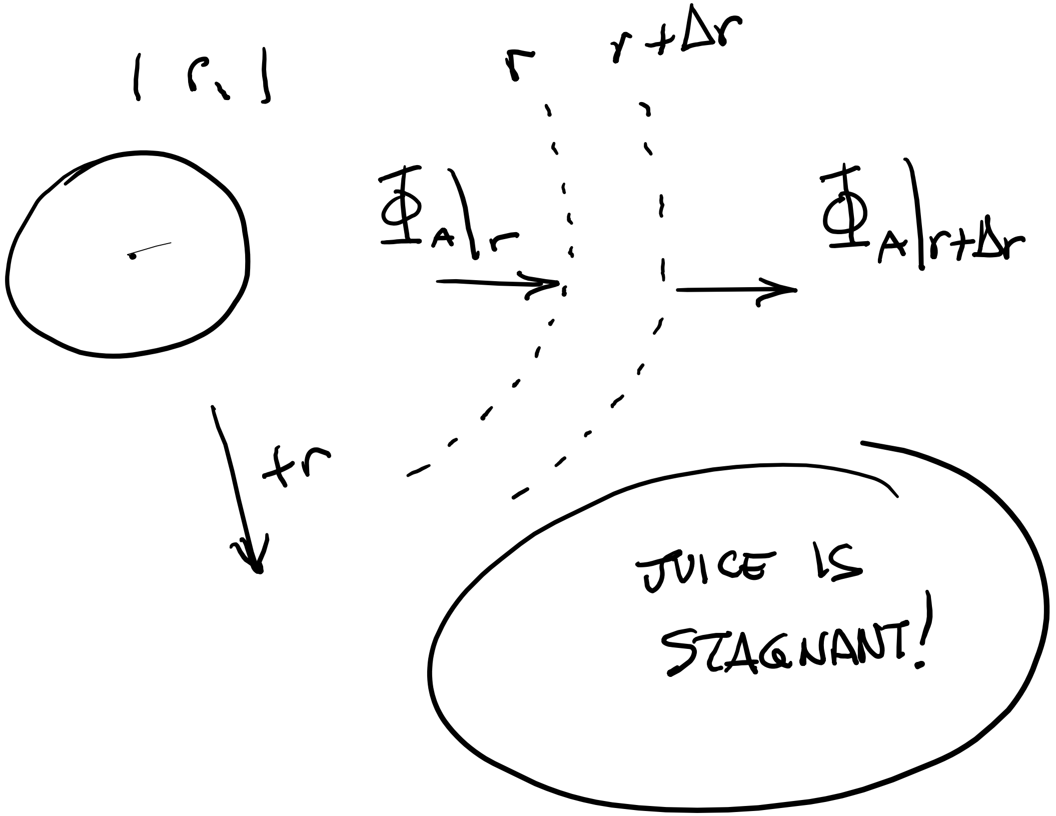
EXAMPLE 2

STEP 1

DRAW & LABEL



BOUNDARY CONDITIONS

$x_A = 0$ @ $r = r_1$ $\quad (r_1 = 1 \times 10^{-4}\ \text{cm})$

$x_A = x_{AEXT}$ @ $r \to \infty$

STEP 2

ACC = IN − OUT + GEN

$$0 = S\Phi_A\big|_r - S\Phi_A\big|_{r+\Delta r} + 0$$

$S = 4\pi r^2$

SURFACE AREA OF SPHERE

$$0 = \left(4\pi r^2 \Phi_A\right)\big|_r - \left(4\pi r^2 \Phi_A\right)\big|_{r+\Delta r}$$

DIVIDE BY $-4\pi\Delta r$

$$0 = \frac{r^2\Phi_A\big|_{r+\Delta r} - r^2\Phi_A\big|_r}{\Delta r}$$

TAKE LIMIT AS $\Delta r \to 0$

$$\boxed{0 = \frac{d}{dr}\left[r^2 \Phi_A\right]}$$

Result of Material Balance.

