

Chapter 2

Mass Transfer Coefficient

2.1 Introduction

The analysis reported in the previous chapter allows to describe the concentration profile and the mass fluxes of components in a mixture by solving local mass balance equations, once the mixture velocity field is known. Such analysis allows the concentration profiles to be evaluated in solids (no velocity) or fluids in laminar flow, when the velocity can be determined via the motion equation (Navier–Stokes equations); the only difficulties in this approach are linked to the mathematical and numerical complexity, which can be important, especially for unsteady state and/or 3D problems. A completely different scenario appears when we deal with turbulent flow, in which elements of fluid do not flow in an orderly manner, one layer over another, but in a chaotic mode, with rapid velocity fluctuations and nonzero instantaneous velocity components, even in the direction perpendicular to the bulk fluid motion. As an example, in the case of turbulent fluid flow past a flat solid surface, eddies with a size several orders of magnitude larger than the mean molecular free path arise and the velocity field shows significant instantaneous components also perpendicularly to the surface; such phenomena contribute significantly to the mass transport process and must be accounted for. If mass transfer between the liquid and the surface occurs in these conditions, thanks to turbulent mixing, the fluid composition varies only slightly with the position in the bulk of fluid, whereas a significant composition gradient may be observed in a thin layer of fluid near the surface.

Considering that:

- even though turbulence is a widely studied topic, we are far from a satisfactory understanding of the turbulent flow mechanism and, as a consequence, of mass transport in turbulent flow
- the mixture composition in the bulk of the fluid in turbulent flow is fairly uniform
- in many relevant engineering applications, a detailed quantitative evaluation of the concentration profile is not required

we turn our attention to lumped-parameter models, aimed at evaluating the mean concentration of the system (in the bulk) and, in some cases, its evolution with time. This simplified analysis requires only the knowledge of the mass fluxes exchanged by the system with the surroundings, through its boundary surface.

Mass transfer coefficients are defined with the aim of evaluating these fluxes in a simple way, with a wise use of theoretical analysis and empirical results.

2.2 Definition of Mass Transport Coefficients

Mass transport coefficient is defined so that

diffusive flux = (mass transport coefficient) \times (concentration difference)

or

$$k_c = \frac{J_A|_s}{c_A^0 - c_{Af}} \quad (2.1)$$

where $J_A|_s$ is the diffusive flux of A on the surface between the system and the surrounding, c_A^0 and c_{Af} are the concentrations of A on the surface and on the bulk of fluid, respectively.¹

Sometimes, the difference in molar fractions or, for a gas phase, in partial pressures between the surface and the bulk of fluid can be considered as the driving force for mass transport; as a consequence, different mass transport coefficient can be also defined as follows:

$$k_x = \frac{J_A|_s}{x_A^0 - x_{Af}} \quad k_p = \frac{J_A|_s}{p_A^0 - p_{Af}} \quad (2.3)$$

Since

$$k_c (c_A^0 - c_{Af}) = k_x (x_A^0 - x_{Af}) = k_p (p_A^0 - p_{Af}) \quad (2.4)$$

it can be easily proved that

$$k_x = k_c \quad k_p = \frac{k_c}{RT} \quad (2.5)$$

¹The bulk concentration is the concentration in the fluid far from the surface or, for flow in conduits, the cup-mixing concentration defined as

$$c_{Af} = \frac{\int_S v c_A dS}{\int_S v dS} \quad (2.2)$$

so that the flow rate of A through the duct section can be given as $c_{Af} \int_S v dS$.

The mass transfer coefficients so defined must account for physical properties of the system (in particular, the diffusivity, \mathcal{D}_{AB} , fluid density, ρ , and viscosity, μ), and for the fluid motion.

