CHE 318 Lecture 10

Unsteady State Mass Transfer (II)

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2026-01-26

Midterm Exam Announcement

- Date: Feb 09, 2026 (Monday)
- Time: 50 min during class
- Question types:
  - Multichoice questions (conceptual, no derivation)
  - Short-answer questions (conceptual, no derivation)
  - Long-answer questions (derivation and / or calculation)
- Formula sheet / calculator policy: refer to course syllabus

Midterm Exam Questions

- Covers up to unsteady state mass transport
- Sample questions to be released this week on Canvas
- Use our AI helper wisely!

Recap

- Unsteady state mass transfer: $\partial c_A / \partial t \neq 0$
  - **Mass balance equation**: [In] - [Out] + [Gen] = [Acc]
  - **Flux equation**: $N_A = J^*_{Az} + c_A / c_T * (N_A + N_B)$
- General expression for U.S.S. M.T. in 3D vector
- Boundary conditions and initial conditions

Learning Outcomes

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

- **Formulate** unsteady-state mass balances with appropriate assumptions and simplifications
- **Identify** accumulation, transport, and generation terms in typical 1D mass transfer problems
- **Interpret** time-dependent concentration profiles in unsteady-state mass transfer examples

B.C. Case 1. Concentration at surfaces

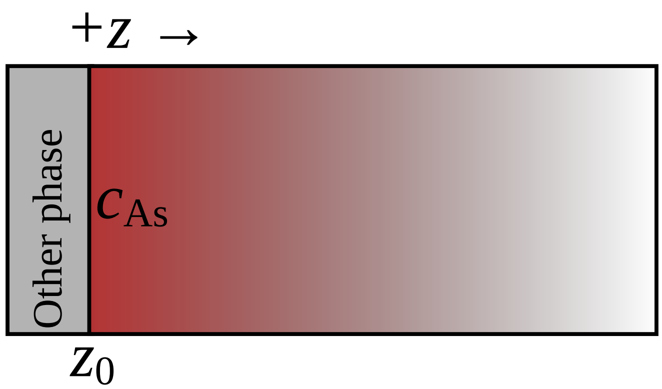

Figure 1: Concentration at phase interfaces

- Interface can be gas|liquid, liquid|solid, gas|solid
- Often assuming equilibrium

$$c_A|_{\text{surf}} = c_{As} \qquad \text{eq. solubility}$$

B.C. Case 2: Chemical Reactions

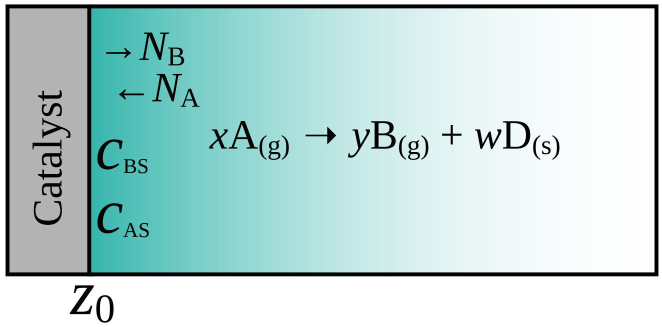

Figure 2: Boundary condition for reaction

$$N_A\big|_{\text{surf}} = \nu_A \, r_A \tag{1}$$

- Surface reaction couples mass transfer and kinetics
- Molar flux at surface determined by reaction rate
- Generally Neumann boundary
- ν_A: stoichiometric ratio

B.C. Case 3: Constant Flux

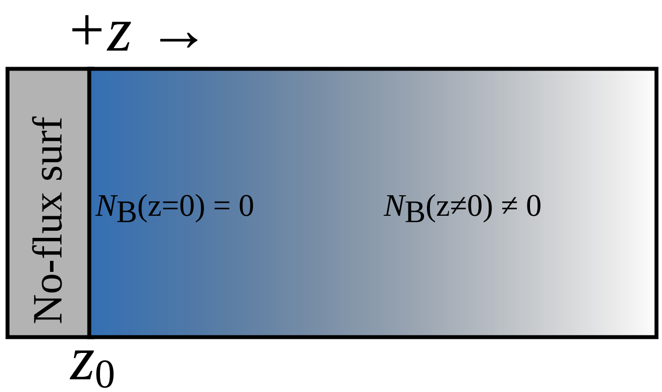

Figure 3: Constant flux B.C.