FROM NEXT PAGE

STEP 3

APPLY FLUX EQUATION.

IN SPHERICAL COORDINATES:

$$\vec{\nabla} x_A = \frac{\partial x_A}{\partial r}\vec{\varepsilon}_r + \frac{1}{r}\frac{\partial x_A}{\partial \theta}\vec{\varepsilon}_\theta + \frac{1}{r\sin\theta}\frac{\partial x_A}{\partial \phi}\vec{\varepsilon}_\phi$$

FLUX IS ONLY IN r DIRECTION

$$\vec{\nabla} x_A = \frac{\partial x_A}{\partial r} = \frac{d x_A}{dr}$$

SO $\quad \vec{\Phi}_A = -cD_{AB}\vec{\nabla} x_A + x_A \sum_{ALL} \vec{\Phi}_j$

NOW: $\quad \Phi_A = -cD_{AB}\dfrac{dx_A}{dr} + x_A \Phi_A \quad (\Phi_B = 0)$ "JUICE"

$$\Phi_A = \frac{-cD_{AB}}{1-x_A}\frac{dx_A}{dr}$$

$$0 = \frac{d}{dr}\left[r^2\left(\frac{-cD_{AB}}{1-x_A}\frac{dx_A}{dr}\right)\right]$$

INTEGRATE ONCE

$$\frac{-cD_{AB}}{1-x_A} r^2 \frac{dx_A}{dr} = C_1$$

$$\frac{-cD_{AB}}{1-x_A} dx_A = \frac{C_1}{r^2} dr$$

INTEGRATE AGAIN ($-cD_{AB}$ IS CONSTANT)

$$-cD_{AB} \int \frac{dx_A}{1-x_A} = C_1 \int \frac{dr}{r^2}$$

$$cD_{AB} \ln(1-x_A) = -\frac{C_1}{r} + C_2$$

STEP 4 — APPLICATION OF BOUNDARY CONDITIONS

i) $x_A = 0$ @ $r = r_1$

$$cD_{AB} \ln(1-0) = -\frac{C_1}{r_1} + C_2$$

$$0 = -\frac{C_1}{r_1} + C_2$$

$$C_2 = \frac{C_1}{r_1}$$

ii) $x = x_{AEXT}$ @ $r \to \infty$

$$cD_{AB} \ln(1 - x_{AEXT}) = \cancel{-\frac{C_1}{\infty}} + C_2$$

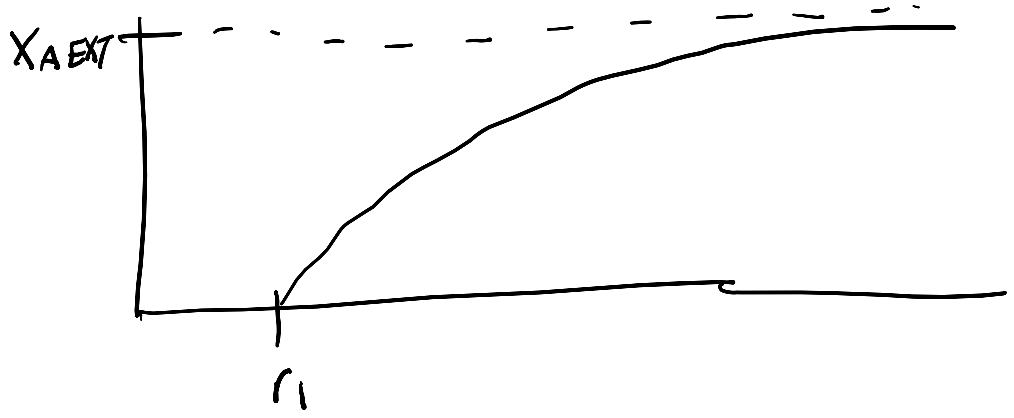
$$C_2 = cD_{AB} \ln(1 - x_{AEXT})$$

$$C_1 = cD_{AB}\, r_1 \ln(1 - x_{EXT})$$

$$c D_{AB} \ln(1 - x_A) = -\frac{r_1}{r} \underbrace{c D_{AB} \ln(1 - x_{A EXT})}_{C_1} + \underbrace{c D_{AB} \ln(1 - x_{A EXT})}_{C_2}$$

