Multiphysics coupling

Component
École Nationale
Supérieure
d'Électrotechnique
d'Électronique

In brief

- **Ametys Code:** N9EM17D
- **Open to exchange students:** No

Presentation

Objectives

- Simulate and analyze in depth (in conjunction with associated theoretical material) coupling configurations between hydrodynamics, transfers and reaction on the basis of DNS-type simulations: (i) transfer around and within a catalyst particle in a flow and (ii) numerical tracing of a reactor.
- Simplify these studies by establishing 1D phenomenological models used in reactor engineering
- Implement a multi-scale simulation on a fixed-bed catalytic reactor configuration based on a coupling between these 1D models.

Description

Teaching method: 3-part project.

The aim of this project is to use COMSOL Multiphysics to solve the equations governing hydrodynamics, transfer and reaction in a single-phase fixed-bed reactor. The problem is complex because of the different phenomena involved and the various scales involved, from the molecular to the reactor scale. Reaction engineering introduces various concepts to simplify the description of the phenomena involved - among them the efficiency factor to correct the reaction rate by limitations due to internal diffusion and external transfer, and the axial dispersion coefficient to correct the deviation of real hydrodynamics from plug flow (perfect fluid flow model). Using problems that first describe the catalyst grain and reactor scales separately, before coupling them together, these different concepts are introduced and their validity discussed by comparison with “exact” solutions solved using the COMSOL tool.

Program/Content

- Coupling between transport phenomena (internal/external) and reaction at the scale of a catalyst particle: “exact” 2D axial simulation and determination of limiting processes; comparison of the resulting global efficiency factor with simplified expressions from reaction engineering (1D particle diffusion-reaction model associated with the film model).

- Numerical tracing within a tubular reactor (vacuum) in laminar flow: introduction to axial dispersion and comparison of Taylor-Aris dispersion and segregated flow regimes; analysis of the Residence Time Distribution and determination of the equivalent axial dispersion coefficient; comparison of the predictions of the 1D piston-dispersion model with the “exact” solution (in the Taylor-Aris regime).

- Multi-scale coupling (catalyst grain / interstitial fluid) within a fixed-bed catalytic reactor.