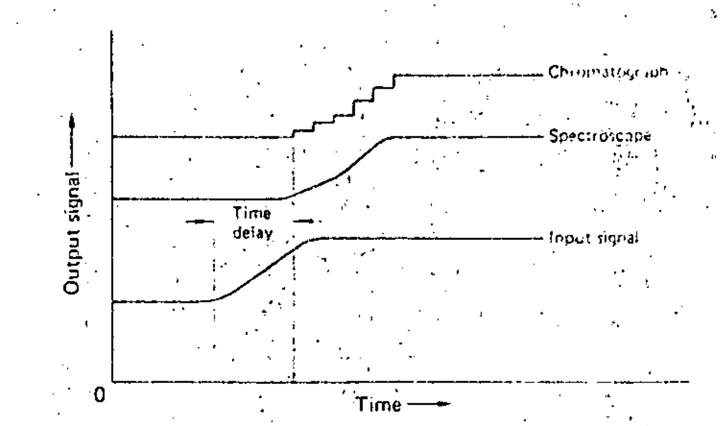
Reset time is sometimes referred to as minutes per repeat, which is the minutes needed to repeat the initial proportional-action change in the controller output. Another popular name for reset time is reset rate, which is the reciprocal of the reset time, and is given in repeats per minute.

Proportional-plus-reset-plus-rate control (PID)—In this controller, a third element has been added, which is termed the derivative control. Derivative control allows a higher proportional gain for higher-order systems. It will anticipate an error by measuring the rate of change of the error, and apply a control action that is proportional to the rate of change. Mathematically, this is:

$$\phi = K_c e + \frac{K_c}{T_i}\int e\,d\theta + K_c T_d\left(\frac{de}{d\theta}\right) \tag{11}$$

Fig. 9 shows a typical controller with the settings for proportional band, reset time, and derivative time.

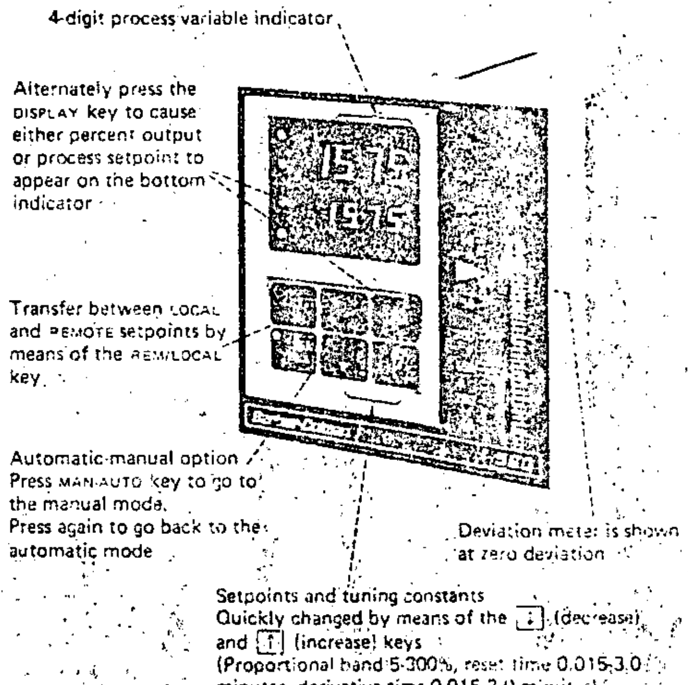
In all types of controllers, we are converting an input signal from a sensing element or measuring device to an output signal that will reposition a control valve or an electrical switch, or that will serve as the input to another controller in a cascaded-control loop. Hopefully, the manipulated variable will produce the desired result in the process so that we may control the process in the way that we intend. The controller itself is the device that receives information from the system, which shows how the system is behaving, and then decides what to do about this information. The controller could be called the central management system of the process control system.



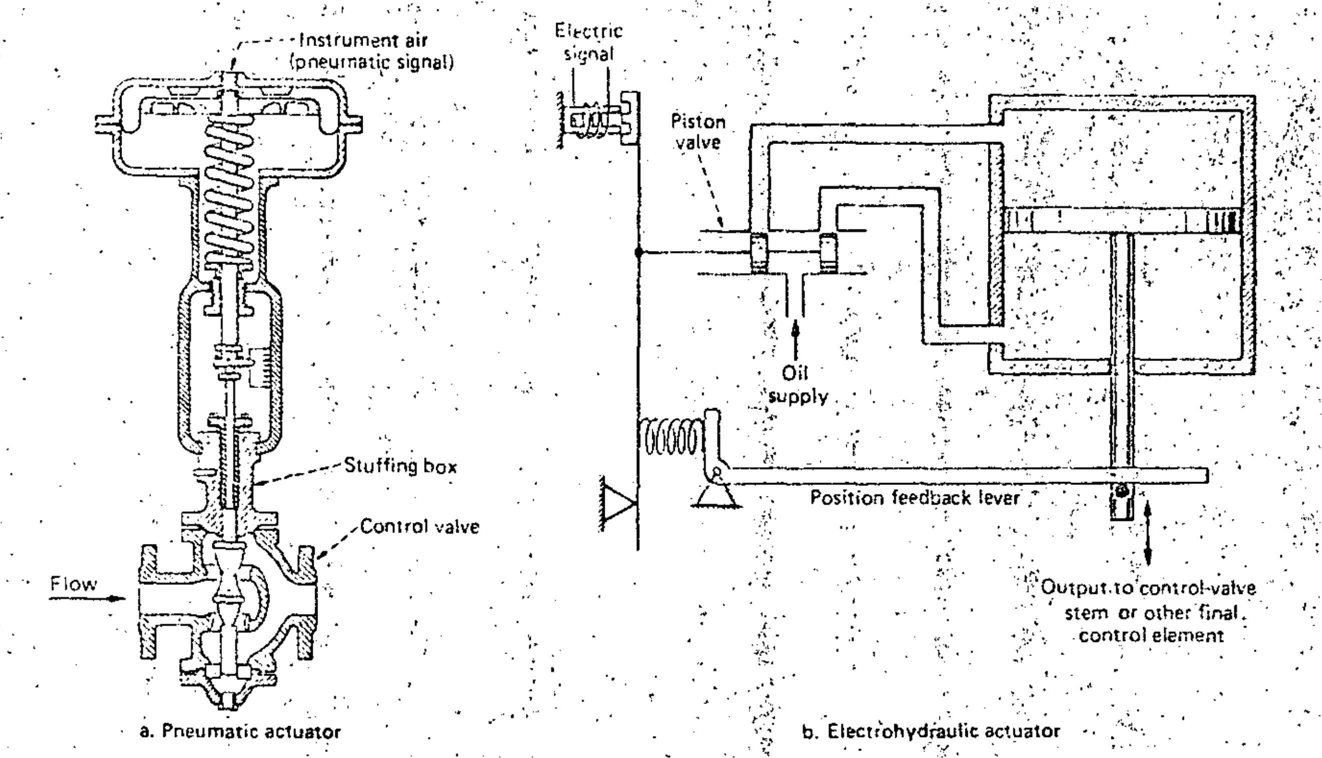
Representative responses of process analyzers Fig. 8

Final control elements

Usually, the final control element is a control valve that receives the output from a controller, and then ad-



Range of settings for process controllers Fig. 9



a. Pneumatic actuator

b. Electrohydraulic actuator

Some actuators for final control elements

Fig. 10

justs the valve position in order to set the flowrate through a pipeline. The resulting change in flowrate produces the desired effect in the process.

Other final control elements include relays to start or stop equipment, and variable-drive motors such as those used to control fan speeds on air-cooled heat exchangers. Fig. 10 shows some typical actuators.

For large valves having appreciable time delay, we can analyze the system, and calculate the time delay between the output signal from the controller and the valve response. Again, the analysis will be from a conservation-of-momentum balance or a force balance around the valve. The result is a second-order differential equation having the same form as Eq. (7).

The equations for flow through a final control valve are [3]:

$$F = AC_v\sqrt{P_1 - P_2} \tag{12}$$

$$F = AC_v\sqrt{(P_1^2 - P_2^2)/2} \tag{13}$$

$$F = 0.601AC_vP_1 \tag{14}$$

where A = fractional opening of valve, C_v = valve capacity, F = flow, P_1 = upstream pressure, and P_2 = downstream pressure. Eq. (12) is for flow of liquids, Eq. (13) for gases in subcritical flow, and Eq. (14) for gases in critical flow.

Sizing of the control valve is primarily concerned with calculating valve capacity, C_v. Though the C_v method is accepted by all valve manufacturers, the equations that are used vary from one manufacturer to another. Therefore, the equations for liquids and gases may vary slightly, and the manufacturer of a particular valve should be consulted when calculating flow.

For gases where the upstream pressure is more than about half the downstream pressure, the gases are considered to be in critical flow (sometimes called sonic flow). Here, the flow is not a function of the downstream pressure.

Applications of the control equations

Let us now return to the hot-water heater of Fig. 1. We will show how the preceding equations can be organized into some systematic form for problem solving.

We will assume that the process has been operating at a steady-state condition. Therefore, all initial conditions (flow, temperature, tank level, stream pressures, etc.) are known. At time θ equal to zero, a change (upset) is imposed on the system. The upset conditions could be a change in flow and/or temperature in the liquid input stream, F_i, a change in temperature in stream S_i, or a change of setpoint in tank-level height or tank temperature. We will derive multiple differential equations, and leave their solutions for a future article.

We can start by deriving the equations to describe the process via material and energy balances:

$$F_i + \boxed{S_i} - \boxed{F_o} = \rho A_T\left(\frac{d\boxed{H}}{d\theta}\right) \tag{15}$$

$$F_iC_pt_i + S_iC_pt_{si} - F_oC_p\boxed{t_o} = \rho A_TH\frac{dt_o}{d\theta} + \rho A_Tt_o\left(\frac{dH}{d\theta}\right) \tag{16}$$

where A_T = tank area, C_p = heat capacity of water (assumed constant), and ρ = density of water (assumed constant).

The unknowns or variables are enclosed in a box the first time they appear in the equations. We must ascertain that we have as many equations as variables—an elementary but important point. For each first-order differential, we must have one initial condition. In this example, the initial conditions are the steady-state tank temperature, t_o, and the tank's liquid-level height, H.

Next, let us look at the temperature-control loop. The temperature-sensing element will be given by Eq. (1). The output from the sensing element, ϕ_t, is related to the temperature input, t_o, by:

$$\tau_t \frac{d\boxed{\phi_{t1}}}{d\theta} = t_o - \phi_{t1} \qquad (17)$$

The initial condition for Eq. (17) is that the output, ϕ_{t1}, equals the tank temperature, t_o. We can convert tank temperature to the actual values of the electrical units (for electronic instruments). We would then convert instrument settings in the controllers to that set of units. Because the conversion is linear, there is no particular advantage in doing this, and the controller and valve responses will be the same. The conversion would add another equation that would only add to the organization and bookkeeping problems. Therefore, we will not apply the conversion because it is actually done in the field equipment.

The output, ϕ_{t1}, from the temperature-sensing device is the input to the temperature controller. We have specified a PID controller whose output, ϕ_{t2}, is given by Eq. (11), and expanded into:

$$\boxed{\phi_{t2}} = K_{ct}(\phi_{t1} - SP_t) + \frac{K_{ct}}{T_{it}}\int (\phi_{t1} - SP_t)d\theta + K_{ct}T_{dt}\frac{d(\phi_{t1} - SP_t)}{d\theta} \qquad (18)$$

If we neglect the control-valve dynamics, we can calculate flowrate S_i from Eq. (12). The output from the controller, ϕ_{t2}, is the fractional opening, A_t, of the valve in Eq. (12). Hence, S_i becomes:

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$$\overset{0-1}{} \quad S_i = A_tC_{vt}\sqrt{P_{1t} - \boxed{P_{2t}}} \qquad (19)$$

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If we wanted to simulate the valve dynamics, we would have a second-order differential equation relating the variables A and ϕ_{t2}. The downstream pressure, P_{2t}, can be calculated from:

$$P_{2t} = g(H) = \rho g h \qquad (20)$$

Eq. (20) shows that the downstream pressure is a function of the tank's liquid-level height.

We now have enough information to calculate the initial condition for the controller output, ϕ_{t2}, because we know the initial flow, S_i. We have *six* equations but *seven* unknown variables. Therefore, we must derive equations in the second control loop.

First, let us look at the cascade control loop in Fig. 1. In many instances, cascade control can be more effective than a simple control-loop system. Without cascade control, the control valve in the outlet line would open (or close) based only on the level of liquid in the tank. If the downstream pressure from the control valve were fairly constant, we could achieve reasonable control of the tank level, H.

For larger variations in the downstream pressure, we might be forced to use the cascade control system to control level in the tank. The flow controller will correct for the variations in the downstream pressure before these can upset the tank level because the flow-control loop measures and corrects the disturbance faster than do the level-sensing element and controller alone.

Cascade control can also anticipate and correct a disturbance in a secondary loop before the upset can disturb the process—for example, in a steam-heated heat exchanger.

The sensing elements for the level and flow controllers have second-order transfer functions, which are:

$$\tau_l^2\left(\frac{d^2\boxed{\phi_{l1}}}{d\theta^2}\right) + 2\zeta_l\tau_l\left(\frac{d\phi_{l1}}{d\theta}\right) + \phi_{l1} = G_lH \qquad (21)$$

$$\tau_F^2\left(\frac{d^2\boxed{\phi_{F1}}}{d\theta^2}\right) + 2\zeta_F\tau_F\left(\frac{d\phi_{F1}}{d\theta}\right) + \phi_{F1} = G_FF_o \qquad (22)$$

Initial conditions for Eq. (21) and (22) are, respectively:

$$\phi_{l1} = H, \ \phi_{F1} = F_o$$

$$\frac{d\phi_{l1}}{d\theta} = \frac{d\phi_{F1}}{d\theta} = 0$$

The output from the proportional level controller is given by:

$$\boxed{\phi_{l2}} = K_{cl}(\phi_{l1} - SP_l) + R \qquad (23)$$

This output becomes the setpoint for the PI (proportional plus integral) flow controller. Output from the flow controller is given by:

$$\boxed{\phi_{F2}} = K_{cF}(\phi_{F1} - \phi_{l2}) + \frac{K_{cF}}{T_{iF}}\int (\phi_{F1} - \phi_{l2})d\theta \qquad (24)$$

We will again neglect the valve dynamics for the flow-control valve. Therefore, the output from the flow controller is the fractional opening, A_F, of the valve, which defines the flowrate, F_o. This relationship is:

$$F_o = \overset{0-1}{A_F}C_{vF}\sqrt{\boxed{P_{1F}} - P_{2F}} \qquad (25)$$

The upstream pressure on the valve will be a function of tank-level height, H, flowrate, F_o, and orifice coefficient, C:

$$P_{1F} = g(H, F_o, C) \rightarrow P = \text{presion de fondo} \qquad (26)$$

We now have *twelve* equations and *twelve* unknowns.

The next article in this CE REFRESHER series will appear in the issue of Nov. 16, and will cover various techniques for solving systems of differential equations.

Steven Danatos, Editor

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Solving the mathematical models for dynamic systems

Separation of variables, integrating factors, variation of variables, and Laplace transforms are techniques for solving the differential equations representing processes and controls.

*John L. Guy Dynamod Enterprises**

☐ A variety of methods are available for solving the differential equations that we obtained when formulating mathematical models for chemical process facilities. These equations were derived by applying chemical engineering fundamentals to processes in Parts 1 and 2 of this series.† Unfortunately, one method does not work best for all problems and conditions.

Basic concepts

Let us review some basic terminology before we begin our study of solving the mathematical expressions.

An ordinary differential equation, ODE, is an expression involving one or more derivatives of an unspecified function (say, the dependent variable Y) with respect to the independent variable (say, time θ). The relationship can contain the terms: Y, constants, and functions of θ. The ODE is of order n if the highest derivative of Y in the equation is the n-th derivative of Y with respect to θ.

An ODE of order n is linear if it can be written as:

$$\frac{d^nY}{d\theta^n} + f_{n-1}(\theta)\frac{d^{n-1}Y}{d\theta^{n-1}} + \cdots + f_1(\theta)\frac{dY}{d\theta} + f_0(\theta)Y = X(\theta) \quad (1)$$

An analytical solution of an ODE for some interval (say, $0 < \theta < \infty$) is a function, $Y(\theta)$, if it is defined and can be differentiated for all values of θ in that interval. The equation reduces to an equality when Y and all derivatives of Y are replaced in the original differential equation.

A general solution for Eq. (1) contains n arbitrary constants. To be independent, the solution cannot be reduced to a form containing less than n such constants. To solve for a particular solution, we must set or solve for the n arbitrary constants (i.e., we must solve the equation n times by substituting n initial values or boundary conditions of the problem into the general solution equation).

A partial differential equation is an expression involving one or more partial derivatives of an unspecified function of each of the two, or more, independent variables.

Let us now proceed to some of the classical mathematical techniques for solving differential equations.

Separation of variables

We have already used the technique of separation of variables for solving the Rayleigh distillation equation (see Part 1), which is:

$$\frac{dX}{d\theta} = \frac{V(KX - X)}{L_0 - V\theta} \quad (2)$$

where K, the equilibrium constant, is a function of X only; L_0 is the initial liquid feed to the system; V, the vapor rate, is a function of time; X is the dependent variable; and θ is time, the independent variable.

We separate the variables X and θ to obtain:

$$\frac{dX}{X(K-1)} = \frac{-V d\theta}{L_0 - V\theta} \quad (3)$$

After the relationship between K and X and between V and θ are defined, we integrate Eq. (2) directly. The initial mole fraction of liquid, X_0, must be calculated independently or stated. For example, if K and V are both constant, the solution of Eq. (3) is:

$$\frac{\ln(X)}{K-1} = \ln(L_0 - V\theta) + I \quad (4)$$

where I is the integration constant. Substituting $X = X_0$ at $\theta = 0$, we solve for I. The final result is:

$$\frac{1}{K-1}\ln\left(\frac{X}{X_0}\right) = \ln\left(\frac{L_0 - V\theta}{L_0}\right) \quad (5)$$

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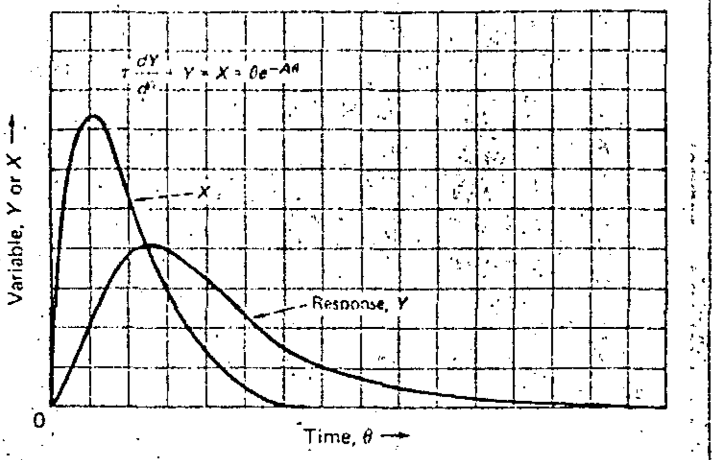
*To meet the author, see *Chem. Eng.*, June 29, p. 80.

†Articles published thus far in this CE REFRESHER: Part 1, June 29, p. 71; Part 2, Aug. 24, p. 111



System response modeled by a first-order equation Fig. 1

Integrating factor

If the variable X is a function of time θ, $X(\theta)$, the equation for the general first-order system can be written as:

$$\tau \frac{dY}{d\theta} + Y = X(\theta) \qquad (6)$$

where X, the forcing function, is a function of θ; Y is the dependent variable; τ is the system time constant; and θ is time, the independent variable.

For this system, we cannot separate the variables directly. However, Eq. (6) represents an equation that we can solve by using an integrating factor. The general form for such equations is:

$$\frac{dY}{d\theta} + f(\theta)Y = X(\theta) \qquad (7)$$

The solution for Eq. (7) is given by:

$$Y(\theta) = e^{+h}\left[\int e^{+h} X(\theta)d\theta + I\right] \qquad (8)$$

$$h = f(\theta)d\theta$$

For example, we can solve Eq. (6) for $X(\theta) = \theta e^{-A\theta}$ by means of Eq. (8) to obtain the general solution, as shown in the following steps:

$$h = \int\left(\frac{1}{\tau}\right) d\theta = \theta/\tau \qquad (9)$$

$$Y(\theta) = e^{-\theta/\tau}\left[\int e^{+\theta/\tau}\theta e^{-A\theta}\, d\theta + I\right] \qquad (10)$$

$$Y(\theta) = e^{-\theta/\tau}\left[\frac{1}{\tau}\int \theta e^{(1/\tau - A)\theta}\, d\theta + I\right]$$

$$Y(\theta) = e^{-\theta/\tau}\left\{\frac{\left(\frac{1}{\tau}\right)e^{(1/\tau - A)\theta}}{\left(\frac{1}{\tau} - A\right)^2}\left[\left(\frac{1}{\tau} - A\right) - 1\right] + I\right\}$$

The initial condition from the steady-state solution of Eq. (6) is $Y(0) = X(0) = 0$. Hence, we can solve for $I = 1/\{\tau[(1/\tau) - A]^2\}$. Therefore, the complete solution to Eq. (6) reduces to:

$$Y(\theta) = \frac{1}{\tau[(1/\tau) - A]^2} \times \left[\frac{\theta}{\tau}e^{-A\theta} - A\theta e^{-A\theta} - e^{-A\theta} + e^{-\theta/\tau}\right] \qquad (11)$$

The response of Y to the upset condition of $X(\theta) = \theta e^{-A\theta}$ is shown in Fig. 1.

Second-order equations

A second-order transfer function was developed in Part 2 (*Chem. Eng.*, Aug. 24, p. 117). This function can be represented as:

$$\tau^2\frac{d^2Y}{d\theta^2} + 2\zeta\tau\frac{dY}{d\theta} + Y = GX \qquad (12)$$

where G is the system gain; X, the forcing function, is a function of θ; Y is the dependent variable; τ is the system time constant; ζ is the damping ratio; and θ is time, the independent variable.

We solve Eq. (12) by (a) equating the left-hand side of the equation to zero to obtain the complementary solution, sometimes called the homogeneous solution, and (b) finding the particular solution by one of many methods. We will discuss only two of these methods here. For a complete discussion, including the theory, refer to textbooks [*1,2*]. The total solution is the sum of the complementary and particular solutions.

The complementary solution to Eq. (12) is:

$$\tau^2\frac{d^2Y}{d\theta^2} + 2\zeta\tau\frac{dY}{d\theta} + Y = 0 \qquad (13)$$

We solve Eq. (13) by assuming a solution, performing the indicated differentiation, and substituting into the original equation. For equations having constant coefficients, we assume an exponential function. We can set up an auxiliary equation by substituting $s^n = d^nY/d\theta^n$. For Eq. (13), we obtain:

$$\tau^2s^2 + 2\zeta\tau s + 1 = 0 \qquad (14)$$

Solving Eq. (14) as a quadratic yields:

$$s_{1,2} = -\frac{\zeta}{\tau} \pm \sqrt{\frac{\zeta^2 - 1}{\tau}}$$

where s_1 and s_2 are the solutions of Eq. (14).

Depending on the relative values of ζ and τ, we obtain an equation in one of the following forms:

1. For unequal, real roots of the auxiliary equation ($\zeta > 1$), the solution to Eq. (13) is:

$$Y = I_1e^{s_1\theta} + I_2e^{s_2\theta} \qquad (16)$$

where I_1 and I_2 are constants of integration.

2. For equal roots of the auxiliary equation ($\zeta = 1$), the solution to Eq. (13) is:

$$Y = (I_1 + I_2\theta)e^{s\theta} \qquad (17)$$

3. For imaginary roots of the auxiliary equation ($\zeta < 1$), the solution to Eq. (13) is:

$$Y = e^{-\zeta\theta/\tau}\left[I_1 \cos\frac{\sqrt{\zeta^2 - 1}}{\tau} + I_2 \sin\frac{\sqrt{\zeta^2 - 1}}{\tau}\right] \qquad (18)$$

The particular solution to Eq. (12) by the method of undetermined coefficients can only be applied to linear

Normal form of particular integrals for second-order differential equations — Table I

$$P\frac{d^2Y}{dX^2} + Q\frac{dY}{dX} + RY = \phi(X)$$

Right-hand side of differential equation, $\phi(X)$	Particular integral	Coefficient values
A constant, C	A constant, K	$K = \frac{C}{R}$
A polynomial, $a_0 + a_1x + \ldots + a_nx^n$	A polynomial, $\alpha_0 + \alpha_1x + \ldots + \alpha_nx^n$	Calculated by substituting in the differential equation and equating coefficients
An exponential, Te^{rx}	An exponential, αe^{rx}	$\alpha = \frac{T}{Pr^2 + Qr + R}$
Trigonometric, $G\sin nx + H\cos nx$	Trigonometric, $L\sin nx + M\cos nx$	$L = \frac{(R - n^2P)G + nQH}{(R - n^2P)^2 + n^2Q^2}$ $M = \frac{(R - n^2P)H - nQG}{(R - n^2P)^2 + n^2Q^2}$

equations having constant coefficients, and only certain forms of the function GX. The procedure follows:

- Assume a form of the particular solution.
- Perform the indicated differentiations, and insert these answers into the original equation.
- Solve the resulting equation for the assumed unknowns, providing that the correct form of the particular solution has been selected.

For example, if $GX = Ge^{\tau_1\theta}$, we can assume a particular solution of:

$$Y_p = \alpha e^{\tau_1\theta} \tag{19}$$

After the appropriate differentiation and substitution into Eq. (12), we solve for α:

$$\alpha = \frac{G}{(\tau^2\tau_1^2 + 2\zeta\tau\tau_1 + 1)} \tag{20}$$

The particular solution for a second-order equation for some forms of GX is shown in Table I [1].

Variation of parameters

Other methods for obtaining the particular solutions are not restricted to linear equations having constant coefficients. However, we have to integrate two expressions to get the solutions.

For example, the method of variation-of-parameters involves replacing the two constants of integration, I_1 and I_2, in the complementary solution with two unknown functions of θ. Before proceeding, we must convert Eq. (12) to the equivalent form:

$$\frac{d^2Y}{d\theta^2} + 2\frac{\zeta}{\tau}\frac{dY}{d\theta} + \frac{1}{\tau^2}Y = \frac{GX}{\tau^2} = R(\theta) \tag{21}$$

where R is a function of θ.

If Y_1 and Y_2 are the two complementary solutions, we can derive the following formulas for the particular solution:

$$Y_p(\theta) = -Y_1\int\frac{Y_2R}{W}d\theta + Y_2\int\frac{Y_1R}{W}d\theta \tag{22}$$

where:

$$W = Y_1\frac{dY_2}{d\theta} - Y_2\frac{dY_1}{d\theta} \tag{23}$$

For the complementary solution via Eq. (16) and the previous value of GX, we proceed with the following steps:

$$Y_1 = e^{s_1\theta} \tag{24}$$

$$Y_2 = e^{s_2\theta} \tag{25}$$

$$dY_1/d\theta = s_1e^{s_1\theta} \tag{26}$$

$$dY_2/d\theta = s_2e^{s_2\theta} \tag{27}$$

$$W = s_2e^{(s_1+s_2)\theta} - s_1e^{(s_1+s_2)\theta} \tag{28}$$

$$\left.\begin{aligned} W &= (s_2 - s_1)e^{(s_1+s_2)\theta} \\ R(\theta) &= Ge^{\tau_1\theta}/\tau^2 \end{aligned}\right\} \tag{29}$$

$$Y_p = -e^{s_1\theta}\int\frac{e^{s_2\theta}Ge^{\tau_1\theta}/\tau^2}{W}d\theta + e^{s_2\theta}\int\frac{e^{s_1\theta}Ge^{\tau_1\theta}/\tau^2}{W}d\theta \tag{30}$$

Eq. (30) reduces to Eq. (19) after performing the indicated calculations.

These methods for obtaining the particular solutions can also be applied to linear equations having variable coefficients. However, the complementary solution will usually involve a series solution. For details, consult appropriate textbooks [1,2].

We can obtain analytic solutions for certain types of second-order nonlinear equations. These are (a) equa-

Laplace transforms of common functions **Table II**

No.	Function of time, $f(\theta)$	Laplace transform, $f(s)$
1.	1	$1/s$
2.	θ	$1/s^2$
3.	$\theta^{n-1}/(n-1)!$	$1/s^n$; $(n = 1, 2, \ldots)$
4.	$e^{-a\theta}$	$1/(s+a)$
5.	$\theta e^{-a\theta}$	$1/(s+a)^2$
6.	$(e^{a\theta} - e^{b\theta})/(a-b)$	$1/(s-a)(s-b)$
7.	$\sin(a\theta)/a$	$1/(s^2+a^2)$
8.	$\cos(a\theta)$	$s/(s^2+a^2)$
9.	$\begin{Bmatrix}(0<\theta<k), f=0\\ (\theta>k), f=1\end{Bmatrix}$	e^{-ks}/s
10.	$\begin{Bmatrix}(0<\theta<k), f=0\\ (\theta>k), f=\theta-k\end{Bmatrix}$	e^{-ks}/s^2
11.	$\begin{Bmatrix}(0<\theta<k), f=0\\ (\theta>k), f=e^{-a(\theta-k)}\end{Bmatrix}$	$e^{-ks}/(s+a)$
12.	$e^{a\theta}\sin(b\theta)/b$	$1/[(s-a)^2+b^2]$
13.	$e^{a\theta}\cos(b\theta)$	$(s-a)/[(s-a)^2+b^2]$

tions where the independent or dependent variable does not occur explicitly; (b) equations that are homogeneous. Again, consult the appropriate textbooks [*1-3*].

Laplace transforms

The Laplace transformation converts an ordinary differential equation, with time as the independent variable, to an equivalent equation that can be solved by purely algebraic methods. The answer to the algebraic equation is the complete solution of the problem, because the initial conditions are included in the process of solving the differential equation.

The procedure is to convert a function of time θ to a function of the Laplace transform variable s in accordance with:

$$\mathfrak{L}[f(\theta)] = \int_0^\infty e^{-s\theta} f(\theta)d\theta \tag{31}$$

Applying Eq. (31) to the first and second derivatives of $f(\theta)$, we obtain:

$$\mathfrak{L}\left[\frac{df(\theta)}{d\theta}\right] = sf(s) - f(0) \tag{32}$$

$$\mathfrak{L}\left[\frac{d^2f(\theta)}{d\theta^2}\right] = s^2f(s) - sf(0) - f'(0) \tag{33}$$

where $f(0)$ and $f'(0)$ are the values of the function and its derivative when θ equals zero. Therefore, we must have initial conditions to be able to use this method directly.

We have now converted a linear ordinary differential equation with the independent variable θ to an algebraic equation with the independent variable s. (Laplace transforms can only be applied to linear or linearized functions.) Table II gives Laplace transforms of some common functions encountered in process and control-system dynamics.

Mathematical manipulations will be reduced if we can set all initial values and their derivatives to zero. Starting from an initial steady-state condition assures us that the derivatives with respect to time are all initially zero. If the dependent variable [such as Y in Eq. (12)] is a difference between the variable as a function of time and the initial (or steady-state) value of that variable, then the initial function value will also be zero.

Let us now solve Eq. (12) with Laplace transforms. Eq. (34) represents Eq. (12) with the function of X previously assumed. We will assume that we have converted Y to a difference between the variable and the initial value, and that we are initially at a steady-state condition.

$$\tau^2\frac{d^2Y}{d\theta^2} + 2\zeta\tau\frac{dY}{d\theta} + Y = Ge^{\tau_1\theta} \tag{34}$$

Converting Eq. (34) to the Laplace domain by transforming each term in the equation, we obtain:

$$\tau^2s^2Y(s) + 2\zeta\tau sY(s) + Y(s) = \frac{G}{(s-\tau_1)} \tag{35}$$

Rearranging and simplifying Eq. (35) yields:

$$Y(s) = \frac{G}{(s-\tau_1)(\tau^2s^2 + 2\zeta\tau s + 1)} \tag{36}$$

$$Y(s) = \frac{G}{(s-\tau_1)(s-s_1)(s-s_2)}$$

where s_1 and s_2 are defined by Eq. (15). After expansion by partial fractions, we obtain:

$$Y(s) = \frac{A}{(s-\tau_1)} + \frac{B}{(s-s_1)} + \frac{C}{(s-s_2)} \tag{37}$$

where:

$$A = \frac{G}{(\tau_1-s_1)(\tau_1-s_2)}\Bigg|_{s=\tau_1}$$

$$B = \frac{G}{(s_1-\tau_1)(s_1-s_2)}$$

$$C = \frac{G}{(s_2-\tau_1)(s_2-s_1)}$$

We calculate the constants A, B and C via expansion by partial fractions. Assume that we can determine functions for A, B and C by expanding the right-hand side of Eq. (36), so that:

$$\frac{G}{(s-\tau_1)(s-s_1)(s-s_2)} = \frac{A}{(s-\tau_1)} + \frac{B}{(s-s_1)} + \frac{C}{(s-s_2)} \tag{38}$$

To find the function A, we multiply each term in Eq. (38) by $(s-\tau_1)$ to obtain:

$$\frac{G}{(s-s_1)(s-s_2)} = A + \frac{B(s-\tau_1)}{(s-s_1)} + \frac{C(s-\tau_1)}{(s-s_2)} \tag{39}$$

By setting $s = \tau_1$, we obtain the value for A. The values for B and C are found in the same manner.

Let us remember that s_1 and s_2 can involve imaginary numbers. However, we can convert functions containing imaginary numbers to their equivalent trigonometfunctions. We can now transform Eq. (37) to a function of θ for the solution:

$$Y(\theta) = Ae^{r_1\theta} + Be^{s_1\theta} + Ce^{s_2\theta} \qquad (40)$$

Applications to automatic control

The design of the automatic control system for a process plant requires formulating the differential equations to describe various systems. We do not always require a complete transient solution to design or to troubleshoot control systems.

For example, if we can describe a control system by a second-order equation such as:

$$A\frac{d^2Y}{d\theta^2} + B\frac{dY}{d\theta} + CY = X(\theta) \qquad (41)$$

where arbitrary constants A, B and C have replaced the coefficients τ, ζ and 2 in Eq. (12), we can transform Eq. (4) to the Laplace domain:

$$Y(s) = \frac{X(s)}{(As^2 + Bs + C)} + \frac{(As + B)X(0) + AX'(0)}{(As^2 + Bs + C)} \qquad (42)$$

The two terms on the right-hand side of Eq. (42) represent two transforms that have some relationship to the control system and to the initial disturbance or forcing function. Therefore, the study of only the first transform (for the control system) may prove to be adequate in many applications.

