



**UNIVERSIDAD NACIONAL AUTÓNOMA  
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Facultad de Ingeniería

**Gas Liquid Transfer with Chemical Reactions**

Proyecto

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UTILIZACIÓN DE GASES OXIDANTES EN LA RECUPERACIÓN DE  
METALES A PARTIR DE MINERALES

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# Gas Liquid Transfer with Chemical Reactions

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# Gas Liquid Transfer with Chemical Reactions

## 1. Introduction

Using industrial gases, oxygen, nitrogen, ozone, and carbon dioxide in the leaching and flotation of sulfide minerals and several effluent treatments, it is important to optimize them technically and economically. The gas dissolution step, previous to chemical reaction is crucial to control the metallurgical process. For example, if mass transfer of oxygen from the bubbles is slow, the leaching rate will depend on the rate of oxygen supply from the gas phase. Because most of these gases, except carbon dioxide, are so sparingly soluble in aqueous solutions, much of our interest in mass transfer lies with the transfer of these gases across the gas–liquid interfaces.

First, the concept of gas diffusivity,  $D_{AB}$ , is discussed. Although it is a slow transfer velocity in an electrolyte, most of the transfer correlation for agitated tanks takes into account the  $D_{AB}$  factor. The flux equations are presented as series of resistances at the interface gas/liquid. Several models are discussed to predict gas transfer as a function of gas diffusivity. Subsequent, is introduced the concept of volumetric mass transfer coefficient,  $k_{LA}$ , which is widely employed in the industry to design agitated tanks. Lastly, the effect of the rate of chemical reaction is reviewed by using the Hatta number and Enhancement factor,  $E$ . At the end of the course, the students will run laboratory tests measuring and comparing the  $k_{LA}$  for two reactors: a flotation cell with a Rushton turbine, and a simple agitation with a magnetic agitator.

The objective of this course is to understand mass transfer fundamentals and identify what operating parameters can optimize the gas transfer.



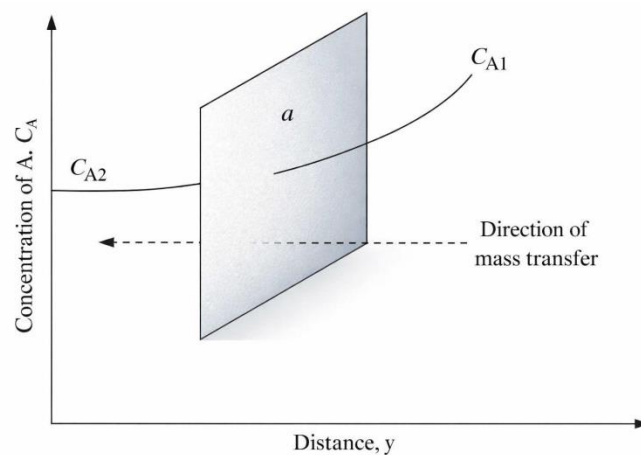
## 2. Molecular diffusion

Is the individual movement of molecules through a substance using its thermal energy. Molecular diffusion is a slow process compared to mixing using a mechanical stirrer (1). For example, if a 75 cm thick layer of water is carefully placed on top of a saline solution of the same thickness, the salt concentration in the upper water layer is reached in 28 years. If the two phases are subjected to mechanical agitation at 20 rpm, the salt concentration becomes uniform in 60 seconds. Mechanical agitation causes the movement of large portions of salt, resulting in eddy currents and turbulent diffusion, which is the opposite of the movement of individual molecules that occurs in molecular diffusion.

The mass transfer by diffusion of A occurs across area  $a$  perpendicular to the direction of diffusion, and it is given by *Fick's law of diffusion*, which states that the mass flux is proportional to the concentration gradient, Fig 1

$$J_A = \frac{N_A}{a} = -D_{AB} \frac{dC_A}{dy} \quad \text{Eq. 1}$$

$J_A$  is the *mass flux* of component A,  $N_A$  is the *rate of mass transfer* of component A,  $a$  is the area across which mass transfer occurs,  $D_{AB}$  is the *binary diffusion coefficient* or *diffusivity* of component A in a mixture of A and B,  $C_A$  is the concentration of component A, and  $y$  is distance,  $dC_A/dy$  is the *concentration gradient*, or change in concentration of A with distance.



