A Novel Computational Approach in Modelling Tubular Fixed Bed Reactors: Aspects of Hydrodynamics and Heat Transfer

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Highlights

- In narrow tubular fixed bed reactors, lateral heterogeneities emerge due to topological constraints imposed by the confining wall.
- A novel approach based on Rigid Body Dynamics (RBD) is adopted to synthesize realistic random packing structures of spherical and cylindrical pellets with $3 < d_t/d_p < 8$.
- CFD simulations of hydrodynamics and heat transfer were performed and validated using literature data.
- The CFD results demonstrate a remarkable influence of local flow maldistribution on the temperature field across the entire radius of narrow beds.

1. Introduction

Fixed bed arrangements find wide applications, particularly in reaction engineering where they are employed as tubular catalytic reactors for the transformation of reactants into desired products. The design of such systems is predominantly rooted in pseudo-homogeneous models with effective parameters extracted from averaged semi-empirical correlations. This prevailing design procedure is inadequate for tubular fixed beds of low to moderate tube-to-particle ratios, say $d_t/d_p \leq 8$, where the role of bed hydrodynamics in propagation of transport scalars is considerable [1,2]. This has persuaded researchers to seek for reliable design procedures, taking into account details of hydrodynamics, as well as the behavior of transport scalars at the pellet scale, in such narrow tubular fixed beds [3,4]. However, the majority of researchers have concentrated on rather simple packing arrangements of spherical pellets, based on inhouse codes, e.g. [5], or even commercial packages such as PFC^{3D} which is a commercial Discrete Element Method (DEM) package, coupling them with supplementary simulation tools such as Computational Fluid Dynamics (CFD) or Lattice Boltzmann (LB). Hence very few works have been devoted to packing of non-spherical pellets and the problem of heat transfer in such packings, e.g. [6]. This stems essentially from the intrinsic complexities connected to packing simulations of non-spherical catalyst pellets and very high computational expenses imposed in heat transfer studies as it is required to create a mesh inside the catalyst objects as well.

The main emphasis of this contribution is centered on the behavior of flow hydrodynamics and lateral heat transfer at the pellet scale for random packing structures of spheres and equilateral solid cylinders.

2. Methods

A novel approach based on Rigid Body Dynamics (RBD) is adopted to generate realistic random packing structures. RBD is an analytical hard-body scheme, capable of simulating the dynamic behaviour of assemblies of objects based on Newton's laws of motion and Lagrangian mechanics. In this work, an inhouse code was developed to generate random packings of spheres and equilateral solid cylinders with $3 < d_t/d_{pv} < 8$. CFD simulations of the flow field and heat transfer were then performed for some of the packing models in laminar, transitional and turbulent flow regimes, for $5 \leq Re_p \leq 3{,}000$, in which the problem of wall-to-bed heat transfer, viz. the wall-heated fixed bed problem, is resolved. The flow is assumed to be compressible and non-isothermal with physical properties of air, and the catalyst pellets are considered as alumina and glass with thermal conductivities of 40 and 1.01 W/mK, repectively. The commercial CFD code adopted here is ANSYS FLUENT V.14.5 in which the governing equations, including the equations of conservation

of total mass (continuity), momentum and energy, in conjunction with auxillary models such as realisable k-ε model coupled with Enhanced Wall Function to cater for turbulent flow regime, are resolved based on a finite volume discretization approach.

3. Results and discussion

The results of the random packing simulations demonstrate the fidelity and robustness of the proposed RBD-code in reproducing the amplitude as well as frequency of the declining oscillation pattern inherent in the radial void fraction distribution (see Figure 1). Furthermore, the CFD simulations results reveal a tremendous influence of local flow maldistribution on the wall-to-bed heat transfer, evidencing the fact that the spatial heterogeneities, inherent in such narrow packing structures, lead to presence of wall efects accross the entirety of the bed cross-section, thereby leading to dominance of localised phenomena in such narrow tubular beds.

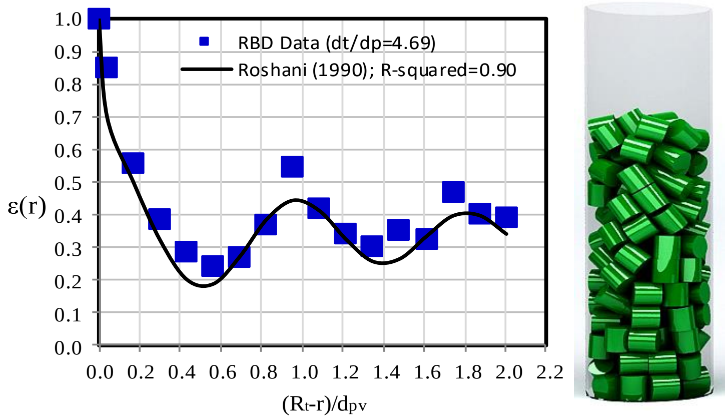

Figure 1. Radial void fraction distribution for the cylindrical packing with $d_t/d_{pv} = 4.1$.

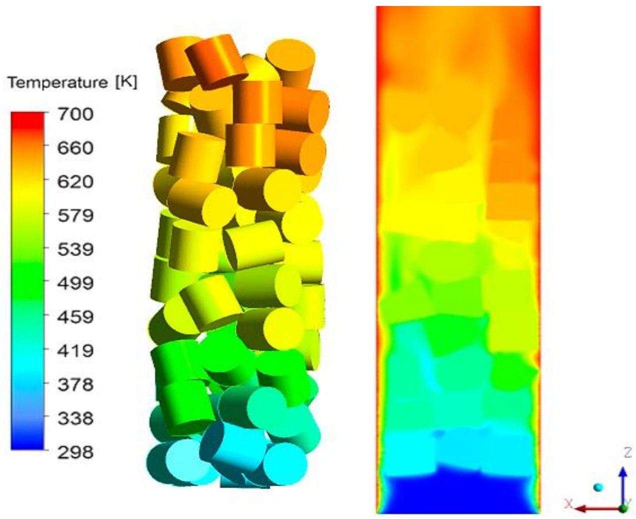

Figure 2. Typical temperature field on the particles and in the central plane, $Re_p = 100$, $d_t/d_p = 3.55$.

4. Conclusions

The results of comparison study for global and local bed properties demonstrates the merits of the proposed code in replicating topological properties of realistic packing structures. Furthermore, it is demonstrated that the coupled RBD-CFD approach for the simulation of random packing structures, mimicking hydrodynamics and transport properties in industrially relevant situations, offers many advantages as compared to conventional design methodologies. This contribution, with the aid of validated data, discusses the merits of our novel approach in improving fixed bed reactor design.

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Keywords

Tubular Fixed Bed Reactors, CFD Simulations, Hydrodynamics, Heat Transfer, Cylindrical Packing Structure