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Direct numerical simulation for flow and heat transfer through random open-cell solid foams: Development of an IBM based CFD model

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ABSTRACT

In the present contribution a sharp interface Immersed Boundary Method (IBM) for flow and heat transfer has been developed to fully resolve highly complex random solid structure on a non-body fitted Cartesian computational grid. A 3D image data set from a Micro-CT (computed tomography) scan of an actual foam geometry is usually converted into a surface mesh of unstructured triangular elements and the current frame work can embed it as an immersed boundary in the CFD domain. A second-order implicit (semi-implicit) method is used to incorporate fluid-solid coupling for flow (heat transfer) at the non-conforming immersed boundary in a structured grid. Both temperature Dirichlet and Neumann boundary conditions, as well as a conjugate heat transfer condition are incorporated at the fluid–solid interface. The proposed method is validated rigorously with existing literature results. The use of a Cartesian grid for flow makes this method robust, computational friendly, and at the same time it avoids the tedious volumetric mesh generation process for very complex shapes. To demonstrate the capability of the current method, it is applied to study flow and heat transfer of a typical foam sample with different flow properties. A closure for pressure drop and heat transfer coefficient are derived for the typical foam sample.

1. Introduction

Traditionally packed bed reactors are randomly filled with particles coated with a thin porous layer containing catalyst. The catalyst inside this layer (washcoat) is accessible only via diffusion through the very fine pores and it drives the design towards smaller particles to obtain a larger specific surface area. At the same time the use of very small particles leads to a large pressure drop and one well known solution to overcome this issue, is to apply slurry reactors that allow for very small particles with minimal pressure drop. Another potential option is to use comparatively large pellets consisting of open structures (open-cell solid foams) where washcoat layers are deposited at the outer surface of the pores inside the solid foam structures. To design and optimize such processes at a large industrial scale with feasible computational cost it is necessary to adopt so called multiscale modeling approach and this is schematically shown in Fig. 1. At the smallest level direct numerical simulation (DNS) are used to fully resolved the pore structures (*micro-scale* or *pore-scale level*) of a small section of solid foam (representative elementary volume, REV), which provides 'closure free' detailed flow and heat transfer characteristics. The results from DNS studies can be used to develop momentum and heat transfer closures. At a *macro-scale* level the external void generated by the randomly packed pellet of different shapes are resolved, but the internal structures of the foams are not resolved and instead are modeled by volume averaging techniques [1] using effective closures developed from DNS studies. Studies at the macro-scale level lead to a phenomenological model for packed bed in large industrial applications where the full bed is represented by a single porosity, sometimes referred as the overall volumetric porosity of the bed.

In this present contribution we are focusing on the very detailed pore-scale level studies of open-cell solid foams for single-phase flow and heat transfer analysis. Due to the random and complex geometrical shapes, most of the numerical work on solid foams is based on idealized representations of the foam unit cell. However, the demand for modeling very complex irregular structures has

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Nomenclature

A_s	Solid surface area, m^2
$\bar{C}$	Convective momentum flux, N/m^3
C_d	Non-dimensional drag coefficient
C_P	Specific heat, *J/(kg-K)*
$\bar{C}_T$	Convective thermal flux, W/m^3
$\bar{d}$	Probe location, *m*
D	Diameter, *m*
d_p	Equivalent particle diameter, *m*
$F_{f\rightarrow s}$	Total force on the solid body, *N*
f	Friction factor
h	Heat transfer coefficient, $W/(m^2\,K)$
k	Thermal conductivity, $W/(m\,K)$
l	Solid surface to probe distance, *m*
Nu	Nusselt number
$\bar{n}$	Surface normal
p	Pressure, *Pa*
Pr	Prandtl number
$\dot{q}$	Wall heat flux, W/m^2
Re	Reynolds number
S_a	Specific surface area, *1/m*
T	Temperature, *K*
t	Time, *s*
u	Velocity, *m/s*
V_s	Solid volume, m^3
$\bar{x}$	Position vector of cell-center, *m*
Δx, Δy and Δz	Grid spacing, *m*
Δt	Time-step, *sec*

Greek symbols

ρ	Density, Kg/m^3
μ	Viscosity, *Pa-s*
δp	Pressure correction, *Pa*
ϕ	Any flow variable
ξ	Dimensionless distance
ε	Porosity

