The **Equation of Species Mass Balance in Terms of Combined Molar quantities** in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B.

The general case, where the combined molar flux with respect to molar velocity ($\underline{N}_A$), is given on page 1.

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In terms of total molar flux, $\underline{N}_A$

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

$$\frac{\partial c_A}{\partial t} = -\nabla \cdot \underline{N}_A + R_A$$

WRF 25-11

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

$$\frac{\partial c_A}{\partial t} = -\left(\frac{\partial N_{A,x}}{\partial x} + \frac{\partial N_{A,y}}{\partial y} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

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

$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r}\frac{\partial (rN_{A,r})}{\partial r} + \frac{1}{r}\frac{\partial N_{A,\theta}}{\partial \theta} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

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

$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r^2}\frac{\partial (r^2 N_{A,r})}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial (N_{A,\theta}\sin\theta)}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial N_{A,\phi}}{\partial \phi}\right) + R_A$$

Fick's law of diffusion, Gibbs notation: $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$

$$= c_A \underline{v}^* - cD_{AB}\nabla x_A$$

WRF 24-22

Fick's law of diffusion, Cartesian coordinates:

$$\begin{pmatrix} N_{A,x} \\ N_{A,y} \\ N_{A,z} \end{pmatrix}_{xyz} = \begin{pmatrix} x_A(N_{A,x} + N_{B,x}) - cD_{AB}\frac{\partial x_A}{\partial x} \\ x_A(N_{A,y} + N_{B,y}) - cD_{AB}\frac{\partial x_A}{\partial y} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB}\frac{\partial x_A}{\partial z} \end{pmatrix}_{xyz}$$

Fick's law of diffusion, cylindrical coordinates:

$$\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,z} \end{pmatrix}_{r\theta z} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB}\frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB}\frac{\partial x_A}{\partial z} \end{pmatrix}_{r\theta z}$$

Fick's law of diffusion, spherical coordinates:

$$\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,\phi} \end{pmatrix}_{r\theta\phi} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB}\frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,\phi} + N_{B,\phi}) - \frac{cD_{AB}}{r\sin\theta}\frac{\partial x_A}{\partial \phi} \end{pmatrix}_{r\theta\phi}$$

NOTES:

- If component A has no sink, $\underline{N}_A = 0$.
- If A diffuses through stagnant B, $\underline{N}_B = 0$.
- If a binary mixture of A and B are undergoing steady equimolar counterdiffusion, $\underline{N}_A = -\underline{N}_B$.
- If, for example, two moles of A diffuse to a surface at which a rapid, irreversible reaction coverts it to one mole of B, then at steady state $-0.5\underline{N}_A = \underline{N}_B$.

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

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

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

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

$\underline{N}_A \equiv c_A\underline{v}_A = \underline{J}_A^* + c_A\underline{v}^* =$ 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)