2.3 Evaluation of Mass Transport Coefficient

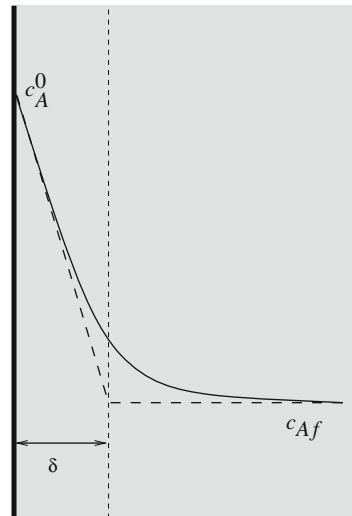
It is evident that, if the mass transport coefficient is known, the evaluation of the flux of A is straightforward, while all the procedure described in the previous section is useless if a method to calculate the mass transport coefficient is not available. Obviously, it is possible to get mass transport coefficient from the results of mass transport experiments, but what we do really need are some correlations of the experimental results that allow to calculate the mass transport coefficient in a variety of conditions. Theoretical considerations, less or more complex, are of paramount utility to wisely build these correlations.

The oldest and most obvious approach is based on the so-called *film model* (see Fig. 2.1). In such model, the entire concentration difference between the bulk of fluid and the surface is considered to be localized in a viscous thin layer (film); within the film, which is adjacent to the surface, solute transport occurs by molecular diffusion, so that the flux of component A is given by:

$$J_A = k_c (c_A^0 - c_{Af}) = \frac{\mathcal{D}_{AB}}{\delta} (c_A^0 - c_{Af}) \quad (2.6)$$

where δ is the film thickness, which is assumed to depend on fluid motion conditions.

Fig. 2.1 Concentration profile near the interface in the film model



The film model does not allow to predict the mass transfer coefficient, since we are unable to evaluate δ , but it predicts that mass transport coefficients for different solutes, under the same fluid flow conditions, are in the same ratio of their molecular diffusivities. Experimental data actually show that mass transport coefficients of different component in the same solvent and in the same fluid dynamic conditions increase with diffusivities to a power ranging from $1/2$ to $1/3$, and, therefore, more complex models must be considered to get fairly good correlations.

More reliable results can be obtained from rigorous dimensional analysis, boundary layer theory or penetration theory: since a deep analysis of mass transport models is out of the aim of an artificial organ engineering book, we only report the main results.

Relations for mass transport coefficients are usually given in terms of dimensionless groups:

- Sherwood number, Sh , is defined as

$$Sh = \frac{k_c \ell}{\mathcal{D}_{AB}} \quad (2.7)$$

where ℓ is a characteristic length of the problem. Comparing the definition of Sherwood to the film model, the physical meaning of Sherwood number can be recognized as the ratio between the characteristic dimension, ℓ , and the film thickness, δ ; usually, Sh is quite a large number, corresponding to a slender film layer;

- Reynolds number, Re , is defined as

$$Re = \frac{\rho v \ell}{\mu} \quad (2.8)$$

which represents the fluid motion conditions;

- Schmidt number, Sc , is defined as

$$Sc = \frac{\mu}{\rho \mathcal{D}_{AB}} \quad (2.9)$$

It is worth noting that Sc only contains fluid properties and represents the ratio between momentum diffusivity, μ/ρ , and diffusivity. For gases $Sc \approx 1$, while for liquids it is in the range $10^2 \div 10^3$.

It can be theoretically proved that mass transport coefficient can be expressed as a function of Re and Sc :

$$Sh = f(Re, Sc) \quad (2.10)$$

Such a function can be obtained by combining theoretical models (boundary layer, penetration theory, etc.) and correlations of experimental data. As an example, for a flow near a solid surface, with high velocity gradient near the surface, boundary layer model suggests a dependence of Sh on $Sc^{1/3}$; on the other hand, for mass transfer