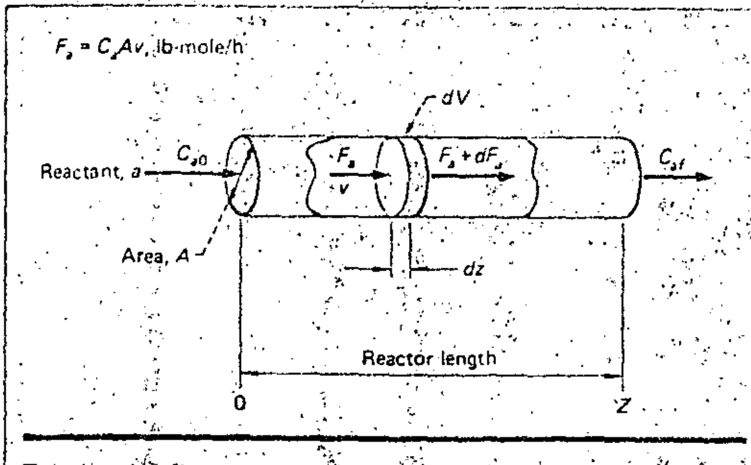
Methods exist for determining the stability of the control system and understanding its response from the transform of the characteristic equation (i.e., the denominator: $As^2 + Bs + C$). Such methods are the root-locus, the Routh test, and the Nyquist diagram.

Also useful in control theory is the frequency-response transform. Substituting $j\omega$ (j is the symbol for the imaginary unit, and ω is the frequency) for s, we obtain an equation in the frequency domain. Such equations again lead to useful methods in the design and analysis of control systems, and provide a procedure for synthesizing the overall differential equation for a control system. These concepts lead to Bode diagrams, polar plots, Nyquist plots, and more-advanced methods of system analysis.

Partial differential equations

Perhaps the most useful application of Laplace transforms involves the solving of partial differential equations. Because we can transform an ordinary differential equation into an algebraic one by using transforms, it follows that we can reduce a partial differential equation with two variables into an ordinary differential equation by using transforms. We must remember that the variable transformed to reduce the equation must have an "open" range because we integrate the Laplace variable to infinity.

In dynamic analysis, time is always one variable. Hence, the transformation can always be applied to the time variable. This procedure will standardize our calculations so that we do not have to spend time analyzing for the type of equation, and can proceed to the solution immediately.



Tubular plug-flow reactor **Fig. 2**

Example illustrates procedures

Let us consider the tubular reactor shown in Fig. 2 where Reactant a is converted to Product b via a first-order kinetic reaction, given by:

$$r = \frac{dC_a}{d\theta} = -kC_a \qquad (43)$$

where C_a is the concentration of Reactant a, lb-mole/ft^3; k is the kinetic rate constant, 1/h; r is rate of reaction, lb-mole/(h)(ft^3); and θ is time, h.

If the conversion of Reactant a is low, or if there is a diluent to absorb and remove heat of reaction so that we can neglect the temperature changes, we can solve the problem without too much trouble.

Neglecting mass diffusion, we can apply a material balance in the differential section of the reactor:

$$\text{Input: } C_aAv$$

$$\text{Reaction: } r_a dV = -kC_a dV = -kC_aAdZ$$

$$\text{Output: } C_aAv + \frac{\partial}{\partial Z}(C_aAvdZ)$$

$$\text{Accumulation: } \frac{\partial(C_aAdZ)}{\partial\theta}$$

where A is cross-section area of reactor, ft^2; v is flow velocity, ft/h; V is reactor volume, ft^3; and Z is reactor length, ft.

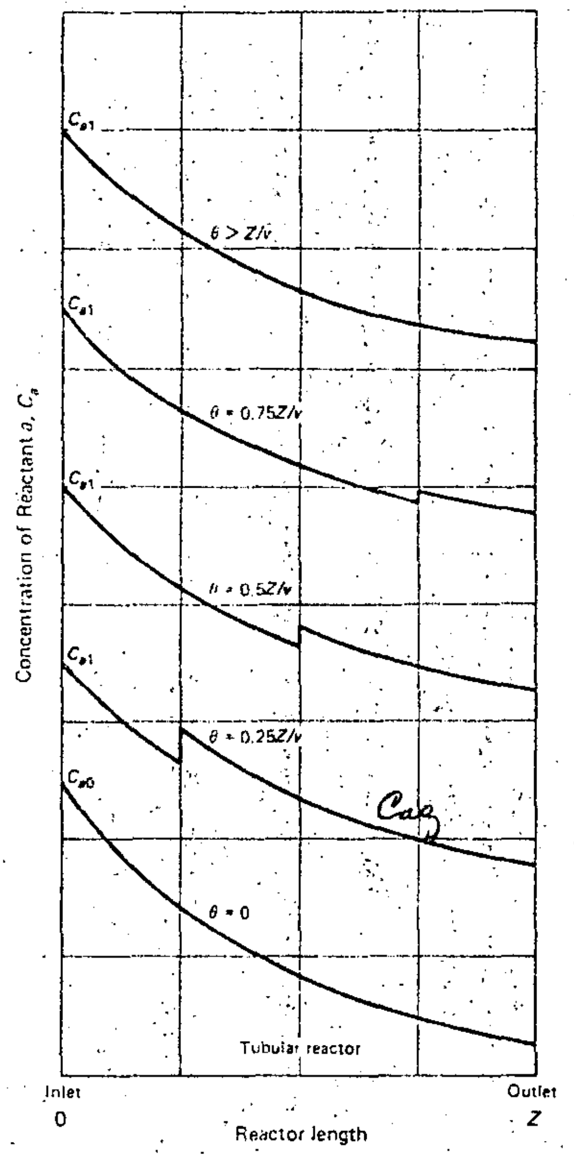
Therefore, the partial differential equation for the material balance is:

$$\frac{\partial(vC_a)}{\partial Z} + \frac{\partial C_a}{\partial\theta} + kC_a = 0 \qquad (44)$$

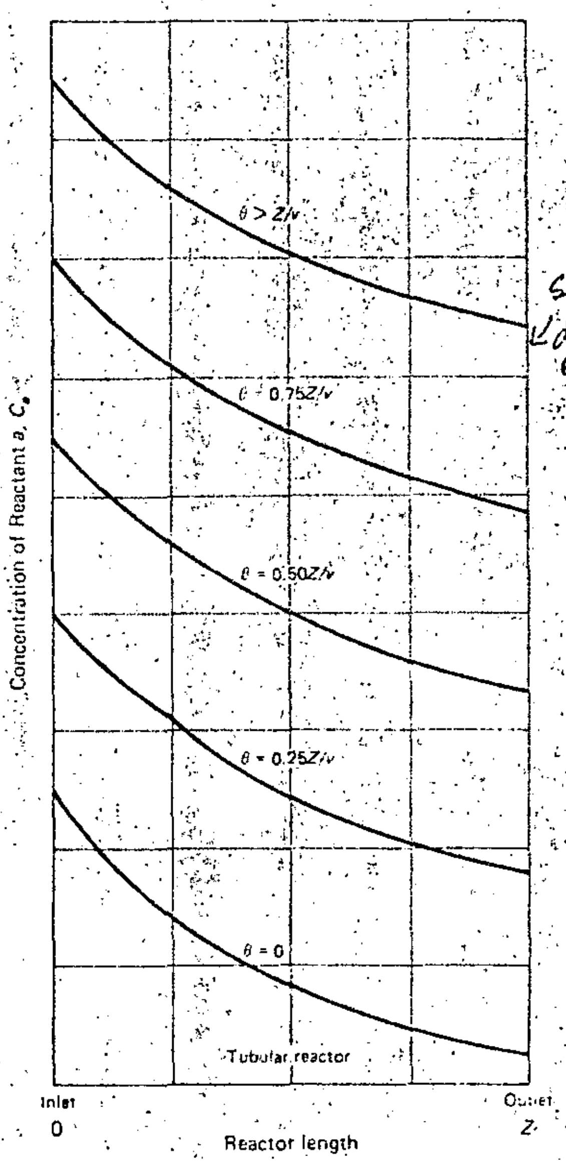
Step change in inlet concentration

If the reactor is initially operating in a steady-state condition, and the inlet concentration changes stepwise from C_{a0} to C_{a1} at some time $\theta = 0$, we can rewrite Eq. (44) as:

$$v\frac{\partial C_a(\theta,Z)}{\partial Z} + \frac{\partial C_a(\theta,Z)}{\partial\theta} + kC_a(\theta,Z) = 0 \qquad (45)$$



Response to step change in inlet concentration Fig. 3



Response to step change in flowrate. Fig. 4

Se produce muy de menor calidad

A bookkeeping problem can arise in applying initial conditions in these types of problems unless we keep track of which independent variables the dependent variable is expressed in [in Eq. (45), C_a is a function of θ and Z].

Solving for the initial conditions, we note that the derivative with respect to time will be zero. Therefore, we will solve:

$$v\frac{dC_a(0,Z)}{dZ} = -kC_a \quad (46)$$

Separating variables [as previously demonstrated by Eq. (2) and (3) for the Rayleigh distillation example] and integrating will yield:

$$\ln C_a(0,Z) = -\frac{kZ}{v} + I \quad (47)$$

The initial conditions are $Z = 0$, $C_a = C_{a0}$. After rearranging, we get:

$$C_a(0,Z) = C_{a0}e^{-(k/v)Z} \quad (48)$$

We will now proceed with the dynamic solution of Eq. (45). Because θ and Z are both independent variables, we find the transform of the first term as:

$$\mathfrak{L}\left[v\frac{C_a(\theta,Z)}{Z}\right] = v\frac{dC_a(s,Z)}{dZ} \quad (49)$$

From Eq. (32), we find that the transform of the second term is:

$$\mathfrak{L}\left[\frac{\partial Ca(\theta,Z)}{\partial\theta}\right] = sC_a(s,Z) - C_a(0,Z)$$

$$\mathfrak{L}\left[\frac{\partial C_a(\theta,Z)}{\partial\theta}\right] = sC_a(s,Z) - C_{a0}e^{-(k/v)Z} \quad (50)$$

The complete transform of Eq. (45) is now written as:

$$v\frac{dC_a(s,Z)}{dZ} + sC_a(s,Z) - C_{a0}e^{-(k/v)Z} + kC_a(s,Z) = 0 \quad (51)$$

Rearranging Eq. (51), we obtain:

$$\frac{dC_a(s,Z)}{dZ} + \frac{(s+k)}{v}C_a(s,Z) = \frac{C_{a0}}{v}e^{-(k/v)Z} \quad (52)$$

We have now reduced Eq. (45) to a first-order equation that can be solved by using an integrating factor. Before applying Eq. (8), we must first calculate the value of the exponent h by substituting the appropriate terms in the equation for h:

$$h = \int \frac{(s+k)}{v} dZ = \frac{(s+k)}{v} Z \quad (53)$$

$$C_a(s,Z) = e^{-(k/v)Z}e^{-(s/v)Z}\left[\frac{C_{a0}e^{(s/v)Z}}{s} + I\right] \quad (54)$$

At $Z = 0$: $\theta > 0$, $C_a(\theta,0) = C_{a1}$, $C_a(s,0) = C_{a1}/s$. Substituting these values into Eq. (54) and rearranging will yield:

$$I = \frac{C_{a1}}{s} - \frac{C_{a0}}{s} \quad (55)$$

← flujo referencia
cambio alimentación
posible

$$C_a(s,Z) = e^{-(k/v)Z}\left[\frac{C_{a0}}{s} + \frac{C_{a1}}{s}e^{-(s/v)Z} - \frac{C_{a0}}{s}e^{-(s/v)Z}\right] \quad (56)$$

Transforming Eq. (56) back to the time domain will yield two answers: one for $\theta < Z/v$, Eq. (57a); the other for $\theta > Z/v$, Eq. (57b):

$$C_a(\theta,Z) = C_{a0}e^{-(k/v)Z} \quad (57a)$$

$$C_a(\theta,Z) = C_{a1}e^{-(k/v)Z} \quad (57b)$$

Step change in feedrate

Let us now look at the response of the system for a step change in the feedrate. The velocity will be constant except for the step change at $\theta = 0$. For this case, the Laplace transform of Eq. (45) is:

$$v\frac{dC_a(s,Z)}{dZ} + sC_a(s,Z) - C_{a0}e^{-(k/v_0)Z} + kC_a(s,Z) = 0 \quad (58)$$

where C_{a0} is the inlet concentration of Reactant a at $Z = 0$, and v_0 is the fluid velocity at the steady-state condition ($\theta < 0$).

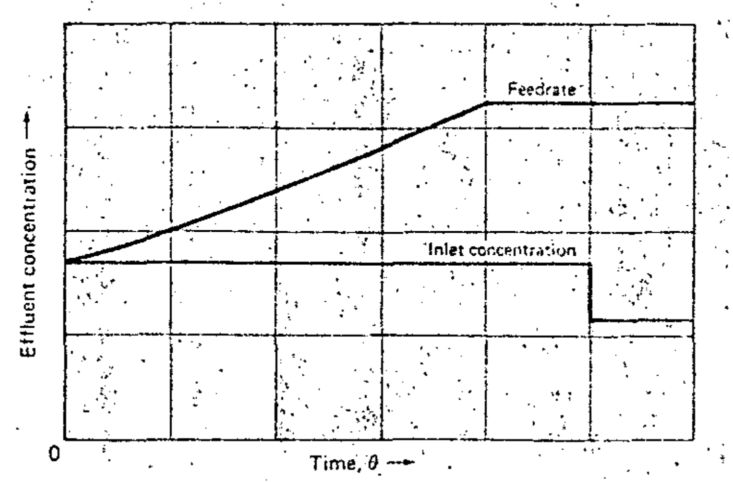
We can again use an integrating factor to solve the equation. The initial condition is $C_a(s,0) = C_{a0}/s$ at $Z = 0$. The solution for Eq. (58) is:

$$C_a(s,Z) = \left[\frac{C_{a0}e^{-(k/v_0)Z}}{\left(s + k - \frac{kv}{v_0}\right)}\right] + \left[\frac{C_{a0}}{s}e^{-(k/v)Z}e^{-(s/v)Z}\right] - \frac{C_{a0}e^{-(k/v)Z}e^{-(s/v)Z}}{s + k - \frac{kv}{v_0}} \quad (59)$$

Converting Eq. (59) to the time domain, we again obtain two answers: one for $\theta < Z/v$, Eq. (60); the other for $\theta > Z/v$, Eq. (61):

$$C_a(\theta,Z) = C_{a0}e^{-(k/v_0)Z}e^{-k[1-(v/v_0)]\theta} \quad (60)$$

$$C_a(\theta,Z) = C_{a0}e^{-(k/v)Z} \quad (61)$$



Tubular reactor response to step changes **Fig. 5**

Fig. 3 and 4 illustrate the concentration profile for the reactor for the two conditions. Fig 5 shows the concentration at the outlet for the two conditions.

A control scheme sensing just the outlet concentration would most likely not be adequate to adjust for the two conditions. The step change in concentration could best be sensed via the inlet concentration that would start to adjust the system reasonably soon after the upset occurred. The same system would not sense a problem for the step change in flowrate by simply measuring the inlet concentration. The final system would have to be adequate to control both upsets if they were considered likely to occur.

Prediction of events likely to occur is one of the most difficult problems in design work and also one of the most critical. After an acceptable control scheme is chosen, a complete model of the system will contain many more equations. Delays in measuring concentration, temperature lag (if temperature were controlling), etc., should be included. However, analyzing the reactor problem at an essentially constant reactant-temperature level can lead to a control concept that we can study in greater depth as design and laboratory-work progress.

The next article in this CE REFRESHER series will appear in the issue of Dec. 28, and will cover techniques for solving the mathematical models of processes and control systems via analog/hybrid computers.

Steven Danatos, Editor

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CE REFRESHER:

Modeling process systems on analog/hybrid computers

Analog simulators perform mathematical operations in parallel at high speeds to solve the differential equations for process systems.

*John L. Guy, Dynamod Enterprises**

☐ In Part 3 of this series,† we developed some manual methods for solving the differential equations for dynamic processes. Such methods, however, have practical limits both in the number of variables to be solved and in the time required for hand computations.

On the other hand, analog and digital computers provide rapid and many solutions for the analyses of dynamic systems. Here, we will show how to simulate and solve the differential equations for complex systems on an analog computer.

Analog computation

Analog computers perform mathematical operations simultaneously by using direct-current (d.c.) electricity. The variables for the analog computer are voltage and time. The variables for chemical process facilities can be represented by electronic components, which can be arranged to simulate even complex systems.

An electronic analog model of the equations describing the physical system can be wired up so that the voltages will represent the dependent variables of the system. After the problem is set up and started on the analog computer, each voltage (representing a dependent variable) is measured. The value of this voltage predicts the value of the dependent variable at a particular time.

Basic operations include summation, integration and function generation. Fig. 1 shows the standard symbols [1] for analog computers, which are used in flowcharting. Circuit diagrams for multiplication, addition and integration, and their mathematical relationships, are shown in Fig. 2.

Hybrid computation

Adding digital computer facilities to an analog computer allows the user to generate complex functions. These can be somewhat difficult to simulate via an analog computer alone. The combined system is called a hybrid computer.

Hybrid facilities allow the user to greatly extend the capacity of the analog machine. The standard analog computer is limited to 26 integrators or 26 first-order differential equations.

By performing calculations sequentially via digital control algorithms, we can program the analog machine to solve the 26 equations repetitively. For example, the equations for solving the tray dynamics for distillation columns require the analog component to be "patched" together on one panel board. The digital machine is then programmed to remember conditions from one time interval to the next and, in this manner, predict the dynamic behavior of the system.

One of the major drawbacks of the analog system is the need to scale variables. Here, the dependent variables (describing the physical system) are scaled as voltage variables whose values range from +10 to −10 V d.c. (the maximum output voltage of most analog devices is ±10 V). Because we can change any of the program steps from a computer terminal console, scaling is no longer the problem that it once was. The technology exists to essentially eliminate this step via instructions from the digital machine. However, a procedure for performing general simulation work is not yet available.

Another drawback of the analog system for process simulation work is the need for electronic wiring (patching) of the panel. The actual process probably takes less time than entering an equivalent digital program via a computer terminal or keypunch, but patching must be done at the location for the analog machine. Each time the same program is rerun, the panel must be rewired. Hence, access to a centralized machine is not possible at different plant and engineering locations. This limitation is recognized by the industry.

Soon, we will be able to access the hybrid computer from a remote location and (via typed commands) generate the wiring of the analog machine [2]. This devel-

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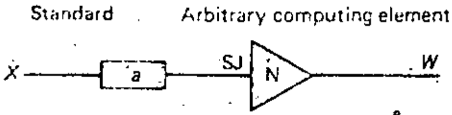
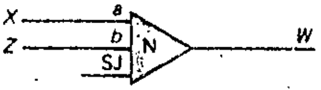
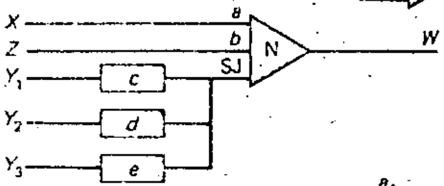
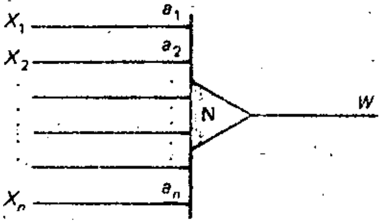
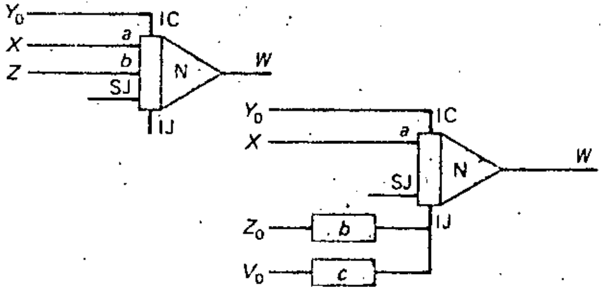
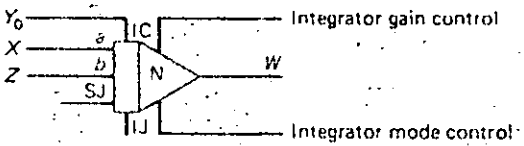
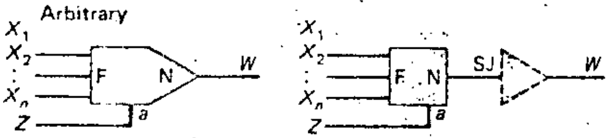
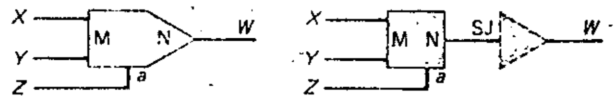
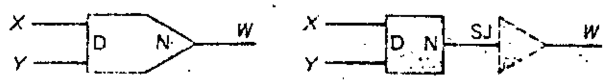
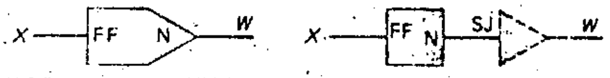
*To meet the author, see *Chem. Eng.*, June 29, p. 80.

†Articles published thus far in this CE REFRESHER: Part 1, June 29, p. 74; Part 2, Aug. 24, p. 111; Part 3, Nov. 16, p. 271.

Summer/Symbol	Function	Notes
	$W = -aX$	1. N = Summer address 2. SJ = Summing junction. This should be designated when used and may appear on all computing elements with patchable summing junctions. 3. The number of inputs to the summer is variable (see different configurations). 4. G = Open-loop gain of the amplifier (G is negative) 5. SM = Saturation magnitude of the high-gain summer.
	$W = -(aX + bZ)$	
	$W = -(aX + bZ + cY_1 + dY_2 + eY_3)$	
	$W = -(a_1x_1 + a_2x_2 + \ldots + a_nX_n)$	

Integrator/Symbol	Function	Notes
Standard configuration 	$W = -(Y_0 - \int_0^T (aX + bZ)dt$ $W = -(Y_0 + bZ_0 + cV_0) - \int_0^T aXdt$	1. N = Integrator address 2. Y_0 = Initial condition (IC) 3. SJ = Summing junction 4. IJ = IC summing junction 5. Integrator gain control changes gain by switching value of feedback capacitor. Integrator gain = $\frac{\text{Output units per second}}{\text{Input units}}$ 6. The integrator mode control selects the analog mode of operation of the integrator.
Mode controlled 	$W = -Y_0 - \int_0^T (aX + bZ)dT$	

Function generator/Symbol	Function	Notes
Arbitrary 	$W = f(X_1, X_2, \ldots, X_n) - aZ$	1. F = Arbitrary function-generator address M = Multiplier D = Divider FF = Fixed-function generator 2. $(X_1, X_2, \ldots, X_n)$ represent functions of 1, 2, . . . , n variables. 3. N = Function generator address 4. The triangular output represents a device with a committed output amplifier. 5. The rectangular output represents a device without a committed amplifier. The device must be connected to the summing junction (SJ) of an amplifier as illustrated by dashed lines. 6. Function generators may be inverting or noninverting.
Multiplier 	$W = -(XY + aZ)$	
Divider 	$W = -X/Y$	
Fixed function 	$W = f(X)$	

Standard symbols for the computing elements for analog and hybrid computers Fig. 1

opment will resolve the rerun setup problem that is inherent in hybrid systems.

uracy and reproducibility

et us compare the accuracy and reproducibility of ults obtained from digital and analog computers.

The digital machine will generate more than six significant figures (based on the data supplied with the problem and if the data contain that many significant figures). The machine reproduces these same figures as many times as the problem is run.

With the analog device, we can only produce about three significant figures. System accuracy will usually extend to three figures. Overall, the accuracy is not as high as with the digital machine.

We should now ask how many figures we need for engineering design work. Probably, three is sufficient for most design work. Because we are accustomed to seeing six or more figures from digital computers, we tend to believe that they all mean something.

The basic design of process equipment may not change. But, change-orders flow through an organization whenever a slight modification arises—say less than 0.1% in a material balance. Some design firms rewrite every equipment specification and the detailed cost estimate for each of the changes. For this reason alone, we might consider the analog machine as better suited for some engineering computations. However, many people would be upset if we hinted that the design was not as exact as they said it was. When a deci- is made to use 6 to 8 significant figures in the com- tations, the next step is to resolve whether overdesign nore than 10 to 20% is adequate to take into account design uncertainties.

Example illustrates procedures

A batch reactor problem will illustrate the procedures involved for simulating with the hybrid machine.

Let us consider a batch-type tank reactor designed to carry out a series reaction having the form:

$$A \rightarrow B \rightarrow C$$

where B is the desired product.

The rate equations for the reaction are:

$$R_A = dC_A/d\theta = -k_1C_A \qquad (1)$$

$$R_B = dC_B/d\theta = k_1C_A - k_2C_B \qquad (2)$$

$$R_C = dC_C/d\theta = k_2C_B \qquad (3)$$

$$k_1 = 10^9 \exp(-9{,}000/T) \qquad (4)$$

$$k_2 = 10^{13} \exp(-12{,}000/T) \qquad (5)$$

where C = concentration of Component A, B or C, lb-mole/ft^3; k = kinetic rate constant, min^{-1}; R = rate of reaction of Component A, B or C, lb-mole/(ft^3)(min); T = temperature, K; and θ = time, min.

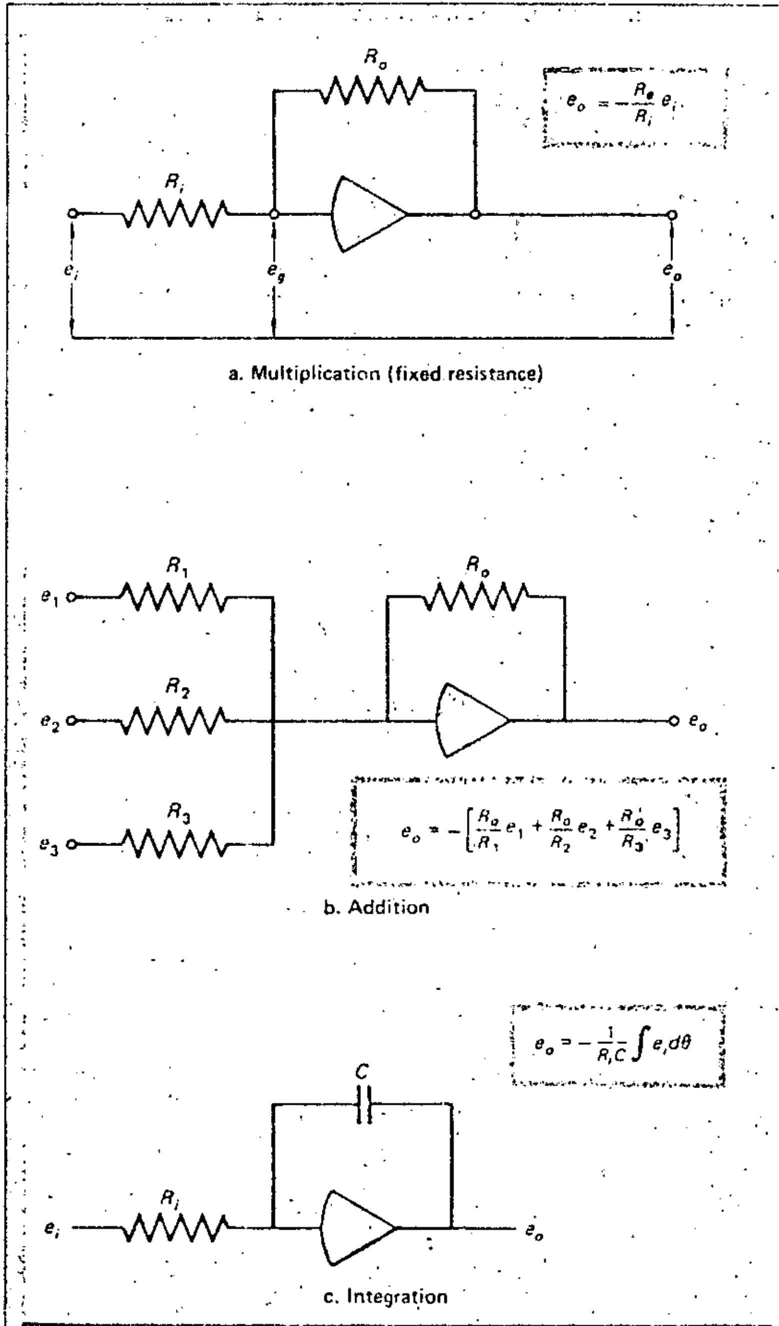
Additional data for this example are:

Heat capacity, C_p, = 50 Btu/(lb-mole)(°F)

sity, ρ, = 0.5 lb-mole/ft^3 ($\sim$ constant)

nperature: 10 to 120°C

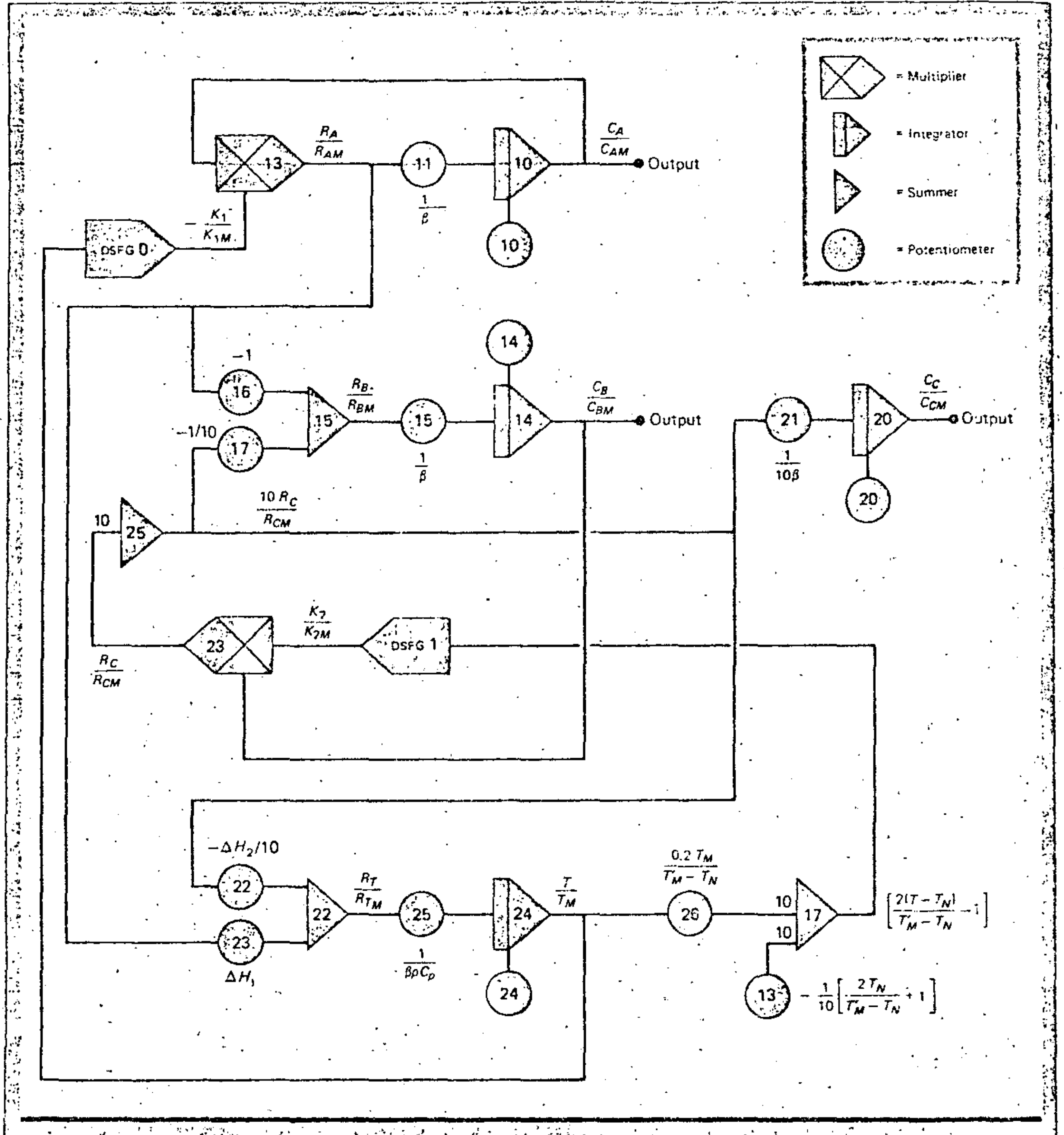
Heat of reaction at 25°C: $\begin{cases}\Delta H_1 = -1{,}800 \text{ cal/mole} \\ \Delta H_2 = -1{,}500 \text{ cal/mole}\end{cases}$



Circuit diagrams for analog computing elements Fig. 2

On hand is a 7,500-gal reactor that is available about one day every three months. Reactant A will be produced as a byproduct in another process at about 500 lb-moles in this period of time. The problem is to determine whether the 7,500-gal reactor will be adequate. Preparation of the reaction mixture and cleanup of the reactor is estimated to take about 12 h. Therefore, reaction time in this equipment will be limited to 12 h. Separation facilities are adequate to recover and refine the product mixture.

The electronic wiring diagram for the hybrid (analog/digital) computer that will simulate this example is shown in Fig. 3. Once the computer is wired up in accordance with this diagram, the problem is solved



Wiring diagram for the batch-series reactor simulation Fig. 3

through conversational computer input/output dialog via a standard keyboard and CRT (cathode ray tube) screen. The final program is listed in Table I.

The exponential reaction rates [Eq. (4) and (5)], are calculated as a function of temperature in the digitally set function generators, DSFG 0 and DSFG 1, as shown in the wiring diagram (Fig. 3). The DSFGs calculate 40 steps in the temperature interval between 100°F and 275°F via a Fortran program. A linear interpolation scheme then generates the reaction-rate constants between these points. Summer 17 (Fig. 3) scales the argument to the DSFGs in order to reduce error resulting from the linear interpolation scheme.

Some scaling must be included in the program to obtain accuracy of results. The procedures shown in the flowchart (Fig. 3) and their implementation on the hybrid computer were synthesized in one day. These do not represent the sophistication that would be required if we had been writing a general-purpose program.

