1 Theorem, Definitions, and Governing Equations

Material derivative: $\frac{\mathrm{D}\vec{f}}{\mathrm{D}t} = \frac{\partial}{\partial t}\vec{f} + \vec{v}\cdot\nabla\vec{a} = \frac{\partial \vec{f}}{\partial t} + \sum_i \frac{\partial \vec{f}}{\partial x_i}\vec{v}_i$

Divergence: $\iiint_V (\nabla\cdot\vec{f})\,dV = \oiint_S (\vec{f}\cdot\hat{n})\,dS$

$$\iiint_V (\nabla\psi)\,dV = \oiint_S (\psi\hat{n})\,dS$$

Reynolds Transport Theorem:

$$\frac{\mathrm{d}}{\mathrm{d}t}\iiint_V \boldsymbol{F}\,dV = \frac{\partial}{\partial t}\iiint_V \boldsymbol{F}\,dV + \iint_A \boldsymbol{F}(\vec{v}\cdot\hat{n})\,dA$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\iiint_V \boldsymbol{F}\,dV = \iiint_V \frac{\mathrm{D}\boldsymbol{F}}{\mathrm{D}t}\,dV$$

$$\frac{\mathrm{D}}{\mathrm{D}t}\iiint_V \alpha\,dV = \iiint_V \left[\frac{\partial\alpha}{\partial t} + \nabla\cdot(\alpha\vec{v})\right]dV = \iiint_V \left[\frac{\partial\alpha}{\partial t} + \sum_i \frac{\partial(\alpha v_i)}{\partial x_i}\right]dV$$

$\alpha \equiv$ volume-specific property

Conservation of mass (continuity), 1 component: $\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\vec{v}) = 0$

Incompressible: $\frac{\mathrm{D}\rho}{\mathrm{D}t} + \rho(\nabla\cdot\vec{v}) = 0 \qquad \nabla\cdot\vec{v} = 0$

Mixture: $\frac{\partial\rho_A}{\partial t} + \nabla\cdot(\rho_A\vec{v}_A) = -\nabla\cdot\boldsymbol{m}_A + \check{R}_A$

Leibniz integral rule: $\frac{\mathrm{d}}{\mathrm{d}x}\int_{a(x)}^{b(x)} f(x,t)\,dt =$

$$\int_{a(x)}^{b(x)} \frac{\partial}{\partial x}f(x,t)\,dt + f(x,b(x))\frac{\mathrm{d}b(x)}{\mathrm{d}x} - f(x,a(x))\frac{\mathrm{d}a(x)}{\mathrm{d}x}$$

2 Diffusion

2.1 Mass Basis with Mass Average Velocity

$\frac{\partial\rho_i}{\partial t} + \nabla\cdot(\rho_i\langle\vec{v}_m\rangle) = -\nabla\cdot\boldsymbol{m}_i + \check{R}_i \qquad \frac{\partial\rho_i}{\partial t} + \nabla\cdot\boldsymbol{\Phi}_{m,i} = \check{R}_i$

$\langle\vec{v}_m\rangle = \sum_i w_i\vec{v}_i \qquad w_i = \frac{\rho_i}{\rho}$

$\boldsymbol{\Phi}_{m,\mathrm{T}} = \sum_i \rho_i\vec{v}_i = \rho\langle\vec{v}_m\rangle$

$\boldsymbol{m}_A = \rho_A(\vec{v}_A - \langle\vec{v}_m\rangle) = \rho_A\vec{v}_A - w_A\boldsymbol{\Phi}_{m,\mathrm{T}}$

$\boldsymbol{\Phi}_{m,A} = \rho_A\vec{v}_A = \boldsymbol{m}_A + \rho_A\vec{v} = \boldsymbol{m}_A + w_A\boldsymbol{\Phi}_{m,\mathrm{T}}$

$\rho\left(\frac{\partial w_A}{\partial t} + \langle\vec{v}_m\rangle\cdot\nabla w_A\right) = -\nabla\cdot\boldsymbol{m}_A + \check{R}_A$

2.2 Molar Basis with Molar Average Velocity

$\frac{\partial c_i}{\partial t} + \nabla\cdot(c_i\langle\vec{v}_n\rangle) = -\nabla\cdot\boldsymbol{n}'_i + \check{r}_i \qquad \frac{\partial c_i}{\partial t} + \nabla\cdot\boldsymbol{\Phi}_{n,i} = \check{r}_i$

$\langle\vec{v}_n\rangle = \sum_i x_i\vec{v}_i \qquad x_i = \frac{c_i}{c}$

$\boldsymbol{\Phi}_{n,\mathrm{T}} = \sum_i c_i\vec{v}_i = c\langle\vec{v}_n\rangle$

$\boldsymbol{n}'_A = c_A(\vec{v}_A - \langle\vec{v}_n\rangle) = c_A\vec{v}_A - x_A\boldsymbol{\Phi}_{n,\mathrm{T}}$

$\boldsymbol{\Phi}_{n,A} = c_A\vec{v}_A = \boldsymbol{n}'_A + c_A\langle\vec{v}_n\rangle = \boldsymbol{n}'_A + x_A\boldsymbol{\Phi}_{n,\mathrm{T}}$

$c\left(\frac{\partial x_A}{\partial t} + \langle\vec{v}_n\rangle\cdot\nabla x_A\right) = -\nabla\cdot\boldsymbol{n}'_A + \check{r}_A - x_A\sum_i \check{r}_i$

3 Maxwell-Stefan Diffusion

3.1 Ideal Gas Mixtures

$\frac{\nabla P_i}{P} = \frac{x_i x_j(\vec{v}_j - \vec{v}_i)}{\mathscr{D}_{ij}} \qquad \vec{d}_i = \frac{\nabla P_i}{P} = \nabla x_i$

$$\nabla x_i = \frac{\mathrm{d}x_i}{\mathrm{d}z} = \sum_{j\neq i}^{n} \frac{x_i\boldsymbol{\Phi}_{n,j} - x_j\boldsymbol{\Phi}_{n,i}}{c\mathscr{D}_{ij}} = \sum_{i\neq j}^{n} \frac{x_i\boldsymbol{n}'_j - x_j\boldsymbol{n}'_i}{c\mathscr{D}_{ij}}$$

Fick's Law: $\boldsymbol{n}' = -c\boldsymbol{B}^{-1}\vec{d}$

$$c\vec{d}_i = -\boldsymbol{n}'_i B_{ii} - \boldsymbol{n}'_j \sum_{j=1,j\neq i}^{n-1} B_{ij}$$

$$B_{ii} = \frac{x_i}{\mathscr{D}_{in}} + \sum_{k=1,k\neq i}^{n} \frac{x_k}{\mathscr{D}_{ik}} \qquad B_{ij} = -x_i\left(\frac{1}{\mathscr{D}_{ij}} - \frac{1}{\mathscr{D}_{in}}\right)$$

Binary: $\boldsymbol{n}'_i = -c\mathscr{D}_{ij}\vec{d}_i$

3.2 Non-ideal Fluid Mixtures

$$\vec{d}_i = \frac{x_i}{RT}\nabla(\mu_i)_{T,P} = \sum_{j=1}^{n-1}\Gamma_{ij}\nabla x_j \qquad \Gamma_{ij} = \delta_{ij} + x_i\left(\frac{\partial\ln\gamma_i}{\partial x_j}\right)_{T,P,x'}$$

$\boldsymbol{n}' = -c\boldsymbol{B}^{-1}\boldsymbol{\Gamma}\nabla\vec{x}$

4 Generalised Fick's Law

Binary: $\boldsymbol{n}'_A = -cD_{AB}\nabla x_A \qquad \boldsymbol{m}_A = -\rho_A D_{AB}\nabla w_A$

n-component: $\boldsymbol{n}'_A = -c\sum_{j=1}^{n-1} D_{ij}\nabla x_j \qquad \boldsymbol{n}'_A = -c\boldsymbol{D}\nabla x$

4.1 Matrix Approximations for Multicomponent Diffusion

$\frac{\partial\vec{x}}{\partial t} + \nabla\cdot(\langle\vec{v}_n\rangle\vec{x}) = \boldsymbol{D}\nabla^2\vec{x} \to \frac{\partial\hat{x}}{\partial t} + \nabla\cdot(\langle\vec{v}_n\rangle\hat{x}) = \hat{\boldsymbol{D}}\nabla^2\hat{x}$

$$\hat{\boldsymbol{D}} \equiv \boldsymbol{P}^{-1}\boldsymbol{D}\boldsymbol{P} \qquad \hat{x} \equiv \boldsymbol{P}^{-1}\vec{x} \qquad \boldsymbol{P} \equiv \begin{bmatrix} 1 & \frac{\lambda_2 - D_{22}}{D_{21}} \\ \frac{\lambda_1 - D_{11}}{D_{12}} & 1 \end{bmatrix}$$

$$\lambda_1 = \frac{1}{2}\left(\mathrm{tr}\,\boldsymbol{D} + \sqrt{\mathrm{disc}\,\boldsymbol{D}}\right) \qquad \lambda_2 = \frac{1}{2}\left(\mathrm{tr}\,\boldsymbol{D} - \sqrt{\mathrm{disc}\,\boldsymbol{D}}\right)$$