- In many cases the flux $N_{A,\text{surf}}$ or $N_{B,\text{surf}}$ can be constant.
- E.g. inpenetratable surface to stagnant gas $N_{B,\text{surf}} = 0$
- **Does not** mean $N_A(z)$ or $N_B(z)$ elsewhere is constant!

U.S.S Example 1: Diffusion Through Stagnant B

We have seen in previous examples how to solve the molar flux of liquid evaporating into stagnant air. Let's see the same system but in unsteady state.

Question: liquid (A) evaporates inside stagnant air (B) inside a vertical tube at constant temperature T and pressure p_T. At the vent of the system dry air is continuous blown. Plot the molar fraction x_A as a function of z and time t. Assume the liquid level is L away from the vent and does not change during the evaporation process.

Step 1: Species Mass Balance (Unsteady, 1D)

For a differential slice $A\,dz$, write the mass balance

$$[\text{IN}] - [\text{OUT}] = [\text{ACC}] \tag{2}$$

$$AN_A|_{z=z} - AN_A|_{z=z+\Delta z} = \frac{\partial}{\partial t}\left(A\,dz\,c_A\right) \tag{3}$$

$$-\frac{\partial N_A}{\partial z} = \frac{\partial c_A}{\partial t} \tag{4}$$

We would have $\frac{\partial c_B}{\partial t} = -\frac{\partial N_B}{\partial z}$

Step 2: Couple With Flux Equation

This is a diffusion through stagnant B case, we can directly write

$$N_A(z,t) = -c_T D_{AB}\frac{\partial x_A(z,t)}{\partial z} + x_A\left[N_A(z,t) + N_B(z,t)\right] \tag{5}$$

- Can we use $N_B = 0$ in this case?
- **No**, N_B changes by z, t!
- $N_B = 0$ only at $z = 0$ (liquid interface)
- **Do not** write the steady state N_A solution!

Step 3: Conservation Equations

Generally, we still need to know the relation between N_A and N_B to solve the mass-balance-flux equations.

The total concentration $c_T = c_A + c_B$ is conserved, therefore we have constrains

$$[\text{In}]_T - [\text{Out}]_T = 0 \tag{6}$$

$$[\text{In}]_A - [\text{Out}]_A = -[\text{In}]_B + [\text{Out}]_B \tag{7}$$

$$\frac{\partial N_A(z,t)}{\partial z} = -\frac{\partial N_B(z,t)}{\partial z} \tag{8}$$

Step 4: Boundary Conditions

Boundary conditions (Left, Right, any time)

- $x_A(0,t) = x_{A0}$ (equilibrium vapor fraction)
- $x_A(L,t) = 0$ (dry air)
- $N_B(0,t) = 0$ (No-flux boundary for B)

The last B.C for $N_B(0,t)$ gives:

$$N_A(0,t) = -\frac{c_T D_{AB}}{1 - x_{A0}} \frac{\partial x_A(0,t)}{\partial z} \tag{9}$$

Step 5: Final solution

- Unsteady state flux equation (stagnant B)

$$N_A = -c_T D_{AB} \frac{\partial x_A}{\partial z} + x_A \left[\frac{-c_T D_{AB}}{1 - x_{A0}} \frac{\partial x_A}{\partial z} \Big|_{z=0} \right] \tag{10}$$

- Governing equation for diffusion through stagnant B, unsteady state:

$$\frac{\partial x_A}{\partial t} = D_{AB} \frac{\partial^2 x_A}{\partial z^2} + \left[\frac{D_{AB}}{1 - x_{A0}} \frac{\partial x_A}{\partial z} \Big|_{z=0} \right] \frac{\partial x_A}{\partial z} \tag{11}$$

