Mathematical modeling of reverse flow reactors for fluid-solid systems

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Highlights

- Reverse flow reactor model was developed and implemented.
- Intraparticle diffusion limitations were included and revealed to be important.
- A sensitivity analysis showed a good predicting power of the model.
- The model was used to predict experimental data retrieved from literature

1. Introduction

The minimization of the energy supply to conduct chemical transformation is one of the fundamental ideologies of process intensification. For exothermic processes, packed bed reactors with periodic flow reversal might be an elegant solution to the problem [1]. Indeed, reverse flow reactors enable to store the heat produced by chemical reactions, which can be employed to heat up the cold feed to the reactor system [2]. Autothermal operation is achieved by carefully calibrating the switching cycle duration and feed temperature, which can be kept much lower than in conventional packed beds. The performance of reverse flow technologies is influenced by the operating conditions, therefore reliable mathematical models to predict the transient and pseudo-steady state behavior of reverse flow reactors are necessary. In the present work, a comprehensive model for reverse flow reactors was developed and implemented. Axial dispersion effects were considered for both the mass and the energy balances to describe non-ideality of the flow pattern of the fluid phase and intraparticle diffusion effects were included. The influence of the main operating parameters was checked via numerical simulations in the parameter space. Finally, the model was tested in predicting the results of van De Beld and Westerterp [3], where a reverse flow reactor was used for air purification purposes.

2. Methods

The reverse flow reactor model was written considering the general mass and energy balance equations valid for packed bed reactors. Both the fluid bulk and the catalytic bed phases were modelled taking into consideration the major non-idealities i.e., axial dispersion in the fluid phase, fluid-solid external heat and mass transfer resistance and intraparticle heat and mass diffusion. The major challenge of the model is the accurate simulation of the reverse flow operation, implying that both boundary conditions and the direction of the flow must be changed periodically. Therefore, the periodical sinusoidal function written as Eq.1 was employed.

$$\alpha = \sum_{n} \frac{4}{\pi(2n+1)} \sin\left(\frac{(2n+1)(\theta)\pi}{p}\right) \tag{1}$$

Equation (1) was multiplied to the convective flux term to simulate the alternation of the fluid flow direction. Moreover, it was used to switch periodically the inlet and outlet positions [4]. A system of partial differential equations appeared in the definition of the system. The computations were conducted using the gPROMS Model Builder v.4 software, using the built-in functions. In particular, the partial differential equations system represented by the mass and energy balance equations of the reactor model, were solved simultaneously using the fully implicit 4th order Runge-Kutta method. The built-in numerical method of lines was employed to discretize both the axial coordinate (50 grid points) of the packed bed reactor and the radial coordinate (20 grid points) of the catalyst pellet.

3. Results and discussion

The performance of reverse flow were compared to classical packed bed reactors operations. It was revealed that the temperature rise is much higher in the case of reverse-flow reactors as the reaction heat is stored in the catalyst bed. As a consequence, the reaction rates are promoted and higher productivities to the desired product can be achieved. Figure 1 displays the key feature of reverse flow reactors; forced non-stationarity eventually results in two, symmetric and oscillating states of the catalyst bed.

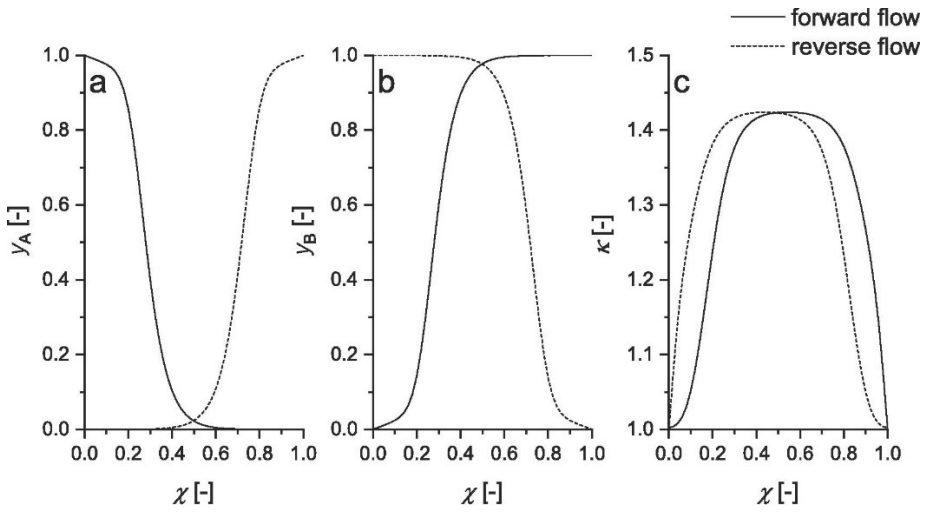

Figure 1. Dimensionless concentration of components a) A, b) B, and c) temperature vs the dimensionless axial coordinate.

For a reversible and exothermic reaction, reverse-flow reactors enable to obtain the optimal temperature profile along the catalyst bed without using several packed beds with intermediate cooling. Mathematical modeling revealed that the optimal productivity can be achieved by carefully calibrating the switching time, which directly affects the temperature profile in the catalyst bed. To further validate the model, the prediction of experimental data retrieved from literature was carried out. The simulation results were in excellent agreement with the experimental data.

4. Conclusions

A complete reverse flow reactor model has been proposed and implemented. The model resulted to be very flexible and efficient in predicting various chemical systems: the effect of several reaction parameters on the transient and pseudo-steady state behavior of the reverse flow reactor was deeply investigated and discussed. The present model was used simulate a real system taken from the literature, ethylene decomposition, demonstrating a good predictive power. In perspective, the model will be applied to optimize the operating conditions of reverse flow operations.

References

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Keywords

Reverse flow reactor; Modeling; Kinetics; Mass and heat transfer