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Anisotropy of effective thermal conductivity analysis of heat transfer coefficient distribution around spherical particles in a packed bed

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Effective thermal conductivity with radiation is analyzed by a homogenization method. The method used can precisely represent the conditions around particles in a packed bed. In this study, the effects of variation in parameters such as heat transfer coefficient distribution around spherical particles in a packed bed, Reynolds number, temperature and particle size on the conductivity were estimated in order to elucidate the heat transfer mechanism of complex packed structures. The results show that it is unnecessary in heat transfer analysis to consider the anisotropic behavior of the flow direction for larger particles, high Reynolds numbers and high temperatures. However, the heat transfer was anisotropic for smaller particle sizes.

Keywords: effective thermal conductivity homogenization method multi-scale analysis microstructure, thermal radiation, packed bed.

Nomenclature

d	–	particle size [m],
f	–	factor to calculate heat transfer distribution [–],
h	–	interfacial thermal conductance [W/(m^{2}K)],
L	–	characteristic macroscopic length [m],
l	–	characteristic microscopic length [m],
Nu	–	Nusselt number [–],
Pr	–	Prandtl number [–],
Re	–	Reynolds number [–],
y	–	dimensionless microscale variable [–],
α	–	ratio of thermal conductivity [–],
β	–	angle from flow direction [–],
χ	–	homogenization function [–],
δ	–	identity matrix,
ε	–	scale parameter (l/L) [–],
ε_r	–	emissivity [–],

Γ – common boundary of the two media,
Λ – dimensionless thermal conductivity [–],
λ – dimensional thermal conductivity [W/(mK)],
Ω – domain.

Superscripts
eff – effective,
g – gas phase,
p – direction of spatial dimension,
q – direction of spatial dimension,
s – solid phase.

1. Introduction

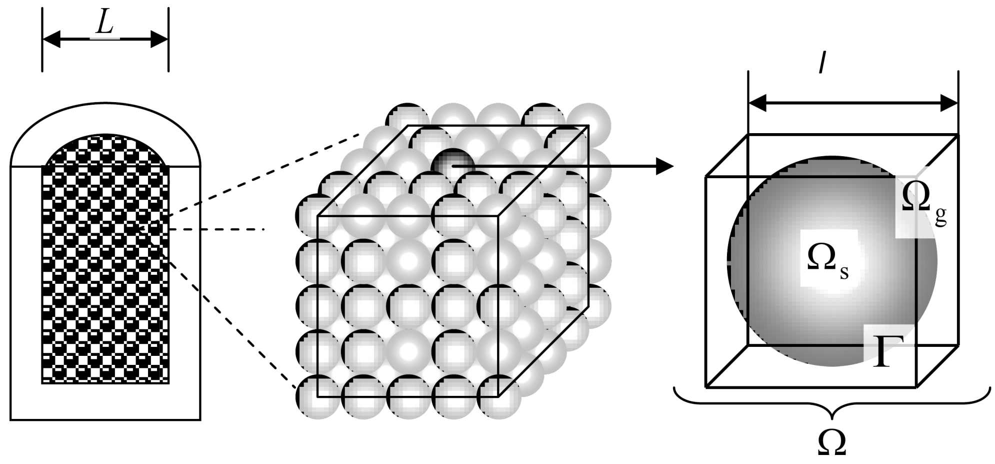
Packed bed reactors have been used in environmental processes such as reducing harmful exhaust gases (e.g. NO_x and SO_x) and producing new energy sources (e.g. generating hydrogen from methane). In catalytic reactors, small particles are tightly packed to create a large surface area. However, mass transfer and heat transfer in the bed are complex. There are many studies of the convection pattern and heat transfer around particles. Ranz and Marshall proposed empirical correlations for calculating the Nusselt number (Nu) around a single spherical particle [1]. However, the Nusselt number is a function of the Prandtl number and Reynolds number (Re), obtained from the measurement of the heat transfer coefficient of a packed bed [2, 3]. Although these models have often been used for simulations, the Prandtl and Reynolds numbers are limited for their application. Moreover, thermal radiation at higher temperatures must be considered separately from heat conduction and convection [4]. Accordingly, a more precise thermal analysis is required to understand heat transfer in a packed bed. A numerical homogenization method is proposed in the current study and used for the thermal analysis of packed beds. The method is very useful because it evaluates precise changes in microstructure and temperature by using a three-dimensional finite element method. This method has been used for structural analysis [5, 6] and heat transfer analysis of composites and fibers [7–13].

