Lecture #11 Modeling of Mass Transport of Chemical Species in Heterogeneous Media

Goal

This lecture introduces students to the fundamentals of mass transport in heterogeneous media, where chemical species move across multiple phases (solid–liquid, solid–gas) or through complex structures such as porous catalysts, porous electrodes, membranes, soils, and geological formations. Compared to homogeneous media, heterogeneous systems require modified modeling approaches to account for porosity, tortuosity, multiphase interactions, and spatial nonuniformity.

Introduction

Mass transport in heterogeneous media is critical to understanding processes such as catalysis, electrochemistry, and environmental transport. Unlike homogeneous media, heterogeneous systems involve multiple phases (e.g., solid-liquid, solid-gas) or complex geometries (e.g., porous materials), making the modeling more challenging and multidimensional.

In heterogeneous systems, the transport of chemical species is affected by the interactions between the phases, as well as the physical structure of the medium.

Mass Transport in Heterogeneous Media

In heterogeneous systems, species move through different phases (e.g., from a liquid phase to a solid phase or through a porous medium). The main transport mechanisms are diffusion, convection, and reaction kinetics, but these can vary significantly depending on the nature of the system.

For porous media, the governing equation often combines the continuity equation with Fick's Law, where the flux is defined as:

$J = -D \nabla C + C v$

Where J is the flux, D is the diffusion coefficient, C is the concentration, and v is the velocity field in the system.

In these cases, the diffusion term may be modified by the porosity and tortuosity of the medium, which alter the effective diffusion coefficient.

Modeling Mass Transport in Porous Media

Porous media, like catalysts or electrodes, are commonly used in many industrial applications. The mass transport in such systems is affected by the pore structure, which introduces heterogeneity in both concentration and flux profiles.

The modified form of the diffusion equation for a porous medium is:

$\partial C/\partial t = \nabla \cdot (D_{eff} \nabla C)$

Where D_eff is the effective diffusion coefficient, which is often reduced due to tortuosity and the complex geometry of the medium.

Electrochemical Systems in Heterogeneous Media

In electrochemical systems, mass transport is often coupled with electrochemical reactions at the electrode surface. The modeling of these systems requires solving coupled equations for current, concentration, and potential. The Nernst-Planck equation is a useful tool in such cases:

$J = -D \nabla C + zFC\mu E$

Where the first term represents the diffusion flux, and the second term accounts for migration due to the electric field.

Example: Electrochemical Reaction in Porous Electrode

Consider a redox reaction occurring at a porous electrode. The concentration of reactants decreases as the reaction proceeds, and the flux of ions is influenced by both diffusion and the electric field. The effective mass transport coefficient can be modeled as:

$D_{eff} = D / (1 + \tau)$

Where τ is the tortuosity factor, which accounts for the path length within the porous structure.

Conclusion

In heterogeneous media, the transport of chemical species is more complex than in homogeneous media due to the interactions between different phases and the structure of the medium. The governing equations need to be adapted to account for the tortuosity and porosity of the medium, as well as for the coupling with electrochemical reactions.

Understanding these systems is crucial for applications in catalysis, battery design, and other electrochemical processes.

Learning Outcomes

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

1. Explain the differences between mass transport in homogeneous and heterogeneous media (related to LO 4, ID 4.5).

2. Apply the modified diffusion equation using effective diffusion coefficients for porous materials (related to LO 4, ID 4.5).

3. Describe how porosity and tortuosity influence mass transport and reaction rates (related to LO 4, ID 4.5–4.6).

4. Model diffusion and migration in porous electrodes, accounting for coupled reaction–transport effects (related to LO 4, ID 4.6).

5. Analyze real-world applications such as catalytic reactors, porous electrodes in batteries, and filtration or environmental systems (related to LO 4, ID 4.6–4.7).

Questions and Self-Study Assignments

1. Explain the difference between homogeneous and heterogeneous media in mass transport.

2. Define porosity and tortuosity. How do they affect the effective diffusion coefficient?

3. Describe the Nernst–Planck flux equation and explain the role of migration.
4. For a porous Li-ion battery electrode, explain how increased tortuosity affects charge/discharge performance.

References

1. Ghasem, N. Modeling and Simulation of Chemical Process Systems. CRC Press, 2015.
— Chapters on diffusion, mass transfer, and heterogeneous systems.
2. Gatzke, E. Introduction to Modeling and Numerical Methods for Biomedical and Chemical Engineers. Springer, 2021.