**Fig 1.** Concentration gradient of component A inducing mass transfer across area a.



The rate of accumulation is the rate of increase of concentration in the element, multiplied by its volume, i.e.,

$$-D \frac{\partial c}{\partial y} + D \left( \frac{\partial c}{\partial y} + dy \frac{\partial^2 c}{\partial y^2} \right) = dy \frac{dc}{dt}$$

Whence

$$D \frac{\partial^2 c}{\partial y^2} = \frac{dc}{dt}$$

When the diffusant reacts with the dissolved species in the liquid, the rate of reaction of diffusant per unit volume,  $r$ , is

$$D \frac{\partial^2 c}{\partial y^2} = \frac{dc}{dt} + dy r$$

### 3. Absorption into Agitated Liquids

When liquid is quiescent, the transport of the dissolved gas is by molecular diffusion alone, and it is very slow. Then, it is unusual to use it in industrial processes. The absorption rate of gases into liquids which are agitated, has several individual flux equations in series

For the Gas Film:  $N_A = k_g(p_{AB} - p_{Ai})$

For the Liquid Film:  $N_A = k_L(C_{Ai} - C_{Ab})$

To find the overall liquid-side coefficient,  $K_L$  we assume that  $C_{Ai} = C_A^*$ , which is the concentration in equilibrium with the bulk gas pressure  $p_{Ab}$ , given by Henry's Law,  $p_A = H C_{Ab}$ . The resistance relationship is

$$\frac{1}{K_L} = \frac{1}{k_g} + \frac{1}{H \cdot k_L}$$

The absorption rate of gases into liquids which are agitated, is given by Whitman's Two-Film Theory, which is an engineering simplification of the boundary layer theory (2).

$$N_A = k(C_{Ai} - C_{Ab})$$



Where,

$N_A$ , is the gas flow rate, mol/m<sup>2</sup>.s

$k$ , is the mass transfer coefficient, m/s

$C_{Ai}$ , is the molar concentration at the interface, and

$C_{Ab}$ , is the molar concentration of A in the bulk liquid.

Because this theory assumes:

A purely stagnant, "dead" layer of liquid of thickness,  $\delta$ .

Zero fluid motion within the film.

Transport is purely molecular diffusion.

The concentration gradient is linear.

The mass transfer coefficient,  $k$ , is expressed as

$$k = \frac{D_{AB}}{\delta}$$

**The Flaw:** It predicts that the mass transfer coefficient,  $k$ , is directly proportional to the diffusion coefficient,  $k \propto D_{AB}^1$ . Experimental data usually shows  $k \propto D^{0.5}$  to  $D^{0.67}$ .

### Other models (3)

- **Boundary Layer Theory: The "Fluid Reality"**

As fluid flows, friction creates a velocity gradient. Simultaneously, a "Concentration Boundary Layer"  $\delta_c$  forms where the concentration goes from the interface value to the bulk value. This theory accounts for both **convection** (fluid motion) and **diffusion**.



Feature	Two-Film Theory	Boundary Layer Theory
Fluid State	Completely Stagnant	Moving (Laminar or Turbulent)
Gradient	Linear: $\frac{dc}{dx} = \text{const}$	Non-linear (Curved)
Dependence	$k \propto D^{1.0}$	$k \propto D^{2/3}$
Thickness, $\delta$	Constant, assumed value	Varies with distance and velocity
Primary Use	Industrial design/Mass transfer unit calcs	Fundamental heat & mass research Computer fluid dynamics

- **Penetration Theory or Higbie's model**

The gas-liquid interface is made up of small liquid elements, which are continuously brought up to the surface from the bulk of the liquid and vice versa and all the surface elements stay at the surface for the same amount of time,  $t_e$ . The mass transfer coefficient,  $k$  is proportional to the square root of diffusivity.

