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Modelling of heat conduction in granular porous media

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1. Introduction

This paper deals with the modelling of the heat transfer in packed bed reactors using their geometric and topological properties. The models used to simulate transport phenomena in granular fixed beds are generally of two types : the process engineering-type models that are either so-called pseudo-homogeneous or heterogeneous models and the Computational Fluid Dynamics (CFD) type which represent the porous medium as either homogeneous with uniform meshing or heterogeneous with complex meshing. Process engineering-type models give acceptable results if the reactor diameter (D) is about 15 times larger than the particle size (d) i.e. $D/d > 15$ [1] and if the chosen models and correlations are suited to the studied problem. But when the $D/d < 15$, like for instance fixed bed reactors used for methane steam reforming where very endothermic chemical reactions take place with high temperature conditions (approximately 800°C), these models cannot accurately simulate the heat transport. As for CFD-type models, they can be precise but require very significant computing resources and time [2].

In this paper, an alternative approach is considered, using graphs derived from tomography as an extension of [3]. Indeed, the packed bed two phases are represented by two dual graphs obtained using X-ray tomography or Discrete element method (DEM) combined with Image Processing using iMorph software. A third solid-fluid coupling graph is built representing the two-phase transfer. The balance equations are written and solved using a pseudo Port-Hamiltonian System (PHS) formulation. The work presented here is limited to the modelling of the heat diffusion in a bed of spherical particles containing stagnant fluid.

2. Methodology

Using iMorph software, the packed bed 3D image (see Figure 1(a)) is constructed and graphs of fluid and solid phases derived (see the solid graph in Figure 1(b) for instance). In the solid graph, nodes and edges are associated to respectively particles and contact surfaces at the interface of two neighboring particles, which can be either solid-solid contacts or solid-fluid-solid contacts as defined in [4]. For the fluid graph, constructed using the Plateau method, one associates nodes and edges to respectively fluid cells and interfaces of two neighboring fluid cells (see Figure 1(c) for illustration). Furthermore, some geometrical properties such as volumes and surfaces of solid and fluid phase elements, are extracted and associated with those of the graphs. The heat transfer in an α -phase (solid or fluid) is described using first order PDE system as :

$$\begin{pmatrix} \partial_t u^\alpha \\ F^\alpha \end{pmatrix} = \begin{pmatrix} 0 & -div \\ -grad & 0 \end{pmatrix} \begin{pmatrix} T^\alpha \\ \phi^\alpha \end{pmatrix} \text{ and } \begin{pmatrix} e_\partial^\alpha \\ f_\partial^\alpha \end{pmatrix} = tr \begin{pmatrix} T^\alpha \\ \phi^\alpha \end{pmatrix} \quad (1)$$

Where u , T and ϕ are respectively the internal energy density, the temperature and the heat flux density. The differential operator in eq. 1 is skew-symmetric then can be considered as Hamiltonian. e_∂ and f_∂ are the port boundary variables and $tr()$ is the trace operator at the domain boundary. The state variables u and T are related through the equation $du = C_V dT$ with C_V the heat capacity in constant volume. The constitutive relations are defined as : $\phi = -\lambda F$ and $F = -gradT$, the thermodynamic

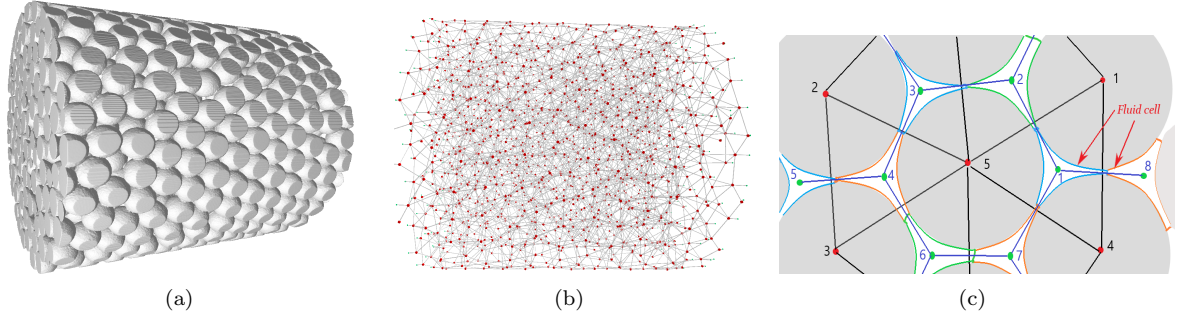


FIGURE 1 – (a)Packed bed X-ray CT image reconstruction (b)Solid graph (1777 solid nodes and 6208 fluid cells) (c) representation of 2D solid and fluid elements

driving force, with λ the actual heat conductivity of the phase.

After discretization of the eq. (1) for the two phases and their coupling via the discrete relationship $\phi_{ij}^{sf} = h_{ij} F_{ij}^{sf}$, representing the heat flux density between a solid element i and a fluid element j , one can derive a finite-dimensional pseudo-PHS for the packed bed filled with stagnant fluid as :

$$\begin{bmatrix} \partial_t \mathbf{U}^s \\ \partial_t \mathbf{U}^f \\ \mathbf{F}^s \\ \mathbf{F}^f \\ \mathbf{F}^{sf} \end{bmatrix} = \begin{bmatrix} 0 & 0 & -D_1^T & 0 & -M_s^T \\ 0 & 0 & 0 & -D_2^T & M_f^T \\ -D_1 & 0 & 0 & 0 & 0 \\ 0 & -D_2 & 0 & 0 & 0 \\ M_s & -M_f & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{T}^s \\ \mathbf{T}^f \\ \Phi^s \\ \Phi^f \\ \Phi^{sf} \end{bmatrix} + \begin{bmatrix} 0 & 0 & -D_{1b}^T & 0 \\ 0 & 0 & 0 & -D_{2b}^T \\ -D_{1b} & 0 & 0 & 0 \\ 0 & -D_{2b} & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{T}^b \\ \mathbf{T}^f \\ \Phi^b \\ \Phi^f \end{bmatrix} \quad (2)$$

With subscripts s , f and b standing for solid, fluid and boundary respectively. \mathbf{U}^s , \mathbf{U}^f , \mathbf{F}^s , \mathbf{F}^f , \mathbf{T}^s , \mathbf{T}^f , Φ^s , Φ^f and Φ^{sf} are vectors collecting the discrete U_i^s , U_j^f , F_{ik}^s , F_{jl}^f , F_{ij}^{sf} , T_i^s , T_j^f , ϕ_{ik}^s , ϕ_{jl}^f and ϕ_{ij}^{sf} , determined by volume-averaging, respectively. D_1 and D_2 , and their transposes D_1^T and D_2^T , represent solid and fluid incidence matrices obtained from dual graphs. The matrices M_s and M_f with their transposes M_s^T are M_f^T are two-phase interconnection matrices.

3. Conclusions & perspectives

We presented in this paper a new approach, for modelling heat diffusion in packed bed containing stagnant fluid, based on a pseudo Port Hamiltonian System formalism. The model was constructed taking into account the actual solid-fluid structure, i.e the topology and geometry. The future work will focus on thermal convection and particle type effect.

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