

INTERPHASE MASS TRANSFER

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Keywords: Turbulent flow, turbulent mass flux, eddy viscosity, eddy diffusivity, Prandtl mixing length, mass flux at the interface, mass transfer coefficient, driving force of mass transfer, film theory, penetration theory, surface renewal theory, von Kármán momentum balance, mass transfer coefficient at high net molar flux, overall mass transfer coefficient, interphase equilibrium, correlations of mass transfer coefficients, , matrix of multicomponent diffusion coefficients, matrix of multicomponent mass transfer coefficients, mass flux in multicomponent systems.

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Summary

In mass transfer processes which constitute the vast majority of industrial processes like absorption, distillation and extraction mass transfer takes place simultaneously by diffusion and convection. Convection is a macroscopic process in which portions of fluid are moved over much larger distances than in diffusion, carrying the transferred component from regions of high concentration to regions of low concentration. This movement is generated by agitation or by eddies and currents of the turbulent flow. Therefore the aim of this chapter is to present the basic concepts of a mass transfer process in which the two phenomena, i.e. diffusion and convection are strictly connected leading to the definition of a resultant mass flux. Consequently, this should enable the design and optimization of mass transfer equipment. At this point it has to be stressed that interphase mass transfer is a substantial part of the fundamentals of Chemical Engineering. As in the majority of mass transfer processes the turbulent flow

is realized, the fundamentals and features of this type of flow were discussed and the equation determining the turbulent mass flux was developed. The main task in designing the mass transfer equipment is the estimation of the mass flux at the interface. To this end the mass transfer models like the film theory, the penetration theory, the surface renewal theory and the boundary layer theory were presented leading to the definition of mass transfer coefficient in one phase. The equation of overall mass transfer coefficient was developed and the method of estimation of the mass flux between the two phases discussed. Special attention was devoted to the multicomponent mass transfer, which, for a long time, was the subject of intensive research. The matrix of multicomponent mass transfer coefficients was defined and the method of calculating its elements presented.

1. Introduction

Mass transfer phenomena can now be encountered in many fields of industry. In particular, separation processes which constitute the vast majority of industrial processes are based on the physics of mass transfer and their design and optimization depends considerably on the knowledge in this field. These problems are the subject of research of the phenomenon named interphase mass transfer which constitutes a substantial part of the fundamentals of Chemical Engineering.

The chapter: “Mass Transfer by Diffusion” is mainly concerned with theoretical treatment of mass transfer in a single phase. However, in most of the industrial processes the species are transported across a phase boundary. For instance, in distillation where a vapor and a liquid phase are brought into contact in special types of columns, the more volatile component is transported from the liquid phase into the vapor phase while the less volatile one in the opposite direction. This is an example of equimolar mass transfer. In absorption the soluble component is transported to the phase boundary, called also the interface, where it dissolves in the liquid and then penetrates into the bulk of the liquid. As the interface is impermeable to the carrier gas (insoluble in the liquid) it is not transferred forming the so called stagnant component. Other examples are liquid – liquid extraction where the solute is transported from one liquid solvent to another, adsorption, drying, membrane processes and heterogeneous chemical reactions.

In all the unit operations mentioned mass transfer takes place simultaneously by diffusion and convection.

Diffusion is a random molecular motion being the consequence of thermally induced translation of molecules. It was discussed in the chapter: “Mass Transfer by Diffusion”.

Convection is a macroscopic process in which portions of fluid are moved over much larger distances than in diffusion. These portions of fluid carry the transferred component from regions of high concentration to regions of low concentration. We should be aware of the fact that the convective flux of fluid transports the whole fluid mixture, so simultaneously all the other components as well. The convective process is generated by agitation or by currents and eddies of the turbulent flow. However, this process is strictly connected with diffusion, as the mass transfer between the adjoining

currents of fluid proceeds by diffusion, thus causing their mixing.

