Lecture #9 Modeling Mass Transport of Chemical Species in Homogeneous Media

Goal

This lecture introduces students to mass transport modeling in homogeneous media, focusing on the fundamental mechanisms—diffusion, convection, and migration—and their mathematical descriptions. Students will learn how to formulate transport equations (Fick's laws, Nernst–Planck equation), apply boundary/initial conditions, and analyze solutions in engineering applications, including reactors, environmental systems, and electrochemical devices.

Introduction

Mass transport refers to the movement of chemical species due to gradients in concentration, pressure, or temperature. It is a fundamental concept in chemical engineering, electrochemistry, and environmental science, essential for understanding reaction kinetics, reactor design, and species distribution in media.

Key transport mechanisms include diffusion, convection, and, for charged species, migration in an electric field. This lecture focuses on modeling these processes in homogeneous media, assuming uniform properties and no phase boundaries.

Fundamental Concepts

Mass transport mechanisms include:

• Diffusion: Movement of species from high to low concentration regions. Governed by Fick's laws:

- Fick's First Law: $J = -D\ \partial C/\partial x$
  J: Flux, D: Diffusion coefficient, $\partial C/\partial x$: Concentration gradient.

- Fick's Second Law: $\partial C/\partial t = D\ \nabla^2 C$
  Describes time-dependent concentration changes.

• Convection: Movement due to bulk fluid flow. Expressed as:

$J = C \cdot v$

where C is the concentration and v is the fluid velocity.

• Migration: For charged species, movement in response to an electric field:

$J_{mig} = zFC\mu E$

z: Charge, F: Faraday's constant, μ: Mobility, E: Electric field strength.

Mathematical Modeling

To model mass transport, we combine the contributions of diffusion, convection, and migration in the Nernst-Planck equation:

$$J = -D\, \partial C/\partial x + Cv + zFC\mu E$$

In homogeneous media, where properties like viscosity are uniform, the modeling equations simplify. For uncharged species or systems without flow, we often use Fick's laws as the governing equations.

Solving Fick's second law requires specifying initial and boundary conditions. For steady-state systems, $\partial C/\partial t = 0$, leading to simpler algebraic solutions. For transient systems, numerical methods or analytical techniques like separation of variables are employed.

Practical Applications

Modeling mass transport is critical in various fields, including:

• Industrial processes: Designing chemical reactors and separation units.

• Environmental science: Predicting pollutant dispersion in water bodies.

• Electrochemistry: Optimizing electrode reactions and battery performance.

Example Problem

Consider a chemical species with a diffusion coefficient $D = 10^{-5}$ cm²/s. Initially, the species concentration is uniform at C_0. At $t = 0$, the concentration at $x = 0$ is fixed at C_s. Determine the concentration profile $C(x, t)$.

Solution:

Using Fick's second law, we solve $\partial C/\partial t = D\, \partial^2 C/\partial x^2$ with boundary conditions:

$C(0, t) = C_s$

$C(\infty, t) = C_0$

Analytical solutions involve error functions or numerical methods.

Summary

Mass transport in homogeneous media involves diffusion, convection, and migration. Modeling these processes provides insights into the behavior of chemical species, enabling applications in industry, research, and environmental studies.

Learning Outcomes

By the end of this lecture, students will be able to:

1. Explain the fundamental mechanisms of mass transport: diffusion, convection, and migration (related to LO 4, ID 4.5).

2. Apply Fick's first and second laws to model concentration gradients and transient diffusion (related to LO 4, ID 4.5).

3. Formulate the Nernst–Planck equation for systems involving diffusion, convection, and ionic migration (related to LO 4, ID 4.5).

4. Solve one-dimensional steady-state and transient diffusion problems using analytical or numerical approaches (related to LO 4, ID 4.5).

Questions and Self-Study Assignments

1. State the three primary mass transport mechanisms and define each one.

2. Derive Fick's first law for one-dimensional steady-state diffusion.

3. Explain the physical meaning of the diffusion coefficient D.

4. Write the full Nernst–Planck equation and describe each term.

5. Describe a real industrial process where mass transport limits reaction rate.

6. Read a recent (≤3 years) research article using diffusion or mass transport modeling. Summarize:
- system studied
- transport equations used
- key findings

References

1.Chemical Reaction Engineering Module User's Guide. – COMSOL, 2020.

2.Ghasem N. Modeling and Simulation of Chemical Process Systems. - CRC Press, 2015. – 518 p.