- Analytical solution exists, but numerical solution is more convenient

U.S.S Diffusion Through Stagnant B: Analytical Solution

$x_A z, t$ has an analytical solution if $L \to \infty$ (See Bird. *Transport Phenomena* Ch 20.1):

$$x_A(z,t) = x_{A0} \frac{1 - \text{erf}(\frac{z}{\sqrt{4D_{AB}t}} - \phi)}{1 + \text{erf}\phi} \tag{12}$$

erf is the **error function**:

$$\text{erf}(\eta) = \frac{2}{\sqrt{\pi}} \int_0^\eta e^{-s^2}\, ds \tag{13}$$

- ϕ: a dimensionless constant depending on x_{A0}, t and D_{AB}
- Scaling combining length and time: $\frac{z}{\sqrt{4D_{AB}t}}$
- Higher D_{AB} faster towards steady state! (Wooclap question 3, L09)
- Penetration depth: $L_p \approx \sqrt{4D_{AB}t}$

Numerical Solutions To Evaporation Problem

The numerical solution using finite difference (FD) methods is beyond CHE 318, but we can briefly breakdown the process into:

- Discretize space: $z \to z_i$
- Approximate spatial derivatives with finite differences
- Convert PDE into a system of ODEs in time
- Integrate in time using standard ODE solvers

U.S.S Diffusion Through Stagnant B: Demo

U.S.S Example 2: Transport Through A Catalyst Wall

Question: A gas mixture containing species A flows through a cylindrical conduit of diameter D with a constant mean velocity v_m. A porous catalytic wall of thickness Δz is located at a fixed axial position inside the conduit. Inside the catalyst region, species A is consumed by a first-order surface reaction:

$$r = k'(c_{A,s} - c_A)$$

Assume:

- surface concentration on catalyst, $c_{A,s}$ is constant
- uniform properties in the radial direction
- constant T, P, and physical properties
- no reaction outside the catalyst region

Step 1: Mass Balance

Consider a differential gas-phase control volume of thickness Δz that intersects the catalytic wall.

$$\text{In} - \text{Out} + \text{Generation} = \text{Accumulation} \tag{14}$$

$$\tag{15}$$

$$\frac{\pi D^2}{4}\left(N_A\big|_z - N_A\big|_{z+\Delta z}\right) + \pi D\,\Delta z\,k'\,(c_{A,s} - c_A) = \frac{\pi D^2}{4}\,\frac{\partial C_A}{\partial t} \tag{16}$$

$$-\frac{\partial N_A}{\partial z} + \frac{4k'}{D}\,(c_{A,s} - c_A) = \frac{\partial c_A}{\partial t} \tag{17}$$

Step 2: Coupling With Flux Equation

Use the convection–diffusion flux (constant v_m):

$$N_A = -\,D_{AB}\,\frac{\partial c_A}{\partial z} + c_A\,v_m \tag{18}$$

When v_m is constant, differentiate over N_A becomes:

$$\frac{\partial N_A}{\partial z} = -\,D_{AB}\,\frac{\partial^2 c_A}{\partial z^2} + v_m\,\frac{\partial c_A}{\partial z} \qquad (v_m = \text{const}) \tag{19}$$

Step 3: General Equation for M.T + Surface Reaction

$$\frac{\partial c_A}{\partial t} = -\left(-\,D_{AB}\,\frac{\partial^2 c_A}{\partial z^2} + v_m\,\frac{\partial c_A}{\partial z}\right) + \frac{4k'}{D}\,(c_{A,s} - c_A) \tag{20}$$

$$= D_{AB}\,\frac{\partial^2 c_A}{\partial z^2} - v_m\,\frac{\partial c_A}{\partial z} + \frac{4k'}{D}\,(c_{A,s} - c_A) \tag{21}$$

Need:

- initial condition $c_A(z, 0)$
- boundary conditions at $z = 0$ and $z = L$

Solve:

- analytical (special cases)
- numerical integration (finite difference)

Summary

- Step-by-step solution to diffusion through stagnant B
- Diffusion and reaction system setup