Numerical simulation of tubular reactor with chemical reactions using OpenFOAM

Dr. Raj Kumar Saini

Ph.D, Indian Institute of Technology, Bombay (IIT Bombay)

M.Tech, Indian Institute of Technology, Madras (IIT Madras)

Email : raj.km.saini@gmail.com

December 11, 2019

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 state. 1D case model is made with blockMesh meshing tool. This study is performed using OpenFOAM-5x. It's a purpose to describe dealing heterogeneous catalysis with chemical reaction and implementation of new solver (tubeChemFoam) with open-source CFD package OpenFOAM. The simulation results are obtained and have been analyzed for the reactants and products.

Keywords: Chemical reaction, Tubular reactor, Laminar flow, Temperature, CFD, OpenFOAM

1 Introduction

The purpose of this case study is to explore and learn OpenFOAM software [1] to the new users and to understand the new solver creation using existing solver in OpenFOAM. It describes the implementation of new equations and solver. This case study demonstrates how to do the following:

- Set up a problem case;
- Creating a 1D mesh by using blockMesh utility;
- solve a unsteady state problem;
- Set up the transport properties;
- Consider the laminar model for laminar flow regime;
- Brief explanation of solver creation;
- To create the species fields and to read the physical properties (createFields.H);
- Modify a existing solver to add temperature equation (tubeChemFoam.C);
- Modify compilation file: dir/Make (files, options), *.C, *.H gedit Make/files.

2 Problem statement

1D tubular reactor with heterogeneous catalysis is on porous media with chemical reaction for transient state in laminar flow regime (Figure 1) [2, 3]. OpenFOAM solves one-dimensional (1D) symmetrical geometry in this case. This case explains setting up OpenFOAM case in the OpenFOAM repository. The Table 1 shows the geometrical parameters and fluid property for the present study.

Table 1: Details of geometry and flow conditions

Geometry details	
Parameters	Value
Length of the tubular reactor (L), cm	100
Width of the tubular reactor (W), cm	20
Depth of the tubular reactor (P), cm	20
Transport Properties	
Dynamic viscosity (μ), kg/m.s	1e-3
Permeability of porous media (κ), m^2	1e-9
Diffusivity (D) m^2/s	1e-6
Kinetic speed of the reaction (v), m^3/s.mol	0.2

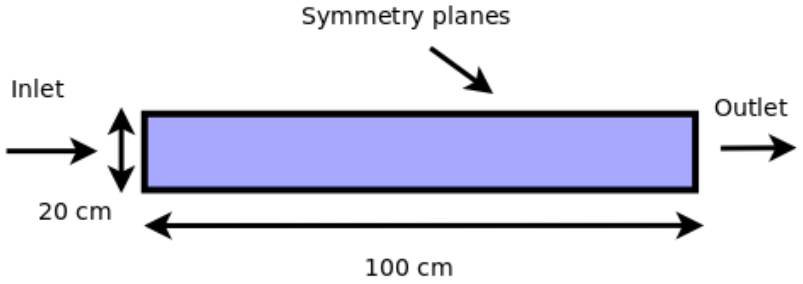


Figure 1: Tubular reactor

3 Mathematical modeling

The chemical reaction considers heterogeneous catalysis on porous media as shown in Equation 1.

$$A + B = C \tag{1}$$

where, A, B and C represent the reactants and products in mol/m^3 respectively.

The governing equations are solving for 1D tubular reactor with heterogeneous catalysis on porous media for the transient state in the laminar flow regime [4]. The solver is mainly solved the following equations (Equations 2-7):

$$\nabla \cdot \vec{U} = 0 \tag{2}$$

$$\vec{U} = -\frac{\kappa}{\mu}\nabla p \tag{3}$$

$$\nabla^2 p = 0 \tag{4}$$

$$\frac{dA}{dt} + \nabla \cdot (\vec{U}A) = D\nabla^2 A - |vAB| \tag{5}$$

$$\frac{dB}{dt} + \nabla \cdot (\vec{U}B) = D\nabla^2 B - vAB \tag{6}$$

$$\frac{dC}{dt} + \nabla \cdot (\vec{U}C) = D\nabla^2 C + vAB \tag{7}$$

where, μ represents dynamic viscosity (kg/m.s), κ permeability of porous media (m^2),D diffusivity (m^2/s), v kinetic speed of the reaction (m^3/s.mol), u velocity of feed (m/s) and p the pressure (Pa). A, B and C concentration of reactants (A=2 & B=1, mol/m^3) and product(C=0, mol/m^3) respectively.

3.1 Boundary conditions

Details of boundary name and corresponding boundary conditions are presented in Table 2.

Table 2: Boundary conditions

Boundary Name	Boundary condition
SymmetryPlanes	symmetry
Iutlet	Velocity
Outlet	Pressure

4 Simulation procedure

This case deals with two-dimensional laminar simulation of fully developed flow. First step in setting up of an OpenFoam case is to copy to present working directory. We need to set all require input parameters before starting the simulation. Mesh generation and implementation of boundary conditions are adopted from a base flange/cavity tutorials (OpenFOAM/(user name)-5.x/run/tutorials/basic/laplacianFoam). This study is considered with unsteady state and laminar flow case.

4.1 Creating geometry and mesh

- Geometry for the present problem is considered 1D dimensional domain. The geometry and mesh are generated by using the 'blockMeshDict' utility. The file is available in 'system' folder in user directory (∼/case/system/).
- Suitable modifications for geometry (length of tubular reactor) have been done in the 'blockMeshDict' file in order to generate geometry.
- Mesh can be generated by using the command 'blockMesh' in the terminal. Figure 2 shows the isometric view of the generated mesh.

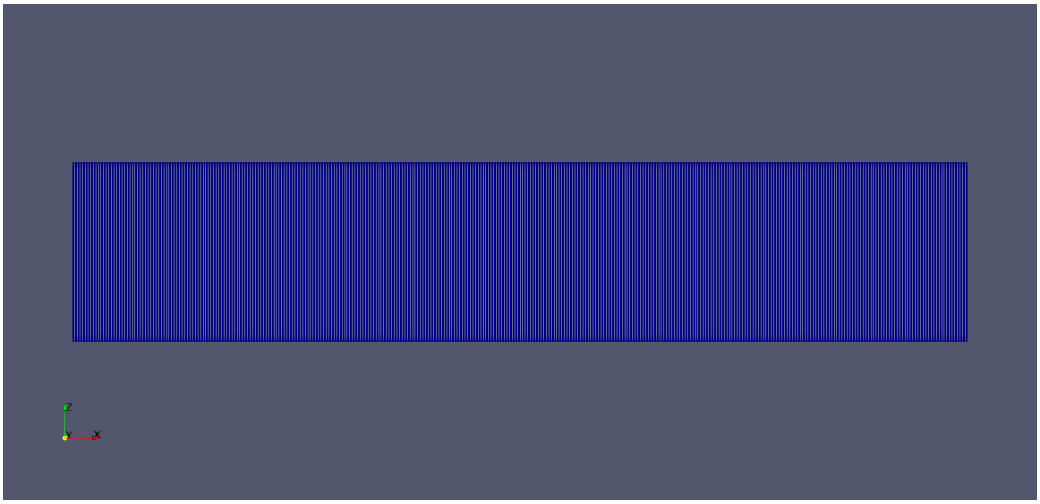


Figure 2: Computational Domain of tubular reactor (1D) with view of mesh after execute command 'blockMesh'

- All modifications for mesh with proper boundary condition with defining inlet and outlet is to be done as velocity patch and its neighbor patch (∼/case/constant/polyMesh/boundary).

4.2 Setting boundary conditions (BC)/Initial conditions (IC)

Files present in '0' folder (∼/case/ has been kept 'p', 'U', 'A', 'B' and 'C' files for laminar and transient flow. Boundaries are assigned and added three boundaries of present case in both the files, i.e. 'p', 'U', 'A', 'B' and 'C'. Details of the boundary conditions are listed in Table 3.

Table 3: Details of boundary conditions

Boundary	p	U	A	B	C
SymmetryPlanes	symmetry	symmetry	symmetry	symmetry	symmetry
Inlet	fixedValue (5e+4)	fixedValue (0.05 m/s)	fixedValue (2)	fixedValue (1)	fixedValue (0)
Outlet	fixedValue (0)	zeroGradient	zeroGradient	zeroGradient	zeroGradient

4.3 Solver details

Transient and laminar flow are considered in the present study. Laminar flow model can be applied in the OpenFoam by using 'simulationType' option in the 'turbulence Properties' file in constant folder. The 'simulationType' option can be used as 'laminar'. In order to run unsteady state simulations, controDict, fvSchemes and fvSolution files are kept in the case directory folder. '**./run**' command executes in terminal to run computations.

This case study also demonstrates to create a new solver using existing solver in OpenFoam. The steps are following:

4.3.1 Solver creation

- Execute 'run' directory: run
- Move to solver directory: cd solvers
- Copy laplacianFoam : cp -r $FOAM_APP/solvers/basic/laplacianFoam solvers/.
- Rename solver directory: mv solvers/laplacianFoam solvers/tubeChemFoam
- Go to the new solver directory: cd tubeChemFoam

4.3.2 Solver creation / modification

- Directory clean: wclean
- Rename solver : mv laplacianFoam.C tubeChemFoam.C
- Change compilation file: gedit Make/files

4.3.3 Solver modification / createFields.H

- Adding the temperature field and related physical properties: gedit createFields.H
- Changes in createFields.H and to create the new fields: gedit createFields.H
- Changes in createFields.H to reading the physical properties: gedit createFields.H
- Solver modification / tubeChemFoam.C
- Modified the solver and add temperature equation: gedit tubeChemFoam.C

4.3.4 Solver compilation

- Directory clean and compile: wclean & wmake
- Go to the cases directory: run

4.3.5 Compilation rules

- Create Make folder: mkdir Make
- Create rule files: gedit Make/files Make/options

4.4 Post-processing

The paraFoam is used to visualize the results. It can be used by typing the following command line in the terminal **paraFoam** to open the paraview software and upload the case.

5 Results and discussion

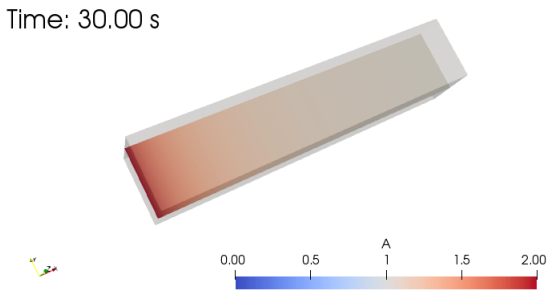
Simulations are performed using OpenFOAM in order to investigate the concentration of reactants and products with a chemical reacting system. Simulation results are analyzed with the help of paraFoam software. Figure 3 - 6 shows the comparison of the fields A, B, C (concentrations of reactant and product) at different velocity and a particular time. The reactant or product is determined by measuring concentrations at different times during the reaction. The concentrations (reactant and product) measure in moles/liter.

Figures 3 & 4 show the concentrations of reactants (A & B) for different inlet velocity of feed, 0.05, 0.10, 0.15 and 0.20 m/s at 30.0 s from starting the reaction. Similar results are shown for the product (C) in Figure 5.

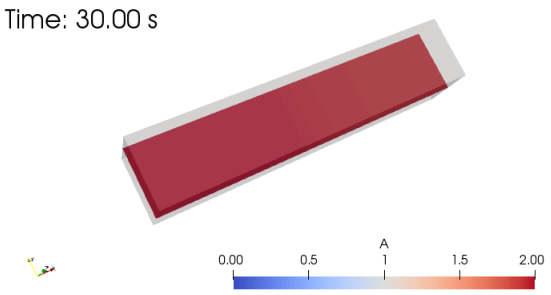
Figure 6 shows the comparison of simulated results of the concentration of reactants and products for different inlet velocity of feed, 0.05, 0.10, 0.15 and 0.20 m/s. The concentration profile of reactants and product change along with the length of the reactor. The concentration of reactant decreases when the concentration of product increases during more reactants molecule react to formed more product.

It can be seen from Figure 6 that the variation in concentration of reactant and product can not be observed when the stationary sate archived.

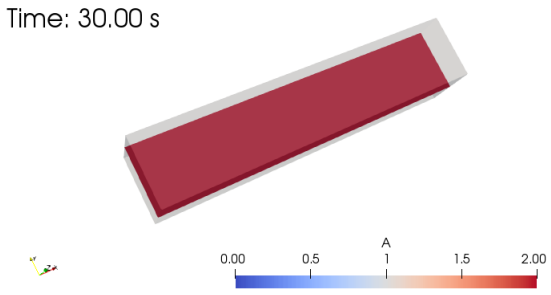
Results are plotted with the help of ‘gnuplot’ (∼/case/gnuplot/gnuplot.gp) and the commands used in plotting gnuplot is available in the file ‘gnuplot.gp’ available in the case directory.