- **Surface renewal theory: Danckwerts model**

In this case, the surface elements do not have equal life, i.e., the probability for a surface element to disappear from the surface in a given interval of time is independent of its age. If  $s$  is the rate of surface renewal, Danckwerts arrived to same dependence of  $k$  proportional to the square root of diffusivity.



- **Comparison of Mass Transfer Theories**

Theory	Key Physical Assumption	Mathematical Relation	DAB Exponent	Best Applied To...
<b>Film Theory</b> (Whitman)	Steady-state diffusion through a stagnant, fixed "dead" layer.	$k = \frac{D}{\delta}$	<b>1.0</b>	Simple industrial design; steady systems.
<b>Boundary Layer</b> (Chilton-Colburn)	Interaction between fluid momentum (viscosity) and molecular diffusion.	$k \propto D^{2/3}$	<b>0.67</b>	Flow in pipes, over flat plates, or through packed beds.
<b>Penetration Theory</b> (Higbie)	Unsteady-state diffusion; fluid "packets" stay at the interface for a fixed time $t_e$	$k = 2 \sqrt{\frac{D}{\pi t_e}}$	<b>0.5</b>	Bubbles rising in a column or falling films with short contact times.
<b>Surface Renewal</b> (Danckwerts)	Fluid "packets" at the interface are randomly replaced by bulk fluid at a rate $s$ .	$k = D * s$	<b>0.5</b>	Highly turbulent systems (stirred tanks, agitated reactors).

Due to the simplicity of the film theory, it is often preferable to use it rather than one of the others

#### 4. Industrial Practice

To use  $k_L$  (m/s), you would need to know the **exact total surface area  $m^2$**  of every single bubble in the tank at any given moment.

**The Reality:** We can't easily measure that area. However, we *can* easily measure the total amount of gas entering the liquid over time.

**The Solution:** We join the velocity  $k$  and the area,  $a$ , into one single measurable value:  **$k_L a$** .

Industry doesn't care about how fast a molecule moves across one square meter; they care about **how many moles of gas enter the entire tank per second**.

The transfer rate equation is:

$$N_A = k_L * a(C_A^* - C_A b)$$

**$k_L$** , is the **speed** of the transfer m/s.





a is the **surface area** available,  $\frac{m^2}{m^3}$

$k_L a$ , the volumetric coefficient, ,  $time^{-1}$

Engineers use empirical power laws to predict  $k_L a$ , based on power input (P/V) and gas superficial velocity ( $u_g$ ) (4):

$$k_L a = C \left( \frac{P}{V} \right)^\alpha (u_g)^\beta$$

## 5. Absorption with Chemical reaction

A combination of mass transfer with chemical reaction is caused when two phases, which are not in equilibrium with one another, are brought into contact. It takes place when:

There is diffusion of the reactant from the interphase to the bulk of the electrolyte.

Chemical reaction in the electrolyte

Diffusion of the residual reagents/products of the reaction within the electrolyte

There are two controls:

Hydrodynamic Control: The Physical Film,  $\delta$ . In the Two-Film Theory, the thickness of the stagnant liquid film,  $\delta$ , is determined by hydrodynamics (stirring speed, flow velocity, and viscosity).

The Reaction Zone,  $\delta_R$ . While the physical film remains constant, a fast chemical reaction changes the **concentration profile** within that film. As the reaction becomes faster, the solute gas (A) is consumed more quickly as it diffuses.

This leads to the concept of the **Hatta Number Ha**, which can be physically interpreted as:

$$Ha = \frac{\text{Physical film thickness, } \delta}{\text{Reaction zone thickness, } \delta_R}$$

**The "Enhancement Factor" (E)**



Because the concentration gradient becomes much steeper (the gas drops to zero over a shorter distance), the mass transfer rate increases. We account for this using the **Enhancement Factor**:

$$N_A = Ek_L(C^* - C_b)$$

Where:

$k_L$ , is the physical mass transfer coefficient,  $\frac{D_{AB}}{\delta}$

E is the multiplier that accounts for the reaction "pulling" more gas into the liquid

### **Acknowledgments**

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