Multi-scale modelling of a fixed bed catalytic reactor: development of a simplified 1D model enhanced with 3D CFD multiphysics simulations.

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Highlights

- A pseudo-periodic 3D comprehensive model of a fixed bed reactor is developed
- Heat transfer in catalytic reactors is impacted by an inlet effect
- A 1D model enhanced with results from a 3D model is developed

1. Introduction

Catalytic fixed bed reactors are widely used in the chemical and process industries. From an industrial and academic point of view, the modelling of fixed bed reactors is important for a better understanding of the coupling between the flow, the heat transfer and the reactions. The present study aims to propose an improved 1D comprehensive model of a monotube fixed bed reactor composed of spherical particles. The 1D model is solved with the software gProms Process, but it is enriched with the results of a 3D model developed with the software Comsol Multiphysics for a finer description. First, the coupling between the laminar flow and heat transfer in the fixed bed reactor is studied and compared with literature. Then the inlet effect and the heat exchange process are studied. Finally, a reaction in the fluid phase is added and a comparison is made between the 1D and the 3D models.

2. Methods

Reduced models and especially 1D models are interesting because they require less computation time and are easy to handle[1]. However, the correlations used in these models are based on the literature and do not necessarily describe the system to be modelled with sufficient accuracy. Therefore, 3D simulations of fixed bed reactors with CFD models coupling flow and heat transfer [2] and sometimes chemical reactions [3] are becoming increasingly useful. The aim of the present work is to develop a 3D model whose simulation results are used to enrich a 1D axial model.

- Geometrical domain

The ratio of the monotube internal diameter over the particle diameter is $\mathrm{N} = \mathrm{d_{cyl}}/\mathrm{d_p} = 5$. The total height of the studied tube is $\mathrm{H_{cyl}} = 54\mathrm{d_p}$. This height corresponds to 10 times the height of the geometric domain, but pseudo-periodic conditions are used in order to simulate the entire monotube. This method allows the simulation of larger geometries, such as industrial configurations, without any loss of quality in the meshing and simulation results[4].

- Multiphysics modeling: coupling laminar flow, heat transfer and chemical reaction

Uniform velocity and temperature ($T_0 = 200°C$) are set at the inlet. The wall temperature is kept constant ($T_w = 300°C$). First, the flow and heat transfer are studied, with heat transfer coming only from the wall side (in a two-way coupling manner, as the fluid properties are temperature dependent). Once this first step is validated, a simple oxidation reaction from species A to B is added: $A + \mathrm{O_2} \rightarrow B + \mathrm{H_2O}$. The boundary conditions are the same as before, but the wall temperature acts as a cooling system because the volumetric reaction is now exothermic. The reaction then affects the heat transfer and therefore also the flow in the reactor (in a three-way coupling).

3. Results and discussion

A preliminary study of mesh independence was carried out and a mesh size of 2.5 million elements for a 15 cm^3 fixed bed tube was selected for the 3D periodic model which contains 109 particles generated by DEM. Flow and heat transfer simulations were first conducted. Different values of the Reynolds number were studied, but only Re_{inlet}=138, corresponding to an inertial dominated flow, is presented here.

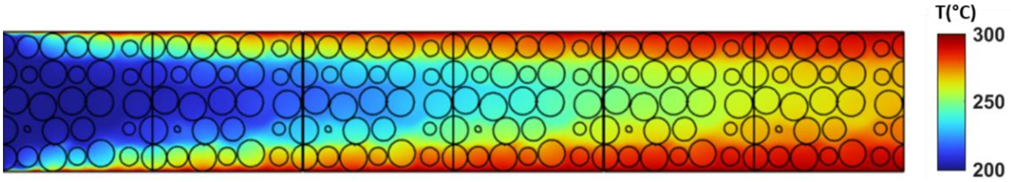

Figure 1. Temperature field at the mid-plane of the reactor for an inlet Reynolds number of 138

The evolution of the pressure drop in the reactor is in good agreement with the correlation of Ergun(1952)[5], so the latter is used in the 1D model to describe the flow. The temperature field from the 3D simulation is similar to previous 3D models in the literature[4][2]. Furthermore, global heat transfer correlations in the literature such as Leva's[6] are in accordance with our results. However, an axial heat transfer correlation that more accurately accounts for the inlet effect is proposed and implemented in the 1D model as shown in Figure 2(a):

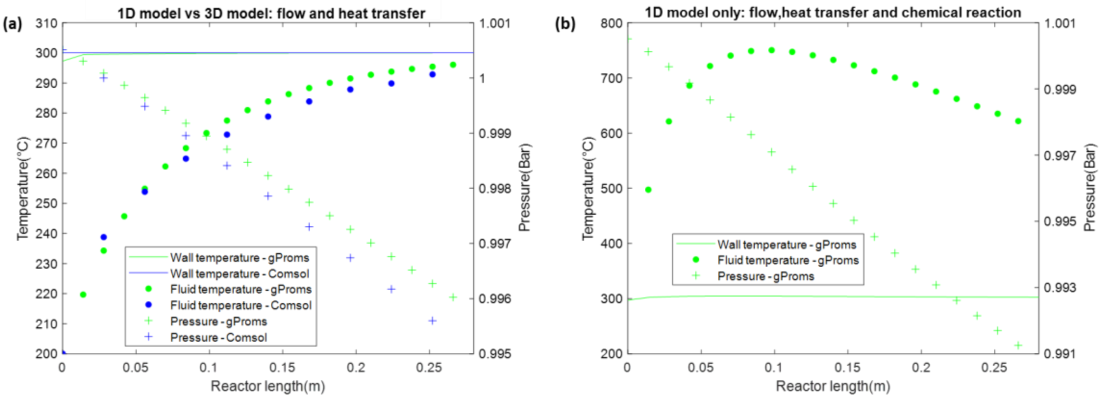

Figure 2. Comparison of average temperature and pressure from 1D and 3D model results:
(a) Coupling of flow and heat transfer, (b) coupling of flow, heat transfer and chemical reaction for 1D model

The pressure and temperature profiles from the simulations of the 1D and 3D models are in good agreement with each other. Figure 2 (b) shows the evolution of the axial temperature in the presence of a chemical reaction, with a significant increase in temperature due to the exothermicity of the reaction, followed by a progressive decrease due the cooling by the wall. 3D CFD Multiphysics simulations involving chemical reactions in a three-way coupling are still in progress for comparison with 1D results.

4. Conclusions

A first study was performed considering only the flow and heat transfer in the fixed bed and the results are in agreement with the literature. Simulation results of the 3D model highlight the inlet effect and led to the formulation of a heat transfer correlation, which was then implemented in the 1D model. Results from both models show excellent agreement between them, confirming that the proposed enriched 1D model is a simplified model of the 3D one, at least for flow and heat transfer. The comparison with the exothermic reaction, which drastically changes the results, will be investigated in the near future.

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Keywords

Reactive Fixed bed, CFD, Heat transfer, 1D modeling