One advantage of the hybrid-computer systems compared with purely analog machines is that a printout of the variables is possible. We can then change any incor-

Table 1 Setup program for simulating reactor problem on hybrid computer

```
/I Executive Subprogram

1.0010)@TT1,1;@TT1,0;
1.0100)"BATCH SERIES REACTOR SIMULATION":
1.0110)SVAR\
1.0200)WA,2000,C:I,U;1,C;
1.0201)"ENTER TIME SCALE - HOURS/SEC":TS=100,TS:TS←
1.0202)"ENTER INITIAL TEMPERATURE":T=100,T:T←
1.0210)BETA=1000/(TS*60)
1.0220);E3,M;
1.0300)"SET PROBLEM CONSTANTS":10,
1.0310)"INITIAL CONDITIONS":12;
1.0400)"SET MAXIMUM VALUES":20;
1.0500)"CALCULATE AND SET COEFFICIENTS":NA;21;WA;21;


Part X. Problem constants

10.0100)"PROBLEM CONSTANTS"
10.0200)DH1 = -3240 "BTU/LB MOLE"
10.0300)DH2 = -2700
10.0400)CPK = 50 "BTU/(LB.MOLE DEGF)"
10.0500)RHO = 0.5 "LB MOLES/FT↑3"


Part XI: Scaled function values

11.0010)"FUNCTION VALUES"
11.0100)I=1,41! DT(I) = TN + (TMP-TN)*(I-1)/40
11.0200)I=1,41! K1T(I) = 1.E9*EXP(-16200/(DT(I)+460))/K1M
11.0300)I=1,41! K2T(I) = 1.E13*EXP (-21600/(DT(I)+460))/K2M


Part XII: Initial conditions for integration

12.0100)"INITIAL CONDITIONS"
12.0200)CA = 0.5 "LB MOLES/FT↑3"
12.0300)CB = 0
12.0400)CC = 0


Part XX. Maximum values for coefficients

20.0100)"MAX VALUES"
20.0200)CAM = 1
20.0300)CBM = 1
20.0400)CCM = 1
20.0500)TM = 300
20.0510)TN = T - 50
20.0520)TMP = T + 125
20.0600)K1M = 1.E9*EXP(-16200/(TMP+460))
20.0700)K2M = 1.E13*EXP(-21600/(TMP+460))
20.1000)RAM = CAM*K1M
20.1100)RBM = 0.1*CBM*K2M + CAM*K1M
20.1200)RCM = CBM*K2M
20.1300)RTM = 3500*(RAM + RCM)

Part XXI: Coefficients

21.0010)"COEFFICIENT SETTINGS"
21.1010)1C10= CA/CAM
21.1011)1C11=-RAM/BETA*CAM)
21.1013)1C13=-(-(2*TN/(TMP-TN)+1)/10)
21.1014)1C14=-CB/CBM
21.1015)1C15=-RBM/(BETA*CBM)
21.1016)1C16=-(-1*RAM/RBM)
21.1017)1C17= (-1*RCM/RBM)/10
21.1020)1C20=-CC/CCM
21.1021)1C21= RCM/(10*BETA*CCM)
21.1022)1C22= (-DH2*RCM/RTM)/10
21.1023)1C23=-(DH1*RAM/RTM)
21.1024)1C24=-T/TM
21.1025)1C25=-RTM/BETA*TM*CPK*RHO)
21.1026)1C26=-(2*TM/(TMP-TN))/10
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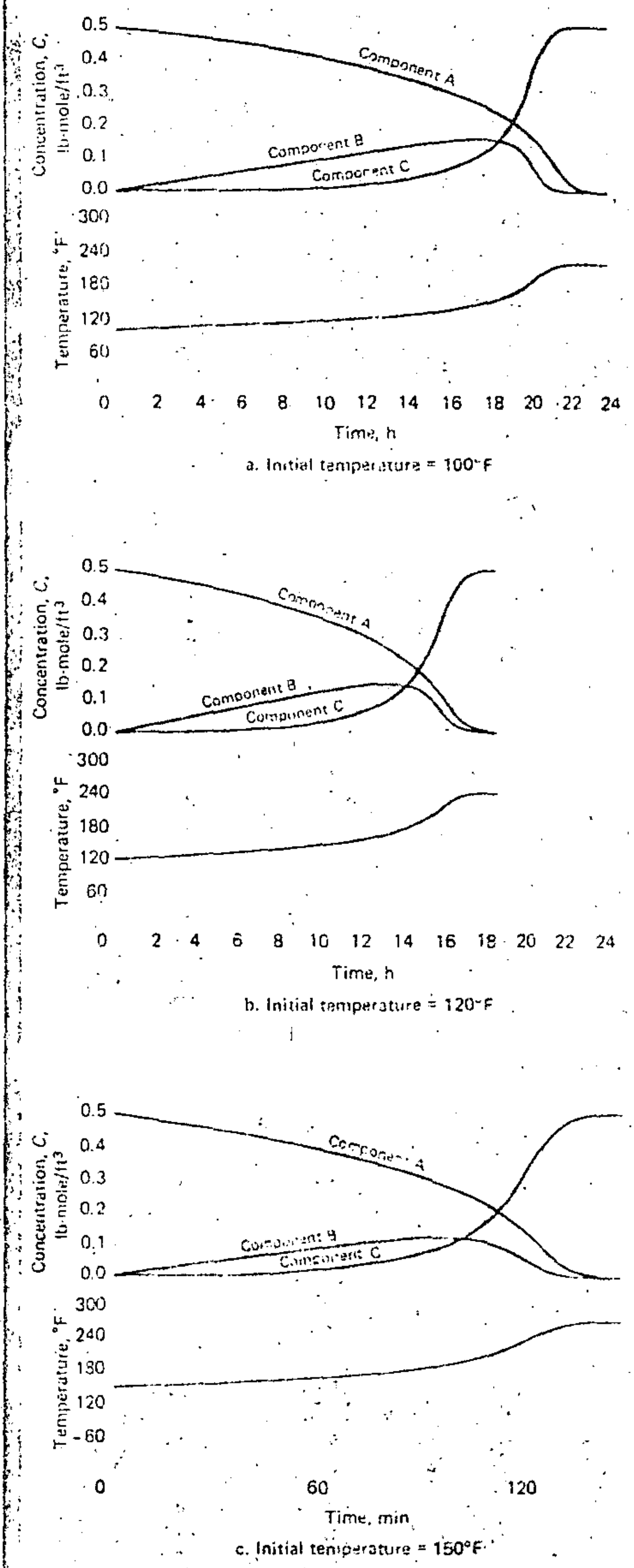

a. Initial temperature = 100°F

b. Initial temperature = 120°F

c. Initial temperature = 150°F

Reactor profiles for adiabatic conditions **Fig. 4**

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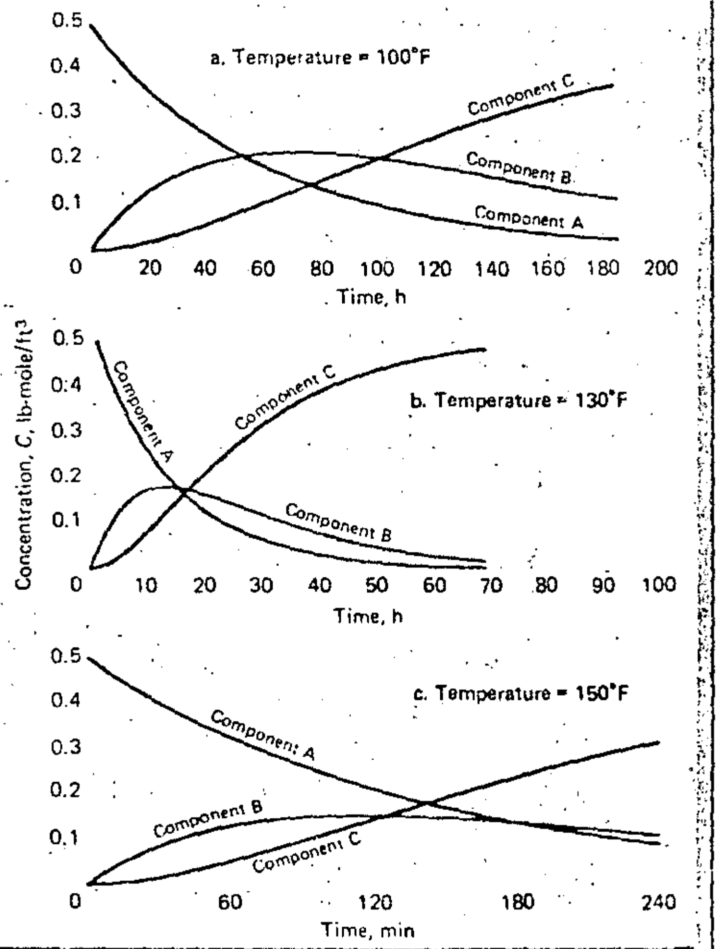

Reactor profiles for isothermal conditions **Fig. 5**

rect or inverted operations at the CRT screen. The program (Table I) is written in the HYTRAN Interpreter language, which runs on the EAI PACER-100 minicomputer. Part I of the program is the executive subprogram that initializes the Model 2,000 analog processor interfaces and executes the other subprograms. Problem constants and initial conditions for integration are set in Parts X and XIII, respectively. Part XX sets the values of the coefficients, and Part XI computes the scaled function values.

Problem interpretation and results

Because the existing reactor is not equipped with heat-exchange equipment, the first step is to determine the concentration profile that we can expect from an adiabatic (i.e., no heat removal) reactor.

Fig. 4 shows the results of the expected reactor profiles at initial temperatures of 100°, 120° and 150°F. The maximum concentration of Component B increases with decreasing temperature. However, we can only reduce the temperature to about 120°F before we also reduce the amount of Component B that is produced within the production time available (i.e., 12 h). A series of runs were obtained by simply changing the initial temperature from the computer console.

If we set the heats of reaction for this example to zero, we can study the reactor profiles for a system operating in an isothermal manner. The reactor profiles obtained from this simulation for three different temperature levels are shown in Fig. 5. The optimum temperature of 130°F (Fig. 5b) produces a maximum concentration of Component B equal to 0.18 lb-mole/ft³ within the reaction time of 12 h.

Actually, we can obtain a greater maximum concentration by decreasing the reactor temperature as the reaction proceeds. We would then obtain higher reaction rates before appreciable amounts of Component B are formed. This result could indicate an interesting dynamic study, but one not justified here because of the short operating time for this process. In a future article of this series, we will provide in-depth studies of reactor systems.

Comparing the results of the studies obtained from the analog simulation to those from a digital computer simulation, we find that the isothermal case agrees exactly with the results from the hybrid computer. However the results of the adiabatic study indicate a slightly different reactor profile. This difference can be traced to the interpolation scheme used in calculating the reaction-rate constants. The use of a "log-x" printed-circuit card [3] would reduce the error, but would probably increase the setup time on the hybrid computer for the problem.

Advantages/limitations

Analog-hybrid computers are a useful tool for dynamic analysis. The integration of differential equations on analog systems is not as difficult a simulation problem as it is with the digital computers. The technology exists to make analog systems as easy to use as the digitals. However, fewer people are developing applications technology for analog machines than for the digitals because of earlier experiences with the analogs.

This lack of effort has hindered the development of canned procedures for analog systems. Hence, programs for analogs are not as plentiful as those for digital machines, and progress in analog methods will continue slowly—at least in chemical engineering applications. However, analog-hybrid processing does produce results conveniently, and perhaps in a shorter period of time than does a purely digital method.

Acknowledgement

I want to express my appreciation to J. Pau Landauer of Electronic Associates, Inc. for his help i preparing this article and performing the compute work.

The next article in this CE REFRESHER series wi appear in the issue of Feb. 22, 1982, and will cov methods for solving problems in process dynamics digital computer methods.

Steven Danatos, Ed

References

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2. Landauer, J. P., Stored Program Hybrid Processing System, *Autom. Pr ing.*
3. Luyben, W. L., "Process Modeling, Simulation and Control for Chem Engineers," McGraw-Hill, New York, 1973.

PROCESS DYNAMICS/5

Modeling process systems via digital computers

The differential equations, representing process systems, must be reduced to linear first-order equations in order to solve initial-value problems by numerical techniques.

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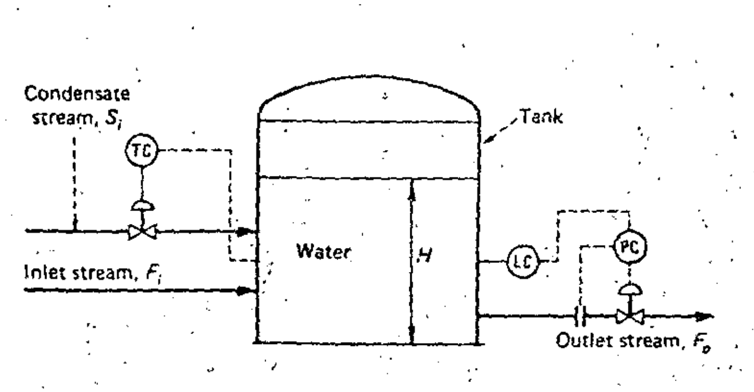
☐ The most powerful tool for solving the differential equations for modeling process-dynamics problems is probably the digital computer. Digital computers eliminate many of the disadvantages of their analog/hybrid counterparts. For example:

- Scaling the variables for time and voltage is not required because digital machines can handle very small numbers (ranging from 10^{-38} for some minicomputers to 10^{-300} for large machines) and very large numbers (10^{38} to 10^{300}).
- Initial setup time is probably lower for the digital machine even with the advances in analog/hybrid computing tools mentioned in Part 4.[†]
- Once a digital program is developed that adequately simulates a certain phenomenon, we can retrieve the program and simulate the phenomenon under different conditions at a later date with less difficulty. (In Part 4, we mentioned that the technology to facilitate re-setup time for analog/hybrid systems is developed, but not advanced to the degree that it is for the digital machines.)
- Reproducibility of results is much greater with the digital computer. Results with from six to eight significant figures can be consistently obtained for the same problem. However, these results usually have more significant figures than the input data for the problem.

Problems arise in solving systems involving differential equations when numerical integration for digital simulation is used instead of the continuous method in analog simulation. The differential equations for the simulation are replaced by difference equations that can cause truncation errors and stability problems.

Systems of differential equations

We derived 12 equations to describe the dynamic response of a hot-water heater (Fig. 1) in Part 2[†] of this series. These equations are reproduced here as the set, Eq. (1). Two new variables have been added—one to normalize the controller output, $(SPAN)$, and the other to determine whether the output should increase or decrease with the error, (AXN). [The variable, (AXN), is limited to values of $+1$ and -1.]



Control systems for water heater **Fig. 1**

$$\frac{dH}{d\theta} = \frac{F_i + S_i - F_o}{\rho A} \tag{1a}$$

$$\frac{dt_o}{d\theta} = \frac{F_i C_p t_i + S_i C_p t_{si} - F_o C_p t_o}{\rho A H} - \left(\frac{t_o}{H}\right)\frac{dH}{d\theta} \tag{1b}$$

$$\frac{d\phi_{t1}}{d\theta} = \frac{t_o - \phi_{t1}}{\tau_t} \tag{1c}$$

$$\begin{aligned}\phi_{t2} = {} & \frac{K_{ct}(AXN)_t(\phi_{t1} - SP_t)}{(SPAN)_t} + \\ & \frac{K_{ct}}{T_{It}}\int \frac{(AXN)_t}{(SPAN)_t}(\phi_{t1} - SP_t)d\theta + \\ & K_{ct}T_{dt}\frac{d\{(AXN)[\phi_{t1} - SP_t]/(SPAN)_t\}}{d\theta}\end{aligned} \tag{1d}$$

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[*] To meet the author, see *Chem. Eng.*, June 29, 1981, p. 86.

[†] Articles published thus far in this CE REFRESHER: Part 1, June 29, 1981, p. 74, Part 2, Aug. 24, 1981, p. 111, Part 3, Nov. 16, 1981, p. 271; Part 4, Dec. 28, 1981, p. 63.

$$S_i = A_l C_{vl} \sqrt{P_{1l} - P_{2l}} \tag{1e}$$

$$P_{2l} = g(H) \tag{1f}$$

$$\tau_l^2 \frac{d^2\phi_{l1}}{d\theta^2} + 2\zeta_l \tau_l \frac{d\phi_{l1}}{d\theta} + \phi_{l1} = G_l H \tag{1g}$$

$$\tau_F^2 \frac{d^2\phi_{F1}}{d\theta^2} + 2\zeta_F \tau_F \frac{d\phi_{F1}}{d\theta} + \phi_{F1} = G_F F_o \tag{1h}$$

$$\phi_{l2} = \frac{K_{cl}(AXN)_l(\phi_{l1} - SP_l)}{(SPAN)_l} + R \tag{1i}$$

$$\phi_{F2} = \frac{K_{cF}(AXN)_F(\phi_{F1} - \phi_{l2})}{(SPAN)_F} + \frac{K_{cF}}{T_{iF}} \int \frac{(AXN)_F(\phi_{F1} - \phi_{l2})}{(SPAN)_F} d\theta \tag{1j}$$

$$F_o = A_F C_{vF} \sqrt{P_{1F} - P_{2F}} \tag{1k}$$

$$P_{1F} = g(H, F_o, C) \tag{1l}$$

Most generalized numerical-integration subroutines are set up to solve equations of the following type (written for n first-order equations):

$$\left.\begin{aligned}
\frac{dY_1}{d\theta} &= f_1(\theta, Y_1, Y_2, \ldots, Y_n) \\
\frac{dY_2}{d\theta} &= f_2(\theta, Y_1, Y_2, \ldots, Y_n) \\
&\;\;\vdots \qquad\qquad \vdots \\
\frac{dY_n}{d\theta} &= f_n(\theta, Y_1, Y_2, \ldots, Y_n)
\end{aligned}\right\} \tag{2}$$

We can reduce the second-order equation to two first-order equations by the following procedure, which is illustrated by the equation for the flowrate-sensing element:

$$\phi'_{F1} = \frac{d\phi_{F1}}{d\theta} \tag{3}$$

$$\frac{d\phi'_{F1}}{d\theta} = \frac{d^2\phi_{F1}}{d\theta^2} \tag{4}$$

Therefore, we obtain two first-order equations:

$$\tau_F^2 \frac{d\phi'_{F1}}{d\theta} + 2\zeta_F \tau_F \phi'_{F1} + \phi_{F1} = G_F F_o \tag{5}$$

$$\frac{d\phi_{F1}}{d\theta} = \phi'_{F1} \tag{6}$$

This procedure can easily be extended to the reduction of one p^{th}-order equation to p first-order equations.

We can rewrite Eq. (1) in the form of Eq. (2) by remembering the relation that if $Y = \int f(\theta)d\theta$, then $dY/d\theta = f(\theta)$. Therefore:

$$\frac{dH}{d\theta} = \frac{(F_i + S_i - F_o)}{\rho A} \tag{7a}$$

$$\frac{dt_o}{d\theta} = \frac{F_i C_p t_i + S_i C_p t_{si} - F_o C_p t_o}{\rho A H} - \left(\frac{t_o}{H}\right)\frac{dH}{d\theta} \tag{7b}$$

$$\frac{d\phi_{l1}}{d\theta} = \frac{t_o - \phi_{l1}}{\tau_l} \tag{7c}$$

$$\frac{d\phi'_{l1}}{d\theta} = \frac{d^2\phi_{l1}}{d\theta^2} = \frac{1}{\tau_l}\left[\frac{dt_o}{d\theta} - \frac{d\phi_{l1}}{d\theta}\right] \tag{7d}$$

$$\frac{d\phi_{l2}}{d\theta} = \frac{K_{cl}(AXN)_l}{(SPAN)_l}\left\{\frac{d\phi_{l1}}{d\theta} + \left[\frac{\phi_{l1} - SP_l}{T_{il}}\right] + T_{dl}\frac{d\phi'_{l1}}{d\theta}\right\} \tag{7e}$$

$$S_i = A_l C_{vl} \sqrt{P_{1l} - P_{2l}} = \phi_{l2} V_{v2} \sqrt{P_{1l} - P_{2l}} \tag{7f}$$

$$P_{2l} = g(H) \tag{7g}$$

$$\frac{d\phi'_{l1}}{d\theta} = \frac{G_l H}{\tau_l^2} - \frac{2\zeta_l \phi'_{l1}}{\tau_l} - \frac{\phi_{l1}}{\tau_l^2} \tag{7h}$$

$$d\phi_{l1}/d\theta = \phi'_{l1} \tag{7i}$$

$$\frac{d\phi'_{F1}}{d\theta} = \frac{G_F F_o}{\tau_F^2} - \frac{2\zeta_F}{\tau_F}\phi'_{F1} - \frac{\phi_{F1}}{\tau_F^2} \tag{7j}$$

$$d\phi_{F1}/d\theta = \phi'_{F1} \tag{7k}$$

$$\phi_{l2} = \frac{K_{cl}(AXN)_l(\phi_{l1} - SP_l)}{(SPAN)_l} + R \tag{7l}$$

$$\frac{d\phi_{l2}}{d\theta} = \frac{K_{cl}(AXN)_l}{(SPAN)_l}\left(\frac{d\phi_{l1}}{d\theta}\right) \tag{7m}$$

$$\frac{d\phi_{F2}}{d\theta} = \frac{K_{cF}(AXN)_F}{(SPAN)_F}\left\{\frac{d\phi_{F1}}{d\theta} - \frac{d\phi_{l2}}{d\theta} + \frac{1}{T_{iF}}(\phi_{F1} - \phi_{l2})\right\} \tag{7n}$$

$$F_o = A_F C_{vF} \sqrt{P_{1F} - P_{2F}} = \phi_{F2} C_{vF} \sqrt{P_{1F} - P_{2F}} \tag{7o}$$

$$P_{1F} = g(H, F_o, C) \tag{7p}$$

We now have a system of 5 algebraic equations and 11 first-order differential equations to solve. However, Eq. (7l) and (7m) are equivalent, so actually we have 15 independent equations to solve.

Eq. (7) can be made exactly into the form of Eq. (2) by substituting the expressions for the derivatives that appear on the right-hand side of the equations. Fortunately, we can forgo the step by arranging our calculations so as to determine the derivatives before we use them on the right-hand side of any equation.

Numerical integration methods

All of the numerical integration methods that we will describe require that a problem have known values of the dependent variables at some time θ, that is usually set equal to zero. This type of problem is called an "initial value problem." We then predict the values of the dependent variables that satisfy our differential equation at successive time intervals via one of several numerical techniques.

Euler method

We can calculate the Point Y_1 at time $(\theta + h)$ by a Taylor series for Eq. (2a) as:

$$Y_1(\theta + h) = Y_1(\theta) + h\frac{dY_1(\theta)}{d\theta} + \frac{h^2}{2}\frac{d^2Y(\theta)}{d\theta^2} + \cdots \tag{8}$$

where h is the step size.

The derivative for $Y_1(\theta)$ is:

$$dY_1(\theta)/d\theta = f_1(\theta, Y_1, Y_2, \ldots, Y_n) \tag{9}$$

Hence by substituting the relationship of Eq. (9) into (8), we obtain the following:

$$Y_1(\theta + h) = Y_1(\theta) + hf_1 + \frac{h^2}{2}\frac{df_1}{d\theta} + \cdots \quad (10)$$

As [illegible] reduce the value for the step size h, we can negl[illegible] the terms containing h^2, ... Therefore, we can calculate the value of Y_1 by:

$$Y_1(\theta + h) = Y_1(\theta) + hf_1 \quad (11)$$

The values for the remaining Ys, i.e., Y_2 through Y_n, are calculated in the same manner.

We call this method "first order" because we truncate all terms that contain more than the first power of h. The omission of these terms will give us a truncation error that is inherent in the method. If h is a small number, the terms including the third and higher powers of h will be small compared with the h^2 term. We then say that the truncation error is of the order of h^2.

The effect of decreasing the step size, h, is shown in Fig. 2 [*1*] for solving the single differential equation:

$$dY/d\theta + Y = 1;\ Y(\theta = 0) = 0 \quad (12)$$

As the step size decreases (Fig. 2), accuracy increases. There also exists a maximum value of h where the method diverges from the true solution for large values of time. This maximum value is 2.0 for Euler's method. Values of h greater than 2.0 will cause the solution to diverge, and the method becomes unstable. Therefore, the stability region for the Euler method ranges from $h = 0$ to $h = 2.0$.

Se[illegible]d-order Runge-Kutta method

The second-order Runge-Kutta method is also known as the modified Euler method. The formulas for calculating values of Y in Eq. (2) by this technique are given by Eq. (13) and (14):

$$Y_1^0(\theta + h) = Y_1(\theta) + hf_1[\theta, Y_1(\theta), \ldots, Y_n(\theta)] \quad (13)$$

$$Y_1(\theta + h) = Y_1(\theta) + \frac{h}{2}[f(\theta + h, Y_1^0, \ldots) + f_1(\theta, Y_1, \ldots)] \quad (14)$$

The truncation error is of the order h^3. Fig. 3 shows the solution to Eq. (12). The stability region for this method again ranges from $h = 0$ to $h = 2.0$. The formulas for this method can also be derived from a Taylor series expansion.

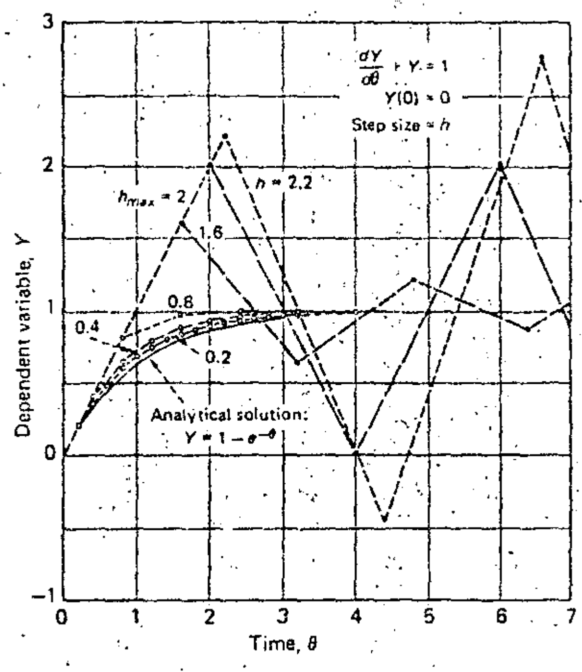
Fourth-order Runge-Kutta method

The formulas for calculating values of Y in Eq. (2) are given by Eq. (15):

$$Y_1(\theta + h) = Y_1(\theta) + \frac{1}{6}(k_{11} + 2k_{21} + 2k_{31} + k_{41}) \quad (15a)$$

$$Y_2(\theta + h) = Y_2(\theta) + \frac{1}{6}(k_{12} + 2k_{22} + 2k_{32} + k_{42}) \quad (15b)$$

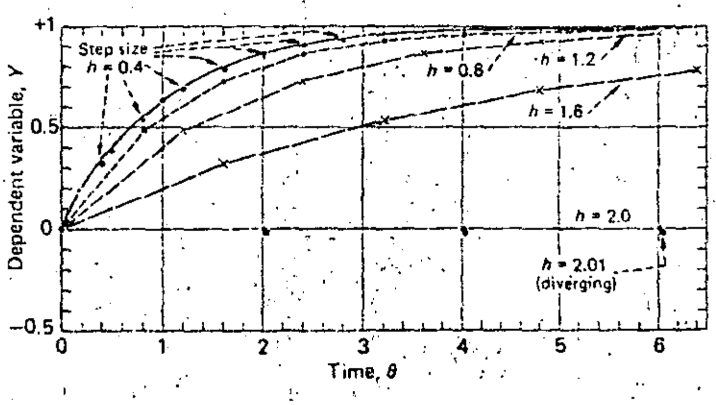
$$Y_n(\theta + h) = Y_n(\theta) + \frac{1}{6}(k_{1n} + 2k_{2n} + 2k_{3n} + k_{4n}) \quad (15c)$$



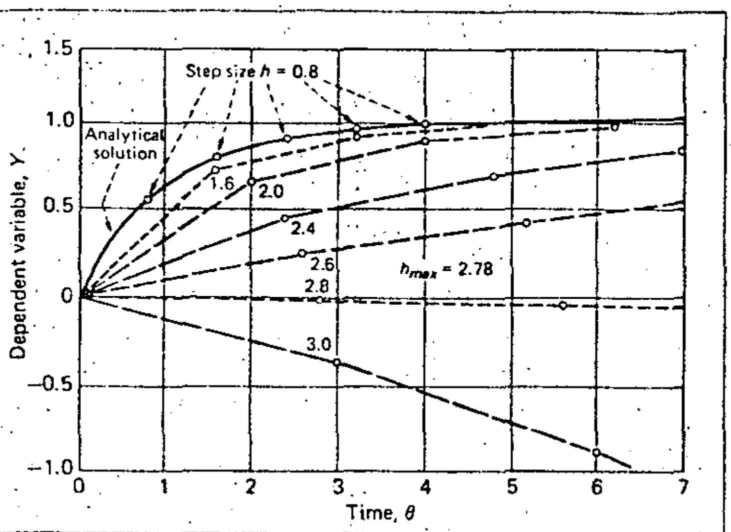
Euler integration: effects of step size Fig. 2

Nomenclature

H	Height of liquid in tank
t_o	Outlet or tank temperature
ϕ_{t1}	Output of temperature sensor
$\dot{\phi}_{t1}$	Derivative of ϕ_{t1}
ϕ_{l1}	Output of liquid-level sensor
$\dot{\phi}_{l1}$	Derivative of $\phi_{l}1$
ϕ_{F1}	Output of outlet flowrate sensor
$\dot{\phi}_{F1}$	Derivative of ϕ_{F1}
ϕ_{t2}	Output of temperature controller
ϕ_{l2}	Output of level controller
ϕ_{F2}	Output of outlet flowrate controller



Modified Euler integration: effects of step size Fig. 3



Runge-Kutta integration: effects of step size **Fig. 4**

where the second subscript in the k terms refers to the subscript of the dependent variable, and:

$$k_{11} = hf_1[\theta, Y_1(\theta), Y_2(\theta), \ldots, Y_n(\theta)] \quad (16a)$$

$$k_{12} = hf_2[\theta, Y_1(\theta), Y_2(\theta), \ldots, Y_n(\theta)] \quad (16b)$$

$$\vdots$$

$$k_{1n} = hf_n[\theta, Y_1(\theta), Y_2(\theta), \ldots, Y_n(\theta)] \quad (16c)$$

$$k_{21} = hf_1\left[\theta + \frac{h}{2}, Y_1(\theta) + \frac{k_{11}}{2}, \ldots, Y_n(\theta) + \frac{k_{1n}}{2}\right] \quad (16d)$$

$$k_{22} = hf_2\left[\theta + \frac{h}{2}, Y_1(\theta) + \frac{k_{11}}{2}, \ldots, Y_n(\theta) + \frac{k_{1n}}{2}\right] \quad (16e)$$

$$\vdots$$

$$k_{2n} = hf_n\left[\theta + \frac{h}{2}, Y_1(\theta) + \frac{k_{11}}{2}, \ldots, Y_n(\theta) + \frac{k_{1n}}{2}\right] \quad (16f)$$

$$k_{31} = hf_1\left[\theta + \frac{h}{2}, Y_1(\theta) + \frac{k_{21}}{2}, \ldots, Y_n(\theta) + \frac{k_{2n}}{2}\right] \quad (16g)$$

$$k_{32} = hf_2\left[\theta + \frac{h}{2}, Y_1(\theta) + \frac{k_{21}}{2}, \ldots, Y_n(\theta) + \frac{k_{2n}}{2}\right] \quad (16h)$$

$$\vdots$$

$$k_{3n} = hf_n\left[\theta + \frac{h}{2}, Y_1(\theta) + \frac{k_{21}}{2}, \ldots, Y_n(\theta) + \frac{k_{2n}}{2}\right] \quad (16i)$$

$$k_{41} = hf_1[\theta + h, Y_1(\theta) + k_{31}, \ldots, Y_n(\theta) + k_{3n}] \quad (16j)$$

$$k_{42} = hf_2[\theta + h, Y_1(\theta) + k_{31}, \ldots, Y_n(\theta) + k_{3n}] \quad (16k)$$

$$\vdots$$

$$k_{4n} = hf_n[\theta + h, Y_1(\theta) + k_{31}, \ldots, Y_n(\theta) + k_{3n}] \quad (16l)$$

The fourth-order Runge-Kutta method can also be derived from a Taylor series. The truncation error is on the order of h^5. Fig. 4 shows the effect of decreasing the step size h to solve Eq. (12). In this method, we have increased the stability region for values of h ranging from zero to about 2.78.

The preceding methods and the corresponding equations use the value at one point to predict the values of the dependent variables at a value of the independent variable (usually time) for a time interval (i.e., time = $\theta + h$). This new value then becomes the one-point value to predict the dependent variables at $\theta + 2h$, etc.

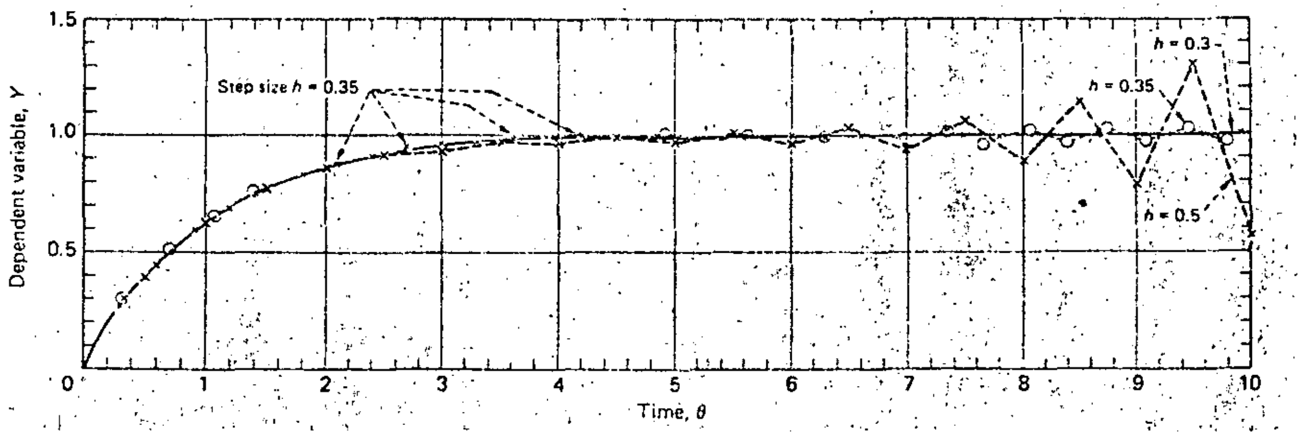
Adams-Bashforth method

The Adams-Bashforth process predicts the variables by using values of the function at four previous points. The formula for the fourth-order process is:

$$Y_1(\theta + h) = Y_1(\theta) + \frac{h}{24}(55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3}) \quad (17a)$$

$$f_n = f_1[\theta, Y_1(\theta), Y_2(\theta), \ldots, Y_n(\theta)] \quad (17b)$$

$$f_{n-1} = f_1[(\theta - h), Y_1(\theta - h), Y_2(\theta - h), \ldots, Y_n(\theta - h)] \quad (17c)$$



Adams-Bashforth integration uses a four-point predictor of model: effects of step size **Fig. 5**

$$f_{n-2} = f_1[(\theta - 2h), Y_1(\theta - 2h), Y_2(\theta - 2h), \ldots, Y_n(\theta - 2h)] \quad (17d)$$

$$f_{n-3} = f_1[(\theta - 3h), Y_1(\theta - 3h), Y_2(\theta - 3h), \ldots, Y_n(\theta - 3h)] \quad (17e)$$

The Adams-Bashforth method can easily be extended to [illegible]iple equations.

Truncation error is on the order of h^5, but the coefficient in the error term is somewhat larger than for the Runge-Kutta method of the same order. Therefore, we must use smaller values of h to achieve the same accuracy. The method is stable over a smaller range of values for h, as shown in Fig. 5.

Unlike the Euler and Runge-Kutta methods, the instability does not appear after one or two time increments. It takes time to develop. We must use the Runge-Kutta method to obtain the initial three values of the dependent variables. The results of solving Eq. (12) by this method are shown in Fig. 5.

Adams-Moulton method

The Adams-Moulton method is an example of a predictor-corrector formula for solving differential equations. The procedure is iterative, and we must specify an acceptable error criterion as well as a step size h. There is also a trade-off between step size and the number of iterations required for convergence. We can use the error estimates to adjust the step size h, but we will defer this discussion until later. The procedure for fixed h is:

Step 1. Compute the initial estimate for $Y_1^0(\theta + h)$ by using Eq. (17).

Step 2. Compute the value for:

$$f_1(\text{[illegible]} h) = f_1[\theta + h, Y_1(\theta + h), Y_2(\theta + h), \ldots, Y_n(\theta + h)]$$

Step 3. Compute the values for:

$$Y_1^k(\theta + h) = Y_1(\theta) + \frac{h}{24}[9f_1(\theta + h) + 19f_1(\theta) - 5f_1(\theta - h) + f_1(\theta - 2h)]$$

where $k = 1, 2, 3, \ldots$

Step 4. Repeat Steps 2 and 3 until the following relationship is satisfied:

$$\left|\frac{Y_1^k - Y_1^{(k-1)}}{Y_r^k}\right| < \epsilon$$

where ϵ is the prescribed error.

The procedure can easily be extended to multiple equations. The accuracy is improved over that provided by Eq. (17). The Adams-Moulton method gives us an estimate of the error with regard to our chosen step size h. However, we obtain this estimate only at the expense of increased computations. The results obtained for Eq. (12) by using this method are shown in Fig. 6, which illustrates the effect of decreasing the step size.

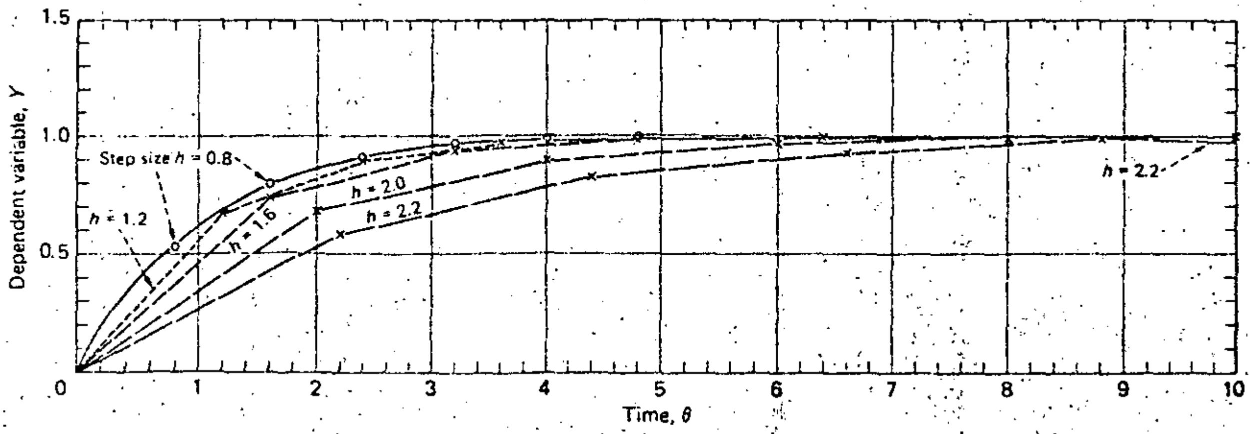
Again, we must use another method to predict the initial three approximations of the functions from the initial given values.

Other methods

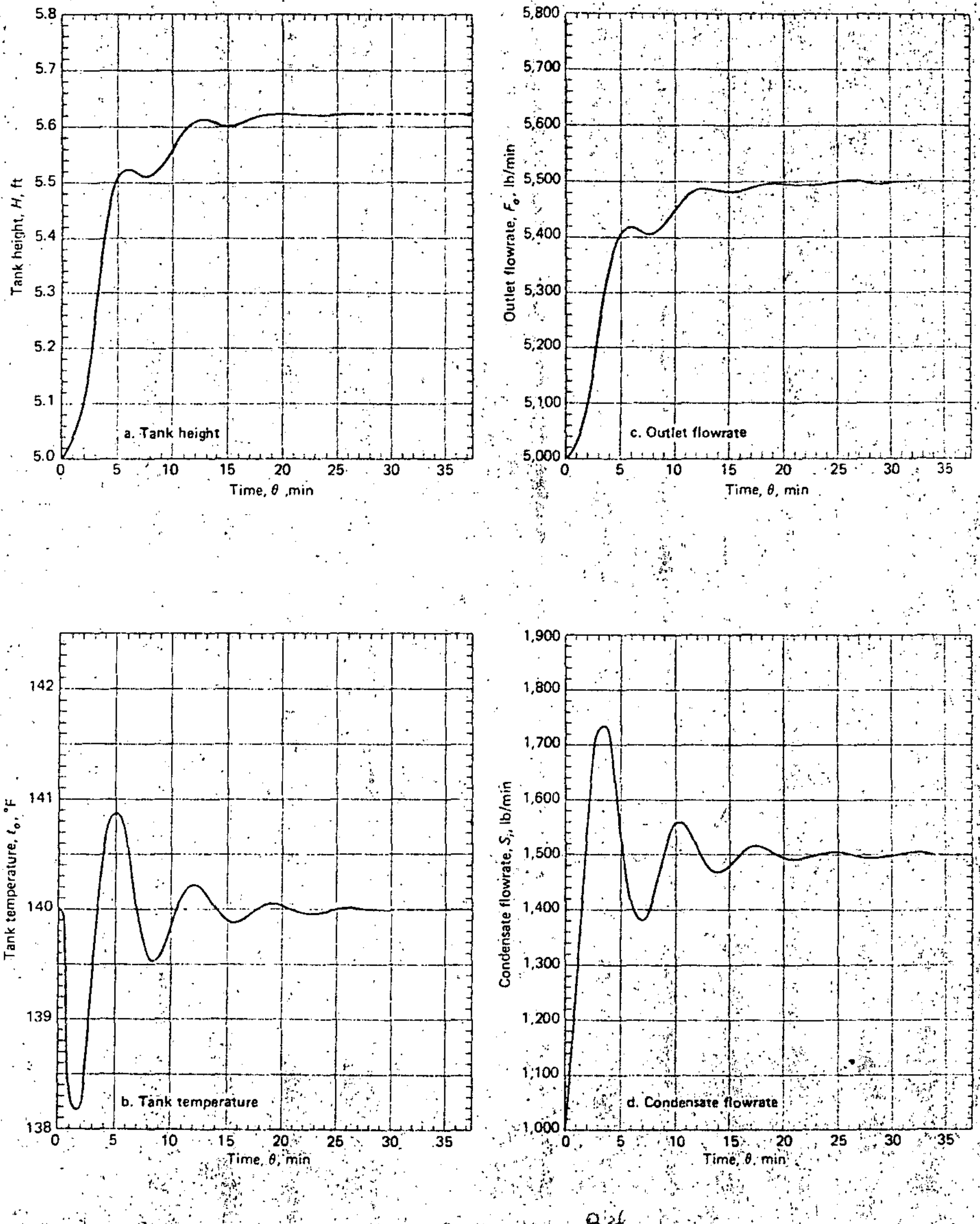
Gear [*2*] describes a general computer program for solving multiple differential equations. The program contains techniques for starting the calculations, changing the step size, and changing the order of the equations. This last refinement can lead to some increase in the efficiency of computation. For details of such procedures, see Gear [*2*].

Stiff systems frequently arise in kinetic studies and distillation-column simulations due to differing rates of exponential decay (referred to as time constants). [We discussed time constants in Part 1 of this series.] By way of example, let us consider the equation $dY/d\theta = \lambda Y$, when $\lambda < 0$. Here, the dependent variable, Y, decays by a factor of e^{-1} in the time θ equal to $-1/\lambda$, the time constant of the equation.

For any system of differential equations, the time constant of each equation will be different. The more the time constants vary, the stiffer the system is. The equations having fast decay rates will control the stability of the method even though the effects of the equations that are negligible in those terms affect phenomena of the system. On the other hand, the truncation error is determined by the equations having slow decay rates.



[illegible]ams-Moulton integration uses a predictor-corrector formula: effects of step size **Fig. 6**


Tank height, H, ft
5.0
5.1
5.2
5.3
5.4
5.5
5.6
5.7
5.8
0
5
10
15
20
25
30
35
Time, θ, min
a. Tank height
Outlet flowrate, F_o, lb/min
5,000
5,100
5,200
5,300
5,400
5,500
5,600
5,700
5,800
Time, θ, min
c. Outlet flowrate
Tank temperature, t_o, °F
138
139
140
141
142
Time, θ, min
b. Tank temperature
Condensate flowrate, S_i, lb/min
1,000
1,100
1,200
1,300
1,400
1,500
1,600
1,700
1,800
1,900
Time, θ, min
d. Condensate flowrate

System [illegible]

Gear has included algorithms for handling stiff systems into the general program for solving multiple differential equations. Other algorithms for handling stiff systems include those of Liniger and Willoughby [3] and Miranker [4].

Water-heater problem

Let us now return to the solution of the water-heater problem, shown in Fig. 1. The tank initially will be operating at steady state. The feed streams are: $F_i = 4{,}000$ lb/min of water at 120°F, and $S_i = 1{,}000$ lb/min of steam condensate at 220°F. The outlet stream $F_o = 5{,}000$ lb/min at 140°F. At time $\theta = 0$, the temperature of the cold feed stream, F_i, decreases to 118°F.

We are now ready to solve the set [Eq. (1)] of equations that describe this system. We can convert Eq. (1) to the general form of Eq. (2). This is time-consuming and unnecessary because we can set up the computer program to solve for the derivatives in the equations.

The computer program will consist of: a section of data (physical data, controller data, etc.), initial conditions (or a subprogram to calculate initial conditions), a subprogram to calculate the functions f, a numerical integration routine, and a master program to monitor the sequence and output the results.

Franks [5] has put together a series of subprograms (Dyflo) to simulate the dynamic operation of many items of process equipment and process control loops.

Once a general computer program is set up, we no longer need to convert each equation to Y and f (which conversion is both tedious and time-consuming), because many operations involve the same physical phenomena. However, to show what is involved in setting up such a computer program, we will convert the equations for the water-heater problem to the following:

Material balance:

$$\frac{dH}{d\theta} = \frac{F_i + S_i - F_o}{\rho A_T} \qquad \text{(A)}$$

Energy balance:

$$\frac{dt_o}{d\theta} = \frac{F_i C_p t_i + S_i C_p t_{si} - F_o C_p t_o}{\rho A_T H} - \frac{t_o}{H}\left(\frac{dH}{d\theta}\right) \qquad \text{(B)}$$

Sensing elements—output is represented by $\phi_{(t,\, l \text{ or } F)1}$ where the first subscript, t, l or F, refers to temperature, level or flow, respectively, and the second subscript "1," stands for output of the sensing element.

Temperature—(first-order transfer function): → φt

$$\frac{d\phi_{t1}}{d\theta} = \frac{t_o - \phi_{t1}}{\tau_t} \qquad \text{(C)}$$

ST φt

SDT

SDDT φt

Level—(second-order transfer function):

$$\frac{d\phi'_{l1}}{d\theta} = \frac{G_l H}{\tau_l^2} - \frac{2\zeta_l}{\tau_l}\phi'_{l1} - \frac{\phi_{l1}}{\tau_l^2} \qquad \text{(D)}$$

ζ =

ω =

$$d\phi_{l1}/d\theta = \phi'_{l1} \qquad \text{(E)}$$

Flow—(second-order transfer function):

SDDF

SF

$$\frac{d\phi'_{F1}}{d\theta} = \frac{G_F F_o}{\tau_F^2} - \frac{2\zeta_F}{\tau_F}\phi'_{F1} - \frac{\phi_{F1}}{\tau_F^2} \qquad \text{(F)}$$

$$d\phi_{F1}/d\theta = \phi'_{F1} \qquad \text{(G)}$$

SDF

Controller output is represented by $\phi_{(t,\, l \text{ or } F)2}$ where the first subscript, t, l or F refers to temperature, level or flow, respectively, and the second subscript, "2," stands for output of the controller.

Temperature—(PID controller*):

$$\frac{d\phi'_{t1}}{d\theta} = \left(\frac{dt_o}{d\theta} - \frac{d\phi_{t1}}{d\theta}\right)\Big/\tau_t \qquad \text{(H)}$$

SDDT

CDT2 PID

$$\frac{d\phi_{t2}}{d\theta} = \frac{K_{ct}(AXN)}{(SPAN)}\left\{\frac{(\phi_{t1} - SP_t)}{T_{it}} + \frac{d\phi_{t1}}{d\theta} + T_d\frac{d\phi'_{t1}}{d\theta}\right\} \qquad \text{(I)}$$

Level—(proportional controller):

$$\phi_{l2} = \left(\frac{K_{cl}(AXN)}{(SPAN)}\right)(\phi_{l1} - SP_l) + R_l \qquad \text{(J)}$$

2LP

$$\frac{d\phi_{l2}}{d\theta} = \frac{K_{cl}(AXN)}{(SPAN)}\left(\frac{d\phi_{l1}}{d\theta}\right) \qquad \text{(K)}$$

CDLP

Flow—(PI controller*):

CFPI

$$\frac{d\phi_{F2}}{d\theta} = \frac{K_{cF}(AXN)}{(SPAN)}\left\{\left(\frac{d\phi_{F1}}{d\theta} - \frac{d\phi_{l2}}{d\theta}\right) + \frac{\phi_{F1} - \phi_{l2}}{T_{iF}}\right\} \qquad \text{(L)}$$

Control valves:

Temperature:

$$P_{2t} = g(H) = [(H - 2)/2.31] + 14.7 \qquad \text{(M)}$$

$$S_i = \phi_{t2} C_{v2}\sqrt{P_{1t} - P_{2t}} \qquad \text{(N)}$$

Flow:

$$P_{1F} = g(H, F_o, C) = [(H - 2)/2.31] + 14.7 \qquad \text{(O)}$$

$$F_o = \phi_{F2} C_{vF}\sqrt{P_{1F} - P_{2F}} \qquad \text{(P)}$$

We must set up our algorithm to solve the differential equations. Then, we solve the algebraic equations because we are predicting the values at $(\theta + \Delta\theta)$ from values at θ in the differential equations. Finally, we can solve the algebraic equations directly at $(\theta + \Delta\theta)$.

A Fortran program was written for this example, which also contained the variable locations for the arrays Y and f of the model. Fig. 7 illustrates the response of the water-heater system for the upset condition and controller settings used to correct for the upset.

The next article in this CE REFRESHER series will appear in the issue of May 3, and will cover modeling and optimization for the control of heat-transfer systems including heat exchangers.

Steven Danatos, Editor

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*PID = proportional + integral + derivative action; PI = proportional + integral action.

CE REFRESHER: PROCESS DYNAMICS/6[†]

Modeling heat-transfer systems

The equations that model heat-transfer systems in batch or continuous equipment must allow for isothermal or nonisothermal heat exchange between process fluids and heat-transfer media.

John L. Guy, Dynamod Enterprises

☐ The dynamic modeling of heat-transfer equipment involves energy flow and temperature, both varying with time at a fixed point in space. We will look at two basic modeling-concepts: (1) the process is intended to rate in the manner so described, i.e., a batch-type cess, and (2) the process is *not* intended to operate with transient variations, i.e., a continuous process undergoing upset.

Batch processes

The reasons, as listed by Kern,* for choosing a batch heat-transfer operation rather than a continuous one are that the:

- Liquid being processed for the product is not continuously available.
- Heating or cooling medium to the equipment is not continuously available.
- Reaction-time or treating-time requirements necessitate holdup.
- Economics of intermittently processing a large batch justify the accumulation of a small continuous stream.
- Cleaning or regeneration procedure takes up a significant part of the total operating period.
- Simplified operation of most batch processes is advantageous.

Let us review some of the common batch operations considered by Kern for which manual calculations are suitable. The heat-transfer coefficients for these are considered constant, and the physical properties are calculated at some average temperature. These examples are all concerned with the heating or cooling of liquid hes. For liquid batches, we will consider the use of thermal and nonisothermal exchange media for jacketed vessels and for external heat-exchangers. Such procedures applied to inherently batch processes are also applicable to the startup of continuous processes.

Jacketed vessel: isothermal medium

The liquid contents of a jacketed tank are being heated by steam condensing in the jacket, as shown in Fig. 1a. The relationships that will be developed are also valid for a heating or cooling coil inside the tank. We can use the same equations for cooling the tank contents via an isothermal boiling fluid—the only change being a negative heat duty that indicates heat transfer is occurring in the opposite direction.

Letting q Btu equal the energy transferred to M lb of liquid having a heat capacity C_p Btu/(lb)(°F), we have:

$$\frac{dq}{d\theta} = MC_p\left(\frac{dt}{d\theta}\right) \qquad (1)$$

where t is temperature of liquid, °F, and θ is time, h.

For an agitated batch, we can assume that the tank temperature varies with time but not with position. For a given time, θ, we can therefore write:

$$dq/d\theta = UA(T - t) \qquad (2)$$

where U is the overall heat-transfer coefficient, Btu/(h)(ft^2)(°F); A is heat-transfer surface, ft^2; and T is temperature in the jacket, °F.

By combining Eq. (1) and (2), we can solve for the time θ to heat the liquid from t_1 to t_2:

$$MC_p(dt/d\theta) = UA(T - t) \qquad (3)$$

$$\int_0^\theta d\theta = \int_{t_1}^{t_2} \frac{MC_p}{UA}\frac{dt}{(T - t)} \qquad (4)$$

$$\left.\begin{aligned}\theta &= -\frac{MC_p}{UA}\ln\left[\frac{T - t_2}{T - t_1}\right]\\ \theta &= \frac{MC_p}{UA}\ln\left[\frac{T - t_1}{T - t_2}\right]\end{aligned}\right\} \qquad (5)$$

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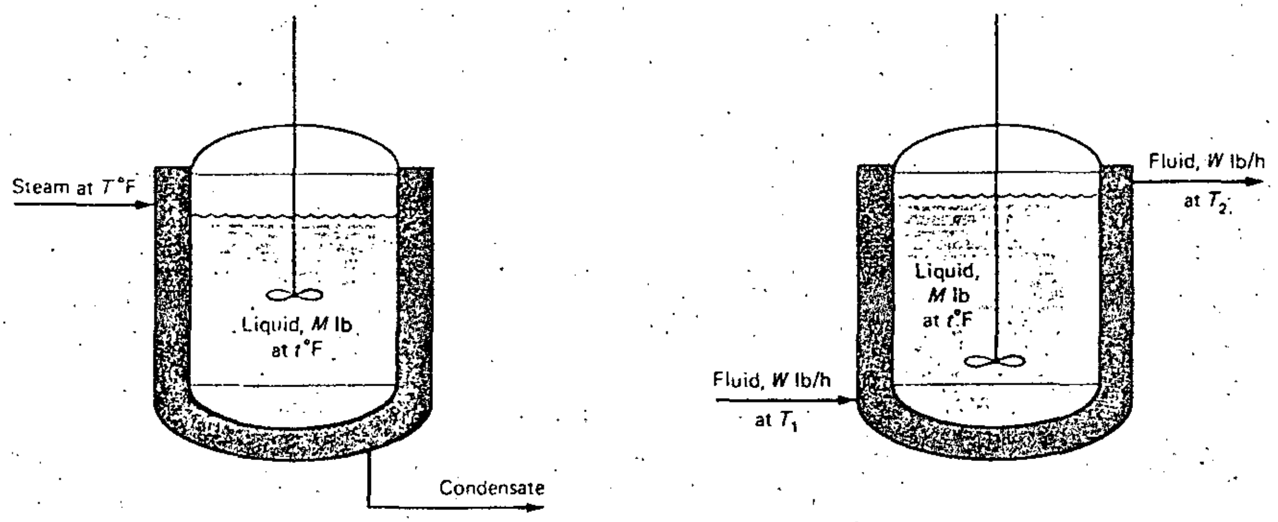
*Kern, D. Q., "Process Heat Transfer," McGraw-Hill, New York, 1950.

[†] Articles published thus far in this CE REFRESHER: Part 1, June 29, 1981, p. 74; Part 2, Aug. 24, 1981, p. 111; Part 3, Nov. 16, 1981, p. 271; Part 4, Dec. 28, 1981, p. 63; Part 5, Mar. 8, 1982, p. 97.



a. Isothermal exchange medium

b. Nonisothermal exchange medium

Heating or cooling a liquid batch in a jacketed vessel **Fig. 1**

Example 1—Let us calculate the time required to cool 10,000 lb of liquid water from 300°F to 250°F by generating atmospheric steam at 212°F—given $U = 100$ Btu/(h)(ft^2)(°F), and $A = 100$ ft^2, and $C_p = 1$ Btu/(lb)(°F).

Substituting the appropriate quantities into Eq. (5), we find:

$$\theta = \frac{(10{,}000)(1)}{(100)(100)} \ln\left[\frac{212 - 300}{212 - 250}\right] = 0.84 \text{ h}$$

We can also calculate the total heat transferred, q, the total steam generated, V, maximum heat transferred, q_{max}, and maximum steam rate, V_{max}, as:

$$q = 10{,}000(1)(300 - 250) = 500{,}000 \text{ Btu}$$
$$V = 500{,}000/970.3 = 515 \text{ lb}$$
$$q_{max} = (100)(100)(300 - 212) = 880{,}000 \text{ Btu/h}$$
$$V_{max} = 880{,}000/970.3 = 907 \text{ lb/h}$$

In these computations, we use 970.3 Btu/lb as the heat of vaporization for steam at 212°F.

Jacketed vessel: nonisothermal medium

The contents of a jacketed tank are being heated or cooled by a circulating fluid (undergoing no phase change) in the jacket, as shown in Fig. 1b. Again, the relationships can be applied to a heating or cooling coil inside a tank. For a constant circulating flowrate, the outlet temperature, T_2, varies with time. A heat balance for the liquid batch and the heat-transfer medium yields:

$$\frac{dq}{d\theta} = MC_{pi}\left(\frac{dt}{d\theta}\right) \qquad (6)$$

$$dq/d\theta = W_o C_{po}(T_2 - T_1) \qquad (7)$$

For a uniform temperature, t, in the tank, we can write:

$$dq/d\theta = UA(LMTD)$$

$$\frac{dq}{d\theta} = UA\left[\frac{(T_1 - t) - (T_2 - t)}{\ln\left(\frac{T_1 - t}{T_2 - t}\right)}\right] \qquad (8)$$

We can eliminate the variable T_2 by equating Eq. (7) and (8) to get:

$$T_2 = t + \frac{T_1 - t}{\exp(UA/W_o C_{po})} \qquad (9)$$

Equating Eq. (6) and (7), substituting the expression for T_2 from Eq. (9), performing the necessary integration, and rearranging, we can obtain the time, θ, that is necessary to heat or cool M lb of liquid from t_1 to t_2 as:

$$\theta = \frac{MC_{pi}}{WC_{po}}\left[\frac{\exp(UA/WC_{po}) - 1}{\exp(UA/WC_{po})}\right] \ln\left[\frac{T_1 - t_1}{T_1 - t_2}\right] \qquad (10)$$

Example 2—Let us calculate the time required to cool the same batch as in Example 1, from 250°F to 120°F, by using cooling water at 90°F and at a circulation rate of 50 gpm (equivalent to 25,000 lb/h). For this example, let $U = 75$ Btu/(h)(ft^2)(°F).

We solve the following terms from Eq. (10):

$$\frac{UA}{WC_{po}} = \frac{75(100)}{25{,}000(1)} = 0.3$$

$$\exp(UA/WC_{po}) = \exp(0.3) = 1.350$$

Using these values and the appropriate data for the example, we substitute them into Eq. (10):

$$\theta = \left(\frac{10{,}000(1)}{25{,}000(1)}\right)\left(\frac{1.35 - 1}{1.35}\right) \ln\left(\frac{90 - 250}{90 - 120}\right) = 0.174 \text{ h}$$

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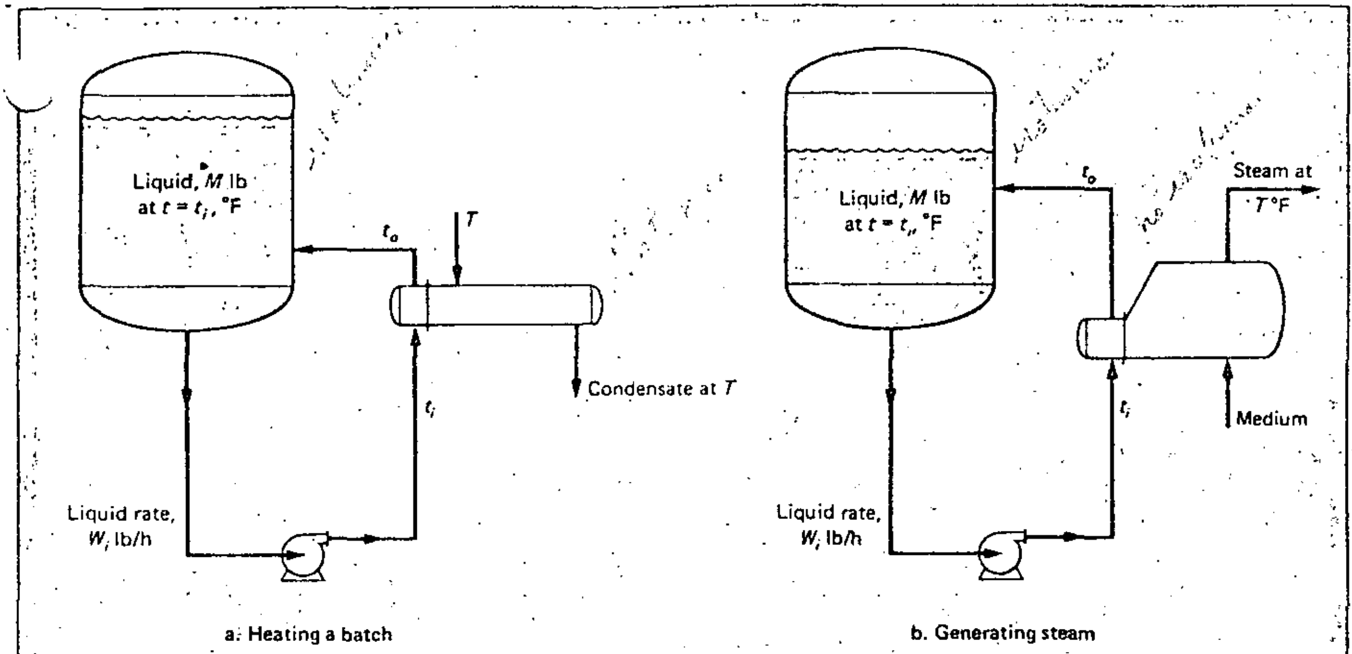


Isothermal heating or cooling with external heat exchanger **Fig. 2**

Next, we obtain the maximum outlet temperature for the cooling water at time θ equal to zero, from Eq. (9):

$$T_2 = 250 + \frac{(90 - 250)}{1.35} = 131.5°\text{F}$$

Based on this outlet temperature, the total annual operating time and the materials of construction, we can now decide whether we need a higher cooling-water circulation rate to reduce the initial temperature rise of the cooling water.

External exchanger: isothermal medium

A batch of liquid in a tank is being heated in an external heat exchanger by a fluid condensing on the shellside of the exchanger, as shown in Fig. 2a. We have now added these variables: the circulation rate of the fluid being heated, W_i, lb/h; and t_i and t_o, the inlet and outlet temperatures to and from the exchanger. The variable t_i is also the temperature in the tank.

We will again start with a heat balance, eliminate the variable t_o, integrate the resulting equations, and rearrange to solve for the time, θ, needed to heat the fluid from t_1 to t_2. The results are:

$$\left.\begin{aligned}\frac{dq}{d\theta} &= MC_{pi}\frac{dt}{d\theta} = W_iC_{pi}(t_o - t_i)\\ \frac{dq}{d\theta} &= UA(LMTD) = UA\left[\frac{(T - t_o) - (T - t_i)}{\ln\left[\dfrac{T - t_o}{T - t_i}\right]}\right]\end{aligned}\right\} \quad (11)$$

$$t_o = T - \frac{(T - t_i)}{\exp(UA/W_iC_{pi})} \quad (12)$$

$$\theta = \frac{M}{W_i}\left[\frac{\exp(UA/W_iC_{pi})}{\exp(UA/W_iC_{pi}) - 1}\right]\ln\left[\frac{T - t_1}{T - t_2}\right] \quad (13)$$

Example 3—We will rework Example 1 for the process shown in Fig. 2b. Let the circulation rate equal 10 gpm (5,000 lb/h), $U = 200$ Btu/(h)(ft^2)(°F), and $A = 100$ ft^2.

We begin by solving the following terms of Eq. (13):

$$\frac{UA}{W_iC_{pi}} = \frac{(200)(100)}{(5{,}000)(1)} = 4$$

$$\exp(UA/W_iC_{pi}) = \exp(4) = 54.6$$

Now, by substituting the numerical values for these terms and other applicable data into Eq. (13), we calculate the required time, θ, initial shellside fluid temperature, $t_{o(init)}$, maximum heat transferred, q_{max}, and maximum steam rate, V_{max}, as:

$$\theta = \frac{10{,}000}{5{,}000}\left(\frac{54.6}{53.6}\right)\ln\left[\frac{212 - 300}{212 - 250}\right] = 1.71 \text{ h}$$

$$t_{o(init)} = 212 - \frac{(212 - 300)}{54.6} = 213.6°\text{F}$$

$$q_{max} = W_iC_{pi}(t_o - t_i)$$

$$q_{max} = 5{,}000(1)(300 - 213.6) = 432{,}000 \text{ Btu/h}$$

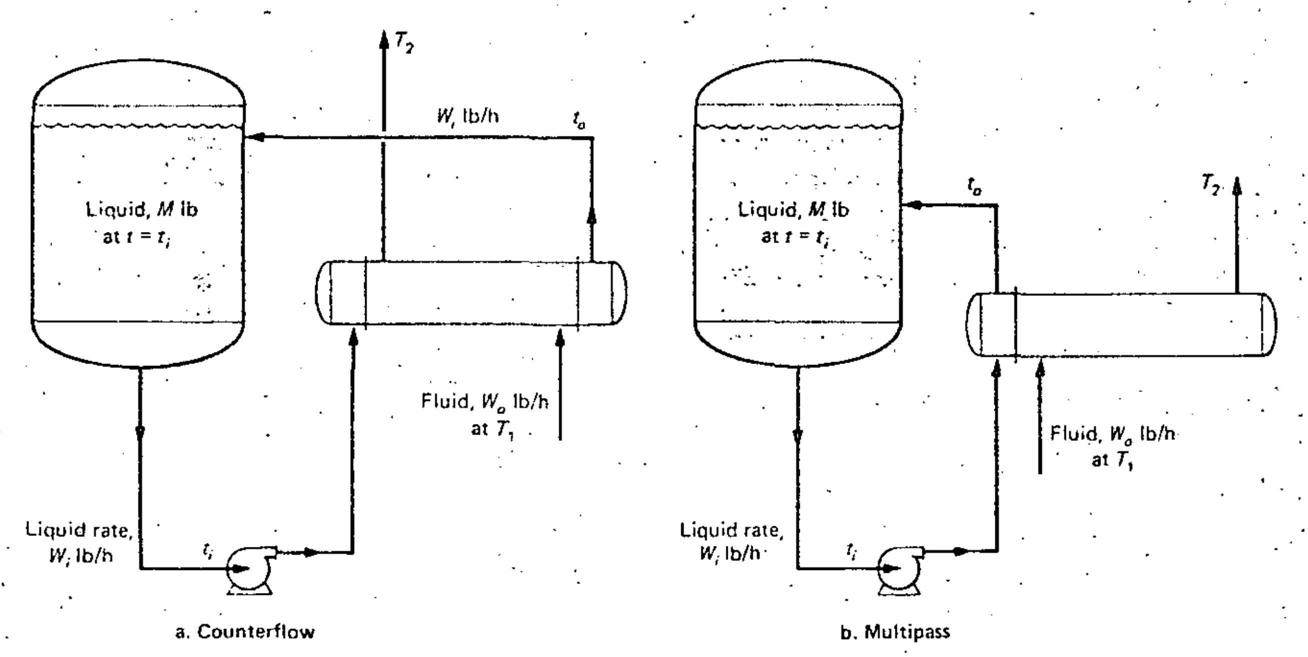
$$V_{max} = 432{,}000/970.3 = 445 \text{ lb/h}$$

If we double the circulation rate, the time to accomplish the total cooling is about the same as for Example 1. (Note: This example does not prove that jacketed vessels are superior to external exchangers.)

External exchanger: nonisothermal medium

For external exchangers using a nonisothermal medium, we will consider two situations: a counterflow arrangement, and a multiple-pass one.

Counterflow—The equipment and its arrangement that we will now simulate is shown in Fig. 3a. The equations that model the system follow. Unfortunately,



a. Counterflow

b. Multipass

Nonisothermal heating or cooling with external exchanger **Fig. 3**

we will have to calculate the outlet temperatures, t_o and T_2, by trial and error from Eq. (15) and (16).

$$\frac{dq}{d\theta} = MC_{pi}\frac{dt}{d\theta} = W_iC_{pi}(t_o - t_i) = W_oC_{po}(T_1 - T_2)$$

$$\frac{dq}{d\theta} = UA\left[\frac{(T_2 - t_i) - (T_1 - t_o)}{\ln[(T_2 - t_i)/(T_1 - t_o)]}\right] \qquad (14)$$

$$\frac{W_iC_{pi}}{UA}(t_o - t_i) = \frac{(T_2 - t_i) - (T_1 - t_o)}{\ln[(T_2 - t_i)/(T_1 - t_o)]} \qquad (15)$$

$$T_2 = T_1 - \frac{W_iC_{pi}}{W_oC_{pi}}(t_o - t_i) \qquad (16)$$

$$\theta = \frac{M}{W_iW_oC_{po}} \times \left[\frac{W_iC_{pi}\left\{\exp\left[UA\left(\frac{1}{W_iC_{pi}} - \frac{1}{W_oC_{po}}\right)\right]\right\} - W_oC_{po}}{\exp\left\{UA\left[\left(\frac{1}{W_iC_{pi}}\right) - \left(\frac{1}{W_oC_{po}}\right)\right]\right\} - 1}\right] \times \ln[(T_1 - t_1)/T_1 - t_2)] \qquad (17)$$

Example 4—Let us solve Example 2 for an external exchanger having a counterflow arrangement. We will assume $U = 150$ Btu/(h)(ft^2)(°F), $A = 100$ ft^2, $W_i = 10$ gpm (5,000 lb/h), and $W_o = 50$ gpm (25,000 lb/h). We calculate the following terms in Eq. (17):

$$UA\left[\frac{1}{W_iC_{pi}} - \frac{1}{W_oC_{po}}\right] =$$

$$150(100)\left[\frac{1}{5{,}000(1)} - \frac{1}{25{,}000(1)}\right] = 2.4$$

$$\exp(2.4) = 11.023$$

We make the necessary substitutions into Eq. (17) to find the required cooling time:

$$\theta = \frac{10{,}000}{5{,}000(25{,}000)(1)} \times \left[\frac{5{,}000(1)(11.023) - 25{,}000(1)}{11.023 - 1}\right]\ln\left(\frac{90 - 250}{90 - 120}\right)$$

$$\theta = 0.402 \text{ h}$$

Solving Eq. (15) and (16) by trial and error, we find the initial temperatures $T_2 \cong 120$°F, and $t_o \cong 102$°F.

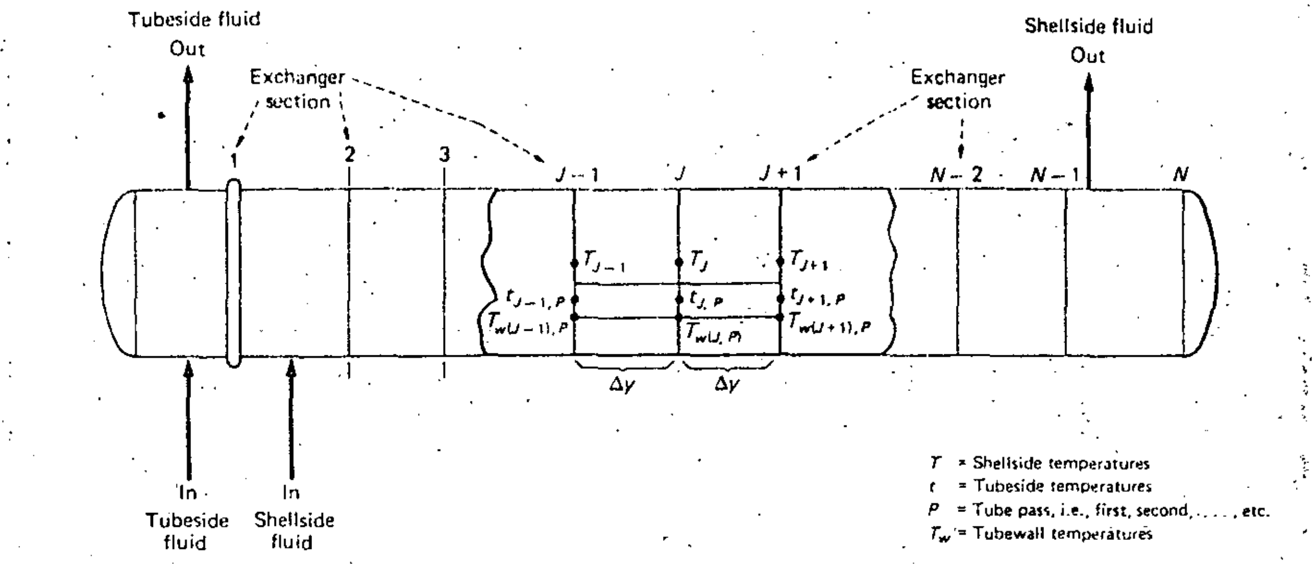
Multipass exchanger—The equipment and its arrangement that we will model is shown in Fig. 3b. We must now add a temperature-correction factor, F, to our calculations (this makes the algebra more tedious). However, we can calculate the time, θ, directly. For the initial exchanger conditions, the solution is again trial and error. We can add the F-factor from charts rather than algebraically to perhaps save some calculation work. The procedure for calculating time, θ, is:

$$\left.\begin{aligned} \frac{dq}{d\theta} &= MC_{pi}\frac{dt}{d\theta} = W_iC_{pi}(t_o - t_i) \\ &= W_oC_{po}(T_1 - T_2) \\ &= UAF\left[\frac{(T_2 - t_i) - (T_1 - t_o)}{\ln\left(\frac{T_2 - t_i}{T_1 - t_o}\right)}\right] \end{aligned}\right\} \qquad (18)$$

$$R = W_iC_{pi}/W_oC_{po} \qquad (19)$$

$$K = \exp\left[\frac{UA}{W_iC_{pi}}\sqrt{R^2 + 1}\right] \qquad (20)$$

$$S = \frac{2(K - 1)}{K(R + 1 + \sqrt{R^2 + 1}) - (R + 1 - \sqrt{R^2 + 1})} \qquad (21)$$



Parameters for modeling a multipass parallel-flow heat exchanger **Fig. 4**

$$F = \frac{\sqrt{R^2+1}\,\ln\left(\dfrac{1-S}{1-RS}\right)}{(R-1)\ln\left\{\dfrac{2-S[(R+1)-\sqrt{R^2-1}]}{2-S[(R+1)+\sqrt{R^2+1}]}\right\}} \quad (22)$$

$$\theta = \frac{M}{SW_i}\ln\left(\frac{T_1-t_1}{T_1-t_2}\right) \quad (23)$$

Example 5—Let us solve Example 4, using a multipass exchanger that increases U to 200 Btu/(h)(ft^2)(°F).

We calculate the values for R, K and S by substituting appropriate values into Eq. (19), (20) and (21), respectively; and get:

$$R = 0.2,\ K = 59.1,\ S = 0.887$$

We can now make the appropriate numerical substitutions into Eq. (23) to calculate the time for cooling:

$$\theta = \frac{10{,}000}{0.887(5{,}000)}\ln\left[\frac{90-250}{90-120}\right] = 3.77\text{ h}$$

In this example, the increased value for the heat-transfer coefficient, U, does not compensate for the temperature correction factor.

Continuous heat-transfer processes

In Part 1 (*Chem. Eng.*, June 29, 1981, p. 77), we derived expressions for a heat-exchanger tube with a sensible liquid being heated on the tubeside by condensing steam on the shellside of the exchanger. The constant temperature of the shellside fluid simplified the derivation of the model because there was one less differential equation than in the sensible-sensible case. If we add a multipass exchanger to the sensible-sensible case, we have increased the computational difficulty even more. The model derived in Part 1 contains two partial-differential equations and is very difficult, if not impossible, to solve manually without creating more complications, however, with computers to perform the calculations, however, we can solve such problems by numerical methods. Using the same derivation as in Part 1, and depending on the service conditions, we can set up the following equations:

- Tubeside: sensible (no phase change)

$$\frac{\frac{\pi}{4}\rho_i d_i^2}{144}C_p\frac{\partial t}{\partial\theta} = \frac{h_i\pi d_i}{12}(T_w - t) - \rho_i v_i\frac{\frac{\pi}{4}d_i^2}{144}C_p\frac{\partial t}{\partial Y} \quad (24)$$

- Tubeside: isothermal condensing or boiling

$$-\lambda\frac{dV}{dY} + h_i\frac{\pi d_i}{12}(T_w - t) = 0 \quad (25)$$

- Shellside: sensible (no phase change)

$$\rho_o A_o C_{po}\frac{\partial T}{\partial\theta} = -\rho_o v_o A_o C_{po}\frac{\partial T}{\partial Y} - \frac{nh_o\pi d_o}{12}(T - T_w) \quad (26)$$

- Shellside: isothermal condensing or boiling

$$\lambda\frac{dV}{dY} + h_o\frac{\pi d_o}{12}(T - T_w) = 0 \quad (27)$$

- Tubewall

$$\rho_w\frac{(d_o^2 - d_i^2)}{4\times 144}C_{pw}\frac{dT_w}{d\theta} = \frac{h_o d_o}{12}(T - T_w) - \frac{h_i d_i}{12}(T_w - t) \quad (28)$$

where A_o = shellside flow area, ft^2; C_p = heat capacity, Btu/(lb)(°F); d = diameter, in.; h = heat-transfer coefficient, Btu/(h)(ft^2)(°F); t = temperature of tubeside fluid, °F; T = temperature of shellside fluid, °F; T_w = temperature of the tubewall, °F; v = fluid velocity, ft/h; V = vapor generated, lb/h; Y = tube length, ft; ρ = density, lb/ft^3; λ = heat of vaporization, Btu/lb; and θ = time, h. And where the subscript i = inside or tubeside, o = outside or shellside, and w = tubewall.

The convention adopted here is that heat is flowing from the shellside to the tubeside. We have also assumed parallel flow in the shellside of the exchanger, and are not modeling the tortuous path that the fluid actually makes in a cross-baffled exchanger. We can extend Eq. (25) and (27) to condensing or boiling a mixture of components. This will cause us to consider changes in the temperature and the individual coefficients as a function of tube length.

The only difficulty with Eq. (24) to (28) is that the steady-state solutions (at $\theta = \infty$) do not agree exactly with the generally accepted design equations. We have omitted the resistance due to the tubewall. While this resistance is not a large percentage of the total resistance to heat transfer, it would be appropriate to remove this slight discrepancy. The exact procedure is to calculate a heat balance across a differential segment of the tubewall. The resulting equation is given by:

$$\frac{dT_w}{d\theta} = \frac{k_w}{C_{pw}\rho_w}\left[\frac{\partial^2 T_w}{\partial R^2} + \frac{1}{R}\frac{\partial T_w}{\partial R}\right] \qquad (29)$$

However, this procedure involves a lot more work in setting up the computer program. In all but the most precise work, the following approach is recommended.

As was indicated in Part 1 of this series, the inside and outside coefficients include a resistance due to fouling. In the same manner, we can include the resistance of the tubewall. If we add half of this resistance to both the inside and outside coefficients, we can calculate (manually or by machine) composite coefficients that will agree with the standard solutions calculated by steady-state methods.

The composite coefficients are given by:

$$h_i = \left[\frac{1}{h_i} + R_{di} + \frac{d_i(d_o - d_i)}{12k_w(d_o + d_i)}\right]^{-1} \qquad (30)$$

$$h_o = \left[\frac{1}{h_o} + R_{do} + \frac{d_o(d_o - d_i)}{12k_w(d_o + d_i)}\right]^{-1} \qquad (31)$$

The most common approach in solving partial-differential equations is to convert the variables, other than time, to finite-difference equations. The resulting equations are then solved by one of several numerical-integration methods such as those discussed in Part 5 (*Chem. Eng.*, Mar. 8, 1982, pp. 98–101).

Let the exchanger shown in Fig. 4 be partitioned into N sections. For each section, we can write the equivalent form of Eq. (24) to (28). For convenience in writing these equations, we will use the following notation:

$A_i = (\pi d_i^2/4 \times 144)\rho_i C_{pi}$
$B_i = h_i \pi d_i/12$
$C_i = (\rho_i v_i \pi d_i^2/4 \times 144)C_{pi}$
P = Pass, i.e., first, second, third, . . . , number of tube passes

$$\frac{dt_{J,P}}{d\theta} = \frac{B_i(T_{w(J,P)} - t_{J,P})}{A_i} + \frac{(-1)^P C_i}{A_i}\left[\frac{t_{J+1,P} - t_{J-1,P}}{2\Delta Y}\right] \qquad (32)$$

$$\frac{dv_i}{dY} = \frac{h_i \pi d_i}{12\lambda}(T_{w(J,P)} - t_{J,P}) \qquad (33)$$

$$\frac{dT_J}{d\theta} = \sum_{P=1}^{N_{Pt}}\left\{\frac{B_o}{A_o}\left[T_J - T_{w(J,P)}\right]n\right\} + \frac{C_o}{A_o}\left[\frac{T_{J+1} - T_{J-1}}{2\Delta Y}\right] \qquad (34)$$

where N_{Pt} = number of tube passes/shell, n = number of tubes/pass, and:

$A_o = \rho_o A_o C_{po}$
$B_o = -(h_o \pi d_o/12)$
$C_o = -\rho_o v_o A_o C_{po}$

$$\frac{dv_o}{dY} = \sum_{P=1}^{N_{Pt}} \frac{h_o \pi d_o}{12\lambda}\left[T_J - T_{w(J,P)}\right]n \qquad (35)$$

$$\frac{dT_{w(J,P)}}{d\theta} = \frac{B_w}{A_w}(T_J - T_{w(J,P)}) - \frac{C_w}{A_w}(T_{w(J,P)} - t_{J,P}) \qquad (36)$$

where:

$A_w = [\rho_w C_{pw}(d_o^2 - d_i^2)]/4 \times 144$
$B_w = h_o d_o/12$
$C_w = h_i d_i/12$

In the last section (N in Fig. 4) of the exchanger, we need to replace Eq. (32) and (34) with the forward difference for the derivative instead of the central difference. These equations become:

$$\frac{dt_{N,P}}{d\theta} = \frac{B_i(T_{w(N,P)} - t_{N,P})}{A_i} + \frac{(-1)^P C_i}{A_i}\left(\frac{t_{N,P} - t_{N-1,P}}{\Delta Y}\right) \qquad (37)$$

$$\frac{dT_N}{d\theta} = \sum_{P=1}^{N_{Pt}}\left\{\frac{B_o}{A_o}\left[T_N - T_{w(N,P)}\right]n\right\} + \frac{C_o}{A_o}\left(\frac{T_N - T_{N-1}}{\Delta Y}\right) \qquad (38)$$

A computer program was written to simulate Example 5. This program handled the numerous trial-and-error computations for solving the model equations, and illustrates the method that we have described for continuous systems.

The next article in this CE REFRESHER series will appear in the issue of June 28, and will cover the modeling and optimization of chemical-reactor systems.

Steven Danatos, Editor

The author

John L. Guy founded Dynamod Enterprises, P.O. Box 240, Swarthmore, PA 19081 [Phone: (215) 328-4545] to market a rigorous dynamic multicomponent-distillation computer program and to provide consulting services to the petrochemical industry. He has had over ten years of industrial experience with Union Carbide Corp. and Atlantic Richfield Co. He has a B.S. in chemical engineering from Ohio State University and an M.S. in chemical engineering from West Virginia University. He is a member of AIChE, and a part-time instructor at Widener University.

Dynamic modeling of tank-type reactor systems

A step-by-step analysis for tank-type reactors, their control and flow systems, and the associated kinetics of the reactions shows how to develop a mathematical model to represent the process.

*John L. Guy, Dynamod Enterprises**

☐ In Parts 3 and 4[†] of this series, when we reviewed the dynamic equations for a plug-flow or pipe reactor and a batch reactor, we did not account for energy balances, or for the dynamics introduced by a control system or external or internal heat-exchange equipment. In those articles, we were essentially involved only with preliminary material-balance calculations. Let us now look at the dynamic modeling of reactor systems.

Tank-type reactor systems

The esterification of an alcohol and an acid proceeds according to the following reaction:

$$A + B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} C + D$$

As an example, let us consider the esterification of ethyl alcohol and acetic acid:

$$C_2H_5OH + CH_3COOH \rightleftharpoons C_2H_5 \cdot OCCH_3 + H_2O$$

The kinetics for the reaction is given by:

$$R = k_1 C_A C_B - k_2 C_C C_D \tag{1}$$

The equilibrium constant, K_e, for the reaction is:

$$K_e = k_1/k_2 \tag{2}$$

Combining Eq. (1) and (2) eliminates the reaction-rate constant k_2, so we obtain:

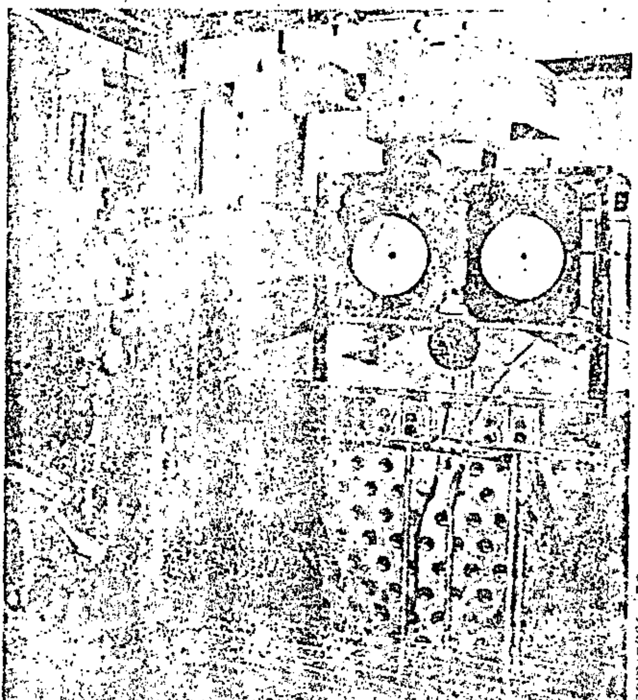
$$R = k_1\left[C_A C_B - \frac{C_C C_D}{K_e}\right] \tag{3}$$

From thermodynamics, we obtain an expression for the equilibrium constant K_e as a function of temperature. We can also express k_1 as a function of temperature. Hence, we can obtain the rate constants as functions of temperature:

$$K_e = f_1(T) \tag{4}$$

$$k_2 = f_1(T) \tag{5}$$

The figure shows a possible control scheme (for the esterification process) that we will use to develop the



Stirred-tank reactors in a process plant

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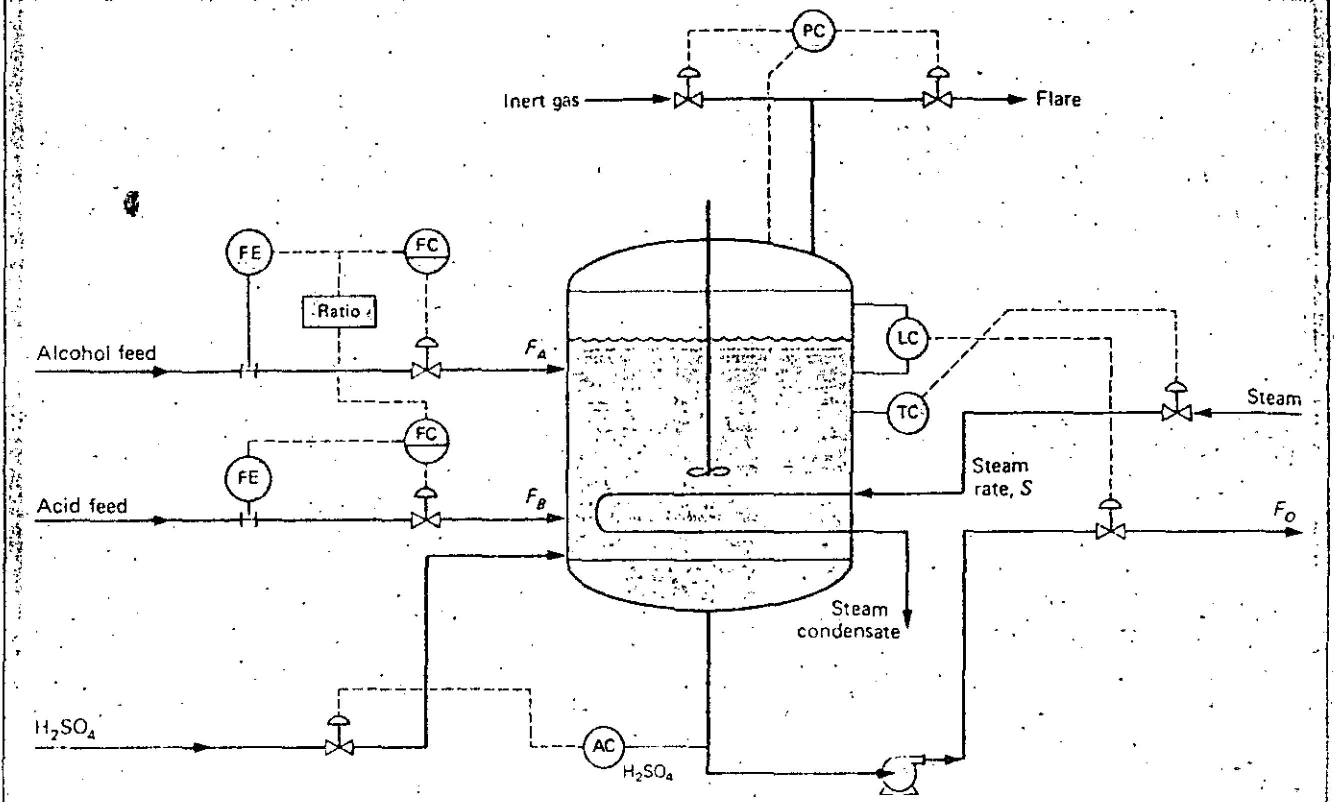
[*] To meet the author, see *Chem. Eng.*, May 3, p. 98.

[†] [illegible] CE Refresher series, see index [illegible] p. 56 of [illegible]



Control scheme for a tank-type reactor system for an esterification process

required equations. A material balance for each component yields:

$$F_A - RV = F_O X_A + \frac{d(V\rho X_A)}{d\theta} \tag{6}$$

$$F_B - RV = F_O X_B + \frac{d(V\rho X_B)}{d\theta} \tag{7}$$

$$+RV = F_O X_C + \frac{d(V\rho X_C)}{d\theta} \tag{8}$$

$$+RV = F_O X_D + \frac{d(V\rho X_D)}{d\theta} \tag{9}$$

By changing the expression for the kinetic rate from a function of concentration X, moles component/ft^3, to mole fraction, x, we obtain:

$$R = \frac{k_1}{\rho^2}\left[x_A x_B - \frac{x_C x_D}{K_e}\right] \tag{10}$$

Simulating the heat-exchanger coil is simplified because of an isothermal condition on both sides of the exchanger. Here, we can assume that the fluid temperatures do not vary with position (but can vary with time). Therefore, we do not have to sectionalize (i.e., use a finite-difference approach) the exchanger bundle. The energy balance equations for the condensing steam (tubeside), the tubewall, and the reaction mixture are given by:

$$-\lambda S + h_i A_i (T_w - t) = 0 \tag{11}$$

$$\frac{n\pi}{4}\left[\frac{(d_o^2 - d_i^2)}{144}\right] L \rho_w C_{pw} \frac{dT_w}{d\theta} = h_o A_o (T - T_w) - h_i A_i (T_w - t) \tag{12}$$

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$$F_AH_A + F_BH_B + h_oA_o(T_w - T) - R\,\Delta H_r = F_OH_O + \frac{d(\rho VC_pT)}{d\theta} \quad (13)$$

Control loop simulations

For each control loop, we can write the differential equations (see Part 2, *Chem. Eng.*, Aug. 24, 1981, p. 111) for the sensing element, the controller, and the control valve. The pressure-control loop will have little effect on the normal operation of this reactor. If we were simulating a reaction that removed one of the components in the vapor phase or in the study of emergency operating conditions, we would not be able to make this simplifying assumption.

The addition of the sulfuric acid catalyst is shown as a control loop, and the process operation might be this sophisticated. Probably, addition of the catalyst will be with a small metering pump adjusted manually. Acid concentration can be measured in the process (online) via a titration apparatus, or sampled hourly and analyzed in the laboratory. This loop is not critical to the reaction system if we maintain a certain minimum acid concentration. However, we do want to measure the amount of acid catalyst supplied to the process because of its cost and the cost of neutralizing it.

Level control

For the level-control system with a PI (proportional and integral) controller, we can derive:

$$\tau_l^2\frac{d^2\phi_l}{d\theta^2} + 2\zeta_l\tau_l\frac{d\phi_l}{d\theta} + \phi_l = G_lH_T \quad (14)$$

$$\phi_l' = d\phi_l/d\theta \quad (14a)$$

$$\tau_l^2[d\phi_l'/d\theta] + 2\zeta_l\tau_l\phi_l' + \phi_l = G_lH_T \quad (14b)$$

$$\phi_{l2} = \frac{K_{cl}(AXN)_l}{(SPAN)_l}[\phi_l - (SP)_l] + \frac{K_{cl}(AXN)_l}{(SPAN)_l}\int\frac{[(\phi_l - (SP)_l]d\theta}{T_{il}} \quad (15)$$

$$\frac{d\phi_{l2}}{d\theta} = \frac{K_{cl}(AXN)_l}{(SPAN)_l}\left[\frac{d\phi_l}{d\theta} + \frac{\phi_l - (SP)_l}{T_{il}}\right] \quad (15a)$$

$$F_O = \phi_{l2}C_{vl}\sqrt{P_{1l} - P_{2l}} \quad (16)$$

where the subscript, *l*, in these equations represents the level-control system.

Temperature control

For the temperature-control loop with a PID (proportional-integral-derivative) controller, we will obtain:

$$\tau_T\frac{d\phi_T}{d\theta} + \phi_T = G_TT \quad (17)$$

$$\frac{d^2\phi_T}{d\theta^2} = \frac{1}{\tau_T}\left[G_T\frac{dT}{d\theta} - \frac{d\phi_T}{d\theta}\right] \quad (17a)$$

$$\phi_{T2} = \frac{K_{cT}(AXN)_T}{(SPAN)_T}\left\{[\phi_T - (SP)_T] + \frac{1}{\tau_{iT}}\int[\phi_T - (SP)_T]d\theta + T_d\frac{d[\phi_T - (SP)_T]}{d\theta}\right\} \quad (18)$$

$$\frac{d\phi_{T2}}{d\theta} = \frac{K_{cT}(AXN)_T}{(SPAN)_T}\left\{\frac{d\phi_T}{d\theta} + \frac{1}{\tau_{iT}}[\phi_T - (SP)_T] + T_d\frac{d^2\phi_T}{d\theta^2}\right\} \quad (18a)$$

$$S = \phi_{T2}C_{vT}\sqrt{[(P_{1T})^2 - (P_{2T})^2]/2} \quad (19)$$

One additional equation is needed to completely describe this control loop. This equation relates the tem-

Nomenclature

A_i	Heat-transfer area, inside	K_e	Equilibrium constant for chemical reaction
A_o	Heat-transfer area, outside	L	Tube length
(AXN)	Controller action	n	Number of tubes in reactor steam coil
C_A	Molar concentration of Reactant A	P_1	Upstream pressure of control valve
C_B	Molar concentration of Reactant B	P_2	Downstream pressure of control valve
C_C	Molar concentration of Product C	R	Rate of reaction
C_D	Molar concentration of Product D	S	Steam rate
C_p	Heat capacity of reactor mixture	$(SPAN)$	Controller span
C_{pw}	Heat capacity of tubewall	t	Steam-chest temperature
C_v	Control valve capacity	T	Reactor temperature
d_i, d_o	Inside and outside diameter	T_w	Tubewall temperature
F_A	Molar flowrate of Reactant A	T_i	Reset time of controller
F_B	Molar flowrate of Reactant B	T_d	Derivative time of controller
F_O	Molar flowrate of output stream	V	Reactor volume
G	Gain of sensing element	x	Mole fraction of Component A, B, C or D
h_i	Inside heat-transfer coefficient	ζ	Damping ratio of sensing element
h_o	Outside heat-transfer coefficient	θ	Time
H_A	Stream enthalpy for Reactant A	λ	Latent heat of steam
H_B	Stream enthalpy for Reactant B	ρ	Density of reaction mixture
H_O	Enthalpy for output stream	ρ_w	Density of tubewall metal
ΔH_r	Heat of reaction	τ	Time constant of sensing element
H_T	Liquid level in reactor	ϕ	Signal to controller from sensing element
k_1, k_2	Reaction-rate constants	ϕ_2	Controller output

perature of the condensing steam to the steam's operating pressure. Neglecting superheat of the steam, we can use the Antoine equation:

$$\ln P_2 = A' + \frac{B'}{t + C'} \quad (20)$$

where A', B' and C' are Antoine coefficients. ✱

Reactant flowrates

The equations for the flowrates of the two reactants are given by the following equations:

$$\tau_{FA}^2 \frac{d^2\phi_{FA}}{d\theta^2} + 2\zeta_{FA}\tau_{FA}\frac{d\phi_{FA}}{d\theta} + \phi_{FA} = G_{FA}F_A \quad (21)$$

$$\phi'_{FA} = d\phi_{FA}/d\theta \quad (21a)$$

$$\tau_{FA}^2[d\phi'_{FA}/d\theta] + 2\zeta_{FA}\tau_{FA}\phi'_{FA} + \phi_{FA} = G_{FA}F_A \quad (21b)$$

$$\phi_{FA2} = \frac{(K_c)_{FA}(AXN)_{FA}}{(SPAN)_{FA}}\left\{[\phi_{FA} - (SP)_{FA}] + \int \frac{[\phi_{FA} - (SP)_{FA}]d\theta}{(T_i)_{FA}}\right\} \quad (22)$$

$$\frac{d\phi_{FA2}}{d\theta} = \frac{(K_c)_{FA}(AXN)_{FA}}{(SPAN)_{FA}}\left\{\frac{d\phi_{FA}}{d\theta} + \frac{1}{T_{iFA}}[\phi_{FA} - (SP)_{FA}]\right\} \quad (22a)$$

$$F_A = \phi_{FA2}C_{vFA}\sqrt{(P_1)_{FA} - (P_2)_{FA}} \quad (23)$$

$$\tau_{FB}^2 \frac{d^2\phi_{FB}}{d\theta^2} + 2\zeta_{FB}\tau_{FB}\frac{d\phi_{FB}}{d\theta} + \phi_{FB} = G_{FB}F_B \quad (24)$$

$$\phi'_{FB} = d\phi_{FB}/d\theta \quad (24a)$$

$$\tau_{FB}^2 \frac{d\phi'_{FB}}{d\theta} + 2\zeta_{FB}\tau_{FB}\phi'_{FB} + \phi_{FB} = G_{FB}F_B \quad (24b)$$

$$(SP)_{FB} = \phi_{FA} \times (\text{Ratio}) \quad (25)$$

$$\phi_{FB2} = \frac{(K_c)_{FB}(AXN)_{FB}}{(SPAN)_{FB}}\left\{[\phi_{FB} - (SP)_{FB}] + \frac{1}{T_{iFB}}\int[\phi_{FB} - (SP)_{FB}]d\theta\right\} \quad (26)$$

$$\frac{d\phi_{FB2}}{d\theta} = \frac{(K_c)_{FB}(AXN)_{FB}}{(SPAN)_{FB}}\left[\frac{d\phi_{FB}}{d\theta} - (\text{Ratio})\frac{d\phi_{FA}}{d\theta} + \frac{\phi_{FB} - \phi_{FA}(\text{Ratio})}{T_{iFB}}\right] \quad (26a)$$

$$F_B = \phi_{FB2}C_{vFB}\sqrt{(P_1)_{FB} - (P_2)_{FB}} \quad (27)$$

Eq. (4) through (27) can be programmed as shown in Part 5 of this series (*Chem. Eng.*, Mar. 8, 1982, p. 97). Initial conditions can be obtained by setting the accumulation terms (i.e., the time-varying terms) to zero. We can further simplify the calculation procedure by assuming that the response of the second-order transfer functions [Eq. (14), (21) and (24)] are very fast in comparison with the other time constants of the system, and we can assume that the system measurements and the signals to the instruments are equal. This eliminates three differential equations.

The next article in this CE REFRESHER series will appear in the issue of Aug. 23, and will cover the dynamic modeling of a tubular reactor system.

Steven Danatos, Edito

Corrections

In Part 6 (May 3rd issue) of the Process Dynamics series, some errors occurred, which a number of readers pointed out by telephone or mail. The correct equations and answers to the examples are:

$$\frac{dq}{d\theta} = -MC_{pi}\left(\frac{dt}{d\theta}\right) \quad (6)$$

$$\theta = \frac{MC_{pi}}{WC_{po}}\left[\frac{\exp(UA/WC_{po})}{\exp(UA/WC_{po}) - 1}\right]\ln\left[\frac{T_1 - t_1}{T_1 - t_2}\right] \quad (10)$$

The time required to cool the batch in Example 2 (bottom of righthand column on p. 91, May 3rd issue) then becomes:

$$\theta = \left(\frac{10{,}000(1)}{25{,}000(1)}\right)\left(\frac{1.35}{1.35 - 1}\right)\ln\left(\frac{90 - 250}{90 - 120}\right) = 2.58 \text{ h}$$

$$\theta = \frac{M}{W_iW_oC_{po}} \times \left[\frac{W_oC_{po}\left\{\exp\left[UA\left(\frac{1}{W_iC_{pi}} - \frac{1}{W_oC_{po}}\right)\right]\right\} - W_iC_{pi}}{\exp\left\{UA\left[\left(\frac{1}{W_iC_{pi}}\right) - \left(\frac{1}{W_oC_{po}}\right)\right]\right\} - 1}\right] \times \ln[(T_1 - t_1)/T_1 - t_2)] \quad (17)$$

The time required to cool the batch in Example 4 (top of p. 96, righthand column) should be calculated by making the following substitutions into Eq. (17):

$$\theta = \frac{10{,}000}{5{,}000(25{,}000)(1)} \times \left[\frac{25{,}000(1)(11.023) - 5{,}000(1)}{11.023 - 1}\right]\ln\left(\frac{90 - 250}{90 - 120}\right)$$

$$\theta = 3.615 \text{ h}$$

$$F = \frac{\sqrt{R^2 + 1}\ln\left(\frac{1 - S}{1 - RS}\right)}{(R - 1)\ln\left\{\frac{2 - S[(R + 1) - \sqrt{R_2 + 1}]}{2 - S[(R + 1) + \sqrt{R_2 + 1}]}\right\}} \quad (22)$$

The equations are numbered as originally shown in Part 6, May 3, 1982.

CE REFRESHER: PROCESS DYNAMICS/8

Dynamic modeling of tubular reactor systems

Interpreting and incorporating the kinetics and thermodynamics of a chemical reaction leads to the development of a mathematical model that includes the flow and control systems for a tubular reactor.

*John L. Guy, Dynamod Enterprises**