Table 2.1 Correlation for mass transport coefficients

Fluid motion	Relations	Characteristic dimension, velocity
Inside circular pipe	$Sh = 0.023Re^{0.83}Sc^{1/3}$	Inner diameter of the pipe; mean velocity in the pipe
Parallel to flat plates	$Sh = 0.664Re^{1/2}Sc^{1/3}$	Plate length; approach velocity of the fluid
Past single solid sphere	$Sh = 2 + 0.6Re^{1/2}Sc^{1/3}$	Sphere diameter; fluid velocity far from the sphere
Past single gas sphere	$Sh = 2 + 0.645Re^{1/2}Sc^{1/2}$	Sphere diameter; fluid velocity far from the sphere
Through fixed beds of pellets	$Sh = 1.17Re^{0.58}Sc^{1/3}$	Pellet diameter; superficial velocity in the bed (volume flow rate divided by the empty bed section)

coefficient in a liquid phase near a gas phase (no velocity gradient in the liquid) penetration theory suggests a dependence of Sh on $Sc^{1/2}$.

Some correlations, referring to the more common flow configurations, are reported in Table 2.1.

2.4 Mass Transfer Between Two Phases

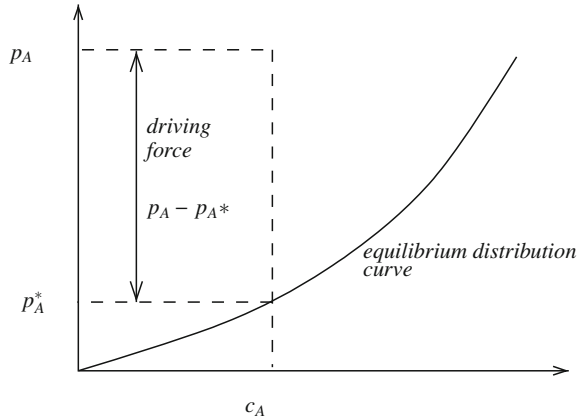
In the previous section, mass transport coefficients have been introduced to describe the mass transport occurring between an interface and the bulk of a homogeneous solution. In practice, we are more often interested in mass transfer between two contacting homogeneous phases; furthermore, in some cases a permeable membrane, offering a resistance to mass transfer, is placed between the two phases. As an example, let us consider oxygen transfer from air to blood, in direct contact or separated by a natural or artificial membrane.

In these cases, it may be desirable to directly describe the mass flux across the interface in terms of an appropriate difference in composition between the two phases and an overall mass transport coefficient. To this aim, we have to face two different problems:

- What is an appropriate difference in composition, to be used as the driving force for mass transfer?;
- How to relate the overall and single-phase mass transfer coefficients?

In the following, we discuss these two problems referring to mass transfer between a gas and a liquid phase in direct contact; we use partial pressure and concentration as composition variables for the gas phase and liquid phase, respectively; the reader can easily follow the same procedure to cope with different situations.

Fig. 2.2 Driving force for mass transfer in a gas–liquid system



As for the suitable composition difference, thermodynamics states that there is no mass transfer if the two phases are in equilibrium and, for a system not in equilibrium, mass transfer occurs to bring the system to equilibrium condition. Equilibrium conditions² are expressed in terms of an equilibrium distribution curve, i.e., a function that relates the composition in the gas phase (e.g., the partial pressure of A) with the composition of the liquid phase (e.g., the concentration of A) at a fixed temperature³

$$p_A = f(c_A) \quad (2.11)$$

Therefore, if we consider a two-phase system, with a gas at partial pressure p_A and a liquid with a concentration c_A (see Fig. 2.2):

- no transfer of A occurs if the partial pressure of A in the gas phase is equal to the partial pressure p_A^* corresponding to the equilibrium with c_A , i.e., if $p_A = p_A^* = f(c_A)$
- the driving force is the difference between p_A and $p_A^* = f(c_A)$; transfer occurs from gas to liquid if $p_A > p_A^*$ (gas absorption) or from liquid to gas if $p_A < p_A^*$ (stripping)⁴
- a suitable way to express the A flux through the interface may be

$$N_A = K_P(p_A - p_A^*) \quad (2.12)$$

²Thermodynamics states that equilibrium conditions are given by the equality of each component chemical potentials in the two phases.