As can be concluded from the above description of industrial applications of mass transfer phenomena the main task and goal of theoretical considerations should lead to the development of expressions which define the mass fluxes at the interface. The rate of mass transfer to the interface depends on the physical properties of the phase, the nature of the fluid flow, the driving force of the process (usually a concentration difference) and the interfacial area. In order to intensify the mass transfer rate the turbulent fluid flow is usually realized in the mass transfer equipment. Turbulent flow is a chaotic motion composed of series of eddies and circulating currents of different sizes (scales) and kinetic energies which cause an intense mixing and, consequently, lead to high mass transfer fluxes. The turbulence of a fluid flowing along a solid surface does not extend to the surface itself. The eddies decay when approaching the solid surface and a laminar sublayer is formed in which the mass transfer proceeds by diffusion.

Therefore the phenomenon called mass transfer to the phase boundary is composed of the transport of the component from the bulk of the fluid phase to the laminar sublayer by convection and of the transport through this layer by diffusion.

As the majority of flows in industrial equipment is turbulent rather than laminar, we will discuss in the next section the nature of turbulent mass transfer and present expressions defining the turbulent mass fluxes.

Unfortunately, the number of analytical solutions of the engineering problems concerning mass transfer is very limited. Therefore, empirical expressions have been elaborated based on approximate models of the mechanism of mass transfer to the interface such as the film theory or the penetration and surface renewal theories as well as the boundary layer theory which simultaneously define the mass transfer coefficient in one phase. This quantity is a parameter in empirical expressions defining the mass transfer flux of a species at the interface. In engineering calculations the mass transfer coefficient is determined mostly from empirical correlations of dimensionless numbers which characterize the problem considered. The method of identifying the dimensionless numbers as well as formulating the correlations was elucidated. The main tool in developing correlations for mass transfer coefficients is the combination of dimensional analysis and experimental data.

The influence of high values of the net total molar flux on the mass transfer coefficient has been discussed and the method of correcting the mass transfer coefficient for high net mass transfer rates developed. The phenomenon plays an important role in processes where simultaneous heat and mass transfer takes place.

In the majority of industrial mass transfer processes the species are transported from one phase into another. The overall mass transfer coefficient has been derived which is a function of the mass transfer coefficients in the two phases as well as of the slope of the equilibrium line.

Special attention has been devoted to the multicomponent mass transfer, which for a long time, has been the subject of intensive research. For an unequivocal determination

of the mass fluxes at the interface in a multicomponent system the film theory has been applied considering the mass transfer process as a steady-state one-dimensional diffusion through a film of constant thickness. Based on this theory the matrix of multicomponent diffusion coefficients as well as multicomponent mass transfer coefficients has been defined and the method of their evaluation explained. These quantities enable the determination of mass transfer fluxes at the interface in a multicomponent system.

2. Turbulent Mass Transfer

In this section we will not discuss the statistical theories of turbulence which try to elucidate the structure of turbulence and the way the turbulent energy is distributed and dissipated. Our main interest is to present the methods which lead to the time-smoothed or Reynolds averaged velocity and concentration profiles.

Turbulent flows are characterized by chaotic fluctuations of velocities. These fluctuations mix the transported quantities such as momentum, energy and species concentration causing their fluctuations as well. It is assumed that the equations of change developed in Section 4 “Generalized Mass Balances” of the chapter “Mass Transfer by Diffusion” can be applied to describe the violently fluctuating motion of turbulent flow.

This is justified by the fact that the sizes of turbulent eddies are several orders of magnitude larger than the mean free path of molecules, and so the assumption of the continuum of the system is fulfilled.

Our considerations concern an isothermal binary system assuming constant density and diffusivity. Thus the mass balance of species *A* will be presented as:

$$\frac{\partial C_A}{\partial t} + \frac{\partial}{\partial x}(w_x C_A) + \frac{\partial}{\partial y}(w_y C_A) + \frac{\partial}{\partial z}(w_z C_A) = D_{AB} \left(\frac{\partial^2 C_A}{\partial x^2} + \frac{\partial^2 C_A}{\partial y^2} + \frac{\partial^2 C_A}{\partial z^2} \right) \quad (1)$$

From the theoretical point of view integrating this equation together with the three momentum balance equations for the velocity components (w_x, w_y, w_z) in time and in space should lead to functions defining the three fluctuating velocities and the fluctuating concentration C_A . This procedure is called Direct Numerical Simulation (DNS). This is a fundamental procedure where no assumptions have been introduced.