☐ The dynamic modeling of reactor systems must take into account the energy balances, the dynamics introduced by a control system and those arising from external or internal heat-exchange equipment, and material balances.

In Part 7† of this series, we developed the model for a tank-type reactor system. Now, we will extend the modeling to a tubular-reactor system.

Tubular-reactor system

We will study the catalytic dehydrogenation of ethyl benzene to styrene via a vapor-phase reaction in a tubular reactor. Heat for the reaction is supplied by a heat-transfer fluid. The flow diagram for the system and its controls is shown in Fig. 1.

The reaction rate, R, is given by:

$$R = k\left[P_e - \frac{P_s P_h}{K}\right] \tag{1}$$

$$k = 12{,}600 \exp[-10{,}000/(t + 273)] \tag{2}$$

$$K = 0.027 \exp[0.021(t - 500)] \tag{3}$$

where P_e = partial pressure of ethyl benzene, P_s = partial pressure of styrene, P_h = partial pressure of hydrogen, and t = temperature, °C.

Other data for this system are listed in the accompanying table.

If we neglect radial gradients in the reactor, we can relate the conversion, x, with the mole fraction of ethyl benzene, Y_e, in the reactor as:

$$Y_e = \frac{1 - x}{1 + x + S};\; x = \frac{1 - Y_e - SY_e}{1 + Y_e} \tag{4}$$

where S = mole steam/mole ethyl benzene.

A material balance for a differential length, ΔZ, of reactor gives:

$$\left(\frac{F}{n}\right)Y_e - \frac{R\pi(d_i)^2\,\Delta Z}{4 \times 144} - \frac{1}{n}\left[FY_e + \frac{\partial FY_e}{\partial Z}\,\Delta Z\right] = \frac{\partial}{\partial\theta}\left[\left(\frac{\rho\pi(d_i)^2}{4 \times 144}\right)\Delta Z Y_e\right] \tag{5}$$

$$-\frac{1}{n}\left[\frac{\partial FY_e}{\partial Z}\right] - \frac{R\pi(d_i)^2}{4 \times 144} = \frac{\partial}{\partial\theta}[\rho Y_e]\frac{\pi(d_i)^2}{4 \times 144} \tag{5a}$$

Equations for the molar flowrate, F, and density, ρ, of the reaction mixture as a function of conversion x are given by:

$$F = F_i(S + 1 + x) \tag{6}$$

$$\rho = \frac{1.8P}{R_g(t + 273)}\left[\frac{(S + 1 + x)}{(S + 1)}\right] \tag{7}$$

The kinetic equation, Eq. (1), as a function of the conversion x is:

$$R = k\left\{\frac{(1 - x)}{(1 + x + S)} - \frac{1}{K}\left[\frac{x^2}{(1 + x + S)}\right]\right\}P\rho_c \tag{8}$$

Energy-balance relationships

We derive the equation for a differential section, ΔZ, of the reactor by an energy balance, as follows:

$$\frac{FC_pt}{n} - R\,\Delta H_R\left[\frac{\pi(d_i)^2\,\Delta Z}{4 \times 144}\right] - \frac{1}{n}\left[FC_pt + \frac{\partial(FC_pt)}{\partial Z}\,\Delta Z\right] + \frac{h_i\pi d_i}{12}\,\Delta Z(T_w - t) = \frac{\partial}{\partial\theta}\left[\frac{\rho\pi(d_i)^2}{4 \times 144}\,\Delta Z C_pt\right] \tag{9}$$

$$-\frac{1}{n}\left[\frac{\partial FC_pt}{\partial Z}\right] - \frac{R\pi(d_i)^2}{4 \times 144}\Delta H_R + \frac{h_i\pi d_i}{12}(T_w - t) = \frac{\pi(d_i)^2}{4 \times 144}C_p\frac{\partial(\rho t)}{\partial\theta} \tag{9a}$$

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*To meet the author, see *Chem. Eng.*, May 3, p. 96.

†Articles published thus far in this CE REFRESHER: Part 1, June 29, 1981, p. 71; Part 2, Aug. 24, 1981, p. 111; Part 3, Nov. 16, 1981, p. 271; Part 4, Dec. 28, 1981, p. 63; Part 5, Mar. 8, 1982, p. 97; Part 6, May 3, 1982, p. 93; Part 7, June 28, 1982, p. 97.

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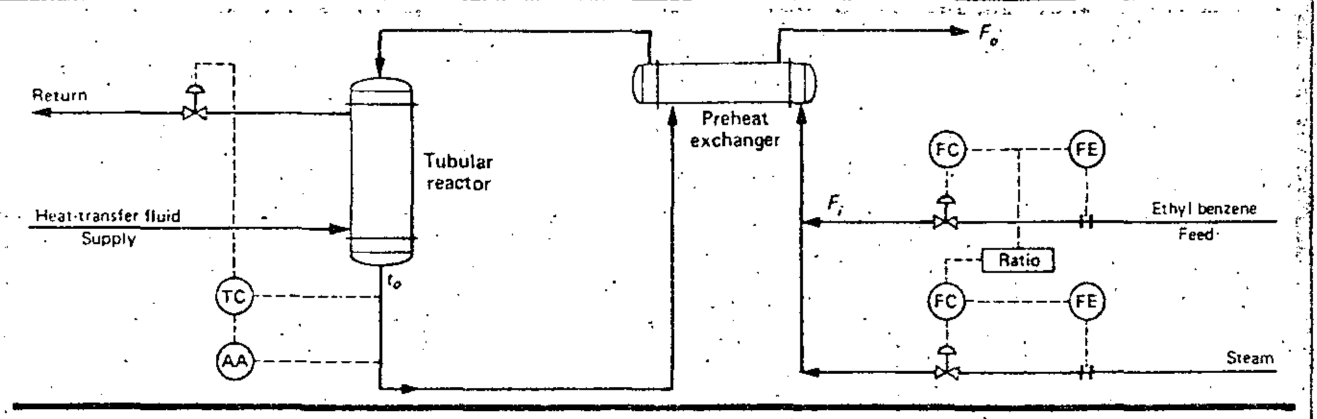

Reactor and control system for vapor-phase catalytic dehydrogenation of ethyl benzene **Fig. 1**

Tubewall and shellside equations for the energy balance are as follows:

$$\rho_o A_o C_{po}\frac{\partial T}{\partial\theta} = -\rho_o v_o A_o C_{po}\frac{\partial T}{\partial Z} - nh_o\frac{\pi d_o}{12}(T - T_w) \quad (10)$$

$$\frac{\rho_w[(d_o)^2 - (d_i)^2]}{4 \times 144}C_{pw}\frac{\partial T_w}{\partial\theta} = \frac{h_o d_o}{12}(T - T_w) - \frac{h_i d_i}{12}(T_w - t) \quad (11)$$

The equations for modeling the energy balance in the preheat exchanger are:

$$\left(\frac{\pi\rho_i(d_i)^2 C_p}{4 \times 144}\right)\frac{\partial t}{\partial\theta} = \frac{h_i \pi d_i}{12}(T_w - t) - \left(\frac{\rho_i v_i \pi(d_i)^2 C_p}{4 \times 144}\right)\frac{\partial t}{\partial Z_1} \quad (12)$$

$$\left(\frac{\rho_w[(d_o)^2 - (d_i)^2]C_{pw}}{4 \times 144}\right)\frac{dT_w}{d\theta} = \frac{h_o d_o(T - T_w)}{12} - \frac{h_i d_i(T_w - t)}{12} \quad (13)$$

$$(\rho_o A_o C_{po})\frac{\partial T}{\partial\theta} = -(\rho_o A_o C_{po} v_o)\frac{\partial T}{\partial Z_1} - \frac{nh_o d_o \pi(T - T_w)}{12} \quad (14)$$

For the steady-state solution, we can use the techniques of Part 5 (*Chem. Eng.*, Mar. 8, p. 97). The independent variables are Z and Z_1 instead of time θ. The steady-state solution gives the initial conditions at each point in the exchanger.

Simulating the control loops

The control loops for this reactor system are shown in Fig. 1. Here, we find that the incoming ethyl benzene and steam are under both flow control and ratio control. The composition analyzer for the product leaving the reactor adjusts the flow of the heat-transfer fluid. Let us now write the expressions (i.e., the differential and algebraic equations) that will model each of the control loops in this process system.

Ethyl benzene flow-control loop

$$\tau_e^2\frac{d^2\phi_e}{d\theta^2} + 2\zeta_e\tau_e\frac{d\phi_e}{d\theta} + \phi_e = G_e F_e \quad (15)$$

$$\phi'_e = d\phi_e/d\theta \quad (15a)$$

$$\tau_e^2\frac{d\phi'_e}{d\theta} + 2\zeta_e\tau_e\phi'_e + \phi_e = G_e F_e \quad (15b)$$

$$\phi_{e2} = \frac{K_{ce}(AXN)_e}{(SPAN)_e}[\phi_e - (SP)_e] + \frac{1}{\tau_{ie}}\int[\phi_e - (SP)_e]d\theta \quad (16)$$

$$\frac{d\phi_{e2}}{d\theta} = \frac{K_{ce}(AXN)_e}{(SPAN)_e}\left\{\frac{d\phi_e}{d\theta} + \frac{1}{\tau_{ie}}[\phi_e - (SP)_e]\right\} \quad (16a)$$

$$F_e = \phi_{e2}C_{ve}\sqrt{[(P_{1e})^2 - (P_{2e})^2]/2} \quad (17)$$

Steam-flow control loop

$$\tau_s^2\frac{d^2\phi_s}{d\theta^2} + 2\zeta_s\tau_s\frac{d\phi_s}{d\theta} + \phi_s = G_s F_s \quad (18)$$

$$\phi'_s = d\phi_s/d\theta \quad (18a)$$

$$\tau_s^2\frac{d\phi'_s}{d\theta} + 2\zeta_s\tau_s\phi'_s + \phi_s = G_s F_s \quad (18b)$$

$$\phi_{s2} = \frac{K_{cs}(AXN)_s}{(SPAN)_s} \times \left\{\left[\frac{\phi_s}{\phi_e} - (SP)_s\right] + \frac{1}{\tau_{is}}\int\left[\frac{\phi_s}{\phi_e} - (SP)_s\right]\right\}d\theta \quad (19)$$

$$\frac{d\phi_{s2}}{d\theta} = \frac{K_{cs}(AXN)_s}{(SPAN)_s} \times \left\{\left[\frac{1}{\phi_e^2}\phi_e\frac{d\phi_s}{d\theta} - \theta_s\frac{d\phi_e}{d\theta}\right] + \frac{1}{\tau_{is}}\left[\frac{\phi_s}{\phi_e} - (SP)_s\right]\right\} \quad (19a)$$

$$S = F_1\phi_{s2}C_{vs}\sqrt{[(P_{1s})^2 - (P_{2s})^2]/2} \quad (20)$$

Analyzer-temperature control loop

$$\phi_A(\theta) = Y_e(\theta - \lambda) \quad (21)$$

where λ is the delay in the analyzer—typically 30 to 90 s for a process-gas chromatograph.

$$\phi_{A2} = \frac{K_{cA}(AXN)_A}{(SPAN)_A} \times \left\{[\phi_A - (SP)_A] + \frac{1}{\tau_{iA}}\int[\phi_A - (SP)_A]d\theta\right\} \quad (22)$$

$$\frac{d\phi_{A2}}{d\theta} = \frac{K_{cA}(AXN)_A}{(SPAN)_A}\left\{\frac{d\phi_A}{d\theta} + \frac{1}{\tau_{iA}}[\phi_A - (SP)_A]\right\} \quad (22a)$$

$$\tau\frac{d\phi_t}{d\theta} + \phi_t = G_t t_o \quad (23)$$

$$\frac{d^2\phi_t}{d8^2} = \frac{1}{\tau_t}\left[\left(\frac{dt_o}{d\theta}\right)G_{to} - \frac{d\phi_t}{d\theta}\right] \quad (23a)$$

$$\phi_{t2} = \frac{K_{ct}(AXN)_t}{(SPAN)_t}\left\{(\phi_t - \phi_A) + \frac{1}{T_{it}}\int(\phi_t - \phi_A)d\theta + T_{dt}\left(\frac{d(\phi_t - \phi_A)}{d\theta}\right)\right\} \quad (24)$$

$$\frac{d\phi_{t2}}{d\theta} = \frac{K_{ct}(AXN)_t}{(SPAN)_t}\left[\frac{d\phi_t}{d\theta} - \frac{d\phi_A}{d\theta} + \frac{1}{T_{it}}(\phi_t - \phi_A) + T_{dt}\left(\frac{d^2\phi_t}{d\theta^2}\right)\right] \quad (24a)$$

$$W_o = \phi_{t2}C_{vt}\sqrt{[(P_{1t})^2 - (P_{2t})^2]/2} \quad (25)$$

Solving the mathematical models

Solution of the equations for this control system does not differ appreciably from that for the control system in Part 5 of this series. Solution for the preheat exchanger is the same as in Part 6 (*Chem. Eng.*, May 3, p. 93). For the reactor, we can use the following summary procedure to describe the reactor at time $(\theta + \Delta\theta)$:

1. Solve for x_m at time θ by using Eq. (4). Here the subscript m refers to the point m in the reactor.
2. Solve for the rate of reaction by Eq. (2), (3) and (8).
3. Expand Eq. (5a) and (9a) to obtain:

$$\frac{\pi(d_i)^2}{4 \times 144}\left[\rho\frac{dY_e}{d\theta} + Y_e\frac{d\rho}{d\theta}\right] = -\frac{1}{n}\left(\frac{dFY_e}{dZ}\right) - R\left(\frac{\pi(d_i)^2}{4 \times 144}\right) \quad (5b)$$

$$\frac{\pi(d_i)^2 C_p}{4 \times 144}\left[\rho\frac{\partial t}{\partial\theta} + t\frac{\partial\rho}{\partial\theta}\right] = -\frac{1}{n}\left[\frac{\partial FC_p t}{\partial Z}\right] - \frac{\pi(d_i)^2}{4 \times 144}R\,\Delta H_R + \frac{h_i\pi d_i(T_w - t)}{12} \quad (9b)$$

4. Expand $\partial\rho/\partial\theta$ by using Eq. (4) and (7) and the following identity:

$$\frac{\partial\rho}{\partial\theta} = \left(\frac{\partial\rho}{\partial x}\right)\left(\frac{\partial x}{\partial Y_e}\right)\left(\frac{\partial Y_e}{\partial\theta}\right)$$

By making the necessary substitutions into this identity, we will obtain:

$$\frac{\partial\rho}{\partial\theta} = \frac{1.8P}{R_g(t + 273)} \times \left\{\frac{(1 + Y_e)(-1 - S) - [1 - Y_e(1 + S)]}{(1 + Y_e)^2}\right\}\frac{\partial Y_e}{\partial\theta} \quad (26)$$

Nomenclature

A_o	Shellside flow area
(AXN)	Controller action
C_p	Heat capacity on tubeside
C_{pc}	Heat capacity on shellside
C_{pw}	Heat capacity of tubewall
C_v	Control valve capacity
d_i, d_o	Inside and outside diameter
F	Molar flowrate inside reactor
F_i	Molar flowrate to reactor
G	Gain of sensing element
ΔH_R	Heat of reaction
h_i, h_o	Inside and outside heat-transfer coefficient
k	Reaction-rate constant
K	Equilibrium constant for chemical reaction
K_c	Gain constant of controller
L	Tube length
n	Number of tubes
P	Pressure
P_1	Upstream pressure of control valve.
P_2	Downstream pressure of control valve
R	Rate of reaction
R_g	Gas constant
$(SPAN)$	Controller span
SP	Controller setpoint
t	Tubeside temperature
T	Shellside temperature
T_w	Tubewall temperature
T_i	Controller reset time
T_d	Controller derivative time
v_o	Shellside velocity
x	Conversion
Y_e	Mole fraction of ethyl benzene
Z, Z_1	Finite distance
ρ_i	Fluid density at inlet
ρ_c	Bulk density of catalyst
ρ_o	Fluid density at outlet
ρ_w	Density of tubewall

Data for catalytic dehydrogenation of ethyl benzene to styrene in a tubular reactor

Bulk density of catalyst	90 lb/ft^3
Operating pressure	1.2 atm
Heat of reaction	60,000 Btu/lb-mol
Specific heat of reaction mixture	0.52
Specific heat of heat-transfer fluid	0.58
Ethyl benzene to reactor	75 lb-mol/h
Steam to reactor	750 lb-mol/h
Reactor data	
Tubes, number	100
Tube diameter (10 gage BWG)	1½ in.
Tube length	6 ft
Inside diameter of shell	23.25 in.
Composite tubeside coefficient	60 Btu/(h)(ft^2)(°F)
Composite shellside coefficient	150 Btu/(h)(ft^2)(°F)
Preheat exchanger	
Tubes, number	376
Tube diameter (14 gage BWG)	¾ in.
Tube length	12 ft
Inside diameter of shell	21.25 in.
Composite tubeside coefficient	100 Btu/(h)(ft^2)(°F)
Composite shellside coefficient	100 Btu/(h)(ft^2)(°F)

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With Eq. (5b), (9b) and (26), we can calculate the derivatives at time θ, and numerically integrate the equations at all points in the reactor to obtain the values of the dependent variables ρ, t and Y_e.

5. Obtain the time derivatives of the temperature variables for the shellside and tubewall from the finite difference relationships of Eq. (10) and (11).

6. Integrate all differential equations numerically.

The final set of difference equations

In order to find solutions for the variables in the example for a tubular reactor, we need numerical data for all the variables at time θ. We will, in using the finite difference technique, consider the reactor as having M sections; and the preheat exchanger, L sections. We will obtain values for the variables at $(\theta + \Delta\theta)$. We will begin with the preheat exchanger.

Preheat exchanger, tubeside

Section 1: $dt_1/d\theta = 0$

Sections $j = 2$ to $j = (L - 1)$:

$$\frac{dt_j}{d\theta} = A(T_{wj} - t_j) - v_i\frac{(t_{j+1} - t_{j-1})}{2\Delta Z}$$

Section L:

$$\frac{dt_L}{d\theta} = A(T_{wL} - t_L) - v_i\frac{(t_L - t_{L-1})}{\Delta Z}$$

where: $$A = \frac{4 \times 12 \times h_i}{\rho_i d_i C_P}$$

Preheat exchanger, shellside

Section L: $dT_L/d\theta = 0$

Sections $j = 2$ to $j = (L - 1)$:

$$\frac{dT_j}{d\theta} = \frac{-v_o(T_{j+1} - T_{j-1})}{2\,\Delta Z_1} - A(T_j - T_{wj})$$

Section 1:

$$\frac{dT_1}{d\theta} = \frac{-v_o(T_2 - T_1)}{\Delta Z} - A(T_1 - T_{w1})$$

where: $$A = \frac{h_i d_i \times 12 \times 4}{\rho_w C_{pw}[(d_o)^2 - (d_i)^2]}$$

(Note: Be careful of the sign of v_o.)

Preheat exchanger, tubewall

Sections $j = 1$ to $j = L$:

$$\frac{dT_{wj}}{d\theta} = A(T_j - T_{wj}) - B(T_{wj} - t_j)$$

where: $$A = \frac{4 \times 12 \times h_o d_o}{\rho_w C_{pw}[(d_o)^2 - (d_i)^2]}$$

$$B = \frac{4 \times 12 \times h_i d_i}{\rho_w C_{pw}[(d_o)^2 - (d_i)^2]}$$

Reactor, shellside and tubewall

Use the same equations as for the preheat exchanger but substitute different values for the physical data, and M instead of L.

Reactor, tubeside

Sections $j = 1$ to $j = M$:

$$x_j = \frac{1 - Y_e(1 + S)}{(1 + Y_e)}$$

$$k_j = 12{,}600 \exp[-11{,}000/(t_j + 273)]$$

$$K_j = 0.027 \exp[0.021(t_j - 500)]$$

$$R_j = k_j\left\{\frac{(1 - x_j)}{(1 + x_j + S)} - \frac{1}{K_j}\left[\frac{(x_j)^2}{(1 + x_j + S)}\right]\right\}P\rho_c$$

$$A_j = \frac{1.8P}{R_g(t_j + 273)}\left[\frac{(x_j + S + 1)}{(S + 1)}\right]$$

$$F_j = F_i(S + 1 + x_j)$$

$$B_j = \rho_j + Y_{ej}A_j$$

$$C_j = B_j D_j$$

$$D_j = \pi(d_i)^2/(4)(144)$$

Section 1:

$$\frac{dt_1}{d\theta} = 0;\ \frac{dY_{e1}}{d\theta} = 0;\ \frac{d\rho_1}{d\theta} = 0$$

Sections $j = 2$ to $j = (M - 1)$:

$$\frac{dY_{ej}}{d\theta} = -\frac{1}{n}\left[\frac{(F_{j+1}Y_{e(j+1)} - F_{j-1}Y_{e(j-1)})}{2C_j\,\Delta Z}\right] - \frac{R_j D_j}{C_j}$$

$$\frac{d\rho_j}{d\theta} = A_j\left(\frac{dY_{ej}}{d\theta}\right)$$

$$E_j = \rho_j + t_j\left(\frac{d\rho_j}{d\theta}\right)$$

$$\frac{dt_j}{d\theta} = \frac{1}{E_j D_j}\left[\left(\frac{C_p}{n}\right)\left(\frac{(F_{j+1}t_{j+1} - F_{j-1}t_{j-1})}{2\,\Delta Z}\right) - R_j D_j\,\Delta H_R + h_i(\pi d_i/12)(T_{wM} - t_M)\right]$$

Section M:

$$\frac{dY_{eM}}{d\theta} = -\frac{1}{n}\left[\frac{(F_M Y_{eM} - F_{M-1}Y_{e(M-1)})}{C_M\,\Delta Z}\right] - \frac{R_M D_M}{C_M}$$

$$\frac{d\rho_M}{d\theta} = A_M\left(\frac{dY_{eM}}{d\theta}\right)$$

$$E_j = \rho_j + t_j\left(\frac{d\rho_j}{d\theta}\right)$$

$$\frac{dt_M}{d\theta} = \frac{1}{E_M D_M}\left[\left(\frac{C_P}{n}\right)\left(\frac{(F_M t_M - F_{M-1}t_{M-1})}{\Delta Z}\right) - R_M D_M\,\Delta H_R + h_i(\pi d_i/12)(T_{wM} - t_M)\right]$$

Instruments—Solve Eq. (15), (16), (18), (19) and (21) through (24) for derivatives.

Integrate all of the derivatives numerically.

Solve algebraic equations—Inlet temperature at the reactor must equal the tubeside outlet temperature of the preheat exchanger. Shellside inlet temperature at the preheat exchanger must equal the tubeside outlet temperature of the reactor. Finally, we compute the flows from Eq. (17), (20) and (25).

The next article in this CE REFRESHER series will appear in the issue of Nov. 19, and will cover the dynamic modeling of distillation systems.

Steven Danatos, Editor

CE REFRESHER: PROCESS DYNAMICS/9

Modeling the phase equilibria in dynamic systems

Developing mathematical models for heat exchangers and the Rayleigh distillation begins by computing equilibrium constants for the liquid-vapor system. The resulting models are then programmed for dynamic simulation on a computer.

*John L. Guy, Dynamod Enterprises**

☐ The modeling of systems involving phase changes in one or more of the components requires calculation of an equilibrium constant before developing the required finite-difference equations. A typical example of such a system is the analysis and control of a distillation tower.

In the first article† of this series, we considered Rayleigh distillation, a one-stage system that involves vapor-liquid phase equilibrium. For that calculation, we can complete an approximate analysis of the process with a desk calculator—although the work becomes tedious. Most problems will be solved via the computer. Typically, this is necessary when a steady-state (or static) solution is required.

For vapor-liquid systems, the equilibrium constant, K, for Component j is given by:

$$K_j = Y_j/X_j \tag{1}$$

(The approach is the same whether considering vapor-liquid systems, or liquid-liquid, liquid-solid, liquid-liquid-vapor, etc., ones)

A wealth of books and articles deal with the computation of the equilibrium constant [1 to 7]. Here, we will simply state that the equilibrium constant, K, is a function of temperature, pressure and composition of the liquid and vapor phases.

Application to heat exchangers

Let us look at the vertical-vapor in-tube condenser that is shown in Fig. 1. In Part 6, we derived equations for isothermal heat transfer plus phase change, and for nonisothermal heat transfer without phase change. In general, we cannot assume isothermal conditions when considering multicomponent systems having phase changes. Here, the following analysis is required:

We can derive Eq. (2) for a differential length of tube, dY_1, via an energy balance by using the general finite-difference analysis.

$$\frac{n_T \pi d_i^2}{4 \times 144}\left[\frac{\partial(\rho_i H_i)}{\partial \theta}\right] = -\frac{\partial(W_i H_i)}{\partial Y_1} + \frac{h_i n_T \pi d_i}{12}(T_w - t) \tag{2}$$

A material balance for Component j and total flowrate, W_i, yields:

$$\frac{n_T \pi d_i^2}{4 \times 144}\left[\frac{\partial(\rho_i Z_j)}{\partial \theta}\right] = -\frac{\partial(W_i Z_j)}{\partial Y_1} \tag{3}$$

Because it is sometimes convenient to use point liquid rates, L_i, and point vapor rates, V_i, and their corresponding mole fractions, X_j and Y_j, we can substitute total and point conditions, Eq. (4), and (5), and the equilibrium relationship given by Eq. (1) into Eq. (3) to obtain Eq. (6).

$$W_i = L_i + V_i \tag{4}$$

$$W_i Z_j = L_i X_j + V_i Y_j \tag{5}$$

$$\frac{n_T \pi d_i^2}{4 \times 144}\left[\frac{\partial(\rho_i Z_j)}{\partial \theta}\right] = -\frac{\partial(L_i X_j)}{\partial Y_1} - \frac{\partial(V_i Y_j)}{\partial Y_1} = -\frac{\partial}{\partial Y_1}(L_i X_j) - \frac{\partial}{\partial Y_1}(W_i - L_i)K_j X_j \tag{6}$$

A total-flow material balance for the differential length of tube dY_1 gives:

$$\left(\frac{n_T \pi d_i^2}{4 \times 144}\right)\frac{\partial \rho_i}{\partial \theta} = -\frac{\partial W_i}{\partial Y_1} \tag{7}$$

For vacuum operation, we can relate the pressure drop in each differential section of the exchanger by an equation [14]. We can then state that change in pressure per differential length, [illegible], is a function of the

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*To contact the author, see *Chem. Eng.*, May [illegible]

†[illegible] Part 1, June 29, 1981, p. [illegible]

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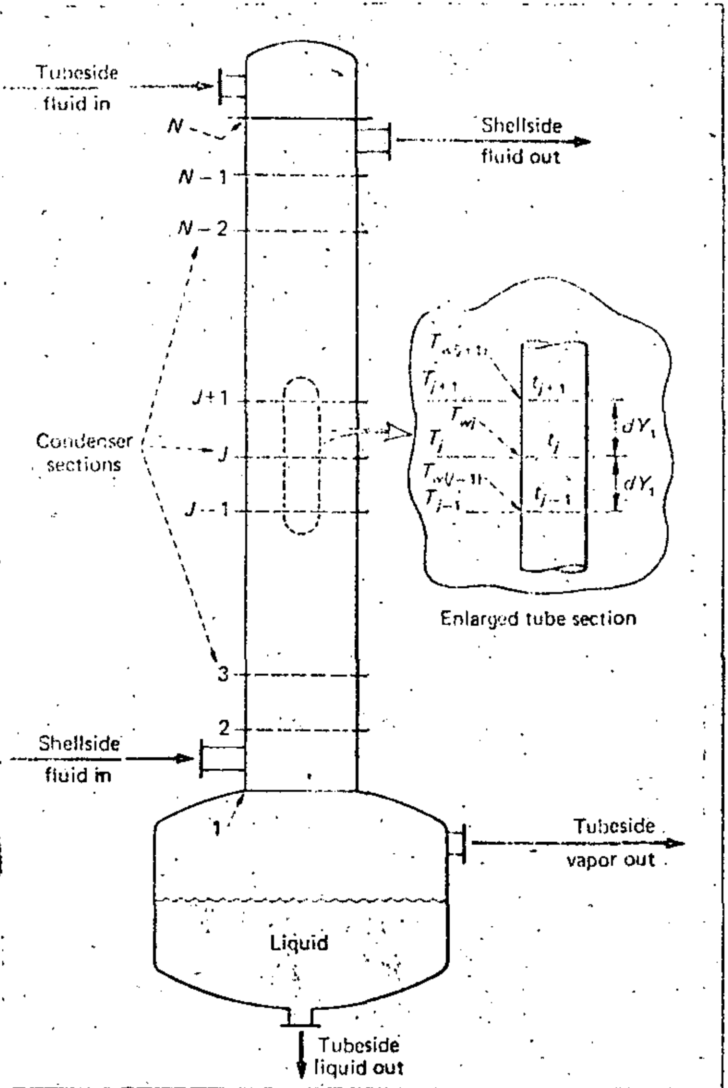
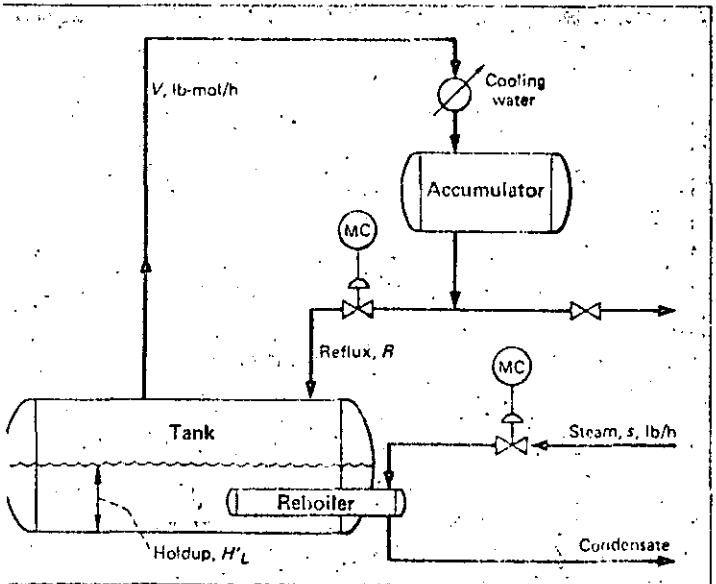


Vertical vapor-in-tube condenser **Fig. 1**



Process arrangement for the example of a Rayleigh distillation **Fig. 2**

Nomenclature

A'_o	Shellside flow area, ft²
C_p	Specific heat
d	Tube diameter, in.
h	Heat-transfer coefficient, Btu/(h)(ft²)(°F)
H	Enthalpy, Btu/lb-mole
H'_L	Liquid holdup, lb-mole
K	Equilibrium constant derived from Eq. (1)
L	Liquid flowrate, lb-mole/h
M	Number of components
n_T	Number of tubes
P	Pressure
Q	Heat-transfer rate, Btu/h
S	Steam rate, lb/h
t	Tubeside temperature, °F
T	Shellside temperature, °F
T_w	Tubewall temperature, °F
T_L	Tube length, ft
V	Vapor flowrate, lb-mole/h
V_L	Liquid volume, ft³
W	Total flowrate (liquid plus vapor), lb-mole/h
X	Mole fraction of liquid
Y	Mole fraction of vapor
Y_1	Tube-length increment, ft
Z	Mole fraction on total-flow basis
θ	Time, h
λ	Latent heat, Btu/lb
ρ	Density, lb/ft³
Subscripts	
i	Tubeside conditions
j	Component number
k	Tube position
L	Liquid
o	Shellside conditions
V	Vapor
w	Tubewall

flowrates; physical properties Φ_i; and tube geometry, Ψ_i; or:

$$dP/dY_1 = f(V_i, L_i, \Phi_i, \Psi_i) \tag{8}$$

Of course, we can use the equation for pressure operation, but the error introduced by the effect of pressure in Eq. (1) decreases as the pressure increases.

To complete the tubeside calculations, we need three additional items:

1. An estimation procedure for calculating the individual heat-transfer coefficients [*10* and *11*], and the composite tubeside and shellside coefficients (see Part 6, *Chem. Eng.*, May 3, 1982, p. 93).
2. An estimation or calculation procedure for determining stream or point enthalpy of the liquid and vapor [*2*, *7*, *8* and *9*].
3. A procedure to estimate the stream densities of the liquid and vapor portions [*2*, *5* and *9*].