Subscripts

c	Center
e	East
IB	Immersed boundary
f	Fluid
S	Surface
s	Solid
sup	Superficial
w	West
∞	Free-stream

increased with the development of X-ray micro computed tomography (μ-CT) imaging [2–4] and available computational resources. This demands the development of closures with a more realistic geometry and decreases the level of uncertainties for the subsequent industrial scale analysis. A 3D image data from a μ-CT scan of an actual foam geometry is usually converted into a surface mesh of unstructured triangular elements and the current article focuses on development of a numerical framework to incorporate such surface mesh as an immersed boundary (IB) in a Cartesian computational domain.

The Immersed Boundary Method [5] is a novel computational technique which is an alternative to the body conformal grid methods for flow over complex shapes. It avoids the challenging high quality grid generation process and the development of a CFD code for unstructured grids. Moreover, simple structured grid based codes are more efficient than unstructured grid codes in terms of memory requirements to store the grid information, computational costs in terms of convergence characteristics and the efforts involved to generate a good quality mesh. At the same time IBM can easily be coupled with other transport equations [6]. On the other hand, body fitted grids have the great ability for local mesh refinement in zones of interest where sharp gradients occur, whereas for the structured meshes grid refinement would be uniform – increasing the total computational cost. There exists a large variety of IBM methods and interested readers may refer to the literature review by Mittal and Iaccarino [7] on different immersed boundary methods. They classified the existing methods in two categories, namely continuous forcing approaches and sharp-interface based approaches. In the continuous forcing approach the no-slip condition for velocity at the immersed boundary was applied by introducing a continuous forcing function as a source term in the momentum equation. The value of this forcing function is maximum at the location of the solid surface and distributed only to the vicinity of the immersed boundary (by means of a smoothed Dirac Delta Function). The major drawback of such formulations, is the smearing of the boundaries due to the spreading nature of the forcing function. On the other side, the discrete (or direct) forcing approach is more elegant where the IB retains a sharp solid interface with no spatial spreading. The extension of the immersed boundary method from momentum to heat transfer or species transfer is quite natural and straightforward when a solid boundary is subjected to a constant temperature or a constant species concentration (Dirichlet) condition. As compared to the Dirichlet condition, heat transfer problems with the Neumann type (given heat flux) boundary condition are comparatively more challenging. To the best of our knowledge, there exist only a few attempts to properly implement Neumann condition in existing IB techniques.

Several authors like Zhang et al. [23], Kim et al. [24], Pacheco et al. [25] and Pan [26] have implemented both the temperature Dirichlet and Neumann-type boundary conditions using a forcing function based IBM. Tseng and Ferziger [27] used polynomial re-constructing techniques to implement the pressure Neumann condition in their ghost-cell IBM. In that sharp interface method they often found numerical instability and boundedness problems due to large negative coefficients in the discretized Poisson equation. In heat transfer analysis often the energy equation needs to be solved simultaneously in both solid and fluid subdomains, this is usually referred to as conjugate heat transfer (CHT). Marella et al. [9] developed a simple CHT model for solidification using a level-set field. Recently, Nagendra et al. [8] proposed a detailed CHT model using ghost cell IB techniques. They extended a ghost-cell immersed boundary method proposed by Gilmanov and Sotiropoulos [28] for different thermal conditions. The aim of this work is to develop an accurate and efficient sharp interface based IBM to simulate flow and heat transfer thought complex porous medium. The present methodology is an extension of the sharp interface, implicit, second order accurate IBM proposed by Deen et al. [5]. The key inclusions in this current contribution are: (a) extension of the method for complex random shaped solid objects, (b) temperature Neumann boundary condition at the solid-fluid interface, and (c) a conjugated heat transfer model.

As discussed earlier, in the chemical process industries solid foams are used as a catalyst support to enhance liquid-solid contacting to facilitate high mass transfer rates. Catalytic reactions are often exothermic or endothermic. Based on the type of reactions and the solid thermal conductivity (i.e. the Biot number), the foam surface exhibits either a constant wall temperature or a constant heat flux condition. For instance, a very fast reaction taking place at the solid surface and/or in the case of very high thermal conductivity of the solid give rise to a uniform temperature inside the solid, i.e. a Dirichlet condition can be assumed for the thermal fluid