To improve the performance of a bed, precise information about the heat transfer around a particle is required. For example, if the flow speed in a reactor is high, the velocity components around a particle, which are related to the heat transfer coefficient, are different between the radial and flow directions. By using the proposed homogenization method, the thermal radiation [4] and the anisotropy of the heat transfer around a particle in a packed bed [14] can be calculated. In this study, to investigate the characteristic behavior of a packed bed for wide range of temperatures and Reynolds numbers the effective thermal conductivity (ETC) is calculated by estimating the heat transfer coefficient distribution around a particle with empirical models. Finally, we quantitatively estimate both thermal radiation and heat transfer at the same time. Simulation method, which can consider some behaviors in packed bed, is the first challenge and the obtained results will provide important insights for designing packed bed reactor.

2. Model

2.1. Homogenization method

To analyze the packed bed shown in Fig. 1a, the simple periodic particle structure in Fig. 1b is considered. Each cell of this periodic structure consists of two domains: solid (Ω_s) and gas (Ω_g), as



a) packed bed b) periodic structure c) unit cell

Fig. 1. Schematic diagram of homogenization method.

shown in Fig. 1c. The subscripts s and g denote the solid and gas components respectively, and Γ denotes the interface between the two domains.

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

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

where ε is a scale parameter and l and L can be understood as the characteristic sizes of the sample at the microscopic and macroscopic scales, respectively. In this analysis, l is the particle diameter of the packed bed and ε ranges from approximately 1×10^{-6} to 1×10^{-4} and homogenization theory can be applied in packed bed because ε is less than 0.01 [15]. Detailed formulation is described in our previous study [4]. Finally, the effective thermal conductivity (ETC) λ_{eff} is obtained as the homogenized property as follows:

$$\lambda_{\text{eff},\,p} = \frac{1}{\Omega} \int\limits_{\Omega} \alpha \left(\delta_{pq} - \frac{\partial \chi_q(y)}{\partial y_p} \right) dy, \tag{2}$$

where $\alpha = 1$ if $y \in \Omega_s$ and $\alpha = \Lambda$ $(= \lambda_g/\lambda_s)$ if $y \in \Omega_g$. $\chi_p(y)$ is homogenization function and corresponds to a unit temperature gradient at microscale y.

Generally, heat transfer coefficient h of the Biot or Nusselt number describes the heat transfer coefficient distribution around the particle [14]. The distribution is calculated from the average heat transfer coefficient and factor f as shown in below. The coefficient is estimated from the Nusselt numbers obtained from the Ranz and Marshall model for a single sphere [7] and Wakao and Kaguei model for linearly aligned spheres [2, 3]

$$\mathrm{Nu} = 2 + 0.6(\mathrm{Pr})^{0.33}(\mathrm{Re})^{0.5} = \frac{hl}{\lambda_g} \cdot (1 < \mathrm{Re} < 10^5), \tag{3}$$

$$\mathrm{Nu} = 2 + 2.11(\mathrm{Pr})^{1/3}(\mathrm{Re})^{0.6} = \frac{hl}{\lambda_g} \cdot (10 < \mathrm{Re} < 10^4). \tag{4}$$

Factor f for the angle of flow direction β is modeled as cosine and sine curves to reproduce the distribution around the single sphere and lined spheres shown in Fig. 2, respectively. In case of lined

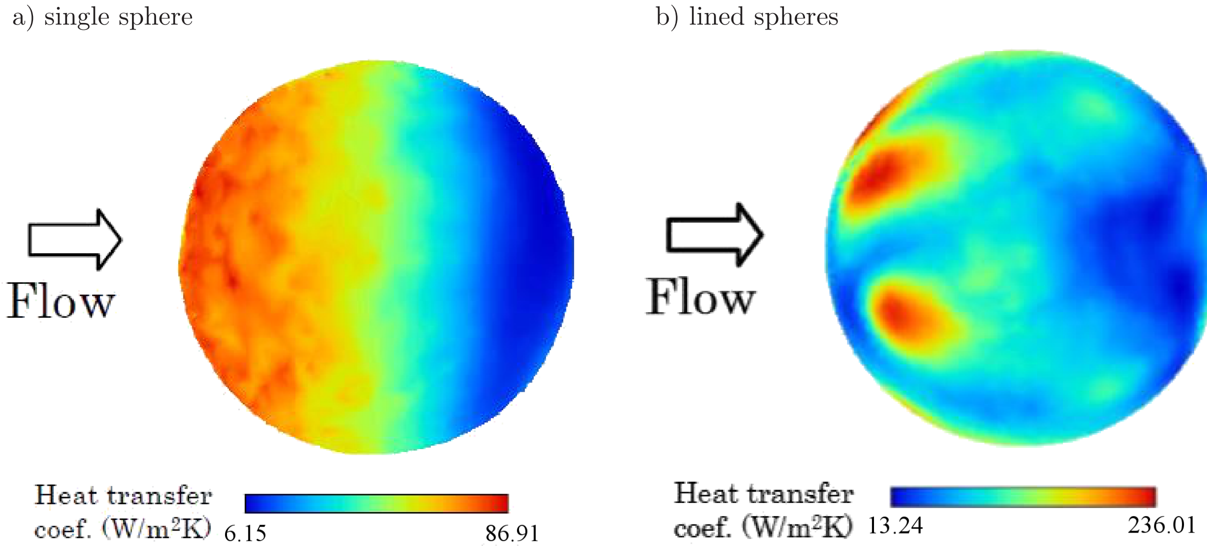


Fig. 2. Heat transfer coefficient distribution around the particle from [14].

spheres with four particles, the coefficient of third sphere from the inlet was chosen because influence from inlet and outlet is the smallest of the four. Multiplying the factor f by the coefficient h in Eqs. (3) and (4) produces distributions similar to those shown in Fig. 2 through the assumption that the distribution pattern is the same in case of lower Reynolds numbers. The average value of the factors for the flow direction is 1 as shown in Fig. 3. Accordingly, the distribution of the heat transfer coefficient, which is similar to the data [14], can be obtained. For example, the local heat transfer coefficient is large at $\beta = 45°$, which is the position of the strongest impinging flow. The anisotropy of the heat transfer can be estimated by using the ETC values λ_1 and λ_2, which are in the flow direction and normal to the flow, respectively, for different Reynolds numbers and particle sizes. Moreover, thermal radiation is considered in order to investigate the effect of heat transfer on the anisotropy at higher temperatures [4].

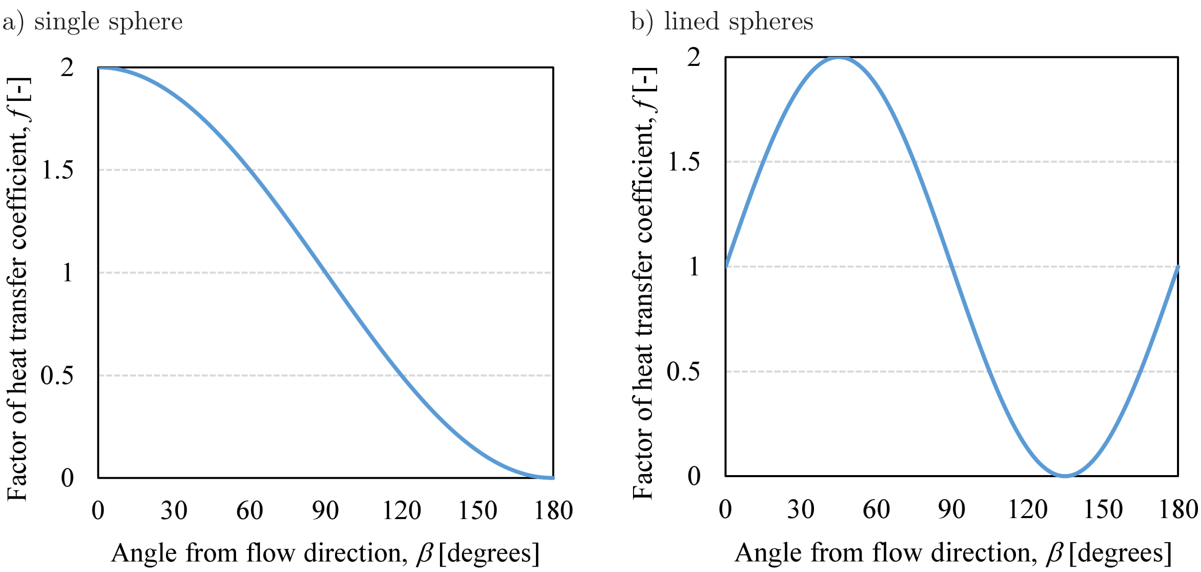


Fig. 3. Assumed relation between local heat transfer coefficient and angle of flow direction around the spheres.

In this homogenization method, finite element meshes of simple packed (SP) geometries are established for packed beds by using Delaunay triangulation to automatically generate a tetragonal mesh [16]. It was confirmed that the number of mesh and element is sufficient (more than 4000). The validity of the code used to implement this model was confirmed by comparison with the solution of Rocha et al. [7] and Kunii et al. for thermal radiation [17].

2.2. Materials

Although the thermal conductivity of materials varies with temperature, λ_s is kept constant ($\lambda_s = 10$) in this study so that the effect of radiation can be examined in isolation.

Thermal conductivity of a gas λ_g depends on the mean free path of the gas molecules; nitrogen was used for this study [4]. Moreover, Prandtl number of nitrogen from Eqs. (3) and (4) is used because the main component of exhaust gas is nitrogen.

3. Results and discussion

3.1. Effect of Reynolds number on effective thermal conductivity for packed beds

The residence time in the bed, determined by operating conditions such as the Reynolds number for the flow rate, is a key factor in process efficiency. Figure 4 shows the effect of the Reynolds number on ETC without thermal radiation for a particle size of $d = 0.1$. The anisotropy of ETC is maintained even at higher Reynolds numbers. The behavior of the ETC for the heat transfer coefficients obtained from single sphere and lined spheres is similar although their absolute values are larger for higher Reynolds numbers. If thermal radiation is not considered at lower temperatures, the anisotropy of ETC in a packed bed must be taken into account for detailed thermal analysis.

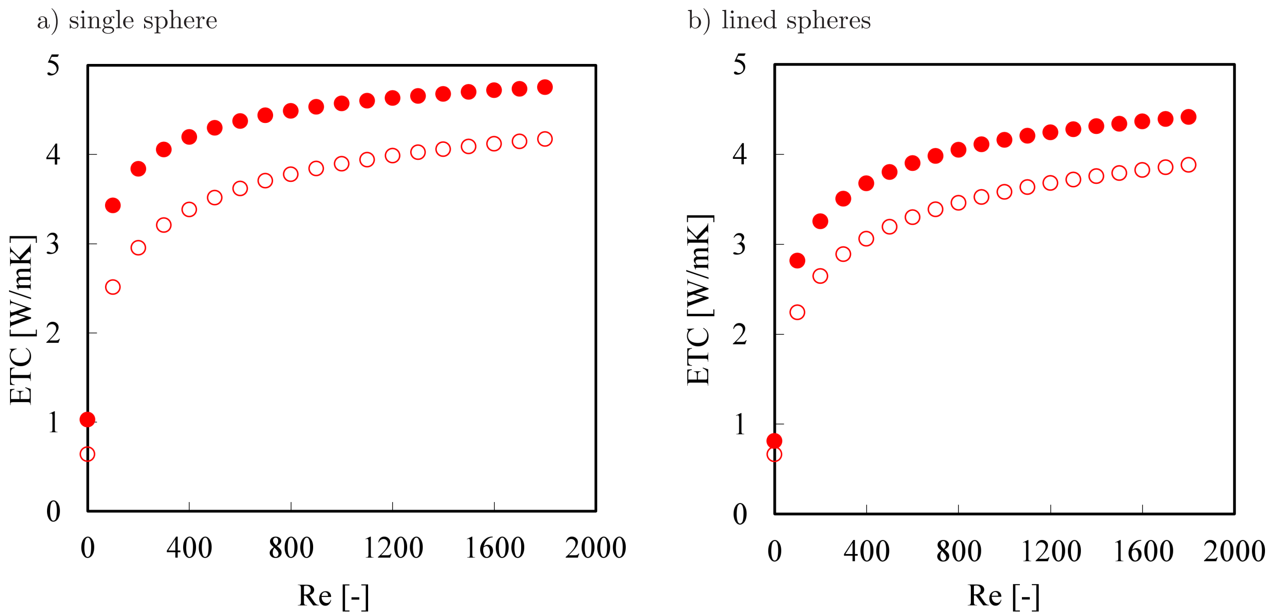


Fig. 4. Effect of Reynolds number on effective thermal conductivity. Filled and unfilled symbols indicate the anisotropy of the ETC values λ_1 and λ_2, respectively.

3.2. Effect of thermal radiation on effective thermal conductivity for a packed bed

The effect of thermal radiation on the ETC is analyzed for the Reynolds number, the temperatures and particle sizes of a single sphere and lined spheres for the emissivity (ε_r) of 0.5 (Figs. 5 and 6). At lower temperatures, the ETC shows anisotropy in the flow direction. However, when the temperature is higher, the anisotropy disappears for larger particles. By contrast, the ETCs for smaller particles are almost constant, and the anisotropy is maintained at lower temperatures because the thermal radiation can be neglected for smaller particle sizes [4]. Therefore, particle size must be taken into account at higher temperatures when the conventional models in Eqs. (3) and (4) are used. This is why the non-dimensional numbers in these equations include the size parameter, which strongly affects the thermal radiation [3, 4]. Overall, the difference in ETC between a single sphere and lined spheres is small and the conventional models are still useful for reducing computational cost and predicting heat transfer under steady conditions. Moreover, combining this analysis with conventional models is helpful for simulating dramatic changes in bed conditions such as temperature, pulverization and thermal expansion of particles.

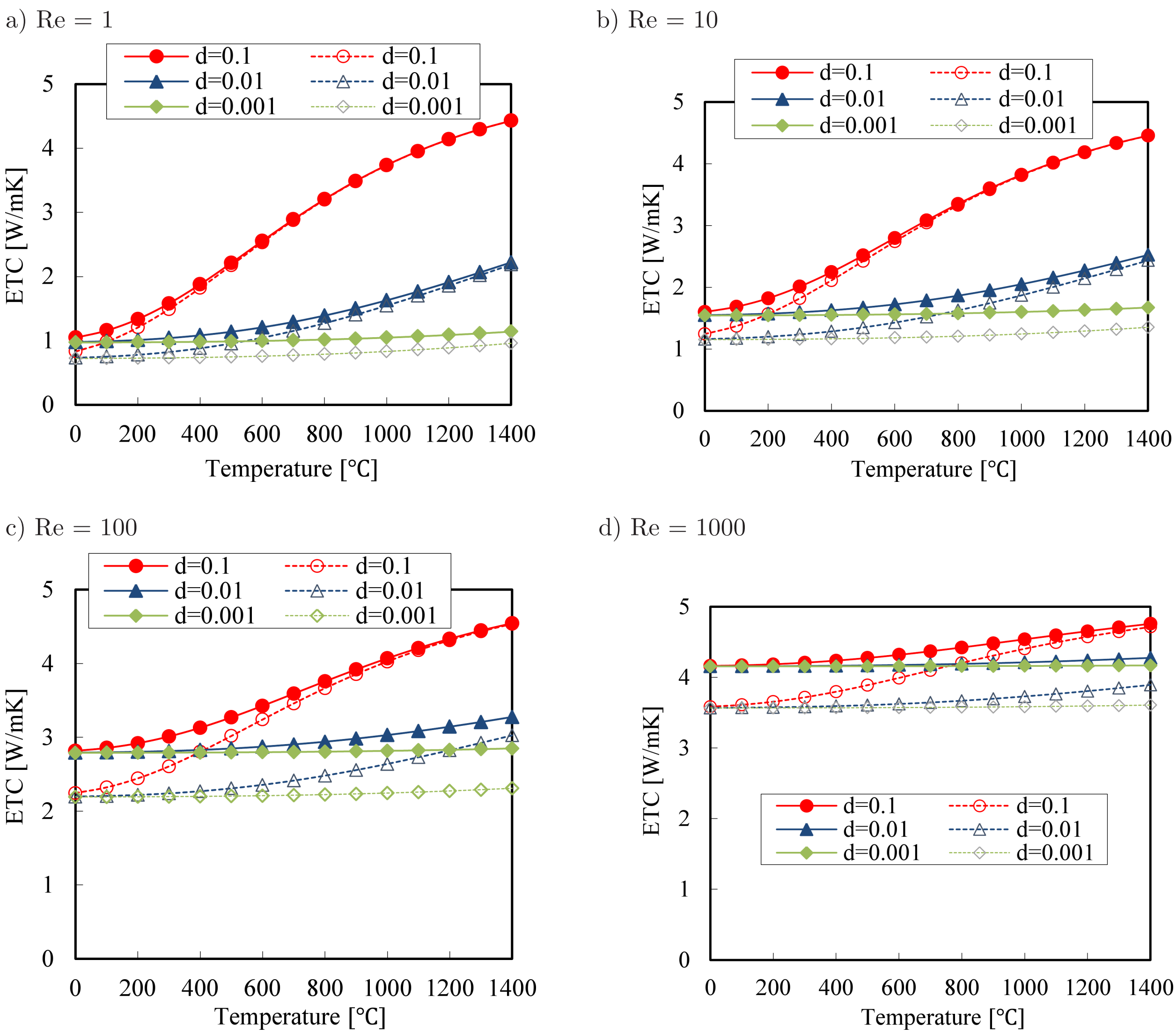


Fig. 5. Effect of temperature on effective thermal conductivity for a single sphere. Filled and unfilled symbols indicate the anisotropy of the ETC values λ_1 and λ_2, respectively.

