THE EFFECT OF RADIATION IN PARTICLE-RESOLVED CFD SIMULATIONS OF FIXED-BED REACTORS

Gregor D. Wehinger
Chemical and Electrochemical Process Engineering
Clausthal University of Technology
Leibnizstr. 17, 38678 Clausthal-Zellerfeld, Germany

Abstract

Many fixed-bed reactors operate at medium to high temperature conditions, where radiation can play an important role in radial heat transfer. The most detailed reactor model are particle-resolved CFD simulations. Most studies have neglected radiation. In this study, the contribution of radiative heat transfer is investigated in a randomly packed bed of 7-hole cylinders. Industrially relevant temperatures and gas-phase mixtures were chosen and tested with two different radiation models. At high temperatures, neglecting radiation can result in temperature differences of up to 40 K. The main driver of radiative heat transfer is surface-to-surface radiation. Whereas the participating media model can be neglected under the investigated conditions.

Keywords

Radiation, CFD simulation, fixed-bed reactor.

Introduction

Fixed-bed reactors (FBR) are widely used in the chemical and process industry. Radial transport of energy plays a paramount role in FBR operation, since this is the direction of cooling (for exothermic reactions) or heating (for endothermic reactions) (Dixon, 2012). Many catalytic reactions occurring in FBRs take place at temperatures > 500 °C. In steam methane reforming, the outer tube wall-temperature can be as high as 1,000 °C (Aasberg-Petersen et al. 2011). The maximum local surface heat-flux $\dot{q}$ at which radiation can be emitted from a surface of a real body is given by the Stefan-Boltzmann equation:

$$\dot{q} = \varepsilon \sigma T_s^4 \qquad (1)$$

Where ε is the emissivity value. Therefore, we can expect an increasing contribution of radiation towards the total heat transfer with increasing temperature. For many catalytic gas-phase reactions in FBRs, the contribution of radiation can become important and its negligence could then lead to conservative temperature predictions or in the case of reacting systems to erroneous estimates.

The most detailed modeling approach for FBRs are particle-resolved CFD simulations, see Jurtz et al. (2018). With this approach, every pellet of the bed is resolved geometrically and the transport phenomena can be modeled with first-principles. Most of the particle-resolved CFD studies have neglected thermal radiation, since lateral mixing was considered to be predominant over radiative heat transfer (Behnam et al. 2012). However, fundamental studies of the effect of radiative heat transfer in FBRs are missing in the current literature.

In this study, the influence of the surface-to-surface and the participating media radiation model is investigated in terms of particle-resolved CFD simulations of FBRs. A bed of randomly packed 7-hole cylinders is considered. Three different temperature levels and the effect of varying surface emissivity values are investigated. The aim of this study is to get aware of radiative heat transfer in modeling FBRs with particle-resolved CFD simulations.

Methods

The randomly packed bed of 7-hole pellets is generated synthetically with a DEM simulation integrated into a workflow presented earlier by Wehinger et al. (2015). The mesh consists of 23 million cells, whereas 9.4 million are for the solid pellet region. Conjugated heat transfer is applied at the conformal interface between solid and gaseous region, see Figure 1.

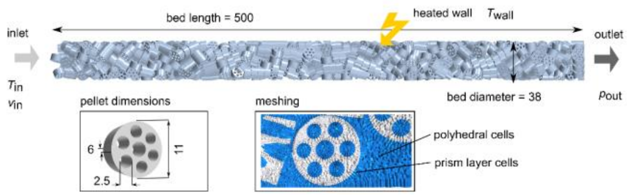

Figure 1. Numerical setup and dimensions.

Two different radiation models are applied. Surface-to-surface (S2S) radiation accounts for thermal radiation exchange only between diffuse surfaces forming a closed set, which is realized with ray-tracing in STAR-CCM+. The Discrete Ordinate Model (DOM) accounts for participating media radiation, which also includes radiative surfaces. Since gas-phase absorption coefficients depend generally on pressure, temperature, and mixture composition, polynomial fits according to Barlow et al. (2001) were implemented in the CFD simulations. Three different temperature levels were investigated, i.e. 400, 600, 800 °C wall temperature with a 150 K lower inlet temperature. The Reynolds number was fixed at 500 and a mass fraction mixture composition of $CH_4/H_2/CO/CO_2/H_2O$: 19.7/0.05/0.07/17.53/62.69 % was chosen to represent a steam reforming-like scenario. However, heat transfer only was applied. All simulations were carried out with Simcenter STAR-CCM+ version 13.04.010 from Siemens PLM software.

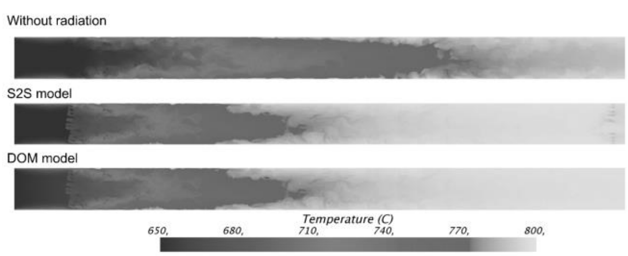

Figure 2. Temperature distribution.

Results and discussion

Figure 2 visualizes the temperature distribution on a plane cut through the bed. It becomes apparent, that the inclusion of a radiation model (S2S or DOM) leads to a significant increase in transferred heat from the wall to the pellets and gas phase, respectively. However, the difference between the DOM and the S2S model is insignificant at these conditions. A quantitative comparison between the different radiation models gives Figure 3 (A). The qualitative findings can be confirmed. At similar axial positions, the temperature with radiation included can be as much as 40 K higher than without modeling radiation. This effect increases/decreases with increasing/decreasing temperature level, respectively. The influence of the surface emissivity value can be as large as 20 K between $\varepsilon = 0.15$ and $\varepsilon = 0.85$, see Figure 3 (B).

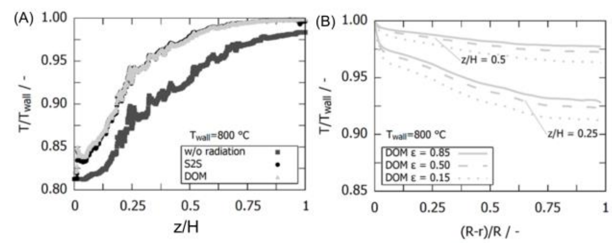

Figure 3. (A) Axial temperature profiles. (B) Radial temperature profile with influence of surface-emissivity values

Conclusion

S2S and DOM radiation were included in particle-resolved CFD simulations. At the present temperature level and mixture composition, the contribution of radiative heat transfer is high. The main contributor is S2S radiation on which the surface emissivity value has a strong influence. The effect of participating media is rather low which shows also much larger computational times. In the future, we will look at different pellet shapes and will include surface reactions to study the effect of radiation on reactive FBRs.

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