³A side effect of this relationship is that we can refer to the composition of a phase α giving the composition of a different phase β in equilibrium with α : In medical field, it is usual to refer to oxygen concentration in the blood in terms of oxygen pressure, i.e., referring to the oxygen partial pressure in a gas phase in equilibrium with the blood.

⁴The driving force can be expressed also in terms of the concentration of A in the liquid phase: no transfer occurs if $c_{AL} = c_A^* = f^{-1}(p_A)$, where f^{-1} stands for the inverse of the function f , and the driving force is a difference between c_A and c_A^* ; absorption occurs if $c_A < c_A^*$.

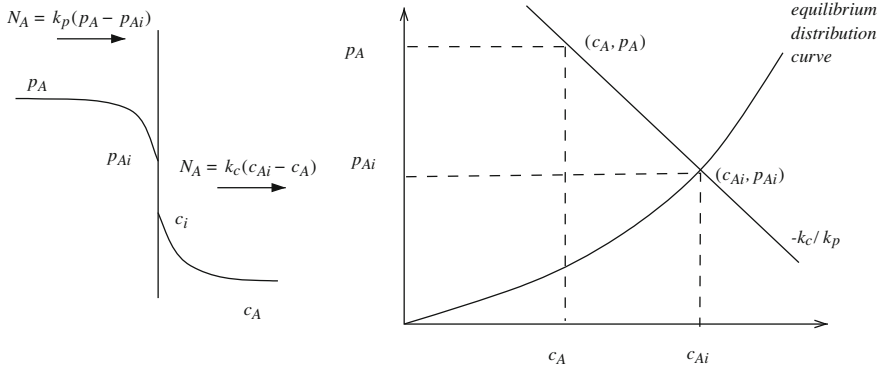


Fig. 2.3 Mass transfer from gas to liquid: flux and compositions at the interface

or

$$N_A = K_c (c_A - c_A^*) \quad (2.13)$$

K_P and K_c are two different overall mass transfer coefficients (with different units), but all of them sum up the resistances to mass transport in both phases. The next step is then related to the overall mass transport coefficient to the mass transport coefficients in gas and liquid phases.

To this aim, let us consider the absorption of A from a gas phase at p_A to a liquid phase at c_A ($p_A > p_A^*$), as in the scheme reported in Fig. 2.3; since A moves from gas to liquid, we have a flux of A from the bulk of the gas phase toward the interface and from the interface to the bulk of the liquid phase; this implies that the partial pressure of A falls from p_A in the bulk of gas to p_{Ai} at the interface, where gas and liquid are in contact; similarly, in the liquid phase, the concentration of A drops from c_{Ai} at the interface to c_A in the bulk of liquid. If the diffusional resistances are only those in the fluid phase, the partial pressure and the concentration of A at the interface (p_{Ai} and c_{Ai}) are in equilibrium, i.e.,

$$p_{Ai} = f(c_{Ai}) \quad (2.14)$$

Furthermore, flux of A from bulk gas to the interface must equal flux of A from the interface to the bulk liquid

$$N_A = k_p(p_A - p_{Ai}) = k_c(c_{Ai} - c_A) \quad (2.15)$$

Equations 2.14 and 2.15 allow to get the interface composition and the flux of A, once the bulk composition and the single-phase mass transfer coefficients are known. The expression of the flux in terms of an overall mass transport coefficient is quite straightforward, if the equilibrium condition is a linear function, i.e., if at equilibrium, $dp/dc = m_{pc}$, with m_{pc} constant at least in the range of pressure and concentration

we are interested in. In this case, it is possible to write

$$p_A - p_A^* = (p_A - p_{Ai}) + (p_{Ai} - p_A^*) = (p_A - p_{Ai}) + m_{pc} (c_{Ai} - c_A) \quad (2.16)$$

and then, considering that $(p_A - p_{Ai}) = N_A/k_p$ and so on,

$$\frac{1}{K_p} = \frac{1}{k_p} + \frac{m_{pc}}{k_c} \quad (2.17)$$

In a similar way, for K_c we get the following:

$$\frac{1}{K_c} = \frac{1}{m_{pc}k_p} + \frac{1}{k_c} \quad (2.18)$$

The above equations show that the overall mass transfer coefficient depends on the single-phase mass transport coefficients and on the slope of the equilibrium distribution curve.

