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Finite element modeling of the transient heat conduction between colliding particles

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Abstract

Finite element method (FEM) is employed to simulate the transient heat conduction during the collision between spherical particles. The total collision time is divided into many small time steps. At each time step, the contact area is evaluated by the Hertz's theory of elastic collision and based on this information, a grid system is generated for FEM computation to determine the temperature distribution in a particle and the heat exchange between particles. The total heat exchange is the sum of the heat exchange at all time steps. The FEM approach and computer code are verified by the good agreement between the numerical and analytical solutions for a well-established case. It is then used to simulate the transient heat transfer process during particle collision. It is shown that the heat exchange is affected by variables related to collision conditions and material properties. The results are qualitatively consistent with those obtained analytically based on the semi-infinite-media assumption. However, the analytical model overestimates the heat exchange, particularly when the Fourier number is high. A modified equation is proposed to overcome this problem based on the present FEM results. The equation is particularly suited for the newly developed particle scale modeling of the heat transfer of multiparticle systems.

Keywords: Finite element method; Heat conduction; Particle collision

1. Introduction

The transient heat conduction during the collision between particles is an important heat transfer mechanism in particle and multiphase systems, such as moving beds, fluidized beds and pneumatic conveying. Although this heat transfer mechanism may be neglected for dilute flow [1], it must be included for dense flow where particles are frequently in contact with their neighbors [2,3]. The study of this problem was pioneered by Soo [4]. He used the theory of elasticity to calculate the area and duration of contact between particles. In his analysis, the thermal conductivities of particles were assumed to be very high so that the temperature of a particle can be regarded uniform at any moment during a collision process. As a result, the resultant model is rather limited and only applicable for particles of large thermal conductivity. To overcome this problem, Sun and Chen [5] conducted both numerical and theoretical analysis of the transient heat conduction due to particle collision and proposed an equation for the calculation of the heat exchange between particles. In their study, the heat conduction between two particles was assumed to be similar to that between two semi-infinite media. This semi-infinite-media assumption is valid if the contact area between particles is very small compared to particle size. However, it may not truly represent the reality if the thermal conductivities of particles are large. More recently, Rong and Horio [6] conducted a numerical study to analyze the thermodynamic characteristics and NO_x emission of burning chars in a fluidized bed, where the particle–particle heat conduction is part of the model they developed. Their model involves various assumptions including the existence of gas layer between particles which could be opened for further investigation.

In recent years, development of a more general and accurate equation to calculate the heat transfer between particles becomes a significant issue, driven by the need to develop a

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Nomenclature

A^*	dimensionless contact area
A_c	maximum contact area (m^2)
A_f	contact area between two colliding particles (m^2)
c	specific heat (J/(kg K))
C	parameter in Eq. (19a)
C'	parameter in Eq. (20)
e	heat exchange given by Eq. (19a) (J)
e'	heat exchange given by Eq. (20) (J)
e_0	heat exchange given by Eq. (19b) (J)
E_i	elastic moduli of particle i (=1 or 2) (Pa)
E_{12}	defined by Eq. (3) (Pa)
Fo	Fourier number, $\alpha_1 t_c/r_c^2$
k	thermal conductivity (W/(m K))
KP	stiffness matrix
m_i	mass of particle i (=1 or 2) (kg)
m_{12}	defined by Eq. (4) (kg)
PM	mass matrix
r	radius coordinate (m)
r_c	maximum contact radius (m)
r_f	contact radius (m)
r_i	radius of particle i (=1 or 2) (m)
r_{12}	defined by Eq. (2) (m)
R	dimensionless radius coordinate
t	time (s)
t_c	time corresponding to r_c or A_c in a collision (s)
T	temperature (°C)
T_{i1}, T_{i2}	initial temperatures of particles 1 and 2, respectively (°C)
V	velocity (m/s)
z	axial coordinate (m)
Z	dimensionless axial coordinate

Greeks letters

α	thermal diffusivity (m^2/s)
ν_i	Poisson ratio of particle i (=1 or 2)
ρ	density (kg/m^3)
τ	dimensionless time, defined by Eq. (5) or (11)
φ	dimensionless temperature, defined by Eq. (11)

better description of heat transfer in particle systems and the connection with the newly developed simulation techniques [7]. For example, discrete particle simulation is now widely used to study the particle or particle-fluid flow at a particle scale (see [8,9] for example). The technique can also be used to study the heat transfer in such a flow system by properly incorporating the heat transfer between particles and structural information in the simulation, as demonstrated in recent studies [6,10–14]. Equations for heat conduction due to collision between particles are an integrated part in such microscopic studies.

