The **Equation of Species Mass Balance** in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B. Two cases are presented: the general case, where the mass flux with respect to mass-average velocity ($\underline{j}_A$) appears (p. 1), and the more usual case (p. 2), where the diffusion coefficient is constant and Fick's law has been incorporated.

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In terms of mass flux, $\underline{j}_A$

Microscopic species mass balance, in terms of mass flux; Gibbs notation

$$\rho\left(\frac{\partial \omega_A}{\partial t}+\underline{v}\cdot\nabla\omega_A\right)=-\nabla\cdot\underline{j}_A+r_A$$

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Microscopic species mass balance, in terms of mass flux; Cartesian coordinates

$$\rho\left(\frac{\partial \omega_A}{\partial t}+v_x\frac{\partial \omega_A}{\partial x}+v_y\frac{\partial \omega_A}{\partial y}+v_z\frac{\partial \omega_A}{\partial z}\right)=-\left(\frac{\partial j_{A,x}}{\partial x}+\frac{\partial j_{A,y}}{\partial y}+\frac{\partial j_{A,z}}{\partial z}\right)+r_A$$

Microscopic species mass balance, in terms of mass flux; cylindrical coordinates

$$\rho\left(\frac{\partial \omega_A}{\partial t}+v_r\frac{\partial \omega_A}{\partial r}+\frac{v_\theta}{r}\frac{\partial \omega_A}{\partial \theta}+v_z\frac{\partial \omega_A}{\partial z}\right)=-\left(\frac{1}{r}\frac{\partial (r j_{A,r})}{\partial r}+\frac{1}{r}\frac{\partial j_{A,\theta}}{\partial \theta}+\frac{\partial j_{A,z}}{\partial z}\right)+r_A$$

Microscopic species mass balance, in terms of mass flux; spherical coordinates

$$\rho\left(\frac{\partial \omega_A}{\partial t}+v_r\frac{\partial \omega_A}{\partial r}+\frac{v_\theta}{r}\frac{\partial \omega_A}{\partial \theta}+\frac{v_\phi}{r\sin\theta}\frac{\partial \omega_A}{\partial \phi}\right)=-\left(\frac{1}{r^2}\frac{\partial (r^2 j_{A,r})}{\partial r}+\frac{1}{r\sin\theta}\frac{\partial (j_{A,\theta}\sin\theta)}{\partial \theta}+\frac{1}{r\sin\theta}\frac{\partial j_{A,\phi}}{\partial \phi}\right)+r_A$$

Fick's law of diffusion, Gibbs notation: $\underline{j}_A=-\rho D_{AB}\nabla\omega_A$

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$$=\rho\omega_A(\underline{v}_A-\underline{v})$$

Fick's law of diffusion, Cartesian coordinates:

$$\begin{pmatrix} j_{A,x}\\ j_{A,y}\\ j_{A,z}\end{pmatrix}_{xyz}=\begin{pmatrix} -\rho D_{AB}\frac{\partial \omega_A}{\partial x}\\ -\rho D_{AB}\frac{\partial \omega_A}{\partial y}\\ -\rho D_{AB}\frac{\partial \omega_A}{\partial z}\end{pmatrix}_{xyz}$$

Fick's law of diffusion, cylindrical coordinates:

$$\begin{pmatrix} j_{A,r}\\ j_{A,\theta}\\ j_{A,z}\end{pmatrix}_{r\theta z}=\begin{pmatrix} -\rho D_{AB}\frac{\partial \omega_A}{\partial r}\\ -\frac{\rho D_{AB}}{r}\frac{\partial \omega_A}{\partial \theta}\\ -\rho D_{AB}\frac{\partial \omega_A}{\partial z}\end{pmatrix}_{r\theta z}$$

Fick's law of diffusion, spherical coordinates:

$$\begin{pmatrix} j_{A,r}\\ j_{A,\theta}\\ j_{A,\phi}\end{pmatrix}_{r\theta\phi}=\begin{pmatrix} -\rho D_{AB}\frac{\partial \omega_A}{\partial r}\\ -\frac{\rho D_{AB}}{r}\frac{\partial \omega_A}{\partial \theta}\\ -\frac{\rho D_{AB}}{r\sin\theta}\frac{\partial \omega_A}{\partial \phi}\end{pmatrix}_{r\theta\phi}$$

The **Equation of Species Mass Balance, constant ρD_{AB}.** For binary systems, and Fick's law has been incorporated. Good for dilute liquid solutions at constant temperature and pressure.

