

Numerical simulation of tubular reactor with chemical reactions using OpenFOAM

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Abstract

This case study demonstrates to learn how to solve with more complex equations. The aim of the present study is to simulate one-dimensional flow in a tubular reactor with heterogeneous catalysis on porous media with chemical reaction in a transient flow. 1D case model is made with blockMesh meshing tool. This study is performed using OpenFOAM-5.x. It's a purpose to describe the dealing of heterogeneous catalysis with chemical reaction and implementation of new solver (tubeChemFoam) with open-source CFD package OpenFOAM. The simulation results are obtained and analyze for the reactants and products.

Problem statement

1D tubular reactor with heterogeneous catalysis is on porous media with chemical reaction for transient state in laminar flow regime (Figure 1).

- Modify compilation file: dir/Make (files, options), *.C, *.H
gedit Make/files , if needed.
- Modify createFields file to create the species fields and to read the physical properties:
createFields.H
- Creating a 1D mesh by using blockMesh
- Set boundary/initial conditions (BC/IC)
- Set physical properties (transportProperties)
- Set numerical schemes, Set solver parameters, Set control parameters
- Solver - **tubeChemFoam**

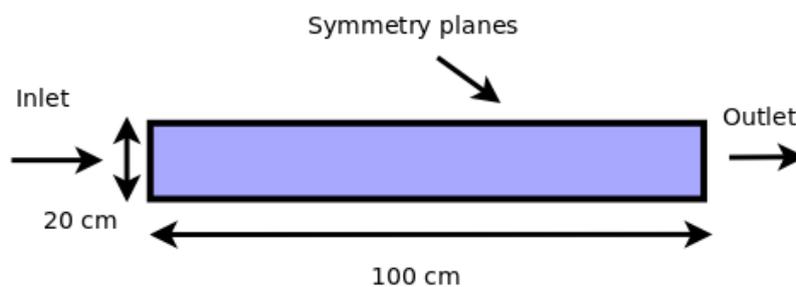


Figure 1: