Integrated multiscale modeling of fixed bed reactors: Studying the reactor under dynamic reaction conditions

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Highlights

- Transient CFD method is implemented into resolved-particle CFD fixed bed simulation.
- Temperature evolution throughout the bed shows lag of particles behind flow.
- A heat wave along the bed shows an increased temperature compared to steady state.

1. Introduction

Chemical reactors are fundamentally multiscale systems. The reaction happens on the catalyst active sites and is a strong function of the particle temperature and species partial pressures which are influenced by the transport and flow patterns in the reactor. Therefore, multiscale resolved particle modeling of fixed bed reactors is essential for improved understanding, design and scale-up. These are the key factors in the American Chemistry Council technology road map[1]. Recently, considerable attention has been drawn to CFD integrated simulation of fixed beds coupled with detailed microkinetics. These studies are mostly focused on reactors operating under steady-state conditions. However, the dynamic behavior of the reactor under the transient conditions such as wrong way behavior and catalyst deactivation are well known issues that also need to be addressed. Furthermore, moving towards renewable sources of energy and raw materials, design and operation of the reactors under dynamic reaction conditions are inevitable.[2] Here, we introduce an approach to extend our previously-developed solid particle CFD method for heterogeneous catalysis[3] to transient simulation of the fixed beds and look into the issues of wrong way behavior and moving hot spot.

2. Methods

The CFD model couples the reaction with transport phenomena in both the solid and fluid phases. The complex reaction mechanisms are initially solved under a wide range of reaction conditions and mapped into multivariate splines. Thus, generic microkinetics libraries for various partial oxidation reactions are constructed. These libraries are integrated into the CFD code to evaluate the reaction rates and surface species coverages during the simulations. Since the surface species concentration reaches steady state much faster than the temperature and partial pressures, it is a common practice to assume they are at steady state even in transient reactor simulations.[4,5] This justifies the use of the generic libraries that are computed by integrating the system of ordinary differential equations of the kinetics mechanisms until it reaches steady state.

The time step (Δt) is evaluated by $\frac{x}{v}$ where x is the smallest mesh size and v is the velocity. The time scale is reduced by factors of 0.25 and 0.5 for the first few iterations to establish the flow simulations. The developed approach is tested for ethylene oxidation on silver catalyst for an illustrative geometry of 25 spherical particles in a cylindrical container. At time zero the reactor temperature is 478 K.

3. Results and discussion

Figure 1. depicts the temperature profile evolution. Inlet and wall temperature are 490 K. At t = 6 s, the particle surface temperatures reach 480 K and the reaction is observable.

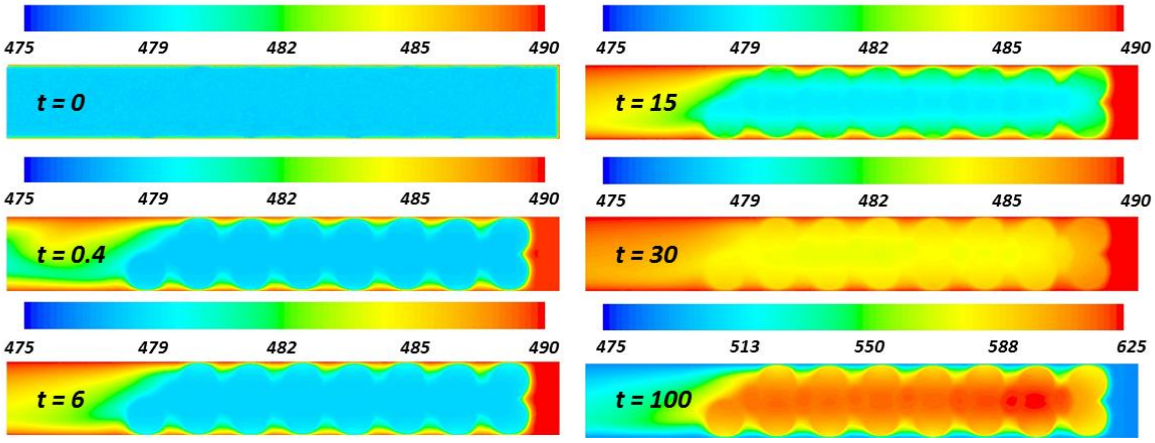

Figure 1. Temperature (K) profile evolution during the first 100 seconds of the simulation. Flow is right to left.

However, even at t = 15, not all sections of the reactor are at the reaction temperature. At t = 30, the reaction is proceeding significantly throughout the catalytic bed and the temperature starts to increase rapidly while the first layer of the catalyst particles is the hottest spot in the reactor. At t = 100, the temperature has raised to 625 K, and the hot spot is moving downstream. The species profiles follow the same pattern as the temperature. At each time step the lowest reactants concentration is at the same spatial location as the highest temperature. For such exothermic reactions under transient conditions the temperature can locally rise to a much higher degree than for steady state. This could lead to an early deactivation of a specific part of the catalytic bed. At t = 100, with a decrease in inlet temperature the hot spot temperature would increase which is clear evidence of wrong way behavior in the reactor.

4. Conclusions

The developed multi-scale approach for transient simulation of the fixed bed enables us to successfully follow the evolution of the temperature and species patterns through the reactor under dynamic conditions. This important feature helps us to understand the loss of selectivity and activity during the transient operating time. Furthermore, the effects of a change in the inlet parameters on the reactors with different configurations under transient conditions will be discussed.

References

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Keywords
Resolved particle; CFD; Transient; Multi-scale.