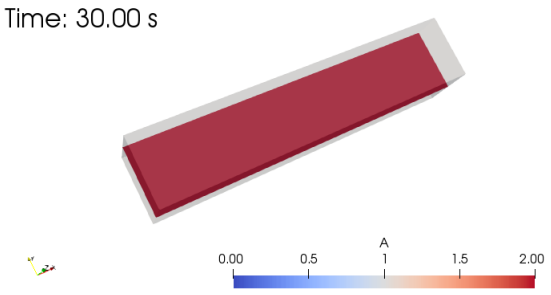
(a) v=0.05 m/s



(b) v=0.10 m/s

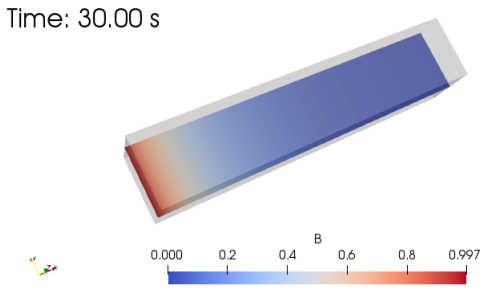


(c) v=0.15 m/s

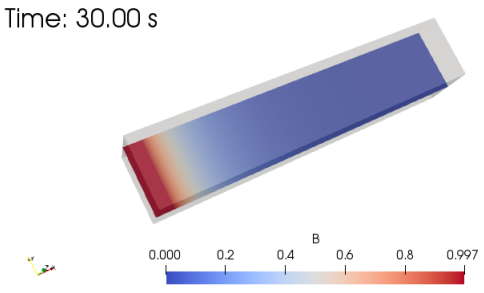


(d) v=0.20 m/s

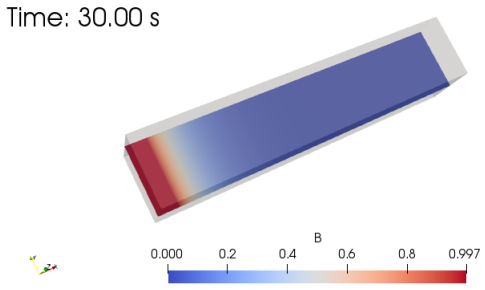
Figure 3: Field 'A', Concentration of A (mol/m^3) for different inlet velocity with length of reactor for different inlet velocity)



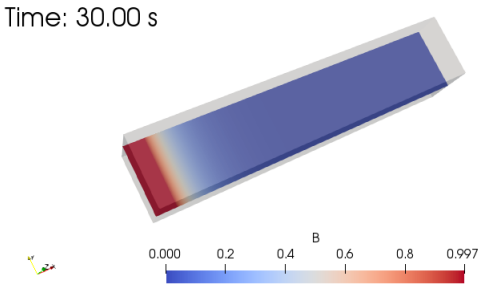
(a) v=0.05 m/s



(b) v=0.10 m/s

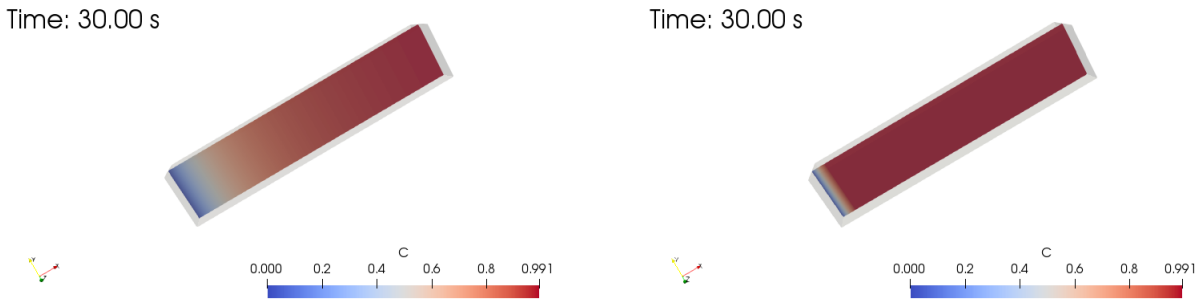


(c) v=0.15 m/s



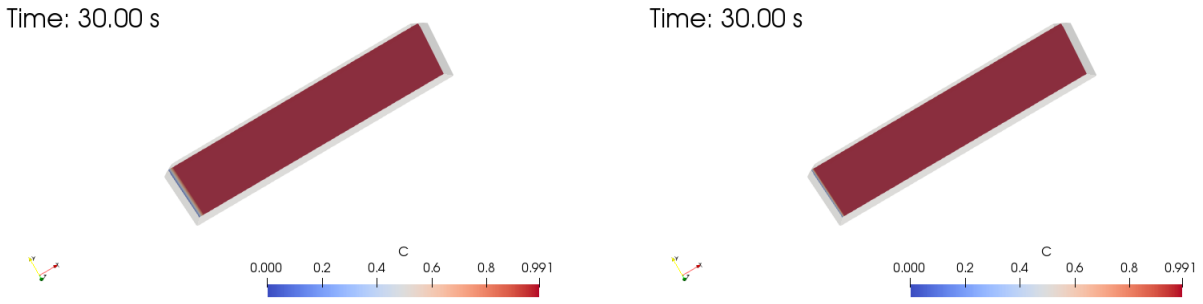
(d) v=0.20 m/s

Figure 4: Field 'B', Concentration of B (mol/m^3) for different inlet velocity with length of reactor for different inlet velocity.



