

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

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

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: $\underline{J}_A^* = -c D_{AB} \nabla x_A$

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

Fick's law of diffusion, Cartesian coordinates: $\begin{pmatrix} J_{A,x}^* \\ J_{A,y}^* \\ J_{A,z}^* \end{pmatrix}_{xyz} = \begin{pmatrix} -c D_{AB} \frac{\partial x_A}{\partial x} \\ -c D_{AB} \frac{\partial x_A}{\partial y} \\ -c D_{AB} \frac{\partial x_A}{\partial z} \end{pmatrix}_{xyz}$

Fick's law of diffusion, cylindrical coordinates: $\begin{pmatrix} J_{A,r}^* \\ J_{A,\theta}^* \\ J_{A,z}^* \end{pmatrix}_{r\theta z} = \begin{pmatrix} -c D_{AB} \frac{\partial x_A}{\partial r} \\ -\frac{c D_{AB}}{r} \frac{\partial x_A}{\partial \theta} \\ -c D_{AB} \frac{\partial x_A}{\partial z} \end{pmatrix}_{r\theta z}$

Fick's law of diffusion, spherical coordinates: $\begin{pmatrix} J_{A,r}^* \\ J_{A,\theta}^* \\ J_{A,\phi}^* \end{pmatrix}_{r\theta\phi} = \begin{pmatrix} -c D_{AB} \frac{\partial x_A}{\partial r} \\ -\frac{c D_{AB}}{r} \frac{\partial x_A}{\partial \theta} \\ -\frac{c D_{AB}}{r \sin \theta} \frac{\partial x_A}{\partial \phi} \end{pmatrix}_{r\theta\phi}$

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.

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

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

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

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

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

$$J_A^* + J_B^* = 0$$

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

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

$\underline{v}_A \equiv$ 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