جهت تخمین ضریب نفوذ مولکولی در مایعات رابطه زیر ارائه شده است:

$$D_{AB} = 0.74 * 10^{-7} \frac{(\Psi_B . M_B)^{0.5} T}{\mu \overline{V}_B^{\ 0.6}} \qquad 29$$

$$D_{AB} \rightarrow molecular\ diffusivity, cm^2 / s$$

$$\Psi_B \rightarrow association\ parameter\ for\ B$$

$$\Psi_A = \begin{cases} 2.6\ for\ water \\ 1.9\ for\ methanol \\ 1\ for\ non-polars \end{cases}$$

$$\overline{V}_A \rightarrow molar\ volume\ of\ A, cm^3 / gmole$$

انتقال جرم در حالت پایدار و در حالت ساکن

اگر سیستم انتقال جرم را دو جزئی فرض نماییم ، سیستم پایدار، انتقال جرم تنها در جهت Z و D_{AB} ثابت می باشد.

$$N_{AZ} = J_{AZ} + x_A \sum N_z$$

$$J_{Az} = -D_{AB} \frac{\partial C_A}{\partial Z} \quad \& \quad X_A = \frac{C_A}{C} \quad \& \quad \sum N_Z = N_{AZ} + N_{BZ}$$

$$\Rightarrow \quad N_{AZ} = -D_{AB} \frac{\partial C_A}{\partial z} + \frac{C_A}{C}\left(N_{AZ} + N_{BZ}\right) \quad \Rightarrow$$

$$N_{AZ} - \frac{C_A}{C}\left(N_{AZ} + N_{BZ}\right) = -D_{AB} \frac{dC_A}{dz} \quad \Rightarrow$$

$$\int \frac{dx}{a+bx} = \frac{1}{b}\ln[a+bx] + c$$

$$\int_{C_{A_1}}^{C_{A_2}} \frac{dC_A}{N_{Az} - \frac{C_A}{C}(N_{Az}+N_{Bz})} = \int_{Z_1}^{Z_2} -\frac{dZ}{D_{AB}} \Rightarrow$$

$$-\frac{C}{N_{Az}+N_{Bz}} ln\left[N_{Az} - \frac{C_A}{C}(N_{Az}+N_{Bz})\right]_{C_{A_1}}^{C_{A_2}} = -\frac{1}{D_{AB}}(Z_2 - Z_1) \Rightarrow$$

$$1 = \frac{1}{N_{Az}+N_{Bz}} \frac{C.D_{AB}}{Z_2 - Z_1} ln\left[\frac{N_{Az} - \frac{C_{A_2}}{C}(N_{Az}+N_{Bz})}{N_{Az} - \frac{C_{A_1}}{C}(N_{Az}+N_{Bz})}\right] \Rightarrow$$

$$1 = \frac{1}{N_{Az}+N_{Bz}} \frac{C.D_{AB}}{Z_2 - Z_1} ln\left[\frac{\frac{N_{Az}}{N_{Az}+N_{Bz}} - \frac{C_{A_2}}{C}}{\frac{N_{Az}}{N_{Az}+N_{Bz}} - \frac{C_{A_1}}{C}}\right] \Rightarrow$$

$\Rightarrow$ طرفين رابطه را در N_{AZ} ضرب ميكنيم $\Rightarrow$

رابطه كلي انتقال جرم :

$$N_{Az} = \frac{N_{Az}}{N_{Az}+N_{Bz}} \frac{C.D_{AB}}{Z_2 - Z_1} \ln \left[\frac{\frac{N_{Az}}{N_{Az}+N_{Bz}} - \frac{C_{A_2}}{C}}{\frac{N_{Az}}{N_{Az}+N_{Bz}} - \frac{C_{A_1}}{C}} \right]$$

$$N_{Az} = \frac{N_{Az}}{N_{Az}+N_{Bz}} \frac{C.D_{AB}}{Z} \ln \left[\frac{\frac{N_{Az}}{N_{Az}+N_{Bz}} - \frac{C_{A_2}}{C}}{\frac{N_{Az}}{N_{Az}+N_{Bz}} - \frac{C_{A_1}}{C}} \right]$$

رابطه كلي انتقال جرم را براي گازها و مايعات مي توان بصورت زير نمايش داد :

