

MODULE 10

MASS TRANSFER

Mass transfer specifically refers to the relative motion of species in a mixture due to concentration gradients. In many technical applications, heat transfer processes occur simultaneously with mass transfer processes. The present module discusses these transfer mechanisms. Since the principles of mass transfer are very similar to those of heat transfer, the analogy between heat and mass transfer will be used throughout this module.

10.1 Mass transfer through diffusion

In Module 2 "Conduction", the Fourier equation was introduced, which relates the heat transfer to an existent temperature gradient:

$$q'' = -k \frac{dT}{dy} \left[\frac{J}{m^2 s} \right] \quad \text{(Fourier's law)} \quad (10.1)$$

For mass transfer, where a component A diffuses in a mixture with a component B an analogous relation for the rate of diffusion, based on the concentration gradient can be used

$$j_A'' = -\rho D_{AB} \frac{d\xi_A}{dy} \left[\frac{kg}{m^2 s} \right] \quad \text{(Fick's law)} \quad (10.2)$$

where ρ is the density of the gas mixture, D_{AB} the diffusion coefficient and $\xi_A = \rho_A / \rho$ the mass concentration of component A.

The sum of all diffusion fluxes must be zero, since the diffusion flow is, by definition, superimposed to the net mass transfer:

$$\sum j_i'' = 0 \quad (10.3)$$

With $\xi_A + \xi_B = 1$ we get

$$\frac{d}{dy} \xi_A = -\frac{d}{dy} \xi_B \quad (10.4)$$

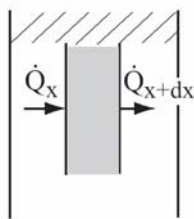
which yields

$$D_{BA} = D_{AB} = D$$

The analogy between diffusive heat transfer (heat conduction) and diffusive mass transfer (diffusion) can be illustrated by considering unsteady diffusive transfer through a layer.

In heat conduction we can calculate the temperature field in a semi-infinite plate, whose surface temperature is forced to suddenly change to a constant value at $t = 0$. The derivation will be repeated here in summarized form.

Heat conduction, unsteady, semi-infinite plate:



$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) \quad (10.5)$$

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c} \frac{\partial^2 T}{\partial x^2} = \alpha \frac{\partial^2 T}{\partial x^2}$$

Fig. 10.1: Unsteady heat conduction

This partial differential equation can be transformed into an ordinary differential equation

$$\frac{d^2 \theta}{d\eta^2} + 2\eta \frac{d\theta}{d\eta} = 0 \quad (10.6)$$

with $\eta = \frac{x}{\sqrt{4\alpha t}}$

and yields

$$\frac{T - T_0}{T_u - T} = 1 - \operatorname{erf} \left(\frac{x}{\sqrt{4\alpha t}} \right) \quad (10.7)$$

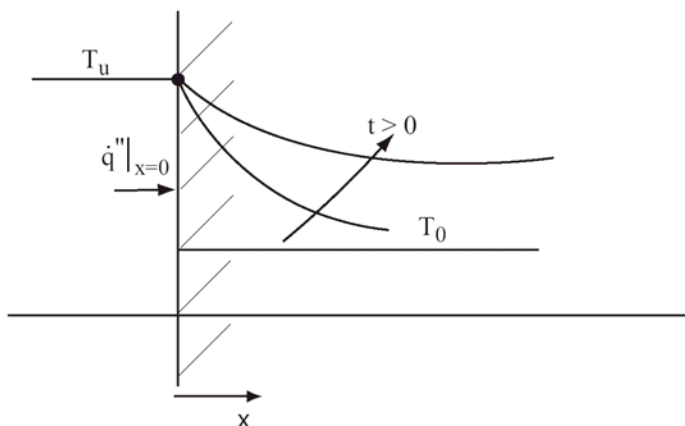


Fig. 10.2 Temperature field

The heat flux at the wall can be calculated from the temperature gradient.

$$\left. \dot{Q} \right|_{x=0} = -k \left. \frac{dT}{dx} \right|_{x=0} = \frac{k}{\sqrt{\pi\alpha t}} (T_u - T_0) = \sqrt{\frac{kc\rho}{\pi t}} (T_u - T) \quad (10.8)$$

The corresponding example in mass transfer is the diffusion of a gas component, which is brought in contact with another gas layer at time $t=0$.

