Powder Technology 291 (2016) 46–51

Contents lists available at ScienceDirect

Powder Technology

journal homepage: www.elsevier.com/locate/powtec

Thermal analysis with contact resistance of packed bed by a homogenization method

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ARTICLE INFO

Article history:
Received 10 June 2015
Received in revised form 2 November 2015
Accepted 3 December 2015
Available online 4 December 2015

Keywords:
Effective thermal conductivity
Homogenization method
Microstructure
Thermal contact resistance
Multi-scale analysis

ABSTRACT

Effective thermal conductivity with contact resistance is analyzed by a homogenization method that can precisely represent the microstructure of a packed bed. The homogenization used in this study explains the heat transfer due to conduction through the solid, the fluid phase, and the contact area between particles, and radiation between solid surfaces. In particular, the effects of parameters, such as the hardness, contact pressure, roughness, temperature, and particle size of the packed bed, on conductivity are estimated in order to clarify the thermal conduction mechanism for the complex packed structure. Heat transfer with thermal contact resistance does not dominate if the Biot number is near 100. In case of larger particle size and no convective heat transfer, the micro-hardness, contact pressure, surface roughness are important factor for effective thermal conductivity. Moreover, thermal radiation in the bed becomes more important for larger particles (>1 mm) and contact resistance can be neglected. However, effective thermal conductivity of pebble bed is dependent on the void fraction.

1. Introduction

Packed beds are used in industrial applications, such as catalytic reactors, heat recovery, heat storage, and insulators. Small particles are usually used to achieve a large surface area. However, as the particle size is reduced, the superficial velocity decreases, which prevents efficient operation. Moreover, if a reaction is endothermic and heat must be added in a catalytic reactor, heat transfer is the most important factor for the bed. Accordingly, heat transfer in the bed must be understood and controlled to enhance performance.

The thermal conductivity of a packed bed becomes anisotropic because temperature distribution causes anisotropy of thermal expansion and contraction, which are related with contact pressure and contact area. Although the contact resistance depends on the contact area between spheres and the gas layer between spheres, unavoidable thermal expansion and temperature rises affect the conduction path and contact area. Moreover, the contact resistance is strongly influenced by the surface roughness of a material and the gas pressure. However, at higher temperatures, thermal radiation must be considered in addition to heat conduction and convection. Accordingly, heat transfer in a bed becomes very complex.

To predict behavior of heat transfer in a packed bed, various types of models, such as the Series and Parallel models and Maxwell-Eucken model were proposed [1,2]. Afterward, finite area contact models between particles and unit cell models were developed as new models [3–6]. On the other hands, in the last decade, although conventional and empirical models have been proposed for the various behaviors of thermal contact resistance [7–10], more precise thermal analysis is required in order to understand heat transfer in a bed. For example, the thermal resistance network model does not always provide satisfactory predictions.

To predict the effective thermal conductivity (ETC) of packed beds precisely, four heat transfer mechanisms must be considered simultaneously: (1) conduction through the solid; (2) conduction through the contact area between particles; (3) radiation between solid surfaces; (4) conduction through the fluid phase; and (5) convective heat transfer between solid and gas. Although DEM approaches [11–13], which can consider wall region effect for the void fraction, convection heat transfer and contact resistance, show good results, their model does not include the thermal radiation. On the other hand, fine and larger particles are mixed to improve the mechanism (1) because the void fraction is reduced. At this time, because the number of contact points becomes larger [14], contact resistance for mechanism (2) must be considered precisely. Moreover, effective thermal conductivity is a function of particle Reynolds number, and fast gas flow rate promotes convective heat transfer [15]. Accordingly, particle size, void fraction, contact resistance, gas glow rate and thermal radiation are important factors for precise analysis in packed bed.

The homogenization method is proposed in this study for thermal analysis of packed beds because the method can evaluate precise changes in microstructure and temperature by using a three-dimensional finite element method [16–22]. In our previous study, thermal radiation

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http://dx.doi.org/10.1016/j.powtec.2015.12.006
0032-5910/

was added to the packed bed model and we succeeded in elucidating the heat transfer of the bed at high temperatures [22]. In this study, thermal contact resistance is added to our analytical model in order to simulate a complex packed bed accurately, and ETC is calculated according to the characteristic behavior of the contact resistance. Moreover, we quantitatively estimate both thermal radiation and thermal contact resistance for various particle sizes and temperatures at the same time. Simulation method, which can consider the radiation and the contact resistance in packed bed, is first challenge and these results obtained from the various parameters will provide important information for understanding heat transfer in packed bed reactor.

2. Model

2.1. Homogenization method

To analyze the packed bed shown in Fig. 1(a), the simple periodic particle structure in Fig. 1(b) is considered. Each cell of this periodic structure consists of two domains: solid, Ω_s, and gas, Ω_g (Fig. 1(c)). The subscripts s and g denote the solid and gas components, respectively, and Γ denotes the interface between their two domains.

The periodic domain Ω is small compared with the characteristic length L at the macroscopic scale:

$$\varepsilon = \frac{l}{L} << 1, \tag{1}$$

where ε is a scale parameter, and l and L can be understood as the characteristic sizes of the sample at the microscopic and the macroscopic scales, respectively. In this analysis, l is the particle diameter of the packed bed and ε ranges from about 1×10^{-6} to 1×10^{-4}.

The multiscale periodic heat conduction problem under steady-state conditions for the medium described above can hence be mathematically expressed as

$$-\frac{\partial}{\partial x_j^*}\left(\lambda_s \frac{\partial T_s}{\partial x_j^*}\right) = g_s \quad \text{in } \Omega_g, \tag{2}$$

$$-\frac{\partial}{\partial x_j^*}\left(\lambda_g \frac{\partial T_g}{\partial x_j^*}\right) = g_g \quad \text{in } \Omega_g, \tag{3}$$

$$-\lambda_s \frac{\partial T_s}{\partial x_j^*}\mathbf{n}_j = -\lambda_g \frac{\partial T_g}{\partial x_j^*}\mathbf{n}_j \quad \text{on } \Gamma, \tag{4}$$

$$-\lambda_s \frac{\partial T_s}{\partial x_j^*}\mathbf{n}_j = h(T_s - T_g) \quad \text{or} \quad = q_t \text{ (See Eq.(25)) on } \Gamma, \tag{5}$$

where λ, T and g are the thermal conductivity, temperature field and volumetric rate of heat generation on a microscopic scale, respectively. Furthermore, $\boldsymbol{n}$ is the outward-pointing unit vector locally normal to the boundary Γ, and h is the interfacial thermal conductance. In case of radiation analysis, q_{rad} is used. Eqs. (2)–(5) are general expressions, and g_s and g_g become zero in the case that the bed is packed.

By defining the following nondimensionalized quantities,

$$y \equiv \frac{x^*}{l}, \quad \theta \equiv \frac{T}{\Delta T}, \quad \Lambda \equiv \frac{\lambda_g}{\lambda_s} \tag{6}$$

in which ΔT is the external temperature difference on the macroscopic scale, we can rewrite Eqs. (2)–(5) as

$$-\frac{\partial}{\partial y_j}\left(\frac{\partial \theta_s}{\partial y_j}\right) = 0 \quad \text{in} \quad \Omega_s, \tag{7}$$

$$-\frac{\partial}{\partial y_j}\left(\Lambda \frac{\partial \theta_g}{\partial y_j}\right) = 0 \quad \text{in} \quad \Omega_g, \tag{8}$$

$$-\frac{\partial \theta_s}{\partial y_j}\mathbf{n}_j = -\Lambda \frac{\partial \theta_g}{\partial y_j}\mathbf{n}_j \quad \text{on} \quad \Gamma, \tag{9}$$

$$-\frac{\partial \theta_s}{\partial y_j}\mathbf{n}_j = \text{Bi}(\theta_s - \theta_g) \quad \text{on} \quad \Gamma. \tag{10}$$

Here, the dimensionless heat generation numbers and the Biot number of convection and radiation with radiation heat transfer coefficient, $h_{r.}$ are given by

$$\text{Bi} \equiv \frac{hl}{\lambda_s} \quad \text{or} \quad \text{Bi} \equiv \frac{h_r l}{\lambda_s}. \tag{11}$$

Multiplying Eqs. (7) and (8) by a weight function ν, integrating over Ω and applying Green's first identity theorem we obtain

$$\int_{\Omega_s} \frac{\partial \nu_s}{\partial y_j}\frac{\partial \theta_s}{\partial y_j} dy - \int_{\Gamma} \nu_s \frac{\partial \theta_s}{\partial y_j}\mathbf{n}_j ds = 0, \tag{12}$$

$$\int_{\Omega_g} \Lambda \frac{\partial \nu_g}{\partial y_j}\frac{\partial \theta_g}{\partial y_j} dy + \int_{\Gamma} \Lambda \nu_g \frac{\partial \theta_g}{\partial y_j}\mathbf{n}_j ds = 0, \tag{13}$$

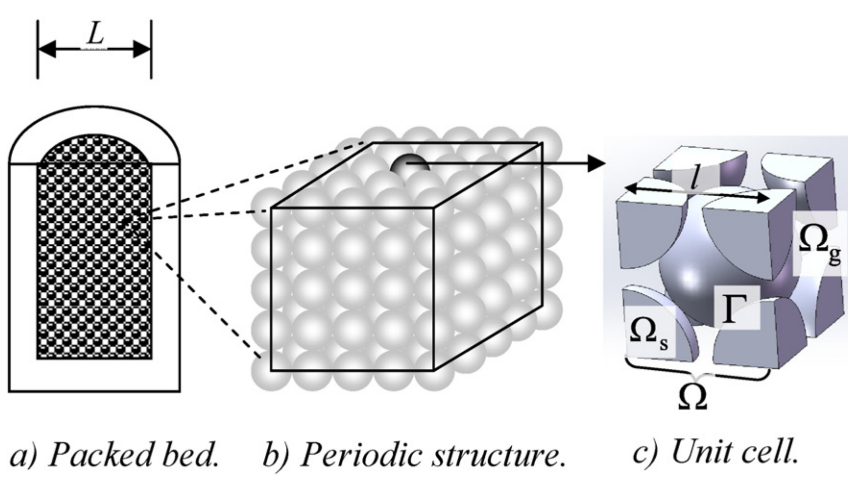

Fig. 1. Schematic diagram of homogenization method. a) Packed bed. b) Periodic structure. c) Unit cell.