$\mathrm{tr}\,\boldsymbol{D} = D_{11} + D_{22} \qquad \mathrm{disc}\,\boldsymbol{D} = (\mathrm{tr}\,\boldsymbol{D})^2 - 4\det\boldsymbol{D}$

$\det\boldsymbol{D} = D_{11}D_{22} - D_{12}D_{21}$

5 Boundary Layer Methods

Solute mass balance: $\boldsymbol{n}' = \frac{\mathrm{d}}{\mathrm{d}t}\int_0^\delta c_A\,dx - c_0\frac{\mathrm{d}\delta}{\mathrm{d}t}$

Continuity: $\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} = 0$

5.1 Momentum Boundary Layer

Von Kármán integral: $\frac{\boldsymbol{\tau}_{\mathrm{wall}}}{\rho} = \frac{\mu}{\rho}\frac{\partial v_x}{\partial y}\Big|_{y=0} = \frac{\mathrm{d}}{\mathrm{d}x}\int_0^{\delta_P}(u_\infty - \vec{v}_x)\vec{v}_x\,dy$

5.2 Concentration Boundary Layer

$\nu = \frac{\mu}{\rho} \qquad \mathrm{Sc} \equiv \frac{\nu}{D} \qquad \frac{\delta_c}{\delta_P} \sim \mathrm{Sc}^{-1/3}$

$k_c(c_{A,\mathrm{sfc}} - c_{A,\mathrm{bulk}}) = \frac{\mathrm{d}}{\mathrm{d}x}\int_0^{\delta_c}\vec{v}_x(c_A - c_{A,\mathrm{bulk}})\,dy$

6 Turbulent Mass Transfer

$\bar{X} \equiv \frac{1}{t_{\mathrm{obs}}}\int_0^{t_{\mathrm{obs}}} X\,dt \qquad X \in \{c, \vec{v}, T, \ldots\} \qquad X_A = \bar{X}_A + X_{A,\mathrm{tb}}$

6.1 Binary Mixture

$\frac{\partial\bar{c}_A}{\partial t} + \nabla(\bar{v}\bar{c}_A) = \nabla\cdot(D\nabla\bar{c}_A) - \nabla\cdot(\bar{v}_{\mathrm{tb}}\bar{c}_{A,\mathrm{tb}}) \qquad \bar{v}_{\mathrm{tb}}\bar{c}_{A,\mathrm{tb}} = -D_{\mathrm{tb}}\nabla\bar{c}_A$

$\frac{\partial\bar{w}_i}{\partial t} + \bar{v}\cdot\nabla\bar{w}_i = -\frac{1}{\rho}\nabla\cdot(\boldsymbol{m}_i + \boldsymbol{m}_{i,\mathrm{tb}})$

6.2 Turbulent Eddy Diffusivity Model in a Tube

$\boldsymbol{\Phi}_{m,i,y} = \boldsymbol{m}_{i,y} + w_i\boldsymbol{\Phi}_{m,\mathrm{T},y}$

$\vec{u}_f \equiv \sqrt{\frac{\tau_{\mathrm{wall}}}{\rho}} = \sqrt{\frac{f}{2}}\bar{u}_f \qquad \overset{*}{y} \equiv \frac{\vec{u}_f\rho}{\mu}y = \frac{\vec{u}_f}{\nu}y$

$\overset{*}{u} \equiv \frac{\vec{u}}{\vec{u}_f} = \sqrt{\frac{2}{f}}\frac{\vec{u}}{\bar{u}} \qquad \overset{*}{R}_{\mathrm{wall}} \equiv \frac{R_{\mathrm{wall}}\vec{u}_f}{\nu} = \mathrm{Re}\sqrt{f/8} \qquad \frac{\nu_{\mathrm{trb}}}{\nu} = \frac{\mathrm{d}\overset{*}{y}}{\mathrm{d}\overset{*}{u}} - 1$