الف) تعميم روابط انتقال جرم براي گازها

براي گازها :

$$\frac{C_A}{C} = \frac{P_A}{P} = y_A \qquad C_A = \frac{P_A}{RT} \qquad C = \frac{P_t}{RT}$$

$$N_{Az} = \frac{N_{Az}}{N_{Az} + N_{Bz}} \frac{P_t . D_{AB}}{RTZ} ln \left[\frac{\frac{N_{Az}}{N_{Az} + N_{Bz}} - \frac{P_{A_2}}{P_t}}{\frac{N_{Az}}{N_{Az} + N_{Bz}} - \frac{P_{A_1}}{P_t}} \right]$$

$$\Rightarrow$$

$$N_{Az} = \frac{N_{Az}}{N_{Az} + N_{Bz}} \frac{P_t . D_{AB}}{RT(Z_2 - Z_1)} ln \left[\frac{\frac{N_{Az}}{N_{Az} + N_{Bz}} - \frac{P_{A_2}}{P_t}}{\frac{N_{Az}}{N_{Az} + N_{Bz}} - \frac{P_{A_1}}{P_t}} \right]$$

ب) تعميم روابط انتقال جرم براي مايعات

براي مايعات :

$$\frac{C_A}{C} = x_i \qquad C_A = \frac{\rho_A}{M} \qquad C = \frac{\rho}{M}$$

$$\Rightarrow N_{AZ} = \frac{N_{AZ}}{N_{AZ} + N_{BZ}} \cdot \frac{D_{AB} * \left(\frac{\rho}{M}\right)_{ave}}{Z_2 - Z_1} \ln\left[\frac{\frac{N_{AZ}}{(N_{AZ} + N_{BZ})} - X_{A_2}}{\frac{N_{AZ}}{(N_{AZ} + N_{BZ})} - X_{A_1}}\right]$$

حالات خاص :

1) نفوذ از میان یک لایه ساکن

در این حالات جزء A از میان جزء ساکن B نفوذ مي کند ، یعنی $N_{BZ}=0$ که در این صورت :

$$N_{BZ} = 0 \quad \Rightarrow \quad \frac{N_{AZ}}{N_{AZ} + \underbrace{\cancel{N_{BZ}}}_{0}} = 1$$

پس خواهیم داشت :

$$N_{AZ} = \frac{C * D_{AB}}{Z} \ln \left[\frac{1 - \frac{C_{A2}}{C}}{1 - \frac{C_{A1}}{C}} \right]$$

براي گازها :

$$N_{AZ} = \frac{P * D_{AB}}{RT\,(Z_2 - Z_1)} \ln\left[\frac{1 - y_{A_2}}{1 - y_{A_1}}\right]$$

براي مايعات :

$$N_{AZ} = \frac{D_{AB} * \left(\frac{\rho}{M}\right)_{ave}}{Z} \ln\left[\frac{1 - x_{A_2}}{1 - x_{A_1}}\right]$$

همچنين براي گازها مي توان نوشت :

$$\begin{cases} P_t = P_{A_1} + P_{B_1} \\ P_t = P_{A_2} + P_{B_2} \end{cases} \Rightarrow P_{A_1} + P_{B_1} = P_{A_2} + P_{B_2} \Rightarrow P_{A_1} - P_{A_2} = P_{B_2} - P_{B_1} \Rightarrow \frac{P_{A_1} - P_{A_2}}{P_{B_2} - P_{B_1}} = 1 \quad 1$$

$$\frac{P_{B_2} - P_{B_1}}{\ln\left(\frac{P_{B_2}}{P_{B_1}}\right)} = P_{BM} \quad 2 \qquad ، \qquad \frac{C_A}{C} = \frac{P_A}{P}$$

$$\Rightarrow \quad N_{AZ} = \frac{P_t * D_{AB}}{RT\,(z_2 - z_1)} \ln\left[\frac{1 - \frac{P_{A_2}}{P_t}}{1 - \frac{P_{A_1}}{P_t}}\right] \quad \Rightarrow$$

$$\Rightarrow \qquad N_{AZ} = \frac{P_t * D_{AB}}{RT(z_2 - z_1)} \ln\left[\frac{P_t - P_{A2}}{P_t - P_{A1}}\right] \qquad \Rightarrow$$

$$\Rightarrow \qquad N_{AZ} = \frac{P_t * D_{AB}}{RT(z_2 - z_1)} \ln \frac{P_{B2}}{P_{B1}} \qquad \Rightarrow$$

