CHE 318 Lecture 09

Introduction to Unsteady State Mass Transfer

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Recap

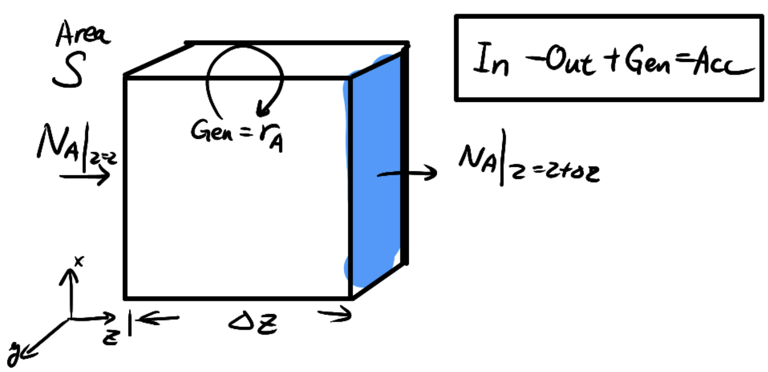
- Solving examples with pseudo steady state assumption
- Conclusion of steady state mass transfer

Learning Outcomes

After today's lecture, you will be able to:

- **Recall** difference between steady and unsteady state solutions
- **Derive** mass balance and flux equations in unsteady state problems
- **Identify** the generation and accumulation terms in typical transport problems
- **Analyze** time-dependent concentration profiles for U.S.S situations.

What Is Unsteady-State Mass Transfer?



[In] - [Out] + [Gen] = [Acc]

- Concentration varies with time $\partial c/\partial t \neq 0$
- Accumulation term is non-zero [Acc] $\neq 0$
- Requires time-dependent mass balances
- Common in transient diffusion, start-up, and response problems
- **More general** than S.S.

Governing Equation for U.S.S M.T.

Consider a control volume in 1D transport, the mass balance equation becomes

$$\begin{aligned}
[\text{Acc}] &= [\text{In}] - [\text{Out}] + [\text{Gen}] \\
S\Delta z \frac{\partial c_A}{\partial t} &= S(N_A|_{z=z} - N_A|_{z=z+\Delta z}) + [\text{Gen}]S\Delta z \\
\frac{\partial c_A}{\partial t} &= -\frac{\partial N_A(z)}{\partial z}|_z + r_A
\end{aligned}$$

where r_A is the generation rate for A (e.g. local reaction). This is the governing equation for all time-dependent mass transfer!

Comparison between Flux equation and Mass Balance

Flux equation

$$N_A = J^*_{Az} + x_A(N_A + N_B)$$

- Amount of material moved **in** and **out** of controled volume
- J^*_{Az}: Fick's first law of diffusion
- Can be used for S.S ($dN_A/dz = 0$) and U.S.S

Mass balance eq

$$\frac{\partial c_A}{\partial t} = -\frac{\partial N_A}{\partial x} + r_A \tag{1}$$

- Change of local c_A over time
- Need flux equation solution first
- Can be used for S.S ($\frac{\partial c_A}{\partial t} = 0$) and U.S.S.

Mass Balance: Extension to 3D

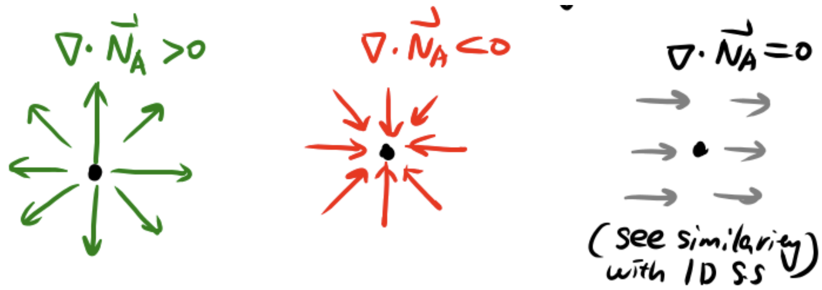


Figure 1: Illustration of divergence

$$\frac{\partial c_A}{\partial t} = r_A - \frac{\partial N_{Ax}}{\partial x} - \frac{\partial N_{Ay}}{\partial y} - \frac{\partial N_{Az}}{\partial z} \tag{2}$$

$$= r_A - \nabla \cdot \vec{N}_A \tag{3}$$

- $\nabla\cdot$ is the **divergence** operator (not Δ, not gradient!)
- $\vec{N}_A$ is generally a 3D vector field

How To Analyze A U.S.S Problem

Unsteady state mass transfer is not intimidating if you follow these steps

1. Draw the scheme
2. Write down the **mass balance** equation ([In] - [Out] + [Gen] = [Acc])
3. Identify the [Gen] and [Acc] terms
4. Choose proper **flux equations** for [In] and [Out] terms
5. Solving analytically or numerically.

Dissecting the General Equation for Mass Balance

$$\begin{aligned} r_A - \frac{\partial c_A}{\partial t} &= \nabla \cdot \left[\vec{J}^*_A + x_A(\vec{N}_A + \vec{N}_B)\right] \\ &= \nabla \cdot \left[\vec{J}^*_A + c_A \vec{v}_m\right] \\ &= \nabla \cdot \left[-D_{AB}\nabla c_A + c_A \vec{v}_m\right] \end{aligned}$$

- We have fluid velocity $\vec{v}_m$ on the R.H.S
- $\nabla\cdot$ creates more nonlinear terms
- Do we know N_A and N_B relation?
- In general this is hard to solve (coupling fluid with mass transfer)
- Often interested in several limiting cases

Special Cases of Unsteady-State Mass Transfer

- Case 1: EMCD for gases at constant p_T, $r_A = 0$ (Fick's second law)
  - There is **no negative sign** in Fick's second law!

$$\frac{\partial c_A}{\partial t} = D_{AB}\nabla^2 c_A \tag{4}$$

- Case 2: Constant D_{AB}

$$\frac{\partial c_A}{\partial t} = D_{AB}\nabla^2 c_A - c_A\nabla\cdot\vec{v}_m - \vec{v}_m\cdot\nabla c_A + r_A$$

- Case 3: Constant ρ and D_{AB} (e.g. imcompressible liquids)

$$\frac{\partial c_A}{\partial t} = D_{AB}\nabla^2 c_A - \vec{v}_m\cdot\nabla c_A + r_A \tag{5}$$

where $\nabla\cdot\vec{v}_m = 0$

What exactly do we solve?

For U.S.S M.T, we typically need

1. Governing equation (PDE) from any limiting case
2. Initial conditions $c_A(z, t = 0)$
3. Boundary conditions (B.C.)
   - Dirichlet B.C. (e.g. $c_A(z = 0) = c_0$)
   - Neumann B.D. (e.g. $N_A(z = 0) = N_{A0}$, constant flux)
4. Solving analytically or numerically
5. Get $c_A(z, t)$, $x_A(z, t)$, $N_A(x, t)$
6. Steady-state solutions often means $c_A(z, t \to \infty)$

Unsteady State Mass Transfer: Calculation Overview

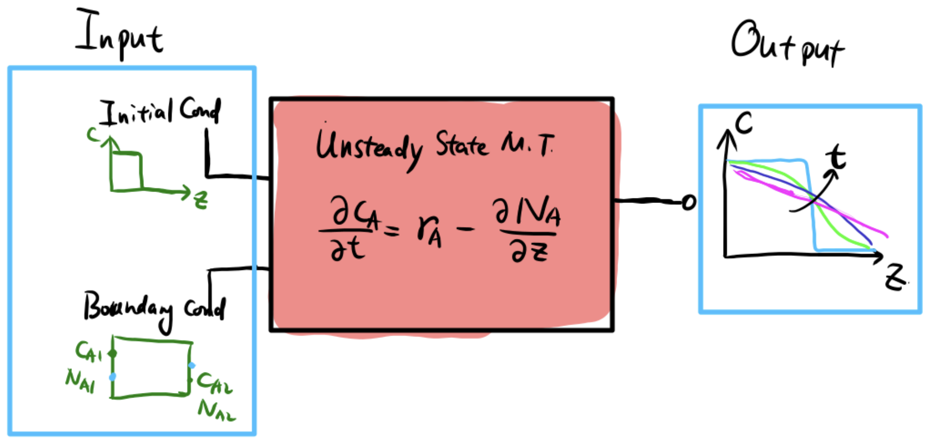


Figure 2: A “solver engine” for unsteady state mass transfer

Summary

- Unsteady state mass transfer governing equation
- Step-by-step solution to diffusion through stagnant B
- Diffusion and reaction system setup