Von Kármán velocity profile:

Viscous, $\{0 \le \overset{*}{y} \le 5\}$: $\overset{*}{u} = \overset{*}{y} \qquad \frac{\mathrm{d}\overset{*}{u}}{\mathrm{d}\overset{*}{y}} = 1 \Rightarrow \frac{\nu_{\mathrm{trb}}}{\nu} = 0$

Buffer, $\{5 \le \overset{*}{y} \le 30\}$: $\overset{*}{u} = 5\ln\overset{*}{y} - 3.05 \qquad \frac{\mathrm{d}\overset{*}{u}}{\mathrm{d}\overset{*}{y}} = \frac{5}{\overset{*}{y}} \Rightarrow \frac{\nu_{\mathrm{trb}}}{\nu} = \frac{\overset{*}{y}}{5} - 1$

Turbulent, $\{30 \le \overset{*}{y}\}$: $\overset{*}{u} = 2.5\ln\overset{*}{y} + 5$

6.2.1 Turbulent Mass Transfer in Binary Fluids

$\mathrm{Sc}_{\mathrm{tb}} \equiv \frac{\nu_{\mathrm{tb}}}{D_{\mathrm{tb}}} \qquad \boldsymbol{m}_{i,y} = -\rho(D_i + D_{\mathrm{tb}})\frac{\mathrm{d}w_i}{\mathrm{d}y}$

Composition profile: $\frac{w_i - w_{i,0}}{w_{i,\mathrm{bulk}} - w_{i,0}} = \frac{1 - e^\psi}{1 - e^\phi}$

$$\psi \equiv \int_0^{\overset{*}{y}} f(\overset{*}{y})\,d\overset{*}{y} \qquad \phi \equiv \int_0^{\overset{*}{y}_{\mathrm{bulk}}} f(\overset{*}{y})\,d\overset{*}{y}$$

6.2.2 Diffusion Flux at Wall

$k_{\mathrm{H}} \equiv \frac{\boldsymbol{\Phi}_{m,\mathrm{T},0}}{\rho}(e^\phi - 1)^{-1} \qquad k_{\mathrm{L}}^{-1} = \int_0^{\overset{*}{y}_{\mathrm{bulk}}} \frac{1}{\vec{u}_f}\left(\mathrm{Sc}^{-1} + \mathrm{Sc}_{\mathrm{tb}}^{-1}\frac{\nu_{\mathrm{tb}}}{\nu}\right)^{-1} d\overset{*}{y}$

$k_{\mathrm{H}} = \Sigma k_{\mathrm{L}} \qquad \Sigma \equiv \frac{\phi}{e^\phi - 1}$

$\mathrm{St} \equiv \frac{k}{\bar{u}} = \sqrt{\frac{f}{2}}\frac{k}{\vec{u}_f}$

$\mathrm{St}_m^{-1} = \frac{2}{f} + \sqrt{\frac{2}{f}}\int_0^{\overset{*}{y}_1}\left(\mathrm{Sc}^{-1} + \mathrm{Sc}_{\mathrm{tb}}^{-1}\frac{\nu_{\mathrm{tb}}}{\nu}\right)^{-1} - \left(1 + \frac{\nu_{\mathrm{tb}}}{\nu}\right)^{-1} d\overset{*}{y}$

6.2.3 Momentum/Mass Transfer Analogies

Reynolds, $\{\mathrm{Sc} = 1, \mathrm{Sc}_{\mathrm{tb}} = 1\}$: $\mathrm{St}_m = \frac{f}{2}$

Chilton-Colburn: $\frac{\nu_{\mathrm{tb}}}{\nu} = 1.77\left(\frac{f}{2}\right)^{\frac{2}{3}}\overset{*}{y}^3 \to \mathrm{St}_m = \frac{f}{2}\mathrm{Sc}^{-\frac{2}{3}}$

Von Kármán, $\{\mathrm{Sc}_{\mathrm{tb}} = 1\}$, viscous/buffer:

$$\mathrm{St}_m^{-1} = \frac{2}{f} + 5\sqrt{\frac{2}{f}}\left(\mathrm{Sc} - 1 + \ln\left[1 + \frac{5}{6}(\mathrm{Sc} - 1)\right]\right)$$

References

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