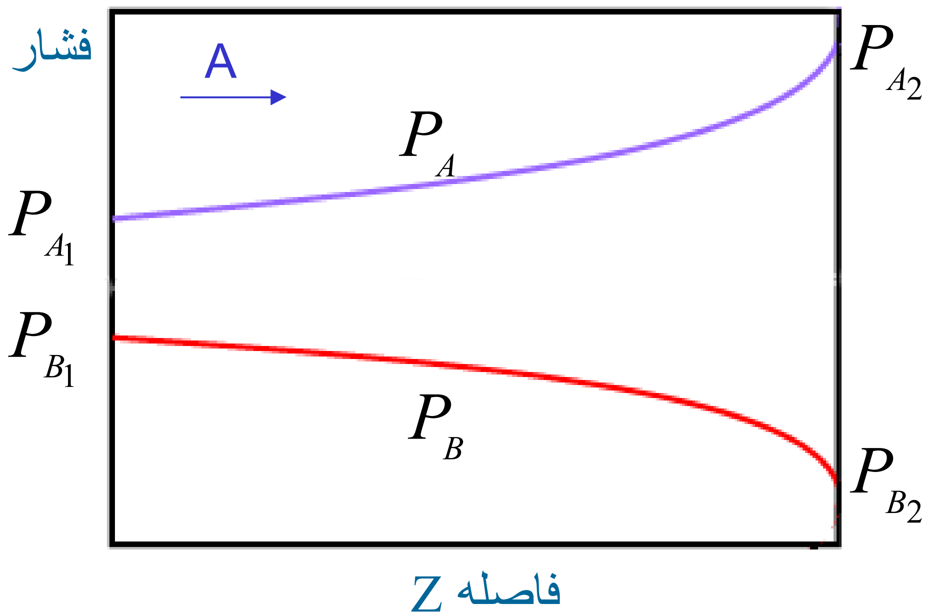
1

$$\Rightarrow \qquad 1 * N_{AZ} = \frac{P_t * D_{AB}}{RT(z_2 - z_1)} \ln \frac{P_{B2}}{P_{B1}} * \frac{P_{A1} - P_{A2}}{P_{B2} - P_{B1}} \qquad \Rightarrow$$

2

$$\Rightarrow \quad N_{AZ} = \frac{P_t * D_{AB}}{RTZ * P_{BM}} (P_{A_1} - P_{A_2})$$

نمودار مربوط به نفوذ جزء A درون جزء B :



2) نفوذ متقابل با شدت مولی معادل در حالت پایا

این حالت اکثرا در عملیات تقطیر مشاهده می شود.در این حالت $N_A=-N_B$ و از معادله کلی قبل نمی توان استفاده نمود.

$$N_{AZ} = J_{AZ} + \frac{C_A}{C}\sum N_Z$$

$$N_{AZ} = -D_{AB}\frac{d_{CA}}{dz} + x_A(N_A + N_B)$$

$$N_{AZ} = -D_{AB}\frac{d_{CA}}{dz} \longrightarrow N_{AZ} = \frac{D_{AB}}{RTZ}(p_{A_1} - p_{A_2})$$

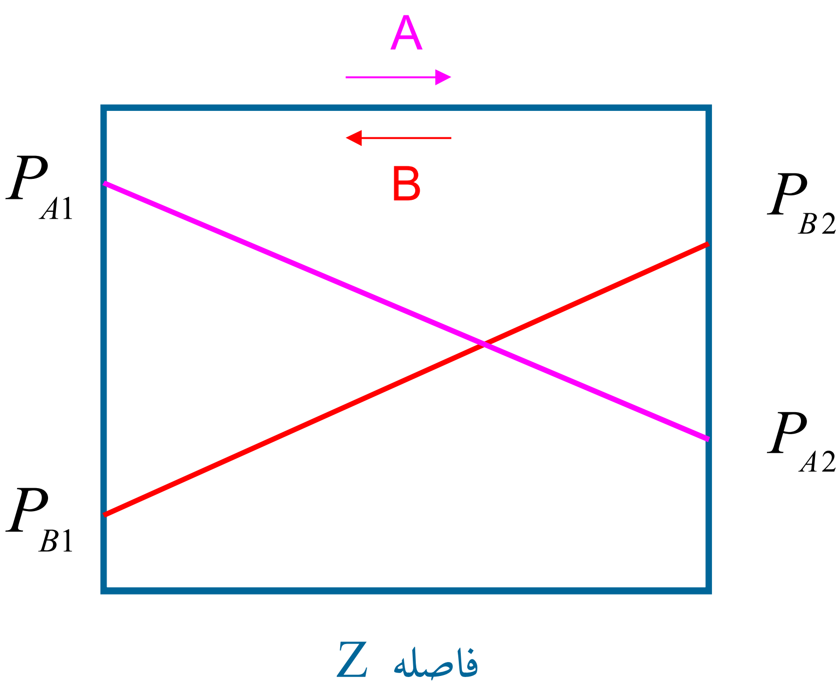
برای گازها:

$$N_{AZ} = \frac{D_{AB}.p}{RTZ}\left(\frac{p_{A1}}{p} - \frac{p_{A2}}{p}\right) = \frac{D_{AB}.p}{RTZ}(y_{A1} - y_{A2})$$

برای مایعات:

$$N_{AZ} = \frac{D_{AB}.(\frac{\rho}{m})_{av}}{Z}(x_{A1} - x_{A2})$$

نمودارمربوط به نفوذ متقابل با شدت مولی مساوی :



Mass Transfer: Diffusion

Fick's First Law

Fluxes

$$ {}_{v}J_{AZ} = -D_{AB}\frac{dC_A}{dz} $$

Flux relative to the volume average velocity

$$ {}_{M}J_{AZ} = -CD_{AB}\frac{dx_A}{dz} $$

Flux relative to the molar average velocity

$$ {}_{m}J_{AZ} = -\rho D_{AB}\frac{d\omega_A}{dz} $$

Flux relative to the mass average velocity

Mass and molar concentrations

$$\rho_\alpha = \text{mass concentration of species } \alpha$$

$$\rho = \sum_{\alpha=1}^{N} \rho_a = \text{mass density of solution}$$

$$\omega_\alpha = \rho_\alpha / \rho = \text{mass fraction of species } \alpha$$

$$c_\alpha = \text{molar concentration of species } \alpha$$

$$c = \sum_{\alpha=1}^{N} c_a = \text{molar density of solution}$$

$$x_\alpha = c_\alpha / c = \text{molar fraction of species } \alpha$$

Fick's First Law

Mass average velocity

$$v_m = \frac{\sum_{i=1}^{n} \rho_i v_i}{\sum_{i=1}^{n} \rho_i}$$

Molar average velocity

$$v_M = \frac{\sum_{i=1}^{n} c_i v_i}{\sum_{i=1}^{n} c_i}$$

Volume average velocity

$$v_v = \sum_{i=1}^{n} \rho_i v_i \left(\frac{\overline{v}_i}{M_i}\right)$$

v_i =velocity of the *ith* species wrt a stationary coordinate

Mass average and molar averages velocity

- Mass average velocity

$$v = \frac{\sum_{a=1}^{N} \rho_a v_a}{\sum_{a=1}^{N} \rho_a} = \frac{\sum_{a=1}^{N} \rho_a v_a}{\rho} = \sum_{a=1}^{N} \omega_a v_a$$

- Molar average velocity

$$v^* = \frac{\sum_{a=1}^{N} c_a v_a}{\sum_{a=1}^{N} c_a} = \frac{\sum_{a=1}^{N} c_a v_a}{c} = \sum_{a=1}^{N} x_a v_a$$

Molecular mass and molar fluxes

- Molecular mass flux, with respect to
  - stationary axes

$$n_\alpha = \rho_\alpha v_\alpha$$

  - mass average velocity

$$j_\alpha = \rho_\alpha \left(v_\alpha - v \right)$$

  - molar average velocity

$$j_\alpha^* = \rho_\alpha \left(v_\alpha - v^* \right)$$

Molecular mass and molar fluxes

- Molecular molar flux, with respect to
  - stationary axes

$$N_\alpha = c_\alpha v_\alpha$$

  - mass average velocity

$$J_\alpha = c_\alpha (v_\alpha - v)$$

  - molar average velocity

$$J_\alpha^* = c_\alpha (v_\alpha - v^*)$$

Summary of mass and molar fluxes

- Equivalent forms of Fick's law of binary diffusion

$$j_A = -\rho D_{AB} \nabla \omega_A$$

$$J_A^* = -c D_{AB} \nabla x_A$$

$$n_A = \omega_A (n_A + n_B) - \rho D_{AB} \nabla \omega_A = \rho_A v - \rho D_{AB} \nabla \omega_A$$

$$N_A = x_A (N_A + N_B) - c D_{AB} \nabla x_A = c_A v^* - c D_{AB} \nabla x_A$$

Maxwell-Stefan equations for Multicomponent diffusion in gases at low pressure

- Maxwell-Stefan equations

$$\nabla x_\alpha = -\sum_{\beta=1}^{N} \frac{x_\alpha x_\beta}{D_{AB}}\left(v_\alpha - v_\beta\right) = -\sum_{\beta=1}^{N} \frac{1}{cD_{AB}}\left(x_\beta N_\alpha - x_\alpha N_\beta\right)$$

$$\alpha = 1,2,3,\ldots..N$$