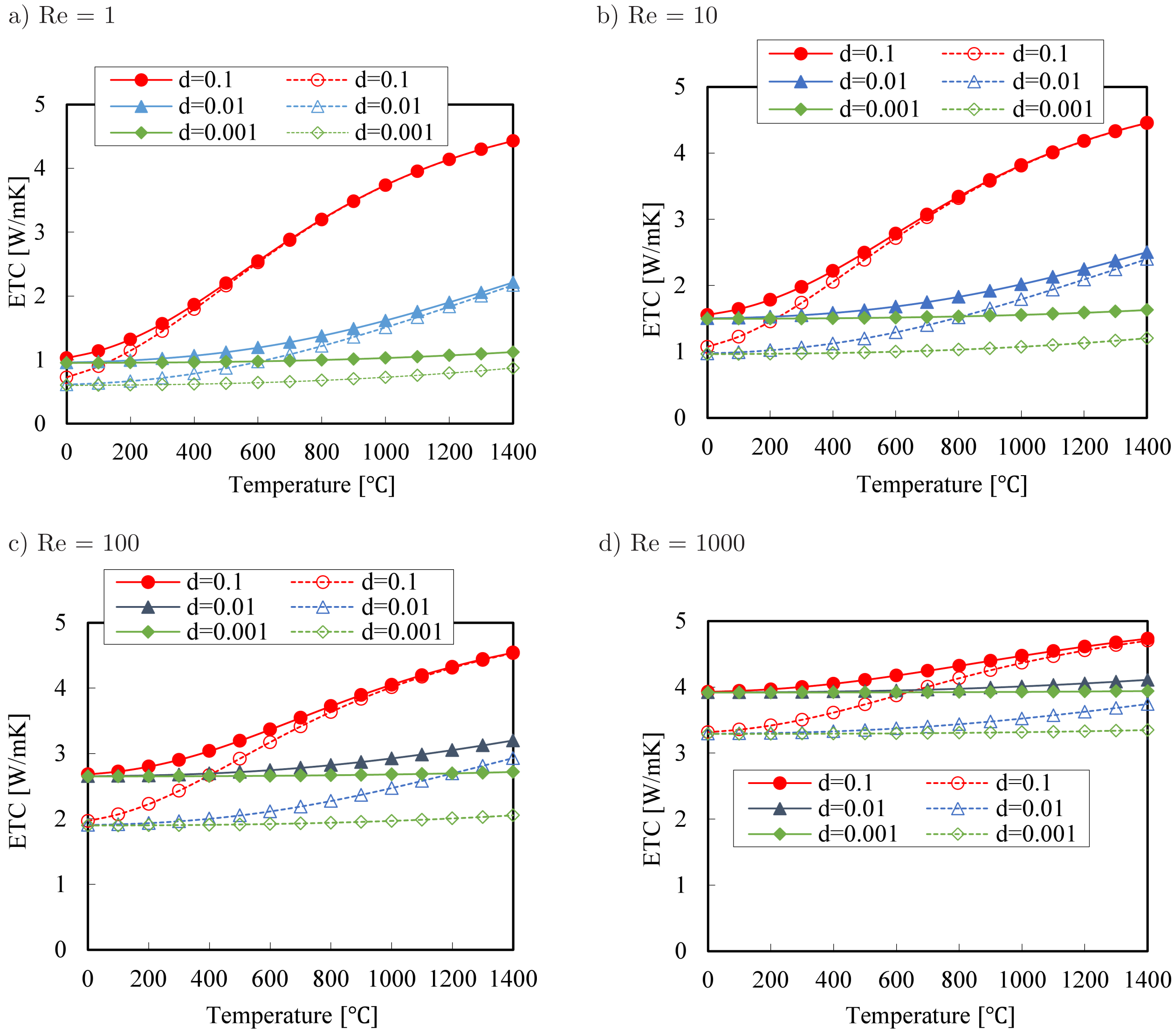


Fig. 6. Effect of temperature on effective thermal conductivity for lined spheres. Filled and unfilled symbols indicate the anisotropy of the ETC values λ_1 and λ_2, respectively.

4. Conclusions

The anisotropy of heat transfer in a packed bed was investigated by using a numerical homogenization method with thermal radiation. The effect of the heat transfer coefficient distribution on ETC was calculated for a single sphere and for lined spheres. Although the absolute values increase with the Reynolds number, the anisotropy of the ETC is maintained even for higher Reynolds numbers. Thermal radiation was also considered for the Reynolds number, particle size and temperature. Thermal radiation dominated for large particles at high temperatures, and the anisotropy of ETC disappeared. However, when the particle size was less than 0.001 m, the radiation transfer in the packed bed was negligible. Accordingly, the anisotropy of ETC was maintained for lower initial temperatures in packed beds with smaller particles, even at higher temperatures. These results highlight the importance of the heat transfer coefficient distribution for ETC at lower temperatures. Homogenization methods can usually provide a quantitative estimate of thermal convection and radiation in a complex system such as a packed bed. Moreover, the proposed method is expected to be a useful tool for modeling heat transfer and can be used in addition to conventional models.

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