Mass Transfer Problem: Shell Balance on a Dissolving Sphere with Reaction — CHE 324 :PhD problem University of Alabama

Sayed Huzaifa Mumit

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Problem Statement

A solid sphere of radius R, composed of substance A, is suspended in a liquid B. Substance A is slightly soluble in B and undergoes a **first-order chemical reaction** in the liquid with rate constant k_1''' (units: s^{-1}). The system is at steady state, and the radius R remains constant during the process. The molar solubility of A in B at the interface (i.e., at $r = R$) is C_{A0}. Assume diffusion is the only mode of mass transfer and that A diffuses radially into the liquid from the surface of the sphere.

Task: *Write the governing assumptions (postulates) and perform a shell mass balance on species A to derive the differential equation for the concentration profile $C_A(r)$ in the liquid. Do not solve for the concentration profile.*

Solution

Postulates (Assumptions)

1. **Steady-state** operation: no accumulation of A in the liquid phase.
2. **Radial symmetry**: concentration depends only on radial distance r.
3. **Constant diffusivity**: D_{AB} is constant throughout the medium.
4. **First-order reaction**: A reacts in the liquid with rate $-k_1''' C_A$.
5. **Constant radius**: The radius R of the solid sphere does not change significantly with time.
6. **Solubility equilibrium at the interface**: $C_A = C_{A0}$ at $r = R$.
7. **Dilute solution**: No bulk convection; only diffusion and reaction occur.

Shell Mass Balance

Consider a thin spherical shell of thickness Δr in the fluid phase, at a distance r from the center of the sphere.

General mass balance:

$$\text{Accumulation} = \text{In} - \text{Out} + \text{Generation}$$

At steady state, accumulation = 0:

$$0 = \text{In} - \text{Out} + \text{Generation}$$

Flux of A due to diffusion:

$$N_A = -D_{AB}\frac{dC_A}{dr}$$

- In at radius r: $4\pi r^2 \left(-D_{AB} \frac{dC_A}{dr} \bigg|_r \right)$
- Out at radius $r + \Delta r$: $4\pi(r + \Delta r)^2 \left(-D_{AB} \frac{dC_A}{dr} \bigg|_{r+\Delta r} \right)$
- Generation due to reaction: $-k_1''' C_A \cdot (4\pi r^2 \Delta r)$

Substituting into the balance:

$$0 = -4\pi r^2 D_{AB}\frac{dC_A}{dr}\bigg|_r + 4\pi(r+\Delta r)^2 D_{AB}\frac{dC_A}{dr}\bigg|_{r+\Delta r} - 4\pi r^2 k_1''' C_A \Delta r$$

Divide through by $4\pi\Delta r$, and take the limit as $\Delta r \to 0$:

$$\lim_{\Delta r \to 0} \frac{(r+\Delta r)^2 D_{AB}\frac{dC_A}{dr}\big|_{r+\Delta r} - r^2 D_{AB}\frac{dC_A}{dr}\big|_r}{\Delta r} = -r^2 k_1''' C_A$$

This becomes a derivative:

$$\frac{d}{dr}\left(r^2 D_{AB}\frac{dC_A}{dr} \right) = -r^2 k_1''' C_A$$

Final Differential Equation

Assuming D_{AB} is constant:

$$\boxed{\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dC_A}{dr} \right) = -\frac{k_1'''}{D_{AB}} C_A}$$

This is the governing equation for the steady-state concentration profile of species A in the surrounding liquid with a first-order reaction.