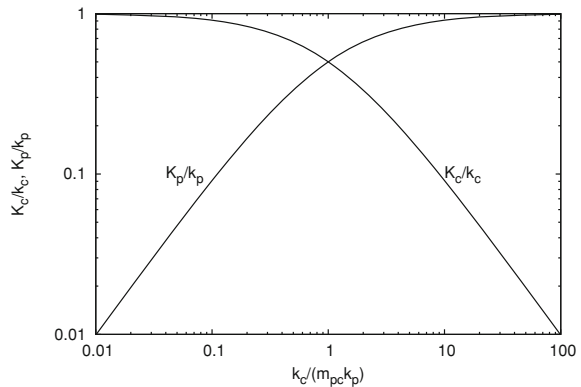
It may be interesting to consider the ratio

$$\frac{k_p}{K_p} = 1 + \frac{m_{pc}k_p}{k_c} \quad \frac{k_c}{K_c} = 1 + \frac{k_c}{m_{pc}k_p} \quad (2.19)$$

The term $m_{pc}k_p/k_c$ accounts for the relative importance of the mass transport resistances in each phase. More specifically:

- if $m_{pc}k_p/k_c \ll 1$ or $k_c/m_{pc}k_p \gg 1$, then $K_p \approx k_p$ while $K_c \approx m_{pc}k_p$ (see Fig. 2.4). In this case, the mass transport resistance in the liquid phase has a little effect on the overall mass transfer rate, i.e., mass transfer is *gas phase controlled*. Under such condition, any effort aimed at increasing the mass transfer rate should be directed to improving the gas-phase mass transport coefficient;

Fig. 2.4 Overall mass transfer coefficient as a function of the ratio $k_c/m_{pc}k_p$



- if $m_{pc}k_p/k_c \gg 1$ $K_c \approx k_c$ and $K_p \approx k_c/m_{pc}$ (see Fig. 2.4). In this case, which occurs more frequently than the previous one, the mass transport resistance in the gas phase has a little effect on the overall mass transfer rate, i.e., mass transfer is *liquid phase controlled*. Under such condition, any effort aimed at increasing the mass transfer rate should be directed to improving the liquid-phase mass transport coefficient;

Symbols

c	Concentration
\mathcal{D}_{AB}	Diffusivity
J_A	Diffusive flux of the component A
k_c	Mass transfer coefficient, based upon concentration driving force
k_p	Mass transfer coefficient, based upon partial pressure driving force
k_x	Mass transfer coefficient, based upon mole fraction driving force
K_c	Overall mass transfer coefficient, based upon concentration driving force
K_p	Overall mass transfer coefficient, based upon pressure driving force
K_x	Overall mass transfer coefficient, based upon mole fraction driving force
ℓ	Characteristic length
m_{pc}	Slope of the equilibrium line, based upon partial pressure (gas phase) and concentration (liquid phase)
P	Pressure
p_A	Partial pressure of the component A
R	Gas constant
Re	Reynolds number
Sc	Schmidt number
Sh	Sherwood number
T	Temperature
v	Fluid velocity
x	Mole fraction
μ	Viscosity
ρ	Density

Subscripts

A	Related to component A
B	Related to component B
f	In the bulk of fluid
i	At the interphase

Superscripts

α	Phase α
β	Phase β
0	On the surface
*	Corresponding to equilibrium conditions

Artificial Organ Engineering

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2017, XV, 265 p. 107 illus., 26 illus. in color., Hardcover

ISBN: 978-1-4471-6442-5