This paper presents a numerical study of the conductive heat transfer between colliding particles by finite element method (FEM). It shows that the applicability of the semi-infinite-media assumption indeed depends on not only the contact area but also other physical parameters such as thermal diffusivity. Based on the present results, to facilitate particle scale modeling of heat transfer in particle systems, an equation is formulated to calculate the heat exchange between colliding particles.

2. Mathematical formulation

2.1. Elastic impact according to Hertz's theory

Consider two elastic smooth spheres of radii r_1 and r_2, elastic moduli E_1 and E_2, Poisson ratios ν_1 and ν_2, masses m_1 and m_2 are moving with a relative velocity V along the line of their centers when they collide. The two spheres are initially at different temperatures T_{i1} and T_{i2}, respectively. According to Hertz's theory of elastic collision, the change rate of the contact area A_f during this collision is given by [15,16]

$$\frac{dA_f}{dt} = \left[(\pi V r_{12})^2 - \frac{4}{5\sqrt{\pi}}\frac{E_{12}}{m_{12}}A_f^{5/2}\right]^{1/2} \tag{1}$$

where

$$r_{12} = \frac{r_1 r_2}{r_1 + r_2} \tag{2}$$

$$E_{12} = \frac{4/3}{(1-\nu_1^2)/E_1 + (1-\nu_2^2)/E_2} \tag{3}$$

and

$$m_{12} = \frac{m_1 m_2}{m_1 + m_2} \tag{4}$$

Integrating Eq. (1) yields

$$\tau = \int_0^{A^*} \frac{dx}{(1-x^{5/2})^{1/2}} \tag{5}$$

where τ is the dimensionless time, defined by

$$\tau = \left(\frac{4E_{12}}{5m_{12}}\right)^{2/5} (r_{12}V)^{1/5} t \tag{6}$$

and A^* is the dimensionless contact area, defined by

$$A^* = \frac{A_f}{A_c} = \frac{r_f^2}{r_c^2} \tag{7}$$

where r_f is the contact radius at time t, A_c and r_c are the maximum contact area and the maximum contact radius, respectively. They are related, given by $A_c = \pi r_c^2$.A_c is calculated by [5,16]

$$A_c = \pi\left(\frac{5m_{12}{r_{12}}^2}{4E_{12}}\right)^{2/5} V^{4/5} \tag{8}$$

and its corresponding time t_c is given as

$$t_c = 2.94\left(\frac{5m_{12}}{4E_{12}}\right)^{2/5} (r_{12}V)^{-1/5} \tag{9}$$

According Eq. (5), the relation between the dimensionless contact area and the dimensionless time can be obtained.

2.2. Heat transfer modeled by finite element method

Since the impact is collinear, an axi-symmetric coordinate system is adopted. The transient heat conduction equation in an axi-symmetrical coordinate system is

$$k\left(\frac{\partial^2 T}{\partial r^2}+\frac{1}{r}\frac{\partial T}{\partial r}+\frac{\partial^2 T}{\partial z^2}\right)=\rho c\frac{\partial T}{\partial t} \tag{10}$$

where k, ρ and c are the thermal conductivity, density and specific heat, respectively. They may take different values for particles 1 and 2.

Non-dimensionalization of Eq. (10) is performed to overcome the difficulty arising from the two quite different length scales (the contact radius is almost 1000 times smaller than the radius of a sphere). Upon introducing the following dimensionless quantities

$$\tau=\frac{at}{r_1^2},\qquad \varphi=\frac{T-T_{i1}}{T_{i2}-T_{i1}},\qquad R=\frac{r}{r_1},\qquad Z=\frac{z}{r_1} \tag{11}$$

Eq. (10) becomes

$$\frac{\partial^2\varphi}{\partial R^2}+\frac{1}{R}\frac{\partial\varphi}{\partial R}+\frac{\partial^2\varphi}{\partial Z^2}=\frac{\partial\varphi}{\partial\tau} \tag{12}$$

In Eq. (11), $\alpha=k/\rho_c$ is the thermal diffusivity. In the present computation, all the boundaries are thermally insulated during the collision process.