However, at this moment it has to be noticed that the time scale of fluctuations is of the order of 0.1ms and the spatial scale of fluctuations is around 30 μ m.

Therefore in the DNS procedure the balance equations are integrated in time on a very

small spatial scale with millions of nodes. A DNS simulation for even a simple problem (such as turbulent flow in a pipe) may take hours on a network of 16 computers. This is an enormous problem demanding very time consuming numerical calculations. It is used only in theoretical considerations and delivers parameters for the simplified empirical turbulent models.

One of the semiempirical simplified models is obtained by applying the Reynolds method of averaging of the instantaneous fluctuating variables (velocity, concentration), which are decomposed into the main mean component and the fluctuating component which is a chaotic deviation from the mean value.

Hence, for the z -component of the fluid velocity we write

$$w_z = \bar{w}_z + w'_z \quad (2)$$

and for the concentration

$$C_A = \bar{C}_A + C'_A \quad (3)$$

The time-averaged concentration profile $\bar{C}_A(x, y, z, t)$ is that estimated experimentally by analyzing the samples of fluid taken from the fluid stream. The intense mixing in the turbulent core generated by the turbulent eddies will cause only slight variations of the time averaged concentration \bar{C}_A with position in this region. The eddies, however, die out approaching the boundary surface of the phase (e.g. tube wall) forming a slowly flowing laminar layer, in which the concentration will change within a small distance from the nearly constant value in the turbulent core to that at the boundary surface. This concentration difference forms the driving force for diffusion in this layer.

The time averaged velocity will then be calculated as follows

$$\bar{w}_z = \frac{1}{\tau} \int_0^{\tau} w_z(t) dt \quad (4)$$

and

$$\bar{C}_A = \frac{1}{\tau} \int_0^{\tau} C_A(t) dt \quad (5)$$

The time period τ must be long enough to encompass a large number of fluctuations and as a result to ensure smooth averaged values of the state variables.

According to definitions (4) and (5) the following relations are obtained

$$\overline{w'_z} = 0; \overline{w_z} = \overline{w_z}; \overline{C'_A} = 0; \overline{C_A} = \overline{C_A}; \frac{\partial \overline{C_A}}{\partial x} = \frac{\partial \overline{C_A}}{\partial x}; \frac{\partial \overline{C_A}}{\partial t} = \frac{\partial \overline{C_A}}{\partial t} \quad (6)$$

It has to be stressed, however, that the quantities $\overline{w'_x C'_A}$, $\overline{w'_y C'_A}$ and $\overline{w'_z C'_A}$ are not zero as the local fluctuations in velocity and concentration are not independent, i.e.:

$$\overline{w'_x C'_A} \neq 0; \overline{w'_y C'_A} \neq 0; \overline{w'_z C'_A} \neq 0 \quad (7)$$

Introducing into Eq. (1) relationships (2) and (3) and performing time averaging with the help of Eqs. (6) and (7) one finally obtains

$$\begin{aligned} \frac{\partial \overline{C_A}}{\partial t} + \frac{\partial}{\partial x} (\overline{w_x C_A}) + \frac{\partial}{\partial y} (\overline{w_y C_A}) + \frac{\partial}{\partial z} (\overline{w_z C_A}) = D_{AB} \left(\frac{\partial^2 \overline{C_A}}{\partial x^2} + \frac{\partial^2 \overline{C_A}}{\partial y^2} + \frac{\partial^2 \overline{C_A}}{\partial z^2} \right) + \\ - \left[\frac{\partial}{\partial x} (\overline{w'_x C'_A}) + \frac{\partial}{\partial y} (\overline{w'_y C'_A}) + \frac{\partial}{\partial z} (\overline{w'_z C'_A}) \right] \end{aligned} \quad (8)$$

Comparison of Eq. (8) with Eq. (1) indicates that in the time averaged Eq. (8) additional terms appeared: $\overline{w'_x C'_A}$, $\overline{w'_y C'_A}$ and $\overline{w'_z C'_A}$. These terms describe the turbulent mass transport, and the i -th (x, y, z) flux with respect to the mass average velocity is defined as

$$J_{Ai}^{(t)} = \overline{w'_i C'_A} \quad i = x, y, z \quad (9)$$

In analogy with Fick's law it is assumed that

$$\mathbf{J}_A^{(t)} = -D_{AB}^{(t)} \nabla \overline{C_A} \quad (10)$$

This equation defines the turbulent diffusivity $D_{AB}^{(t)}$ called also eddy diffusivity. The eddy diffusivity is not a physical property of the fluid mixture like D_{AB} but depends on the character of flow, mainly intensity of turbulence and on the position in the system varying considerably from the turbulent core to the phase boundary.

Introducing Eq. (10) into Eq. (8) we finally obtain the mass balance of component A determining the time-averaged concentration $\overline{C_A}(x, y, z, t)$ in turbulent flow

$$\frac{\partial \overline{C_A}}{\partial t} + \nabla \cdot (\overline{\mathbf{w} C_A}) = \nabla \cdot \left[\left(D_{AB} + D_{AB}^{(t)} \right) \nabla \overline{C_A} \right] \quad (11)$$

In this equation an effective mass diffusivity appears which is the sum of the molecular diffusivity D_{AB} and eddy diffusivity $D_{AB}^{(t)}$. This quantity is a strong function of position and as mentioned before its values vary considerably.

The quantities like momentum, energy and concentration are transported by turbulent eddies, hence by the same mechanism, so there should be a correlation between the parameters appearing in their flux equations. Applying the Reynolds analogy between the turbulent momentum transfer and the turbulent mass transfer a dimensionless number is defined called the turbulent Schmidt number

$$Sc^{(t)} = \frac{\nu^{(t)}}{D_{AB}^{(t)}} \quad (12)$$

where $\nu^{(t)}$ is the eddy kinematic viscosity $\nu^{(t)} = \mu^{(t)} / \rho$.

In the Computational Fluid Dynamics (CFD) many turbulence models have been developed which enable the determination of the eddy viscosity $\nu^{(t)}$.

Among them the standard $k - \varepsilon$ model has gained primary significance because of its possibilities of practical use in engineering calculations. It is a semiempirical model connecting phenomenological considerations and experimental data. The turbulent or eddy viscosity $\nu^{(t)}$ is computed as a combination of the turbulent kinetic energy k and its dissipation rate ε .

$$\nu^{(t)} = \frac{\mu^{(t)}}{\rho} = C_{\mu} \frac{k^2}{\varepsilon} \quad (13)$$

where $C_{\mu} = 0.09$.

The turbulent kinetic energy k and its rate of dissipation ε are calculated from additional transport equations for k and ε . The recommended value of the turbulent Schmidt number is 0.7.

The $k - \varepsilon$ model takes also into account the steep velocity and concentration profiles in the boundary layers near the solid surface by an analytical function called the logarithmic wall function.

Let us now sum up the previous considerations and present a computational procedure which would enable the estimation of the time-averaged concentration profile. In order to do this we have to solve the following partial differential equations:

- The mass balance of species A for turbulent flow
- Three momentum balance equations for the three components of velocity

- The transport equation for the turbulent kinetic energy
- The transport equation for the rate of dissipation of the turbulent kinetic energy

As can be seen this is an enormous problem demanding laborious and very time consuming numerical calculations, providing in some very complex cases convergence difficulties. Fortunately, there exist commercial CFD codes called Fluent which considerably facilitate the computational procedure. Nevertheless it has to be stated that in many engineering problems this method is impractical.