The transient field of concentration with pure diffusion results from a balance of component i

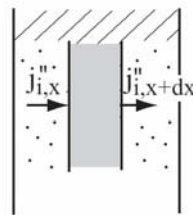


Fig. 10.3: Transient diffusion

$$\begin{aligned} \frac{\partial \rho_i}{\partial t} &= \rho D \frac{\partial^2 \xi_i}{\partial x^2} \\ \frac{\partial \xi_i}{\partial t} &= D \frac{\partial^2 \xi_i}{\partial x^2} \end{aligned} \quad (10.9)$$

The initial and boundary conditions for the semi-infinite fluid layer with a fixed concentration at the interface are:

$$\begin{aligned} \xi_i(t=0, x) &= \xi_{i,o} \\ \xi_i(t > 0, x=0) &= \xi_{i,u} \\ \xi_i(t > 0, x \rightarrow \infty) &= \xi_{i,o} \end{aligned} \quad (10.10)$$

The solution, i.e. the field of concentration, is analogue to the one above.

$$\frac{\xi_i - \xi_{i,o}}{\xi_{i,u} - \xi_{i,o}} = 1 - \operatorname{erf}\left(\frac{x}{\sqrt{4Dt}}\right) \quad (10.11)$$

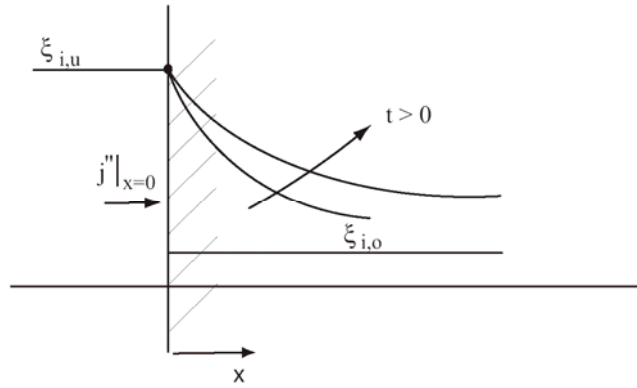


Fig. 10.4 Concentration field

The diffusive mass flux of component i at the interface can be derived as

$$j''_{i,x=0} = \frac{\rho D}{\sqrt{\pi D t}} (\xi_{i,Ph} - \xi_{i,o}) \quad (10.12)$$

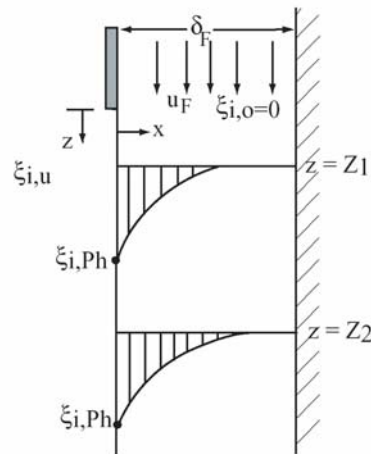


Fig. 10.5 Gas absorption in a falling film

A practical example from chemical engineering is the absorption of a gas component i in a falling film. Considering a large film thickness or short contact times the theoretical results (penetration theory) can be used.

The absorbed mass flux is

$$\begin{aligned} m_i &= A j''_{i,x=0} \\ &= A \frac{\rho D}{\sqrt{\pi D t}} (\xi_{i,Ph} - \xi_{i,o}) \end{aligned} \quad (10.13)$$

Finally, the contact time can be calculated from the film velocity and the film length:

$$t = \frac{L_f}{u_f} \quad (10.14)$$

10.2 Mass transfer in a flowing medium

If we balance the net masses flowing in and out of a control volume of a fluid mixture, i.e. the sum of the convective and diffusive mass flows of the component i

$$n_i'' = n_{i,conv}'' + n_{i,diff}'' = \xi_i \rho u + j_i'' \quad (10.15)$$

we get for a steady state flow without sources the conservation equation for the component i under investigation:

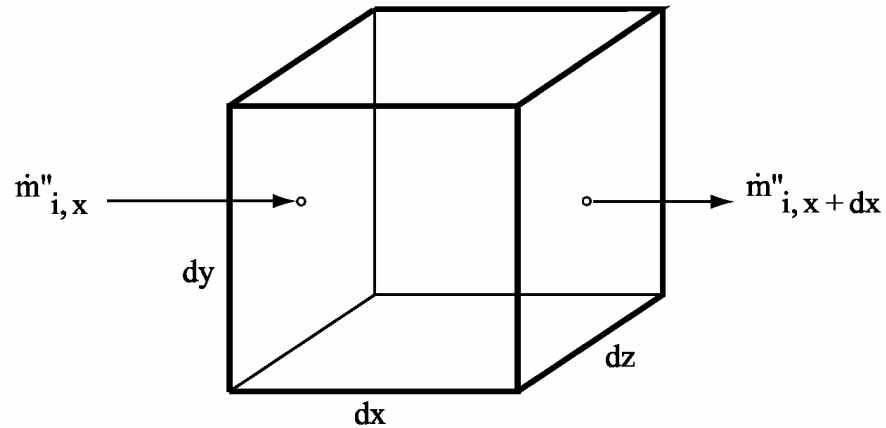


Fig. 10.6 Balance of mass flows on a control volume

$$\frac{\partial}{\partial x} (\xi_i \rho u + j_{i,x}'') + \frac{\partial}{\partial y} (\xi_i \rho v + j_{i,y}'') + \frac{\partial}{\partial z} (\xi_i \rho w + j_{i,z}'') = 0 \quad (10.16)$$