$$\ln(1 - x_A) = \ln(1 - x_{A EXT})\left(1 - \frac{r_1}{r}\right)$$

$$x_A = 1 - (1 - x_{A EX})^{(1 - r_1/r)} \leftarrow \text{EXPONENT}$$



$$\Phi_A = \frac{c_1}{r^2} = \frac{c D_{AB}\, r_1 \ln(1 - x_{AEXT})}{r^2} \qquad \Phi_A = f(r)$$

FLUX AT SURFACE

$$\Phi_A \Big|_{r_1} = \frac{c D_{AB} \ln(1 - x_{AEXT})}{r_1}$$

MOLAR FLOWRATE AT SURFACE

$$\dot{n}_A \Big|_{r_1} = S\Big|_{r_1} \Phi\Big|_{r_1}$$

$$= \left(4\pi r_1^2\right)\left(\frac{c D_{AB} \ln(1 - x_{AEXT})}{r_1}\right)$$

$$\boxed{\dot{n}_A \Big|_{r_1} = 4\pi c D_{AB}\, r_1 \ln(1 - x_{AEXT})}$$

REAL NUMBERS

$r_i = 1\times10^{-4}\,\text{cm}$ (1 μm)

$r = 2\times10^{-4}\,\text{cm}$ (1 μm FROM SURFACE)

$\rho = 1.06\,\text{g/cm}^3$

$c = \rho / \bar{M}$

$\bar{M} = (0.05)(180) + (0.95)(18) = 26.13\,\text{g/mol}$

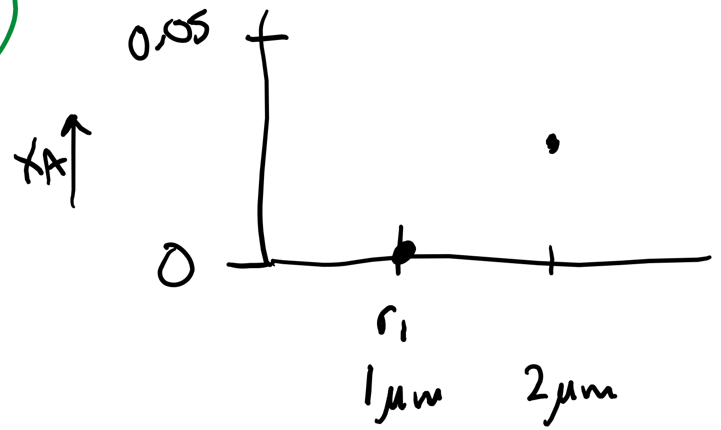
$c = 0.0406\,\text{mol/cm}^3$

$x_{A\,EXT} = 0.05$

EXPONENT

$$x_A = 1 - (1 - 0.05)^{\left(1 - \frac{1\times10^{-4}}{2\times10^{-4}}\right)}$$

$$\underline{x_A = 0.0253}$$



$$\dot{n}_A\Big|_{r_1} = 4\pi c D_{AB} r_1 \ln(1 - x_{AEXT})$$

$$= 4\pi(0.0406)(0.69 \times 10^{-5})(1 \times 10^{-4}) \ln(1 - 0.05)$$

$$\dot{n}_A\Big|_{r_1} = -1.81 \times 10^{-4}\ \mathrm{mol/s}$$

NEGATIVE SIGN MEANS FLOW IS IN $-r$ DIRECTION OR TOWARD CELLS.