BASED ON MASS FRACTIONS

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

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

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

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

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

$\underline{j}_A + \underline{j}_B = 0$, 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

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

BASED ON MOLE FRACTIONS

The **Equation of Species Mass Balance in Terms of Molar quantities** in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B. Two cases are presented: the general case, where the molar flux with respect to molar 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 molar flux, $\underline{J}_A^*$

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

$$c\left(\frac{\partial x_A}{\partial t} + \underline{v}^* \cdot \nabla x_A\right) = -\nabla \cdot \underline{J}_A^* + (x_B R_A - x_A R_B)$$

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

$$c\left(\frac{\partial x_A}{\partial t} + v_x^* \frac{\partial x_A}{\partial x} + v_y^* \frac{\partial \omega_A}{\partial y} + v_z^* \frac{\partial x_A}{\partial z}\right) = -\left(\frac{\partial J_{A,x}^*}{\partial x} + \frac{\partial J_{A,y}^*}{\partial y} + \frac{\partial J_{A,z}^*}{\partial z}\right) + (x_B R_A - x_A R_B)$$

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

$$c\left(\frac{\partial x_A}{\partial t} + v_r^* \frac{\partial x_A}{\partial r} + \frac{v_\theta^*}{r}\frac{\partial x_A}{\partial \theta} + v_z^* \frac{\partial x_A}{\partial z}\right) = -\left(\frac{1}{r}\frac{\partial (r J_{A,r}^*)}{\partial r} + \frac{1}{r}\frac{\partial J_{A,\theta}^*}{\partial \theta} + \frac{\partial J_{A,z}^*}{\partial z}\right) + (x_B R_A - x_A R_B)$$

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

$$c\left(\frac{\partial x_A}{\partial t} + v_r^* \frac{\partial x_A}{\partial r} + \frac{v_\theta^*}{r}\frac{\partial x_A}{\partial \theta} + \frac{v_\phi^*}{r\sin\theta}\frac{\partial x_A}{\partial \phi}\right) = -\left(\frac{1}{r^2}\frac{\partial (r^2 J_{A,r}^*)}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial (J_{A,\theta}^* \sin\theta)}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial J_{A,\phi}^*}{\partial \phi}\right) + (x_B R_A - x_A R_B)$$

Fick's law of diffusion, Gibbs notation: $\underline{J}_A^* = -cD_{AB}\nabla x_A$

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$$= c x_A(\underline{v}_A - \underline{v}^*)$$

Fick's law of diffusion, Cartesian coordinates:

$$\begin{pmatrix} J_{A,x}^* \\ J_{A,y}^* \\ J_{A,z}^* \end{pmatrix}_{xyz} = \begin{pmatrix} -cD_{AB}\frac{\partial x_A}{\partial x} \\ -cD_{AB}\frac{\partial x_A}{\partial y} \\ -cD_{AB}\frac{\partial x_A}{\partial z} \end{pmatrix}_{xyz}$$

Fick's law of diffusion, cylindrical coordinates:

$$\begin{pmatrix} J_{A,r}^* \\ J_{A,\theta}^* \\ J_{A,z}^* \end{pmatrix}_{r\theta z} = \begin{pmatrix} -cD_{AB}\frac{\partial x_A}{\partial r} \\ -\frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta} \\ -cD_{AB}\frac{\partial x_A}{\partial z} \end{pmatrix}_{r\theta z}$$

Fick's law of diffusion, spherical coordinates:

$$\begin{pmatrix} J_{A,r}^* \\ J_{A,\theta}^* \\ J_{A,\phi}^* \end{pmatrix}_{r\theta\phi} = \begin{pmatrix} -cD_{AB}\frac{\partial x_A}{\partial r} \\ -\frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta} \\ -\frac{cD_{AB}}{r\sin\theta}\frac{\partial x_A}{\partial \phi} \end{pmatrix}_{r\theta\phi}$$

The **Equation of Species Mass Balance in Terms of Molar Quantities, constant cD_{AB}.** For binary systems, and Fick's law has been incorporated. Good for low density gases at constant temperature and pressure.

In terms of Diffusivity, D_{AB}

Microscopic species mass balance, constant thermal conductivity; Gibbs notation

$$c\left(\frac{\partial x_A}{\partial t} + \underline{v}^* \cdot \nabla x_A\right) = cD_{AB}\nabla^2 x_A + (x_B R_A - x_A R_B)$$

Microscopic species mass balance, constant thermal conductivity; Cartesian coordinates

$$c\left(\frac{\partial x_A}{\partial t} + v_x^*\frac{\partial x_A}{\partial x} + v_y^*\frac{\partial x_A}{\partial y} + v_z^*\frac{\partial x_A}{\partial z}\right) = cD_{AB}\left(\frac{\partial^2 x_A}{\partial x^2} + \frac{\partial^2 x_A}{\partial y^2} + \frac{\partial^2 x_A}{\partial z^2}\right) + (x_B R_A - x_A R_B)$$

Microscopic species mass balance, constant thermal conductivity; cylindrical coordinates

$$c\left(\frac{\partial x_A}{\partial t} + v_r^*\frac{\partial x_A}{\partial r} + \frac{v_\theta^*}{r}\frac{\partial x_A}{\partial \theta} + v_z^*\frac{\partial x_A}{\partial z}\right) = cD_{AB}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial x_A}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 x_A}{\partial \theta^2} + \frac{\partial^2 x_A}{\partial z^2}\right) + (x_B R_A - x_A R_B)$$

Microscopic species mass balance, constant thermal conductivity; spherical coordinates

$$c\left(\frac{\partial x_A}{\partial t} + v_r^*\frac{\partial x_A}{\partial r} + \frac{v_\theta^*}{r}\frac{\partial x_A}{\partial \theta} + \frac{v_\phi^*}{r\sin\theta}\frac{\partial x_A}{\partial \phi}\right)$$
$$= cD_{AB}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial x_A}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial x_A}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 x_A}{\partial \phi^2}\right) + (x_B R_A - x_A R_B)$$

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

$\underline{J}_A^* \equiv$ molar flux relative to a mixture's molar average velocity, $\underline{v}^*$ $\left(\text{units: } \underline{J}_A^*[=]\frac{mole}{area\cdot time}\right)$

$= c_A(\underline{v}_A - \underline{v}^*)$

$\underline{J}_A^* + \underline{J}_B^* = 0$

$\underline{N}_A \equiv c_A\underline{v}_A = \underline{J}_A^* + c_A\underline{v}^* =$ combined molar flux relative to stationary coordinates

$\underline{N}_A + \underline{N}_B = c\underline{v}^*$

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

$\underline{v}^* = x_A\underline{v}_A + x_B\underline{v}_B \equiv$ molar average velocity

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