This equation can be differentiated partially and rewritten applying the equation of continuity. This yields the form of the conservation equation for component i (the index i will be disregarded further on):

$$\rho u \frac{\partial \xi}{\partial x} + \rho v \frac{\partial \xi}{\partial y} + \rho w \frac{\partial \xi}{\partial z} = \frac{\partial}{\partial x} \left(\rho D \frac{\partial \xi}{\partial x} \right) + \frac{\partial}{\partial y} \left(\rho D \frac{\partial \xi}{\partial y} \right) + \frac{\partial}{\partial z} \left(\rho D \frac{\partial \xi}{\partial z} \right) \quad (10.17)$$

Assuming constant material properties and introducing the **Schmidt number**

$Sc = \frac{\mu}{\rho D}$, we get the simplified form:

$$\rho u \frac{\partial \xi}{\partial x} + \rho v \frac{\partial \xi}{\partial y} + \rho w \frac{\partial \xi}{\partial z} = \frac{\mu}{Sc} \left(\frac{\partial^2 \xi}{\partial x^2} + \frac{\partial^2 \xi}{\partial y^2} + \frac{\partial^2 \xi}{\partial z^2} \right) \quad (10.18)$$

which in analogy to the energy equation of the Module 6 on convection, can be made dimensionless by introducing dimensionless parameters. In a physical

sense, $Sc = \frac{\mu}{\rho D} = \frac{\nu}{D} = \frac{\text{Momentum diffusivity}}{\text{Mass diffusivity}}$

If we define

$$x^* = \frac{x}{L}; \quad y^* = \frac{y}{L}; \quad z^* = \frac{z}{L}; \quad u^* = \frac{u}{u_\infty}; \quad v^* = \frac{v}{u_\infty}; \quad w^* = \frac{w}{u_\infty}; \quad \xi^* = \frac{\xi - \xi_w}{\xi_\infty - \xi_w}$$

we get the dimensionless equation of mass conservation

$$u^* \frac{\partial \xi^*}{\partial x^*} + v^* \frac{\partial \xi^*}{\partial y^*} + w^* \frac{\partial \xi^*}{\partial z^*} = \frac{1}{ReSc} \left(\frac{\partial^2 \xi^*}{\partial x^{*2}} + \frac{\partial^2 \xi^*}{\partial y^{*2}} + \frac{\partial^2 \xi^*}{\partial z^{*2}} \right) \quad (10.19)$$

from which can be concluded that the scaled concentration field must depend on the dimensionless coordinates and the dimensionless numbers Re and Sc:

$$\xi^* = f(x^*, y^*, z^*, Re, Pr) \quad (10.20)$$

Note the analogy to heat transfer, where in Module 6 "Convection", for the temperature field, the following was valid:

$$T^* = f(x^*, y^*, z^*, Re, Pr) \quad (10.21)$$

10.3 Diffusive mass transfer on a surface

The heat flux was determined in Module 6 "Convection" from the gradient of the temperature at the wall:

$$\mathcal{Q}_w = -k \frac{\partial T}{\partial y} \Big|_{y=0} = -k \frac{T_\infty - T_w}{L} \frac{\partial T^*}{\partial y^*} \Big|_{y^*=0} \quad (10.22)$$

This heat flux was represented using an empirical equation for the heat transfer coefficient:

$$q_w'' = h(T_w - T_\infty) \quad (10.23)$$

which written in dimensionless form was introduced as the Nusselt number Nu:

$$\frac{hL}{k} = Nu = \left. \frac{\partial T^*}{\partial y^*} \right|_{y^*=0} = f(\text{Re}, \text{Pr}) \quad (10.24)$$

For many practical cases, the Nusselt laws are written in the form:

$$Nu = C \text{Re}^m \text{Pr}^n \quad (10.25)$$

We will proceed accordingly to describe mass transfer.