In terms of Diffusivity, D_{AB}

Microscopic species mass balance, constant thermal conductivity; Gibbs notation

$$\rho\left(\frac{\partial\omega_A}{\partial t}+\underline{v}\cdot\nabla\omega_A\right)=\rho D_{AB}\nabla^2\omega_A+r_A$$

Microscopic species mass balance, constant thermal conductivity; Cartesian coordinates

$$\rho\left(\frac{\partial\omega_A}{\partial t}+v_x\frac{\partial\omega_A}{\partial x}+v_y\frac{\partial\omega_A}{\partial y}+v_z\frac{\partial\omega_A}{\partial z}\right)=\rho D_{AB}\left(\frac{\partial^2\omega_A}{\partial x^2}+\frac{\partial^2\omega_A}{\partial y^2}+\frac{\partial^2\omega_A}{\partial z^2}\right)+r_A$$

Microscopic species mass balance, constant thermal conductivity; cylindrical coordinates

$$\rho\left(\frac{\partial\omega_A}{\partial t}+v_r\frac{\partial\omega_A}{\partial r}+\frac{v_\theta}{r}\frac{\partial\omega_A}{\partial\theta}+v_z\frac{\partial\omega_A}{\partial z}\right)=\rho D_{AB}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\omega_A}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2\omega_A}{\partial\theta^2}+\frac{\partial^2\omega_A}{\partial z^2}\right)+r_A$$

Microscopic species mass balance, constant thermal conductivity; spherical coordinates

$$\begin{aligned}\rho&\left(\frac{\partial\omega_A}{\partial t}+v_r\frac{\partial\omega_A}{\partial r}+\frac{v_\theta}{r}\frac{\partial\omega_A}{\partial\theta}+\frac{v_\phi}{r\sin\theta}\frac{\partial\omega_A}{\partial\phi}\right)\\&=\rho D_{AB}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\omega_A}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\omega_A}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\omega_A}{\partial\phi^2}\right)+r_A\end{aligned}$$

$cx_A=c_A=\frac{1}{M_A}(\rho_A)=\frac{1}{M_A}(\rho\omega_A)$ $\quad\left(\text{units: }c[=]\frac{mol\ mix}{vol\ soln};\rho[=]\frac{mass\ mix}{vol\ soln};c_A[=]\frac{mol\ A}{vol\ soln};\rho_A[=]\frac{mass\ A}{vol\ soln}\right)$

$\underline{j}_A\equiv$ mass flux of species A relative to a mixture's mass average velocity, $\underline{v}$ $\quad\left(\text{units: }\underline{j}_A[=]\frac{mass\ A}{area\cdot time}\right)$

$\quad=\rho_A(\underline{v}_A-\underline{v})$

$\underline{j}_A+\underline{j}_B=0$, i.e. these fluxes are measured relative to the mixture's center of mass

$\underline{n}_A\equiv\rho_A\underline{v}_A=\underline{j}_A+\rho_A\underline{v}=$ combined mass flux relative to stationary coordinates

$\underline{n}_A+\underline{n}_B=\rho\underline{v}$

$\underline{v}_A\equiv$ velocity of species A in a mixture, i.e. average velocity of all molecules of species A within a small volume

$\underline{v}=\omega_A\underline{v}_A+\omega_B\underline{v}_B\equiv$ mass average velocity; same velocity as in the microscopic momentum and energy balances

Reference: R. B. Bird, W. E. Stewart, and E. N. Lightfoot, *Transport Phenomena*, 2nd edition, Wiley, 2002.
(p. 515, 584)