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Multiscale modelling of packed bed chemical looping reforming

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Abstract

A comparison of reactive flows on two distinct scales is presented here (i) Particle resolved direct numerical simulation (PR-DNS), and (ii) 1D packed bed model. The PR-DNS geometry is meshed with polyhedral elements both inside and outside the particle to directly resolve the phenomena of intra particle diffusion and external heat and mass transfer. In contrast, the 1D packed bed model incorporates appropriate closure models to compare against the PR-DNS solutions at a computational cost several magnitudes less. Simulations are performed for endothermic steam methane reforming reactions (SMR) over a range of inlet temperatures. The comparison of the results between the two approaches shows that the 1D model can adequately replicate the PR-DNS results with appropriate modifications to the closures. The resulting verified 1D model was then used to simulate the reforming stage of an industrial scale packed bed chemical looping reforming reactor.

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Keywords: CFD-DEM; Direct Numerical Simulation (DNS); heat transfer; multiscale; packed bed; reaction rate; steam methane reforming

1. Introduction

Packed bed reactors are extremely relevant to the chemical and process industry, with wide variety of uses in adsorption, heat exchangers, chemical reforming, etc. With the development in the field of computational resources, it is now possible to obtain resolved 3D CFD simulations of flow around arrays of packed particles.

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PR-DNS can provide insight into the local phenomena of velocities and void fractions in the packed beds, which cannot be obtained from experiments. There have been several attempts to model the intra particle diffusion, but most of studies used the particles as the porous regions [1]. The detailed review of several works done for intra particle diffusion is given by Dixon [2]. Dixon [2] presented the most recent work with 3D CFD simulations for heterogeneous catalytic reactions in a tube packed bed ($3 \leq N \leq 10$), having reactions inside the catalytic particle and not just confined to the exterior surface for steam methane reforming (SMR) endothermic reaction.

The objective of the current work is to evaluate the prediction of endothermic steam methane reforming (SMR) on two distinct scale. Firstly, PR-DNS is used on a geometry of ~100 densely packed mono-disperse spherical particles ($\varepsilon = 0.355$) extracted in a way shown in our previous works [3, 4]. Secondly, computationally affordable 1D packed bed model which is based on appropriate models for effectiveness factor [5] and external heat and mass transfer [6]. The comparison between both the approaches for specie concentration and temperature differences are documented and the verified 1D model is used to an industrial-scale simulation of reforming in a packed bed chemical looping reforming (PBCLR) reactor.

Nomenclature

Greek Symbols		Nu	Nusselt number ($h\ d_p/k_g$)
α	Volume fraction	P	Pressure [Pa]
ε	Void fraction	Pr	Prandtl number ($\mu\ C_p/k_g$)
ϕ	Thiele modulus (Th)	R	Gas constant [8.314 J/mol/K]
η	Effectiveness factor	r	Radius [m]
ρ	Density (kg/m^3)	Re	Reynolds number ($\rho\ u_s\ d_p/\mu$)
Latin Symbols		Sc	Schmidt number ($\mu/\rho\ D$)
a	Characteristic length of spherical particle ($r_p/3$)	T	Temperature [K]
C_p	Specific heat capacity of gas [J/kg·K]	u_s	Superficial velocity of the gas [m/s]
E_a	Activation energy [J/mol]	*Sub/superscripts*	
h_e	effective heat transfer coefficient [W/m^2·K]	g	Gas
k_0	Arrhenius constant [1/s]	p	Particle
kg	Thermal conductivity of gas [W/m·K]		

2. Methodology

2.1. PR-DNS simulation setup

The realistically packed bed of monodisperse spherical particles ($\varepsilon = 0.355$) is generated using discrete element method (DEM) in *ANSYS FLUENT* as explained in detail in our previous works [3, 4].

The SMR reaction takes place inside the porous particles (grain model [7]) according to Eq. (1)-(3). The simulation parameters used are given in Table 1. The reactions were modeled using the kinetic model of Langmuir-Hinshelwood methodology proposed by Xu and Fremont [8] with appropriate kinetic and equilibrium constants from [9].

$$CH_4 + H_2O \leftrightarrow CO + 3H_2 \quad Rx1 \tag{1}$$

$$CO + H_2O \leftrightarrow CO_2 + H_2 \quad Rx2 \tag{2}$$

$$CH_4 + 2H_2O \leftrightarrow CO_2 + 4H_2 \quad Rx3 \tag{3}$$

Simulations are completed for three different values for inlet temperature (Table 1). The molecular diffusivity and gas thermal conductivity are obtained according to the kinetic theory of gases.