For the diffusive mass flow rate, Fick's Law is rewritten using dimensionless quantities:

$$j_A'' = -\rho D \left. \frac{\partial \xi}{\partial y} \right|_{y=0} = -\rho D \frac{\xi_\infty - \xi_w}{L} \left. \frac{\partial \xi^*}{\partial y^*} \right|_{y^*=0} \quad (10.26)$$

and compared to an empirical equation using the **mass transfer coefficient**

$$h_{mass} \left[\frac{kg}{m^2 s} \right]$$

$$j_A'' = h_{mass} (\xi_w - \xi_\infty) \quad (10.27)$$

By the comparison, we get the dimensionless mass transfer number, the **Sherwood number** Sh:

$$\frac{h_{mass} L}{\rho D} = \text{Sh} = \left. \frac{\partial \xi^*}{\partial y^*} \right|_{y^*=0} = f(\text{Re}, \text{Sc}) \quad (10.28)$$

Sherwood number correlations, in turn, can be written using appropriate dimensionless numbers

$$\text{Sh} = C \text{Re}^m \text{Sc}^n \quad (10.29)$$

Since the type of the mass conservation equation and energy equation are the same, the constants C and the exponents m and n of both relationships must be equal for comparable boundary conditions.

It seems like we need one more dimensionless number to represent the relative magnitudes of heat and mass diffusion in the thermal and concentration boundary layers. That is the **Lewis number**, defined as

$$\text{Le} = \frac{\text{Sc}}{\text{Pr}} = \frac{\alpha}{D} = \frac{\text{Thermal diffusivity}}{\text{Mass diffusivity}}$$

10.4 Analogy between heat and mass transfer

Comparing the correlation for the heat and mass transfer, we can find their ratio

$$\frac{Sh}{Nu} = \left(\frac{Sc}{Pr} \right)^n \quad (10.30)$$

and hence

$$\frac{h_{mass}}{h/c_p} = \left(\frac{Sc}{Pr} \right)^{n-1} \quad (10.31)$$

For gases, the Prandtl and the Schmidt number are almost equal. In this case a simple approximation for the relationship between the mass and heat transfer coefficient can be derived, which is the so-called Lewis relation

$$\frac{h_{mass}}{h/c_p} = 1 \quad \text{Lewis relation} \quad (10.32)$$

10.5 Evaporation on a liquid surface

When vapour from the surface of the liquid A enters the surrounding gas mixture, consisting of the component A and B, then this process is called evaporation. This mass transfer is determined by diffusive processes, i.e. diffusive resistances. The process differs from that of vaporisation, since in the latter the transferred vapour component is transferred to a pure vapour environment. Diffusion resistances are not relevant for the process of vaporisation.

The net mass flow of component A from the liquid surface to the gas consists of a convective and diffusive part

$$n_A'' = n_{A,conv}'' + n_{A,diff}'' = \xi_A \rho v + j_A'' \quad (10.33)$$

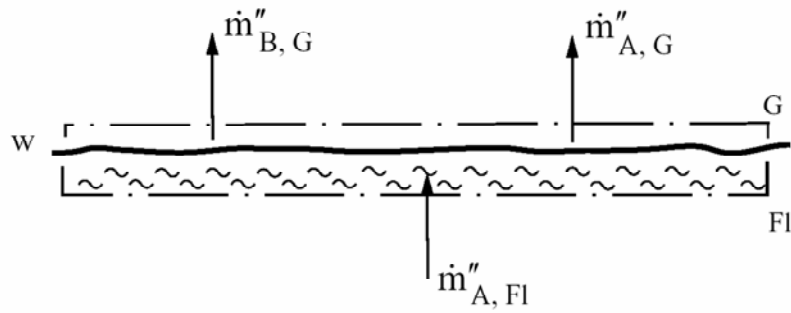


Fig. 10.7 Mass balance on a liquid surface

Usually, it is assumed that the gas component B cannot penetrate the liquid surface, hence for the net flow of component B:

$$n_B'' = n_{B,conv}'' + n_{B,diff}'' = \xi_B \rho v + j_B'' \quad (10.34)$$

With $j_A'' + j_B'' = 0$ and $\xi_A + \xi_B = 1$ we get the net evaporation flow on the surface

$$n'' = n_{A,w}'' = \frac{1}{1 - \frac{\xi_{A,w}}{F}} j_{A,w}''$$

The net mass flow is obviously increased by the factor F, the Stefan factor, compared to the diffusion flow. This factor takes into account that the wall is only permeable for the evaporating component A ("semi-permeable wall").

If we express the diffusive flow by equation 10.27, by the mass transfer coefficient and the concentration difference, we get:

$$n'' = h_{mass} \frac{\xi_w - \xi_\infty}{1 - \xi_w} \quad (10.35)$$

or in dimensionless form

$$\frac{n''}{\rho u_\infty} = \frac{Sh}{ReSc} \frac{\xi_w - \xi_\infty}{1 - \xi_w} \quad (10.36)$$

with ξ as the mass concentration of the transferred component and B the driving potential for the mass transfer.