Determination of effective parameters for pseudo homogeneous packed bed reactor modelling using particle resolved CFD simulations

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Highlights

- CFD Simulation of heat and mass transfer in packed beds used to determine effective parameters of heat transfer and conductivity for pseudo homogeneous modelling.
- Multiple methods for determining effective parameters from CFD implemented.
- Methods rated in respect to replicating temperature profile from CFD.

1. Introduction

Chemical processes often rely on heterogeneous reactions using catalysts. Especially, for highly endothermal and exothermal processes slender packed bed reactors consisting of catalytic pellets are used. For simulations of these industrial reactors usually pseudo-homogeneous models are employed, which do not resolve the pellets but their effect on flow, heat and mass transfer are modeled by employing effective parameters. The pseudo homogeneous model approach [1] is described by

$$G \cdot c_p \cdot \frac{\partial T}{\partial z} = \lambda_R \cdot \frac{1}{r} \cdot \frac{\partial}{\partial r}\left(r \frac{\partial T}{\partial r}\right), \qquad \text{eqn. (1)}$$

neglecting axial conductivity. In order to create the required effective parameters α_{Wall} and λ_{Radial}, particle resolved modelling using computational fluid dynamics (CFD) together with discrete element methods (DEM) is be used.

2. Methods

Using DEM simulations, a packed bed of spheres is created, as shown in figure 1. After meshing and setup of required submodels like e.g. wall contact model, a CFD simulation to model heat transfer in the packed bed is done. Based on the CFD model, several methods to extract effective parameters for wall heat transfer and effective conductivity were investigated.

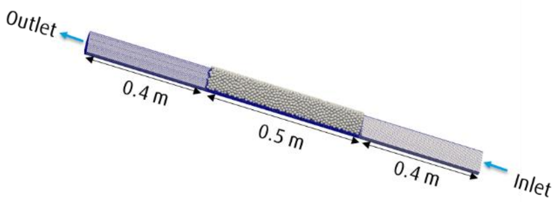

Figure 1: CFD domain for a packed bed of spheres

The methods investigated were an optimization of parameters of a pseudo homogenous model, direct readout of wall heat fluxes and temperature differences from CFD and two methods which rely on the analytic solution to the partial differential equation [1]:

$$\frac{T_{\text{Wall}} - T}{T_{\text{Wall}} - T_0} = 2 \sum_{n=1}^{\infty} \frac{J_0\left(\frac{a_n r}{r_{\max}}\right) \cdot \exp\left(-a_n^2 \cdot y\right)}{a_n \cdot \left[1 + \left(\frac{a_n}{B}\right)\right] \cdot J_1(a_n)} \qquad y = \lambda_{\text{Radial}} \cdot \frac{z}{G \cdot c_p \cdot r_{\max}^2} \qquad B = \frac{\alpha_{\text{Wall}} \cdot r_{\max}}{\lambda_{\text{Radial}}} \qquad \text{eqn. (2)}$$

According to Wakao and Kaguei [1] the methods for optimization and evaluation of equation 2 were implemented. Additionally, the CFD model allows to directly read the effective parameters as wall fluxed and temperatures as all positions are known:

$$\alpha_{\text{Wall}} = \frac{q_{\text{Wall}}}{(T_{\text{Wall,fluid}} - T_{\text{Wall}})} \qquad \text{eqn. (3)}$$

$$\lambda_{\text{Radial}} = \frac{q_{\text{Wall}} \cdot (R_{1,\text{fluid}} - R_{\text{Wall}})}{(T_{1,\text{fluid}} - T_{\text{Wall,fluid}})} \qquad \text{eqn. (4)}$$

with values having index 1 are located slightly away from the wall. The effective parameter determined form all methods were then used to calculate temperature profiles using the pseudo homogeneous model and temperature values from the CFD model were compared against. An average error according to

$$\epsilon = \left\{\frac{1}{N} \cdot \sum_{n=1}^{N} \left[\frac{(T_{\text{CFD}} - T_{\text{calc}})_n}{T_W - T_0}\right]^2\right\}^{0.5} \quad \text{eqn. (5)}$$

was defined to rate the agreement of the two models and hence, rate the different methods to determine effective parameters.

3. Results and discussion

The resulting errors for the different evaluation methods were displayed in table 1.

Table 1: Mean temperature error of pseudo homogeneous model to particle resolved CFD model for different methods to determine effective parameters

Method	$\alpha_{\text{Wall}} \left[\frac{W}{m^2 \cdot K}\right]$	$\lambda_{\text{Radial}} \left[\frac{W}{m \cdot K}\right]$	$\epsilon[K]$
Optimization	48.5	1.38	1.1
Center T Linearization [a1 over mixed mean T]	47.5	1.20	2.1
Center T Linearization [a1 Intercept]	38.3	2.52	4.0
CFD Heat Flux Evaluation	47.5	2.29	3.2

It is found that the numeric optimization of the pseudo homogeneous model by varying α_W and λ_R results in the best agreement with the particle resolved CFD model. This agrees with literature [1]. The direct readout of α_{Wall} and λ_{Radial} as a new method to evaluate the CFD is possible but provides results with worse agreement than the optimization.

4. Conclusions

Multiple methods to derive effective parameters for pseudo homogeneous packed bed models based on CFD/DEM simulations are created. It is found that optimization-based approach gives the least difference from CFD temperature profile to temperature profile of pseudo homogeneous model, hence, it should be used.

References

[1] N. Wakao and S. Kaguei, Heat and mass transfer in packed beds, Gordon and Breach, 1982

Keywords
Packed bed reactors, Heat transfer, CFD