(a) v=0.05 m/s

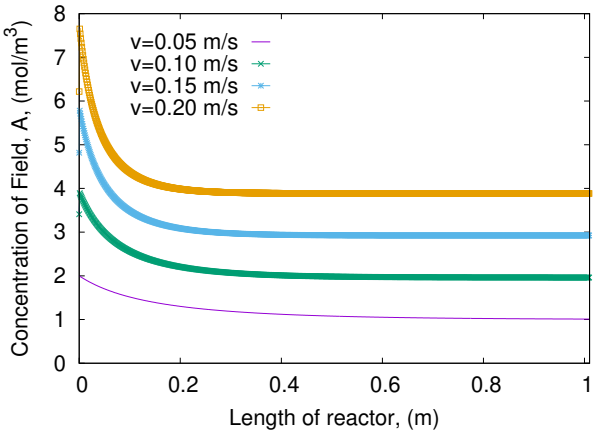
(b) v=0.10 m/s



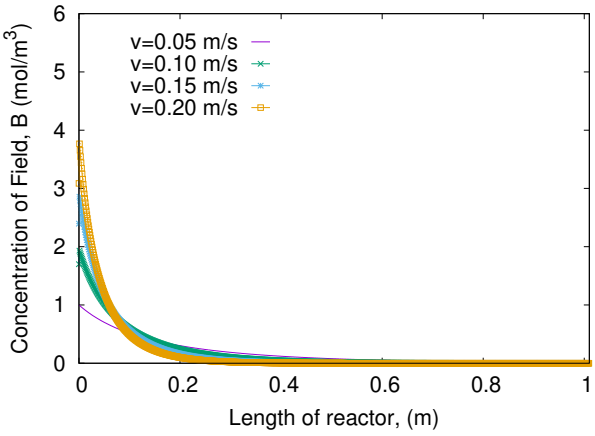
(c) v=0.15 m/s

(d) v=0.20 m/s

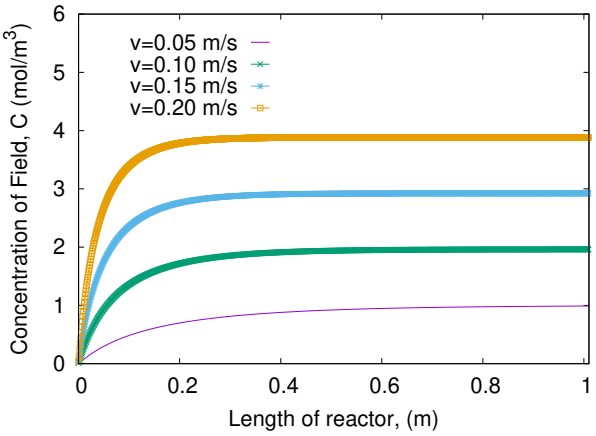
Figure 5: Field 'C', Concentration of C (mol/m^3) for different inlet velocity with length of reactor for different inlet velocity.



(a)



(b)



(c)

Figure 6: Field 'A', 'B' and C, Concentration of reactants and product (mol/m^3) varies with length of reactor for different inlet velocity.

References

[1] C. J. Greenshields, *OpenFOAM: The OpenFOAM Foundation. User Guide Version 5*. CFD Direct Limited, July. 2017.

[2] M. J. Nieves-Remacha, A. A. Kulkarni, and K. F. Jensen, "Openfoam computational fluid dynamic simulations of single-phase flows in an advanced-flow reactor," *Industrial & Engineering Chemistry Research*, vol. 54, no. 30, pp. 7543–7553, 2015.

[3] L. Yin, Y. Jia, X. Guo, D. Chen, and Z. Jin, "Flow behaviors and heat transfer characteristics of liquid film during the pyrolysis process of molten plastics using openfoam," *International Journal of Heat and Mass Transfer*, vol. 133, pp. 129 – 136, 2019.

[4] M. Mottaghi and S. Kuhn, "Numerical investigation of well-structured porous media in a milli-scale tubular reactor," *Chemical Engineering Science*, vol. 208, p. 115146, 2019.