We can then use the finite-difference technique derived from Eq. (1) through (8) to simulate tubeside conditions in the exchanger. The resulting equations are also valid, if more complicated than necessary, for single-phase systems and multiphase single-component systems.

The finite-difference equations from Part 6 of this series for the shellside and tubewall temperature profiles complete the model for the condenser. These equations are:

$$\frac{dT_k}{d\theta} = \frac{B_o}{A_o}(T_k - T_{wk})n_T + \frac{C_o}{A_o}\left(\frac{T_{k+1} - T_k}{\Delta Y_1}\right) \quad (9)$$

where:

$$A_o = \rho_o A_o' C_{po}$$

$$B_o = -(h_o \pi d_o/12)$$

$$C_o = -\rho_o v_o A_o C_{po}$$

$$\frac{dT_{wk}}{d\theta} = \frac{B_w}{A_w}(T_k - T_{wk}) - \frac{C_w}{A_w}(T_{wk} - t_k) \quad (10)$$

where:

$$A_w = \rho_w C_{pw}(d_o^2 - d_i^2)/(4 \times 144)$$

$$B_w = h_o d_o/12$$

$$C_w = h_i d_i/12$$

The dynamic model

After setting the time derivatives to zero to obtain a steady-state solution, we complete the dynamic solution by performing the following:

Step 1—Computing tubeside and shellside composite coefficients by the methods given in Part 6 of the series. We can also compute these coefficients at various points in the exchanger and recompute them as the vapor and/or liquid flowrates and compositions vary. These additional computations usually do not appreciably alter the results. However, we can and probably should recompute the coefficients if the total flowrates change appreciably.

Step 2—Calculating the derivatives in Eq. (9) and (10).

Step 3—Integrating numerically the resulting finite-difference form of Eq. (3) or (6) to obtain new values at time $(\theta + \Delta\theta)$ of the quantity $\rho_i Z_j$ at Points $k = (N - 1), (N - 2), \ldots, 2, 1$. The finite-difference form of Eq. (3) is:

$$\frac{d(\rho_{i,k}Z_{j,k})}{d\theta} = \frac{W_{i,(k+1)}Z_{j,(k+1)} - W_{i,k}Z_{j,k}}{[n_T \pi d_i^2/(4 \times 144)]\Delta Y_1} \quad (11)$$

For the number of components in the system, M, the mole fraction, $Z_{j,k}$, must sum to 1, or:

$$\sum_{j=1}^{M} Z_{j,k} = 1 \text{ for } k = N-1, N-2, \ldots, 2, 1 \quad (12)$$

Thus, we can obtain the total component mole-fractions at each point in the exchanger by normalizing, as shown by:

$$Z_{j,k} = \frac{\rho_{i,k}Z_{j,k}}{\sum_{j=1}^{M}(\rho_{i,k}Z_{j,k})} \quad (13)$$

This procedure allows us to calculate $\rho_{i,k}$ directly, and to estimate the derivative $d\rho_{i,k}/d\theta$.

Step 4—Obtaining values of $(\rho_{i,k}H_{i,k})$ and, with the value of $\rho_{i,k}$ from Step 3, obtaining the value of $H_{i,k}$ by numerically integrating the finite-difference form of Eq. (2), which is:

$$\frac{d(\rho_{i,k}H_{i,k})}{d\theta} = \left(\frac{4 \times 144}{n_T \pi d_i^2}\right)\left\{\left(\frac{W_{i,(k+1)}H_{i,(k+1)} - W_{i,k}H_{i,k}}{\Delta Y_1}\right) + (h_i n_T \pi d_i/12)(T_{wk} - t_k)\right\} \quad (14)$$

The procedure is now iterative.

Step 5—Assuming a temperature, t_k, at each point, k, in the exchanger, we can now solve for the fraction of vapor by means of the Rachford and Rice equation [*12*] from:

$$f\left(\frac{V_{i,k}}{W_{i,k}}\right) = \sum_j \frac{Z_{j,k}(K_{j,k} - 1)}{(K_{j,k} - 1)(V_{i,k}/W_{i,k}) + 1} = 0 \quad (15)$$

This procedure is also iterative.

We can now calculate the point compositions for the calculated (i.e., new) liquid and vapor compositions from the following equations [*13*]:

$$\left(\frac{L}{V}\right)_{i,k} = \frac{(L/W)_{i,k}}{(V/W)_{i,k}} = \frac{1 - (V/W)_{i,k}}{(V/W)_{i,k}} \quad (16)$$

$$Y_{j,k} = \frac{Z_{j,k}[(L/V)_{i,k} + 1]}{1 + (L/V)_{i,k}/K_{j,k}} \quad (17)$$

$$X_{j,k} = Y_{j,k}/K_{j,k} \quad (18)$$

We use our selected enthalpy-estimation procedure to calculate a point enthalpy based on the above composition values.

We can now iterate via our selected temperature until we obtain a value for the difference in the stream enthalpy (as calculated in Steps 4 and 5) that is less than some prescribed error.

Step 6—Integrating the derivatives calculated in Step 2 numerically, we obtain new temperature profiles for the tubewall and the shellside stream.

Step 7—Integrating Eq. (7) numerically, we obtain new values of $W_{i,k}$ (for $k = N - 1, N - 2, \ldots, 2, 1$); or, using the algebraic form of Eq. (7) [as given by Eq. (19)], we obtain the new values for $W_{i,k}$. The derivatives, $d\rho_{i,k}/d\theta$, have been calculated in Step 3.

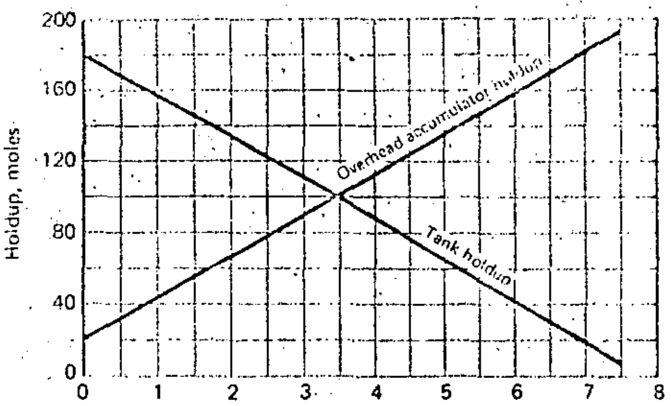
$$W_k = W_{k+1} - \frac{n_T \pi d_i^2}{4 \times 144}\left(\frac{d\rho_{i,k}}{d\theta}\right)\Delta Y_1 \quad (19)$$

Step 8—Returning to Step 1, we proceed to the next time interval, θ.

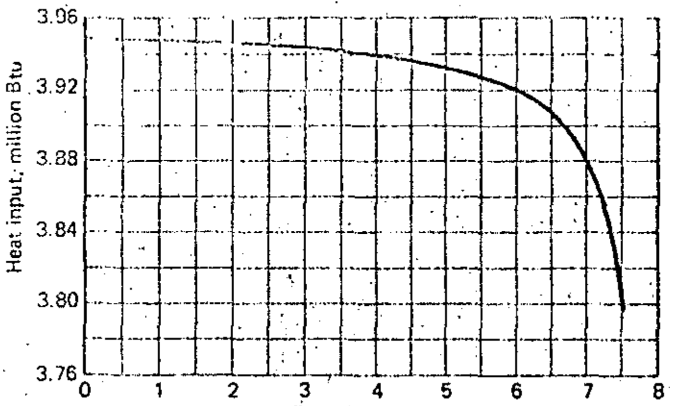
The same procedure can be used for multicomponent phase change on the shellside, or, multicomponent phase change on both sides of the exchanger. (Indeed, I have developed a computer program based on the above procedures.)

Rayleigh distillation

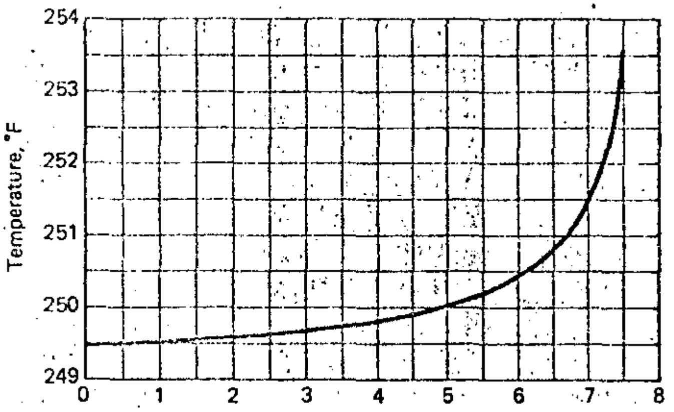
We discussed shortcut methods for simulating Rayleigh distillation (an inherently time-varying batch process) in Part 1 of this series. Let us turn our attention to problems that are not so easy to simplify because (a) the system is multicomponent, or (b) the equilibrium



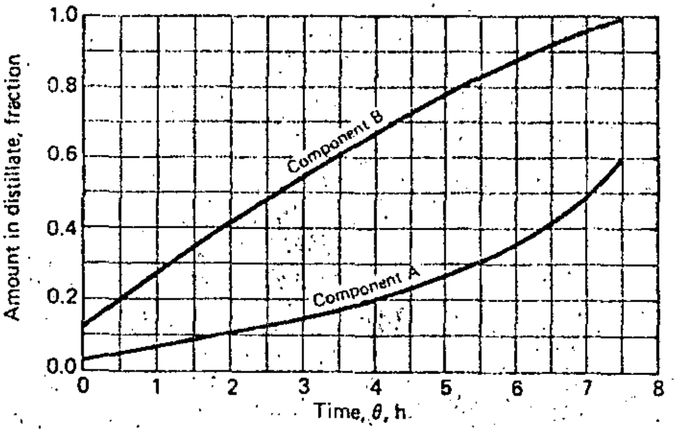
a. Molar holdup



b. Reboiler heat input



c. Reboiler temperature



d. Reboiler recoveries

Results from computer modeling of Rayleigh distillation problem — Fig. 3

4

constant K is not constant nor is the relative volatility. Let us consider the following problem:

In an inherently batch process, we have an equal molar mixture of components A and B. Component A is the more volatile one, but we desire to leave this component in the tank and distill the less volatile one overhead. The addition of water to the mixture forms an azeotrope with Component B, and we can concentrate Component A and the excess water in the tank. Addition of water to the reaction mixture is required in the next step of the batch procedure so we are not presented with the additional expense of separating water and Component A.

The system shown in Fig. 2 is initially at total reflux. At some time, we will close the reflux valve and start withdrawing product from the system.

With condensing steam supplying the energy to vaporize the material in the tank, we can write the equation for the energy balances on the tubeside and the tubewall. Because we are considering an isothermal phase change on both sides of the exchanger, we do not need to sectionalize (i.e., use finite-difference procedures) the tube bundle. The equations are:

$$S = \frac{h_i n_T \pi d_i T_L}{12\lambda}(t - T_w) \tag{20}$$

$$\frac{dT_w}{d\theta} = \frac{B_w}{A_w}(T - T_w) - \frac{C_w}{A_w}(T_w - t) \tag{21}$$

The total material-balance equation for the tank fluid is:

$$d(\rho_i V_L)/d\theta = -V \tag{22}$$

or simply:

$$d(H'_L)/d\theta = -V \tag{23}$$

Eq. (23) allows us to avoid a density calculation. In some problems, the decrease in molar holdup, H'_L, and therefore the decrease in liquid level, decreases the heat-transfer surface, and we must use Eq. (22).

The material balance for Component j is given by:

$$d(H'_L X_j)/d\theta = -VY_j \tag{24}$$

Substituting Eq. (1) into Eq. (24) and expanding:

$$\frac{dX_j}{d\theta} = \frac{-X_j[VK_j + (dH'_L/d\theta)]}{H'_L} \tag{25}$$

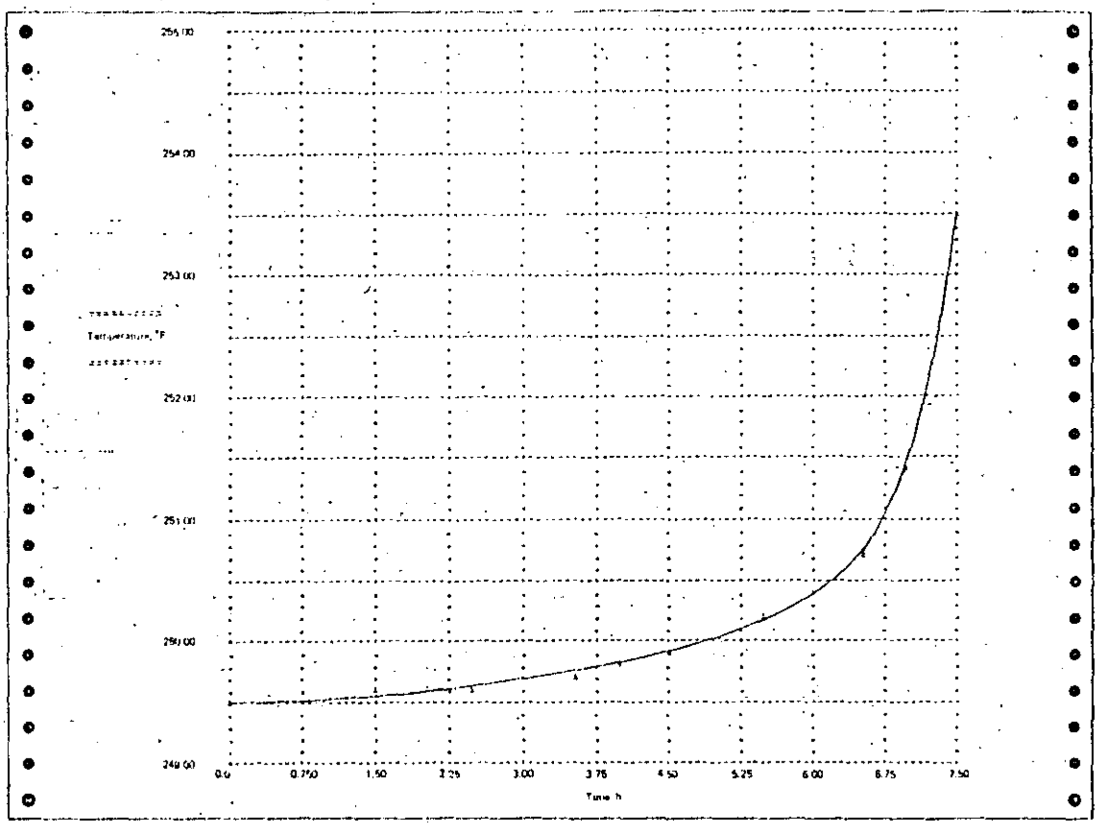
The energy balance for the tank system is given by:

$$Q_s = \frac{h_{oNT} \pi d_o T_L}{12}(T_w - T) \tag{26}$$

$$\frac{dH_L}{d\theta} = \frac{Q_s - VH_V - H_L(dH'_L/d\theta)}{H'_L} \tag{27}$$

A bubblepoint calculation relates the composition of the liquid and the tank temperature. For equilibrium existing between the liquid in the tank and the vapor leaving the tank, the temperatures of the two phases are equal. We can calculate liquid and vapor enthalpies by a suitable procedure.

For the example, we are collecting the distillate in the overhead accumulator. We can calculate the time lags between the inlet and outlet streams to the condenser. However, there is little interest in them. We will specify for this example that the condenser will condense and



Computer-derived plot for tank temperature produced by a line printer from the program **Fig. 4**

subcool the overhead vapor to 100°F. We can then rate the condenser by a separate calculation.

In our process (Fig. 2), we do not have a control system for adjusting steam flow to the reboiler. We do show a manual valve in the steam line. As the tank temperature increases, the steam condensing in the tubes decreases, and the corresponding flow reducation reduces the pressure drop across the manual valve. The temperature of the steam increases with pressure. This relationship between the steam temperature and an equation to model the control valve (see Part 2 of this series) supplies the necessary equations to complete the analysis.

Computer results

These procedures can be modeled with a computer program developed by me. The results, as a function of time, from the program are shown in Fig. 3 and 4. Fig. 3a represents the molar holdup in the tank and overhead accumulator. Fig. 3b and 3c show the reboiler heat input to the system and the tank temperature, respectively. Fig. 4 also shows the tank temperature as plotted by a line printer from the program. Such computer-oriented plots, which are usually necessary for design analysis, eliminate much engineering time used for manual plotting.

F[illegible] shows the removal of components A and B [illegible] significant reduction. A method for reducing the loss of Component A proposes the placing of additional stages between the tank and the overhead system. We will show the procedure for analyzing this in the next article that will appear in the issue of Jan. 10, 1983.

Steven Danatos, Editor

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REFRESHER: PROCESS DYNAMICS/10

Modeling batch distillation in multitray columns

Packed or tray columns can improve separation efficiency for batch distillations. The modeling of such systems via a computer simulation enables rapid evaluation of many alternative techniques.

*John L. Guy, Dynamod Enterprises**

☐ In the separation of a two-component system of A and B via a Rayleigh distillation, the addition of water for[illegible] an azeotrope in which Component B (the less vo[illegible]e one) is distilled overhead. In Part 9† of this series, we modeled such a system. While we can remove essentially all of Component B from the tank (95% in seven hours of operation for our example), we lose 49% of the more volatile Component A.

To reduce these losses, we can consider adding stages (either as trays or as packings) between the tank and condenser. The system with trays is shown in Fig. 1. We need additional equations to describe the added trays in order to model the system.

Developing the model

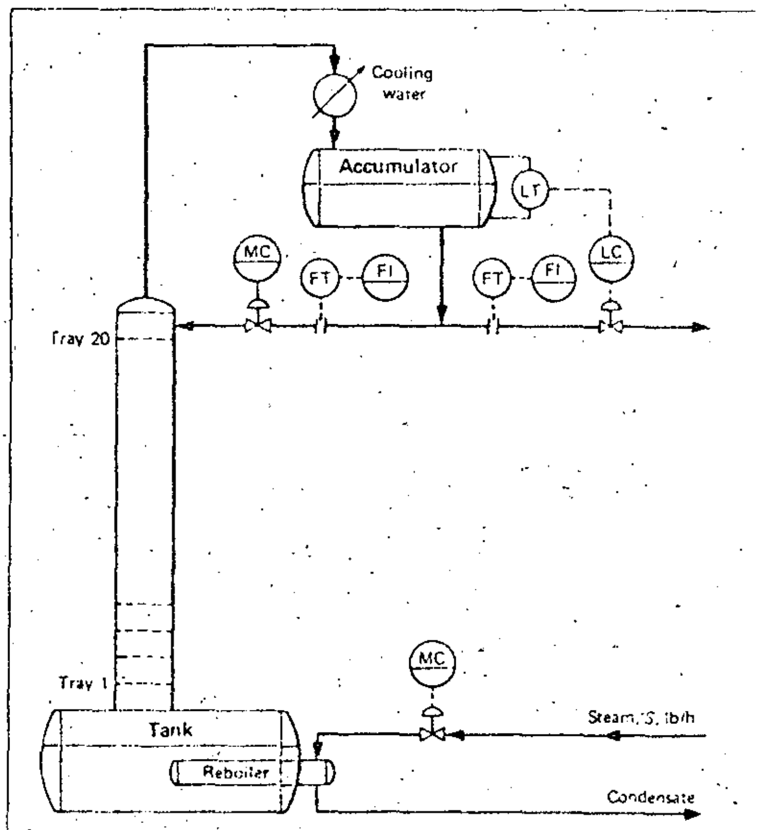
Fig. 2 shows a cross section of the tray column, the flow relationships for the liquid and vapor streams, and the holdups on the tray and in the downcomer. A total material balance around Tray number k yields:

$$\frac{d(\rho_L H_L)_k}{d\theta} + \frac{d(\rho_V H_V)_k}{d\theta} = V_{k-1} + L_{k+1} - V_k - L_k + F_k - DL_k - DV_k \quad (1)$$

Assuming that we can neglect vapor-phase holdup, Eq. (1) can be simplified to:

$$\frac{d(\rho_L H_L)_k}{d\theta} = V_{k-1} + L_{k+1} - V_k - L_k + F_k - DL_k - DV_k \quad (2)$$

[illegible]e simplest procedure [1] is to assume a constant [illegible]ar holdup, H'_L, and to assume an equilibrium stage. Because we know that the outlet flowrate does not change instantly when molar holdup is kept constant, we can approximate the stage hydraulics by estimating a hydraulic time constant, H_{TC}. (This procedure can



Process arrangement for the example of a batch distillation

Fig. 1

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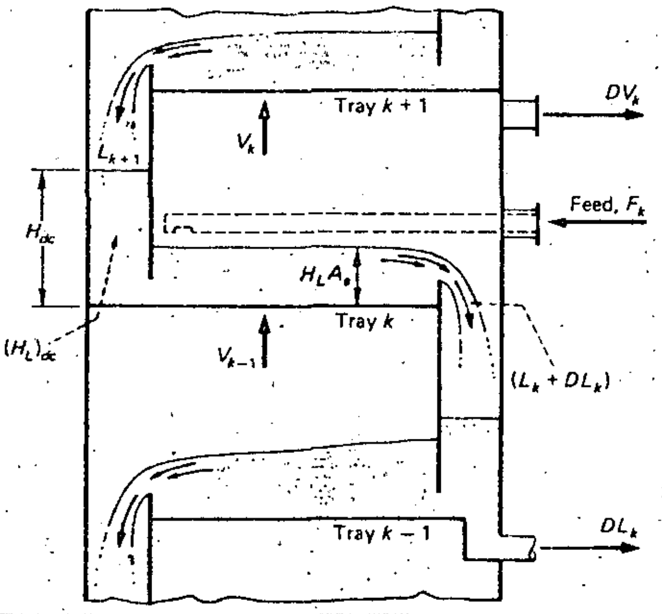
* To meet the author, see *Chem. Eng.*, May 3, 1982, p. 96.

†Articles published thus far in this CE REFRESHER: Part 1, June 29, 1981, p. 74; Part 2, Aug. 24, 1981, p. 111; Part 3, Nov. 16, 1981, p. 271; Part 4, Dec. 28, 1981, p. 63; Part 5, Mar. 8, 1982, p. 97; Part 6, May 3, 1982, p. 93; Part 7, June 20, 1982, p. 97; Part 8, Aug. 23, 1982, p. 91; Part 9, Nov. 29, 1982, p. 75.

Nomenclature

A_a	Active area of tray, ft^2
A_{dc}	Downcomer area, ft^2
DL_k	Liquid draw from Tray k, lb-mol/h
DV_k	Vapor draw from Tray k, lb-mol/h
F_k	Feed to Tray k, lb-mol/h
H	Stream enthalpy, Btu/lb-mol
H_{dc}	Liquid height in downcomer, in.
H_L	Liquid holdup, ft^3
H'_L	Liquid Holdup, lb-mol
H_{uD}	Head loss under downcomer, in. liquid
H_V	Vapor holdup, ft^3
H_w	Weir height, in.
H_{TC}	Hydraulic time constant, h
K_j	Equilibrium constant for Component j
K_1 K_2 K_3	Pressure-drop coefficients
L_k	Liquid flow from Tray k, lb-mol/h
L_{wi}	Outlet weir height, in.
t_m	Valve thickness, in.
v_H	Hole velocity, ft/s
X_j	Mole fraction of liquid for Component j
Y_j	Mole fraction of vapor for Component j
ΔP	Tray pressure drop, in. liquid
ΔP_{dry}	Dry-tray pressure drop, in. liquid
θ	Time, h
η	Tray efficiency
ρ_L	Liquid density, lb/ft^3 or lb-mol/ft^3
ρ_m	Valve-metal density, lb/ft^3
ρ_V	Vapor density, lb/ft^3 or lb-mol/ft^3



Flow relations existing on a typical tray of the column **Fig. 2**

also be used for packed towers.) In equation form, we obtain the following relationship:

$$\frac{dL_k}{d\theta} = \frac{1}{(H_{TC})_k}\Big[V_{k-1} + L_{k+1} - V_k - L_k + F_k - DL_k - DV_k\Big] \quad (3)$$

With the preceding simplification, we can derive a material balance for Component j as it is processed on Tray k:

$$\frac{d(H'_L X_j)_k}{d\theta} = V_{k-1}Y_{(k-1),j} + L_{k+1}X_{(k+1),j} + F_k Z_{k,j} - (V_k + DV_k)Y_{k,j} - (L_k + DL_k)X_{k,j} \quad (4)$$

We eliminate Y_j^* from Eq. (5) by substituting the following definition of the equilibrium constant:

$$Y_j^* = K_j X_j \quad (5)$$

Making the substitution, and after some manipulation, we obtain:

$$\frac{dX_{k,j}}{d\theta} = \frac{1}{H'_L}\Big[V_{k-1}Y_{(k-1),j} + L_{k+1}X_{(k+1),j} + F_k Z_{k,j} - X_{k,j}(V_k K_{k,j} + DV_k K_{k,j} + L_k + DL_k)\Big]. \quad (6)$$

An energy balance around Stage k yields:

$$\frac{d(H_L)_k}{d\theta} = \frac{1}{H'_L}\Big[V_{k-1}(H_v)_{k-1} + L_{k+1}(H_L)_{k+1} + F_k(H_F)_k - (V_k + DV_k)(H_V)_k - (L_k + DL_k)(H_L)_k\Big] \quad (7)$$

Simulating an equilibrium stage

We now have sufficient equations to simulate an equilibrium stage. The procedure for getting a solution is:

Step 1—Integrate the set of equations, as given by Eq. (6)—i.e., one equation for each component.

Step 2—Normalize the calculated mole fractions.

Step 3—Calculate a stage temperature and an equilibrium vapor composition from a bubblepoint (the temperature of initial boiling) computation.

Step 4—Calculate a liquid enthalpy from the temperature and liquid composition in steps 2 and 3.

Step 5—Integrate Eq. (3) to solve for liquid flowrate leaving the stage.

Step 6—Rearrange Eq. (7) by assuming that the change in liquid enthalpy is small (this assumption reduces the computation time), and then solve for the outlet vapor rate directly from:

$$V_k = [V_{k-1}(H_V)_{k-1} + L_{k+1}(H_L)_{k+1} + F_k(H_F)_k - DV_k(H_V)_k - L_k(H_L)_k - DL_k(H_L)_k]/(H_V)_k \quad (8)$$

Modeling real trays

We can simulate the operation of tray decks with a more sophisticated procedure, and the following is recommended for more-exacting work. We will simulate a "real" tray instead of an ideal stage.

The composition of the vapor leaving the tray can be derived from the definition of a Murphree tray efficiency, which is:

$$\eta_{k,j} = \frac{Y_{k,j} - Y_{(k-1),j}}{Y^*_{k,j} - Y_{(k-1),j}} \quad (9)$$

Rearranging Eq. (9), we obtain the following for:

$$Y_{k,j} = Y_{(k-1),j} + \eta_{k,j}(Y^*_{k,j} - Y_{(k-1),j}) \qquad (10)$$

Theoretically, the efficiency, $\eta_{k,j}$, varies with each component on each stage. We can calculate the change in $\eta_{k,j}$ as the liquid rates, vapor rates and physical properties on each stage change via some suitable method. However, we should determine how precise we can calculate these numbers before proceeding. In the example that will be discussed later in this article, we have assumed a constant tray efficiency, and proceeded without additional computations.

We can rewrite Eq. (2):

$$\frac{d(\rho_L H_L)_k}{d\theta} = V_{k-1} + L_{k+1} - V_k - L_k + F_k - DL_k - DV_k \qquad (11)$$

The calculation for tray hydraulics relate the liquid volume holdup, H_L, with the outlet liquid flowrates, L_k. First, we calculate a dry-tray pressure drop via the maximums of Eq. (12) and (13) for valve trays [2], and via Eq. (14) for sieve trays [3]. The dry-tray pressure drop is a function of the vapor flowrate and physical properties from tray $(k - 1)$. The liquid-density factor converts the calculated pressure-drop value to inches of liquid:

For valve trays:

$$\Delta P_{dry} = 1.35 t_m \left(\frac{\rho_m}{\rho_L}\right) + K_1(v_H)^2 \left(\frac{\rho_V}{\rho_L}\right) \qquad (12)$$

$$\Delta P_{dry} = K_2(V_H)^2[\rho_V/\rho_L] \qquad (13)$$

For sieve trays:

$$\Delta P_{dry} = K_3 V_H(\rho_V/\rho_L) \qquad (14)$$

The total tray pressure-drop is given by:

$$\Delta P = \Delta P_{dry} + 0.4(gpm/L_{wi})^{2/3} + 0.4\mathrm{H}_w \qquad (15)$$

The downcomer backup (inches of liquid column) is given by:

$$H_{dc} = H_w + 0.4\left(\frac{gpm}{L_{wi}}\right)^{2/3} + (\Delta P_{dry} + H_{uD})\left(\frac{\rho_L}{\rho_L - \rho_V}\right) \qquad (16)$$

Liquid holdup by volume in the downcomer (ft^3) is the product of the downcomer backup (ft) multiplied by the downcomer area (ft^2), or:

$$(H_L)_{dc} = H_{dc}(A_{dc}/12) \qquad (17)$$

Liquid holdup by volume on the tray deck itself is the product of the liquid height (ft) on the tray, as given by Eq. (18), and the active area (ft^2). Eq. (18) neglects any liquid gradient on the tray.

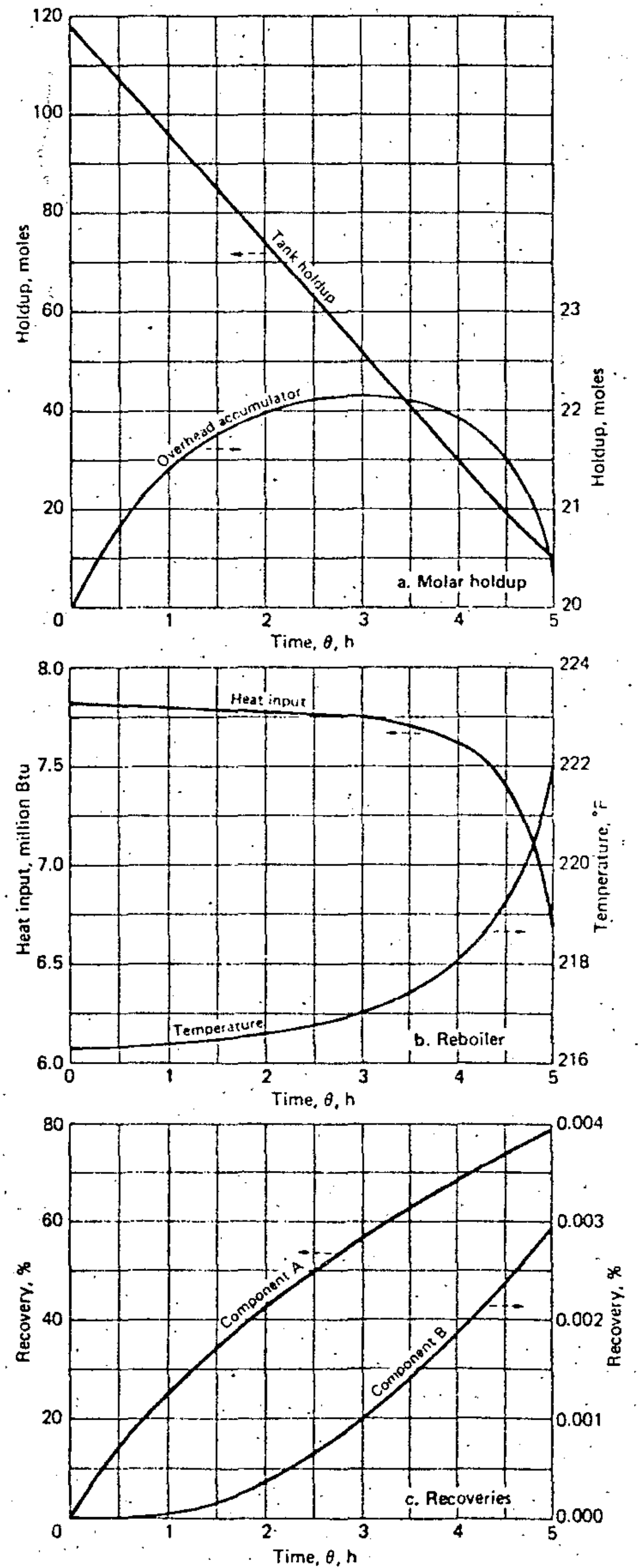
$$(H'_L)_{Aa} = H_w + 0.119(pph/L_{wi}\rho_L)^{2/3} \qquad (18)$$

where *pph* is flow in lb/h.

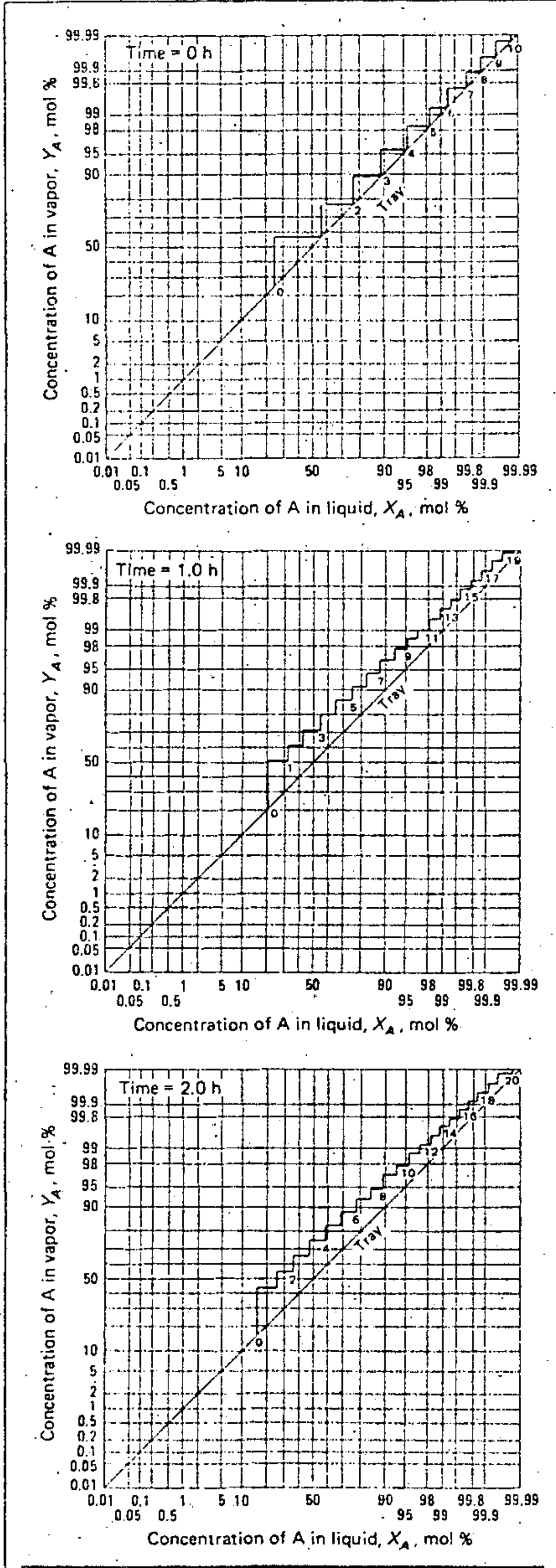
The total tray holdup is the sum of the liquid in the downcomer and on the tray deck, or:

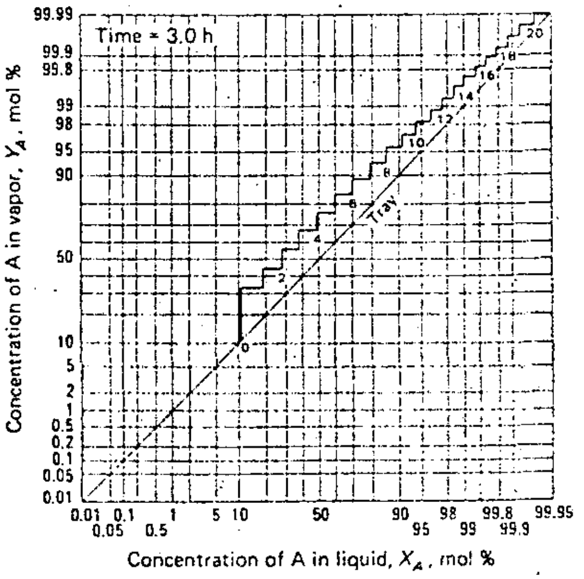
$$H'_L = (H_L)_{Aa}(A_a/12) + (H_L)_{dc} \qquad (19)$$

With reference to Fig. 2, we can make the simulation



Results from computer modeling of batch distillation problem. **Fig. 3**





Pseudo-McCabe-Thiele diagrams trace course of the batch distillation

Fig. 4

even more sophisticated by calculating the component and total material balances around the downcomer and the tray decks individually. However, this degree of sophistication is ignored in the following discussion.

For variable molar holdup in the liquid phase, Eq. (4) becomes:

$$\frac{d(\rho_L H_L X_j)_k}{d\theta} = V_{k-1}Y_{(k-1),j} + L_{k+1}X_{(k+1),j} + F_k Z_{k,j} - (V_k + DV_k)Y_{k,j} - (L_k + DL_k)X_{k,j} \qquad (20)$$

Substituting Eq. (10) into Eq. (20) yields:

$$\frac{dX_{k,j}}{d\theta} = \Big\{[V_{k-1} - (V_k + DV_k)(1 - \eta_{k,j})]Y_{(k-1),j} + L_{k+1}X_{(k+1),j} + F_k Z_{k,j} - x_{k,j}\Big[L_k + DL_k + (V_k + DV_k)\eta_{k,j}K_{k,j} + \frac{d(\rho_L H_L)}{d\theta}\Big]\Big\}/\rho_L H_L \qquad (21)$$

For this case, the procedure for solution is:

Step 1—Calculate the derivatives in Eq. (11) and (21). There will be one solution for each component.

Step 2—Integrate Eq. (21) to calculate the mole fraction of each component, and normalize.

Step 3—Calculate the tray liquid temperature via a bubblepoint calculation.

Step 4—Calculate the actual vapor composition from Eq. (10) by using the equilibrium vapor composition from Step 3. Calculate the vapor temperature by a dewpoint computation.

Step 5—Integrate Eq. (11) in order to calculate the change in molar holdup. By using a suitable procedure for estimating density, we can estimate the volume of liquid holdup on the tray deck and in the downcomer.

Step 6—Solve for the liquid flowrate from the tray by using the results of Step 5 and Eq. (12) through (19).

Step 7—Estimate the vapor enthalpy by some suitable procedure, using the values of the vapor composition and temperature from Step 4.

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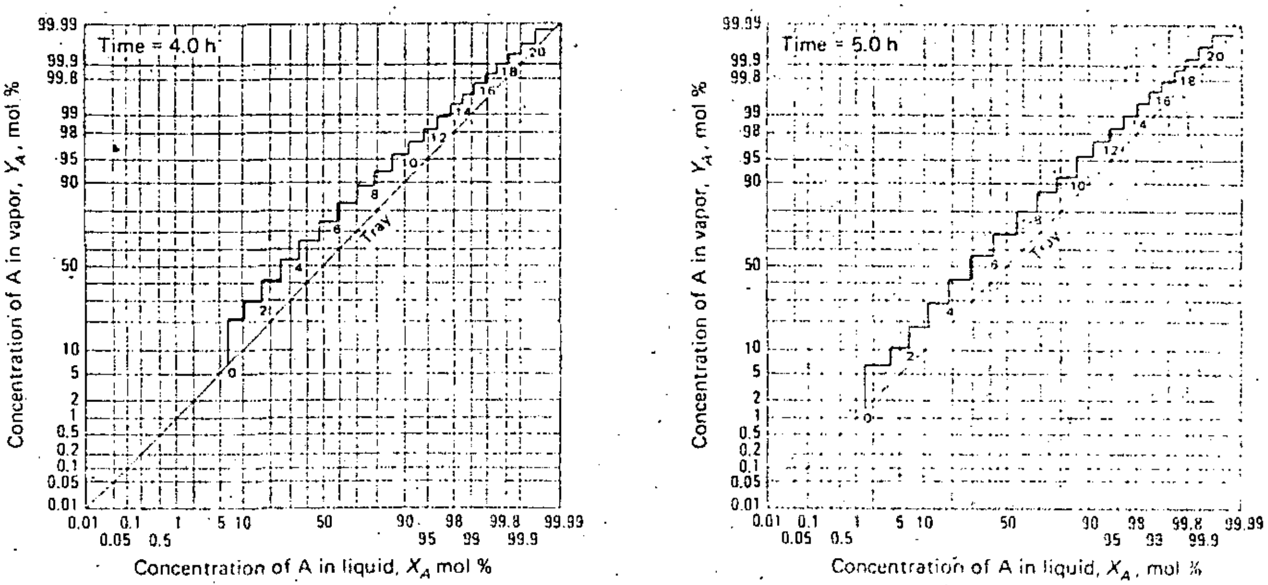

Step 8—Solve for the vapor rate from the tray via Eq. (8).

Application to multitray towers

The solution procedure can be applied to multitray towers. However, with more-sophisticated integration methods, there are advantages in solving all the trays simultaneously as opposed to solving each stage separately. The advanced integration methods are usually more economical because of the stiffness of the system* due to the tray-hydraulic calculation and, in some instances, due to the integration of the liquid composition. The stiffness for the latter factor can be quantified by a $(L + KV)/H'_L$ factor [4]. This factor controls the step size for integration, which is used in the simulation.

Rayleigh distillation problem

In Part 9 (*Chem. Eng.*, Nov. 29, 1982, pp. 78–79), we used a Rayleigh distillation to separate an equal molar mixture of components A and B. Component A was the more volatile one, but we desired to leave it in the tank and distill the less volatile one overhead. By adding water to the mixture, an azeotrope was formed with B. Thereby, Component A and the water were concentrated in the tank. After performing the simulation, we discovered that 95% of Component B was recovered, but that 49% of Component A was lost.

Since the loss of Component A is significant, we will now model this separation by adding 20 trays. We will use an assumed tray efficiency of 80% between the reboiler tank and the condenser, and provide reflux to the resulting tower, as shown in Fig. 1. An initial reflux ratio of 1.0 is assumed.

These modifications increase the sharpness of the separation. However, we do not achieve a complete recovery of Component A. We will lose very little of Component B. A higher reflux ratio, additional trays, or a change in operating procedures such as additional water in the system—all or any may be necessary to recover more than 70–85% of Component A.

These procedures, along with the routines developed for the reboiler and overhead system in Part 9, can be modeled with a computer program that I have developed. Fig. 3a represents the molar holdup in the tank and overhead accumulator. A level-control loop in the overhead system can be modeled with the equations developed in Part 2 of this series. Fig. 3b shows the reboiler heat input and the reboiler temperature.

Fig. 3c shows the recovery of components A and B. We recover about 64–79% of Component A in the product tank after five hours of operation. Assuming that we transfer the liquid from the overhead accumulator to the product tank at this time, we will have recovered about 70–85% of Component A. We have significantly reduced the losses of Component B, since the program predicts losses of only 0.003%. Unfortunately, we do not have the option of continuing the distillation because the reboiler tank is almost empty (for the conditions chosen for this problem).

Fig. 4 shows the progress of the distillation as plotted on a pseudo-McCabe-Thiele diagrams. Such plots can be generated by the program. Such plots can suggest changes in column conditions that can give the required recovery of Component A. For further study, each reader can decide the variable to be changed.

We will continue looking at distillation in the next article, which will appear in the issue of Mar. 21. Here, the emphasis will be on continuous tower operation.

Steven Danatos, Editor

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*See Part 5 of this series, *Chem. Eng.*, Mar. 8, 1982, p. 101.

Dynamic modeling of continuous-distillation and emergency systems

This final article contains the procedures for simulating continuous distillation, and describes the methods for modeling emergency, startup and shutdown conditions in process plants.

*John L. Guy, Dynamod Enterprises**

☐ For the dynamic analysis of continuous towers, we need a more sophisticated steady-state program than as required for the batch-distillation program that we discussed in Part 10† for modeling trays. The steady-state program enables us to determine initial values for the column variables.

Example illustrates procedures

Let us consider the distillation tower shown in Fig. 1. The column is designed to remove three light-key components overhead, and to remove a stream containing only the heavy-key component from the bottom.

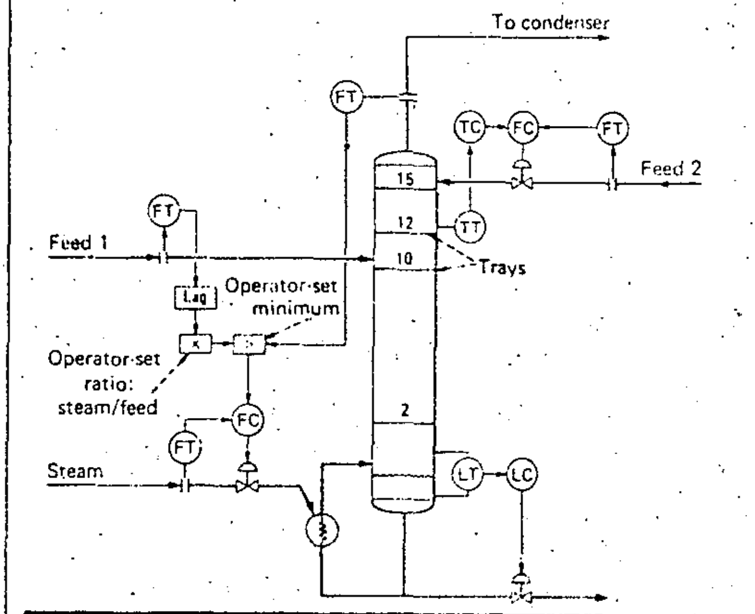
The four-component system can be simulated with a modified van Laar activity-coefficient estimation method. In our example, we will use 15 ideal trays (i.e., tray efficiency = 100%) to show the difference in simulating actual valve trays and estimating the tray hydraulics by means of the hydraulic time constant (see Part 10 of this series for the details.).

We will begin by reviewing the required procedures and equations in order to simulate this four-component, fifteen-tray system. In parts 9 and 10, we simulated tank- or kettle-type reboiler systems, respectively. In this example, we find a natural-circulation reboiler system. This can be modeled but generally not quite as simply as the tank-type reboiler.

The natural-circulation reboiler has a circulation rate dependent on vapor- and liquid-phase rates and densities. The temperature profile depends on the vapor-liquid equilibria, as well as on local temperature differences and exchanger geometry. The shellside and tubewall temperature profiles can be calculated as described in the previous articles—especially Part 6.

The tubeside calculation procedure begins with the multicomponent phase-change that we considered in Part 9. In addition to the equations in Part 9, we must derive equations for the fluid-flow hydraulics to determine the total flowrate through the exchanger tubeside. Fair [1] presents a procedure that can be extended to dynamic systems.

The bottom of the tower can be simulated with mate-



Distillation system separates four components in a 15-tray tower

Fig. 1

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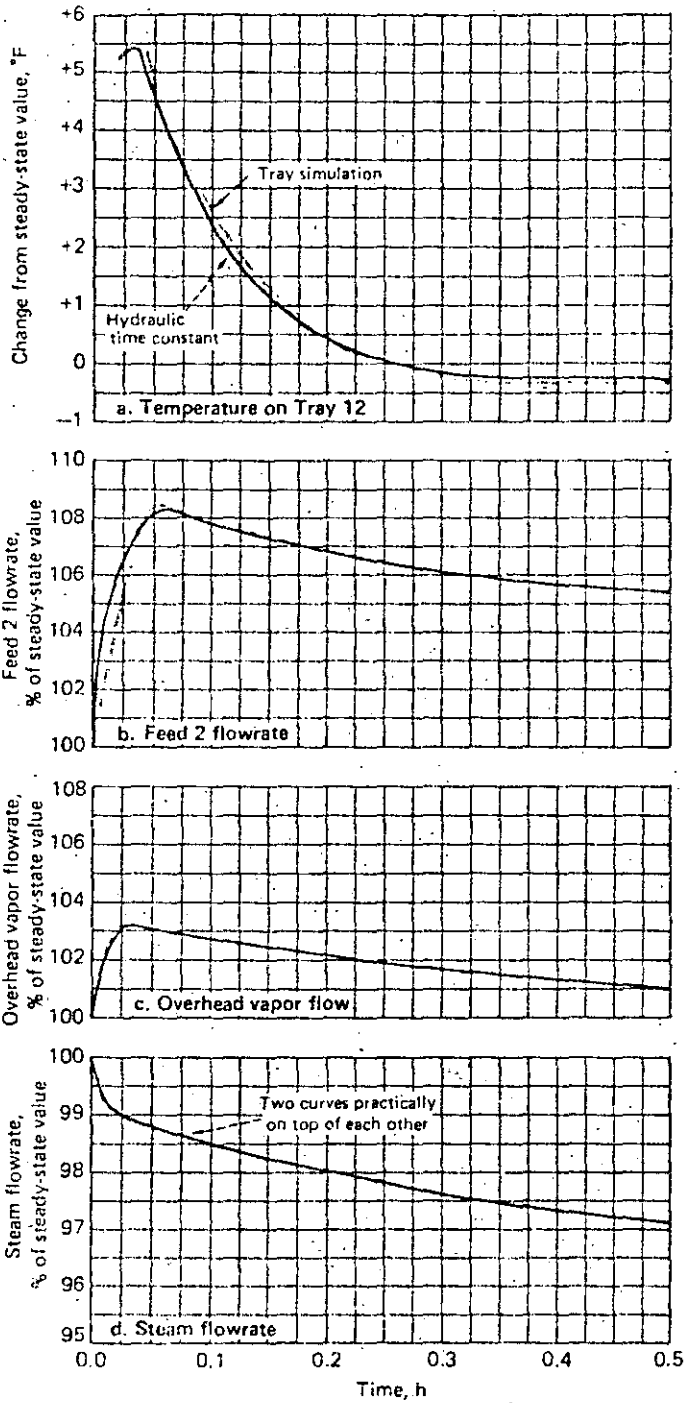
*To meet the author, see *Chem. Eng.*, May 3, 1982, p. 96.

†Articles published in this CE REFRESHER: Part 1, June 29, 1981, p. 74; Part 2, [illegible], p. 111, Part 3, Nov. 16, 1981, p. 271, Part 4, Dec. 28, 1981, p. 83, Part 5, Mar. 8, 1982, p. 97; [illegible], p. 92; Part 7, June 28, 1982, p. 97; Part 8, [illegible], p. 91; Part 9, Nov. 29, 1982, p. 75, Part 10, Jan. 10, 1983, p. 99.



Results from tray simulations, with models using variable- and constant-holdup tray hydraulics Fig. 2

rial and energy balances. The inlet streams to the bottom are liquid from the bottom tray and liquid from the reboiler. The outlet streams are product flow and liquid to the reboiler. The amount of material in the bottom of the tower must be taken into account because the difference in the liquid-level height and the top tubesheet of the exchanger (or, some other convenient reference point in the exchanger) has a direct effect on the circulation rate, pressure balance and vapor-liquid equilibrium of the reboiler.

For single-component systems, we can make reasonable assumptions provided they are not forgotten when we start to analyze the results. If we maintain the liquid level and the pressure fairly constant in the bottom of the tower, and if the exchanger has only a small preheat section so that the major mechanism of heat transfer is nucleate boiling, the system will tend to behave as a tank-type reboiler. These assumptions should be verified by simulating the natural-circulation system at various times during the column simulation. This procedure saves much computer time and work.

The equations for each tray were discussed in Part 10 of this series. The two methods—constant stage holdup and variable stage holdup—and their results will be compared later in this article

Modeling the control loops

The control loops (Fig. 1) can be simulated by the methods given in Part 2 of this series. For the level-control loop at the bottom of the tower, the level transmitter can be described by a second-order transfer function. Alternatively, we can neglect the computation and save calculation time because there is no appreciable time lag. The controller can be described by the equation for a PI (proportional + integral) type of controller. The control-valve equation for a liquid is also given in Part 2.

For the temperature-control loop that regulates the flow of Feed 2, the flow-sensing element can be described by a second-order transfer function, or we can neglect the computation. The temperature-sensing element can be described by a first-order transfer function. The temperature controller can be described by the equation for a proportional + integral + derivative (PID) controller. The flow controller can be described by the equation for a PI controller with its setpoint equal to the output of the temperature controller. The control-valve equation has been given in Part 2.

The third control loop (Heat input/Feed 1/Overhead vapor rate) requires the type of analysis given in Part 2. We must be careful to compare inputs by using the same dimensions when simulating the decision unit.

In this example, we are looking for the maximums for three quantities: (1) the signal from the sensing element for Feed 1 multiplied by a set ratio, (2) the signal from the overhead-vapor flow-sensing element, and (3) a manual operator input. I have converted all inputs to the decision unit to percent of the range of the steam-flow controller. The time-lag or time-delay function after the flowrate-sensing element for Feed 1 compensates for the time that the change in feed flowrate affects flow hydraulics in the reboiler system. The equation is:

$$Y(\theta) = X(\theta - \tau) \quad (1)$$

or, expressing Eq. (1) as a Laplace transform:

$$Y(s) = X(s)e^{-s\tau} \quad (2)$$

where Y is the output from the unit, X is the input to the unit, and τ is the time that the signal is delayed.

The flow-sensing elements for the overhead vapor, Feed 1, and steam to the reboiler, can be described by second-order transfer functions, or again we can neglect this computation. The steam controller with its setpoint

Echo print of input data **Table I**

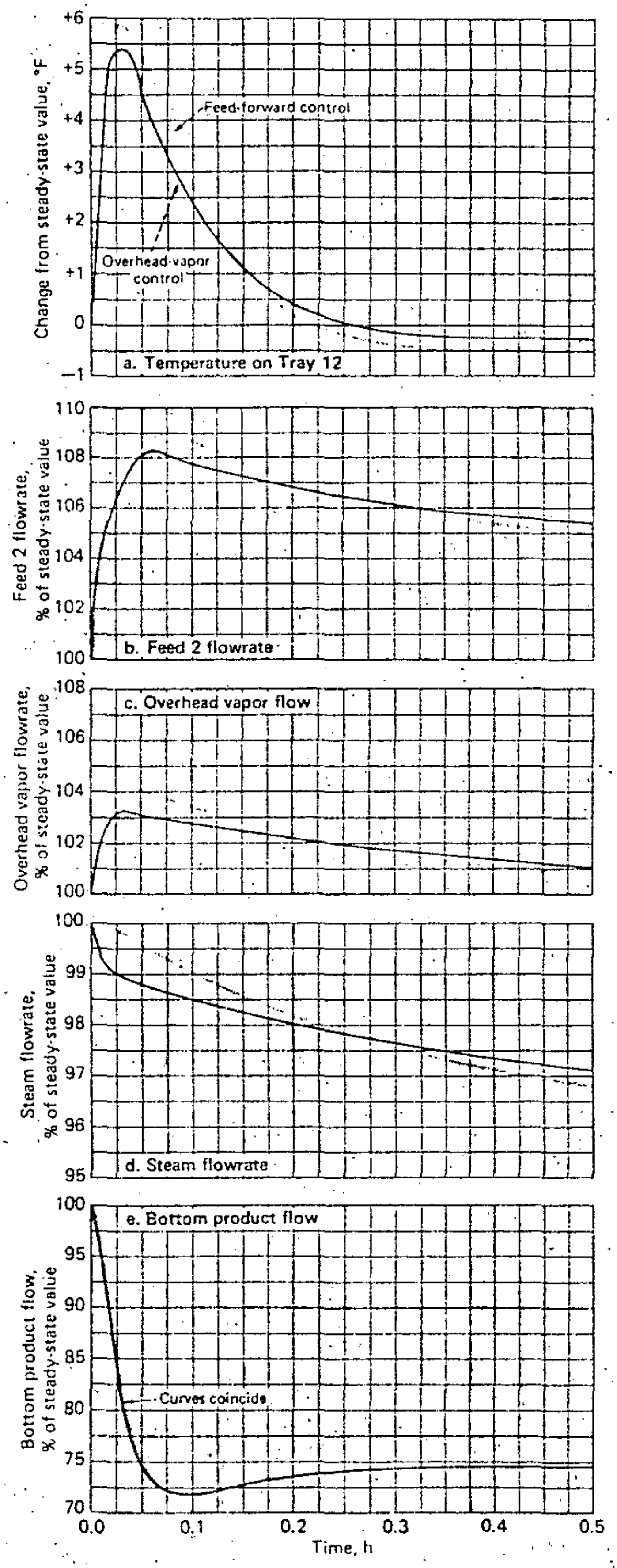
```
DYNA  .001, .5, .025, 1, 1, 25.2, 190.4, 0.001
TRAY  0, 1, 1, 10, 62.3, 5, 6, 2, 1.5, 0
TRAY  0, 1, 11, 15, 62.3, 5, 6, 2, 1.5, 0
CONM  SECOND    FEED   1, 202, 21, 0, 1., 0.001
CONM  CONTROL  TEMP   2, 12, 22, 0, 1., 0.008
CONM  OVHD      FLOW   3, 15, 21, 1, 1
CONM  FIRST     FEED   4, 201, 21, 0, 0.01162, 0.005, 0, 0.01
CONM  MANUAL    SET    5, 0, 0, 0, 200
CONM  STEAM     FLOW   8, 198, 21, 0, 1, 0.001
CONM  BOTTOM    LEVEL- 6, 0, 25, 0, 1
CONX  106, 0, 4, 0, 0, 0, 74.93
CONX  105, 0, 5, 0, 0, 2, 0.04
COND  104, 3, 0, 1, 3, 0, 4, 0, 5
CONC  CONTROL  TEMP  2, 2, 0, 2, 122, 212, 100, 1, 0.1
CONC  OVHD     FLOW  3, 3, 0, 2, 0, 446, 400, -1, 0.1
CONC  BOTTOM   LEVEL 6, 6, 0, 1, 160, 234, 100, 1, 0.1
CONC  STEAM    FLOW  7, 8, 3, 2, 0, 478, 200, -1, 0.001
CONC  SECOND   FEED  1, 1, 2, 2, 0, 374, 200, -1, 0.001
CONV  STEAM    FLOW  7, 198, 0, 2, 75, 70, 18, 0.02
CONV  BOTTOM   FLOW  6, 0, 1, 2, 35, 33.5, 2487, 0.02
CONV  SECOND   FEED  1, 202, 1, 2, 25, 20, 2487, 0.02
CONR  14.3578, --6869.59, 376.636, 16344, 540, 112874
UPST  1, 0, 15, 3
FDCH  1, 10, 0, 1, 18280, 25, 185
FRCH  1, 0.6634, 0,-10.4252, 88.9114
KEYV  21, 100
KEYV  22, 9
KEYV  22, 10
KEYV  22, 11
KEYV  22, 12
KEYV  22, 13
KEYV  22, 15
KEYV  21, 202
KEYV  21, 198
KEYV  4, 15, 1
KEYV  21, 15, 1
KEYV  4, 15, 1
KEYV  21
KEYV  25
KEYV  4
PLOT  1, 8
PLOT  1, 9
PLOT  6, 2, 3, 4, 5, 6, 7
```

from the decision unit can be described via the equation for a PI controller. The equation for the steam-control valve was given in Part 2.

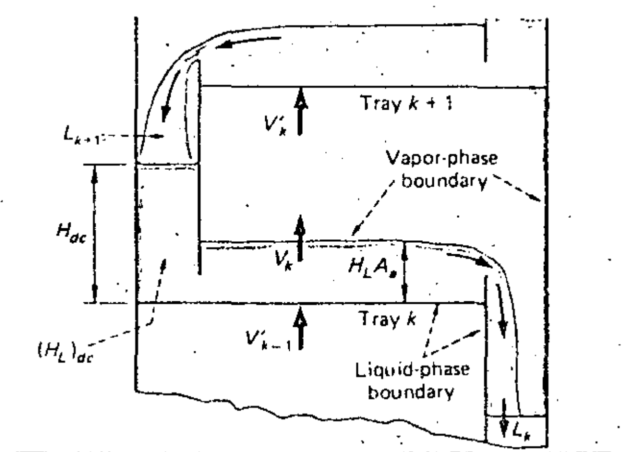
Results of the simulation

Input data that describe the dynamic parameters are listed in Table I. These lines describe tray data, measurements units (or sensing elements), algebra units, decision unit, controllers, control valves, reboiler unit, upset condition, feedstream changes, and requests for summary results in tabular and graphical form. For our example, the upset to the tower was taken as a 25% [illegible]uction in the Feed 1 rate to the tower.

Fig. 2 shows the results of the simulations for one set of control-loop parameters. The graphs show the difference between a method for simulating the valve trays rigorously with variable holdup, and one for estimating the constant-holdup tray hydraulics via the hydraulic



Tower response when steam is controlled via overhead-vapor flowrate or via Feed 1 **Fig. 3**



Models for a typical tray consider the liquid-phase and vapor-phase boundaries **Fig. 4**

time constant. Fig. 2a shows the variation in temperature on Tray 12 (used to change flowrate of Feed 2) vs. time. Fig. 2b shows the variation in flowrate for Feed 2. Fig. 2c shows the variation in the overhead-vapor flowrate, while Fig. 2d shows the change in the steam flowrate to the reboiler.

The purpose of the curves is to demonstrate that there is little real difference between the two correlations used for this simulation. However, we should use the correlation for trays in towers where a pressure-control problem is suspected or anticipated. Hence, the change in pressure on tower equilibrium can be included in the calculations. This correlation should also be used for a large change in internal flowrates.

Fig. 3 shows the results of two simulations that differ in control-loop parameters. One curve shows the response of the tower when steam to the reboiler is controlled by the sensing element for the overhead-vapor flowrate; and the other shows the tower response with the steam being controlled by the flowrate for Feed 1. The curves show the changes in the tower variables:

Variable	Fig.
Controlled stage temperature	3a
Flowrate for Feed 2	3b
Overhead-vapor flowrate	3c
Steam flowrate	3d
Product stream from bottom of tower	3e

The results in Fig. 3 show that either set of parameters gives a stable, reasonably fast response to the upset condition. However, we do not get this fast response without a penalty, because the reduction of 25% in the primary feed stream (Feed 1) did not yield a corresponding reduction in energy consumption.

We will now consider some applications of dynamic modeling to emergency systems usually found in the chemical process industries.

Pressure relief systems

In order to reduce the size of, and investment in, emergency relief systems, it is becoming increasingly important to simulate them via dynamic modeling.

For example, overpressure in a distillation tower results in the release of vapor to a flare system. As processes have become larger, these flare systems have been required to increase in size. Now some systems have become large enough to cause concern because of increasing land costs, etc.

Dynamic modeling can reduce these costs by enabling the development of novel operating procedures and more-sophisticated (as opposed to redundant) methods of instrumentation.

Modeling a distillation tower for such considerations requires additional computations. A common assumption that we made was that vapor-phase holdup was negligible. While holdup in the vapor phase may be small in comparison to that in the liquid phase, the pressure change in a tower depends directly on the change in molar holdup of the vapor phase.

Let us look at a typical tray, as shown in Fig. 4. In this analysis, we will consider two systems: The first will consist of the liquid-phase boundary (lower left), the second will consist of the vapor-phase boundary (upper right).

If we consider a stage having no external feed and no side-stream withdrawals (these can be applied as additional input and output streams without much additional work), we can derive component and total-material balances. For the liquid phase, we obtain:

$$\frac{d(\rho_L H_L)}{d(\theta)} = L_{k+1} + V'_{k-1} - L_k - V_k \qquad (3)$$

$$\frac{dX_{k,j}}{d\theta} = \Big\{[V'_{k-1} - V_k(1 - \eta_{k,j})]Y'_{k-1} + L_{k+1}X_{(k+1),j} - X_{k,j}\Big[L_k + V_k\eta_{k,j}K_{k,j} + \frac{d(\rho_L H_L)}{d\theta}\Big]\Big\}\Big/\rho_L H_L \qquad (4)$$

For the vapor phase, we obtain:

$$\frac{d(\rho_V H_V)}{d\theta} = V_k - V'_k \qquad (5)$$

$$\frac{dY'_{k,j}}{d\theta} = \Big[V_k Y_{k,j} - V'_k Y'_{k,j} - Y'_{k,j}\frac{d(\rho_V H_V)}{d\theta}\Big]\Big/\rho_V H_V \qquad (6)$$

The volumetric holdup in the vapor and liquid phases (H_V and H_L) will be a constant, and we could add another equation to account for this. However, because the volume of the vapor holdup is usually much greater than the volume of the liquid holdup, we introduce hardly any error by assuming that the holdup for vapor volume is essentially constant.

The second consideration is that Eq. (6) is only exact for a completely mixed vapor phase, where the vapor composition to the tray above equals the average composition of the total volume holdup. This is analogous to the tank problem that we considered in parts 2 and 5.

At the other extreme, we could consider the flow analogous to a pipe flow, where:

$$Y_{k,j}(\theta) = Y_{k,j}(\theta - \tau) \qquad (7)$$

where τ is a time-delay function that depends on the vapor rate and the tray layout.

In an actual column, we could be at either extreme, or somewhere in between. While we could develop equations for each situation, we cannot describe tower operation that precisely, or even say that we have that requirement. Even the expression for liquid holdup and flowrate (developed in Part 10) is an approximation.

For comparison, an actual tray [2] is shown in Fig. 5. To completely describe the tray's operation, we would take into account: the liquid distribution at all points on the tray; entrainment of liquid to the tray above, and weeping to the tray below; changes in tray efficiency during operation; and secondary physical-property changes such as surface tension and viscosity. After doing so, we could possibly obtain "better answers."

We could also complicate the model and never be able to make recommendations because we would either not get any answers, or the modeling costs would become prohibitive. Therefore, we prefer to use simplified models so that we can reach some decisions about problems—understanding that the model is not perfect.

We can calculate the number of moles in the vapor space as a function of time from Eq. (5). For the system pressure above a tray, we can use a pressure-volume relationship such as:

$$P_k = Z\eta_T RT/H_V \tag{8}$$

We can calculate a vapor temperature from an energy balance, but this probably is not necessary. The only remaining item is to arrange our calculations so that the vapor rate from a tray to the tray above depends on the material balance in the vapor space, as well as the tray pressure drop across the tray. I have developed a model for this but have not been able to mpare the results with an actual tower operation. owever, the model could be used in the process design and safety design for such systems.

Systems involving reactions

If we have kinetic rate data, we can simulate distillation and other operations involving chemical reactions. These could be intended operations or unintended operations such as inadvertently routing a chemical to a piece of equipment that acts as a catalyst.

For a plate distillation tower (possibly the most difficult system to simulate), we can add a reaction term to the material balance, as given by Eq. (3) and (4) for liquid-phase reactions.

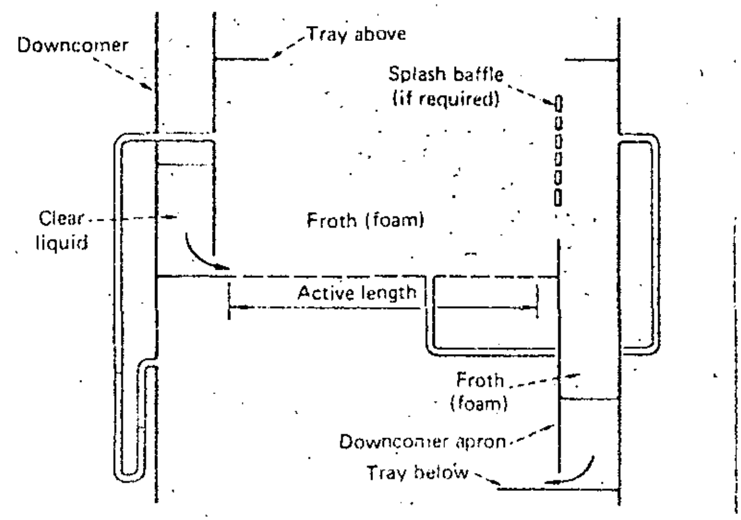
The analysis can be used to simulate the possible overpressure in a piece of equipment, design a relief system, design an instrumentation system, or design a different system at different operating conditions.

Loss of condenser coolant

Loss, or severe reduction, of condenser cooling water (or loss of air circulation for air-cooled units) can result in either loss of reflux to a tower or loss of cooling for a reactor, to create an emergency condition. This analysis is probably routinely made because we have already developed the necessary equations for the simulation, and because we do not need additional kinetic data.

artup and shutdown

The same type of "What would happen if . . . ?" questions applied to the normal operations of processes can also be asked about the procedures for starting up or shutting down the facilities. Again, dynamic analysis will play an important role in answering such questions.



Flow patterns and liquid phases occurring on an actual tray Fig. 5

Other situations and design aspects

It is impossible to discuss every situation that can lead to a plant emergency. Each situation and each process must be analyzed during the design phase. It is better to look at situations before constructing the facility. The question arises: "How much engineering time and money are enough?" Ultimately, every engineer will have to answer this question, but dynamic analysis will become more important in the design of facilities.

Additionally, dynamic modeling can also be applied to situations where catastrophic results are not likely outcomes. For example:

- Can we revise procedures to assure that a particular valve is not open during shutdown (or at other times) so as to cause the abnormal discharge of pollutants to a waterway?
- Can we design processes in such a way so as not to produce byproducts that will create disposal hazards?
- Can we design processes that are more energy-efficient and maintain good safety and reliability?

Obviously, there are no answers for every situation and no recipes for success. However, if the reader thinks about situations where dynamic analysis can lead to safer, more-efficient designs, this series will have achieved its purpose.

Steven Danatos, Editor

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2. King, C. J., "Separation Processes," McGraw-Hill, New York, 1971.

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