Therefore, many simpler empirical expressions have been developed for the eddy diffusivity. One of them is based on the mixing length theory of Prandtl. The mixing length is analogous to the concept of the mean free path of gas molecules and is a distance which an eddy must travel before it is dissipated by the surrounding fluid. Hence Prandtl proposed the following relationship for the molar turbulent flux:

$$J_{Ay}^{(t)} = -l^2 \left| \frac{d\bar{w}_x}{dy} \right| \frac{d\bar{C}_A}{dy} \quad (14)$$

where l is the mixing length and $l^2 \left| \frac{d\bar{w}_x}{dy} \right|$ corresponds to $D_{AB}^{(t)}$.

The approximate expression for l in wall turbulence is

$$l \cong ky \quad (y - \text{distance from the wall}) \quad (15)$$

where k is a constant usually assumed as 0.4.

The value $l^2 \left| \frac{d\bar{w}_x}{dy} \right|$ also defines the eddy viscosity and the eddy heat conductivity in the equations of momentum and heat flux, thus fulfilling the Reynolds analogy.

Unfortunately, to calculate $D_{AB}^{(t)}$ we need to know the velocity profile $\bar{w}_x(y)$. This profile can be obtained on the basis of the universal velocity profile which distinguishes the following regions in the flow along a solid surface:

- The laminar sublayer in which eddies have vanished and only molecular transport takes place
- The buffer layer where the molecular transport and the turbulent transport are of comparable magnitude
- The inertial sublayer at the beginning of the turbulent core, in which the molecular transport plays a minor role

- (d) The turbulent core, in which the turbulent transport is so prevailing that the molecular transport can be completely neglected.

In some engineering calculations (e.g. computing the average velocity in a pipe) it is helpful to use equations which in an approximate way describe the velocity profile in the whole region from the wall to the turbulent core.

They are:

the logarithmic profile

$$\frac{\overline{w}_x}{w_*} = 2.5 \ln \left(\frac{yw_*}{\nu} \right) + 5.3 \quad (16)$$

and the power law profile

$$\frac{\overline{w}_x}{w_*} = \left(\frac{1}{\sqrt{3}} \ln Re + \frac{5}{2} \right) \left(\frac{yw_*}{\nu} \right)^{3/(2 \ln Re)} \quad (17)$$

where $w_* = \sqrt{\tau_0 / \rho}$ has the dimension of velocity and is called the friction velocity; τ_0 is the shear stress at the wall.

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Biographical Sketch

Andrzej Burghardt was born in 1928 in Warsaw, Poland. He received his B.Sc. in 1952 and finally graduated in Chemical Engineering from the Silesian Technical University, Gliwice, Poland obtaining M.Sc. degree. In 1962 he received his Ph.D. while in 1965 the degree Doctor in Technical Sciences from the same university. In 1971 he was awarded a title of Professor in Technical Sciences by the President of the Republic of Poland while some years later, in 1983, he was elected as a member of the Polish Academy of Sciences. In the years 1987-2003 he was a chairman of the Committee of Chemical Engineering at the Polish Academy of Sciences.

Currently he is a member of the Presidium of the Polish Academy of Sciences and of the Scientific Council at the Ministry of Science and Informatics. He is also an active member of the Working Party on Chemical Reaction Engineering of the European Federation of Chemical Engineering.

In the years 1954-1966 he was engaged at the Silesian Technical University, Gliwice, Poland as an Assistant Professor lecturing in Distillation, Mass Transfer and Chemical Reaction Engineering. Then, in 1966, he moved to the Institute of Chemical Engineering of the Polish Academy of Sciences where he was designated to the post of director holding this post until 2002. His field of research focuses mainly on the theory of mass transfer in multicomponent and multiphase systems as well as on chemical reaction engineering with special interest in dynamics of chemical reactors. He is author and co-author of nearly 200 scientific publications in refereed journals and of following books and chapters in collective editions: *Chemical Reactors' Engineering Vol. I and II, Examples of Reactor Design, Dynamics of Processes in a Porous Catalyst Pellet, Mass Transfer in Multicomponent Systems, Condensation of Multicomponent Mixtures in VDI-Wärmeatlas (Three Ed. in German one in English)*. He is also a member of Editorial Boards in several journals