Example 1: Unsteady State Evaporation, the Arnold Cell

We wish to predict the rate at which a volatile liquid A evaporates into pure B in a tube of infinite length. The liquid level is maintained at $z = 0$ at all times. The temperature and pressure are assumed constant, and the vapors of A and B form an ideal gas mixture. Hence the molar density c is constant throughout the gas phase, and $\mathfrak{D}_{AB}$ may be considered to be constant. It is further assumed that species B is insoluble in liquid A, and that the molar average velocity in the gas phase does not depend on the radial coordinate.

Solution:

C.E. for mixture
$$\frac{\partial c}{\partial t} = -\nabla \cdot c v^* + \sum_{\alpha=1}^{N} R_\alpha$$

for a mixture with constant total concentration

$c =$ const. and no reactions $\Rightarrow \nabla \cdot v^* = 0$

$$\Rightarrow \frac{\partial v_z^*}{\partial z} = 0 \quad \Rightarrow v_z^* = v_{z0}(t) \neq f(z)$$

@ $z = 0$

From table 17.8-1
$$v_z^* = \frac{N_{Az0} + \cancel{N_{Bz0}}^{\,0}}{c}$$

Table 17.8-2 $\longrightarrow$
$$= -\frac{D_{AB}}{1 - x_{A0}} \left.\frac{\partial x_A}{\partial z}\right|_{z=0}$$

B insoluble

E 19.1-17:
$$c\left(\frac{\partial x_A}{\partial t} + v^* \cdot \nabla x_A\right) = c D_{AB} \nabla^2 x_A + (x_B R_A - x_A R_B)$$

$$\therefore \quad \frac{\partial x_A}{\partial t} - v_z^* \frac{\partial x_A}{\partial z} = D_{AB} \frac{\partial^2 x_A}{\partial z^2}.$$

$$\frac{\partial x_A}{\partial t} - \left(\frac{D_{AB}}{1 - x_{A0}} \left.\frac{\partial x_A}{\partial z}\right|_{z=0}\right) \frac{\partial x_A}{\partial z} = D_{AB} \frac{\partial^2 x_A}{\partial z^2}.$$

$t = 0 \qquad x_A = 0$

$z = 0 \qquad x_A = x_{A0}$

$z \to \infty \qquad x_A = 0.$

similarity transformation: scaling

$$\frac{1}{t} \sim \frac{D_{AB}}{z^2} \quad \Rightarrow \quad \eta = \frac{z}{\sqrt{t D_{AB}}}$$

$$\frac{\partial x_A}{\partial t} = \frac{d x_A}{d\eta}\frac{\partial \eta}{\partial t} = -\frac{1}{2}\frac{\eta}{t}\frac{d x_A}{d\eta}$$

$$\frac{\partial x_A}{\partial z} = \frac{d x_A}{d\eta}\frac{\partial \eta}{\partial z} = \frac{1}{\sqrt{t D_{AB}}}\frac{d x_A}{d\eta}$$

$$\frac{\partial^2 x_A}{\partial z^2} = \frac{d^2 x_A}{d\eta^2}\left(\frac{\partial \eta}{\partial z}\right)^2 = \frac{1}{t D_{AB}}\frac{d^2 x_A}{d\eta^2}$$

$$-\frac{1}{2}\frac{\eta}{\cancel{t}}\frac{d x_A}{d\eta} - \left(\frac{\cancel{D_{AB}}}{1-x_{A0}}\frac{1}{\sqrt{\cancel{t D_{AB}}}}\left.\frac{d x_A}{d\eta}\right|_{\eta=0}\right)\frac{d x_A/d\eta}{\sqrt{\cancel{t D_{AB}}}} =$$

$$\cancel{D_{AB}}\frac{1}{\cancel{t D_{AB}}}\frac{d^2 x_A}{d\eta^2}.$$

let $X = \frac{x_A}{x_{A0}}$,

$$\Rightarrow \frac{d^2 X}{d\eta^2} + \left[\frac{1}{2}\eta + \frac{x_{A0}}{1-x_{A0}}\left.\frac{d x_A}{d\eta}\right|_{\eta=0}\right]\frac{dX}{d\eta} = 0.$$

$$\frac{d^2 X}{d\eta^2} + \frac{1}{2}(\eta - \beta)\frac{dX}{d\eta} = 0, \quad \beta = -\frac{2 x_{A0}}{1-x_{A0}}\left.\frac{d x_A}{d\eta}\right|_{\eta=0}$$

$\eta = 0 \qquad X = 1$

$\eta \to \infty \qquad X = 0.$

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let $Y = \frac{dX}{d\eta}$ $\Rightarrow$ $\frac{dY}{d\eta} + \frac{1}{2}(\eta - \beta) Y = 0$.

$$\Rightarrow \ln(Y) = -\frac{1}{2}\int (\eta - \beta)\, d\eta$$

let $u = \eta - \beta$, $\Rightarrow du = d\eta$.

$$\Rightarrow \ln(Y) = -\frac{1}{4}(\eta - \beta)^2 + C_1'.$$

$$\frac{dX}{d\eta} = Y = C_1 e^{-\frac{(\eta-\beta)^2}{4}}$$

$$X = C_1 \int_0^{\eta} e^{-\frac{(\bar{\eta}-\beta)^2}{4}} d\bar{\eta} + C_2$$

BC1 $\Rightarrow$ $C_2 = 1$

BC2 $\Rightarrow$ $C_1 = \frac{1}{\int_0^{\infty} e^{-\frac{(\bar{\eta}-\beta)^2}{4}} d\bar{\eta}}$

$$\Rightarrow X = 1 - \frac{\int_0^{\eta} e^{-\left(\frac{\bar{\eta}-\beta}{2}\right)^2} d\bar{\eta}}{\int_0^{\infty} e^{-\left(\frac{\bar{\eta}-\beta}{2}\right)^2} d\bar{\eta}}$$

$\alpha = \frac{\eta - \beta}{2}$.

$$X = 1 - \frac{\cancel{2} \int_{-\frac{\beta}{2}}^{\frac{\eta-\beta}{2}} e^{-\alpha^2} d\alpha}{\cancel{2} \int_{-\beta/2}^{\infty} e^{-\alpha^2} d\alpha}.$$

$$X(\eta) = 1 - \frac{\operatorname{erf}\left(\frac{\eta-\beta}{2}\right) + \operatorname{erf}\left(\frac{\beta}{2}\right)}{\underbrace{\cancel{\operatorname{erf}(\infty)}}_{1} + \operatorname{erf}\left(\frac{\beta}{2}\right)}$$

$$= \frac{1 + \cancel{\operatorname{erf}\left(\frac{\beta}{2}\right)} - \operatorname{erf}\left(\frac{\eta-\beta}{2}\right) - \cancel{\operatorname{erf}\left(\frac{\beta}{2}\right)}}{1 + \operatorname{erf}\left(\frac{\beta}{2}\right)}$$

$$= \frac{1 - \operatorname{erf}\left(\frac{\eta-\beta}{2}\right)}{1 + \operatorname{erf}\left(\frac{\beta}{2}\right)}.$$

recall $\beta = -\frac{2 X_{A0}}{1 - X_{A0}} \left.\frac{dX_A}{d\eta}\right|_{\eta=0}.$

$$= -\frac{2 X_{A0}}{1 - X_{A0}} \cdot \frac{-1}{1+\operatorname{erf}\left(\frac{\beta}{2}\right)} \left[\frac{d}{d\eta}\left(\operatorname{erf}\left(\frac{\eta-\beta}{2}\right)\right)\right]_{\eta=0}$$

$$= \frac{2 X_{A0}}{1 - X_{A0}} \frac{1}{1+\operatorname{erf}\left(\frac{\beta}{2}\right)} \frac{\cancel{2}}{\sqrt{\pi}} \left(e^{-\left(\frac{\eta-\beta}{2}\right)^2}\right) \frac{1}{\cancel{2}} \Bigg|_{\eta=0}.$$

$$\beta = \frac{2 X_{A0}}{1 - X_{A0}} \frac{1}{1+\operatorname{erf}\left(\frac{\beta}{2}\right)} \frac{1}{\sqrt{\pi}} e^{-\frac{\beta^2}{4}}$$

Example 2: Gas absorption with Chemical Rapid Chemical Reaction

Gas A is absorbed by a stationary liquid solvent S, the latter containing solute B. Species A reacts with B in an instantaneous irreversible reaction according to the equation $aA + bB \rightarrow$ Products. It may be assumed that Fick's second law adequately describes the diffusion processes, since A, B, and the reaction products are present in S in low concentrations. Obtain expressions for the concentration profiles.

Solution:

In this problem there will be a plane parallel to the interface at a distance z_R inside the liquid, which seperates two regions one containing only A and another containing only B. Also,

$z_R = f(t)$. For A & B:

$$\frac{\partial c_A}{\partial t} = D_{AS} \frac{\partial^2 c_A}{\partial z^2} \qquad 0 \le z \le z_R(t)$$

$$\frac{\partial c_B}{\partial t} = D_{BS} \frac{\partial^2 c_B}{\partial z^2} \qquad z_R \le z < \infty$$

$t = 0$ $\qquad c_B = c_{B\infty} \qquad c_A = 0$.

$z = 0$ $\qquad c_A = c_{A0}$.

$z = z_R$ $\qquad c_A = c_B$

$z = z_R$ $\qquad -\frac{1}{a} D_{AS} \frac{\partial c_A}{\partial z} = \frac{1}{b} D_{BS} \frac{\partial c_B}{\partial z}$

$z \to \infty$ $\qquad c_B = c_{B\infty}$.

$$\frac{c_A}{c_{A0}} = C_1 + C_2 \, \mathrm{erf}\left(\frac{z}{\sqrt{4 D_{AS} t}}\right) \qquad 0 \leq z \leq z_R .$$

$$\frac{c_B}{c_{B\infty}} = C_3 + C_4 \, \mathrm{erf}\left(\frac{z}{\sqrt{4 D_{BS} t}}\right) \qquad z_R \leq z < \infty$$

see 12.1-3 for solution.

applying BC (this will be next HW!).

⋮

$$\frac{c_A}{c_{A0}} = 1 - \frac{\mathrm{erf}(z/\sqrt{4 D_{AS} t})}{\mathrm{erf}(z_R/\sqrt{4 D_{AS} t})}$$

$$\frac{c_B}{c_{B\infty}} = 1 - \frac{1 - \mathrm{erf}(z/\sqrt{4 D_{BS} t})}{1 - \mathrm{erf}(z_R/\sqrt{4 D_{BS} t})}$$

and BC3 gives:

$$1 - \mathrm{erf}\sqrt{\frac{\gamma}{D_{BS}}} = \frac{a \, c_{B\infty}}{b \, c_{A0}} \sqrt{\frac{D_{BS}}{D_{AS}}} \, \mathrm{erf}\sqrt{\frac{\gamma}{D_{AS}}} \, \exp\left(\frac{\gamma}{D_{AS}} - \frac{\gamma}{D_{BS}}\right)$$

where $\gamma = \frac{z_R^2}{4t}$.

see Fig 20.1-2