Since an axi-symmetric coordinate system is adopted, only half of the domain needs to be discretized. To capture the drastic temperature gradient near the contact point, the mesh near the contact area is much denser than the other areas. The coordinate system and the mesh at each time step are schematically shown in Fig. 1. The mesh is generated automatically according to the contact area at each time step.

In the mesh shown in Fig. 1, the whole domain is divided into many "small elements". In this study, there are 833 node points in total, involving 722 quadrilateral elements and 118 triangular elements. In each element, the temperature distribution is approximated in terms of its nodal values, e.g., φ_1, φ_2 and φ_3 for a triangular element, through the so-called "shape functions", N_1, N_2 and N_3

$$\varphi\cong N_1\varphi_1+N_2\varphi_2+N_3\varphi_3 \tag{13}$$

If using tensor notation, Eq. (13) can be expressed as

$$\varphi\cong N_i\varphi_i \tag{14}$$

Using the above-mentioned "shape functions" N_i as the weighted functions, the Galerkin weighted residual expression of the dimensionless heat conduction equation in an element is [17]

$$\int_e\!\!\int N_i\left[\frac{\partial^2(N_j\varphi_j)}{\partial R^2}+\frac{1}{R}\frac{\partial^2(N_j\varphi_j)}{\partial R^2}+\frac{\partial^2(N_j\varphi_j)}{\partial Z^2}\right]R\mathrm{d}R\mathrm{d}Z = \int_e\!\!\int N_i\frac{\partial(N_j\varphi_j)}{\partial\tau}R\mathrm{d}R\mathrm{d}Z \tag{15}$$

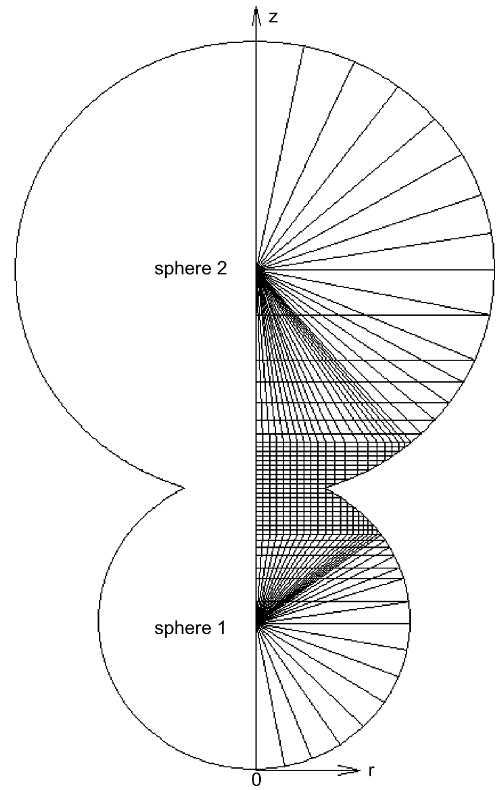

Fig. 1. The coordinate system and space discretization.

Applying the principle of integration by parts to the second-derivative term, the weighted residual expression becomes

$$\mathbf{KP}\boldsymbol{\varphi}+\mathbf{PM}\frac{\mathrm{d}\boldsymbol{\varphi}}{\mathrm{d}\tau}=0 \tag{16}$$

where $\boldsymbol{\varphi}$ is the vector of dimensionless temperature φ, **KP** is called "stiffness matrix" whose terms are of the form

$$\mathbf{KP}_{ij}=\int_e\!\!\int R\left[\frac{\partial N_i}{\partial R}\frac{\partial N_j}{\partial R}+\frac{\partial N_i}{\partial Z}\frac{\partial N_j}{\partial Z}\right]\mathrm{d}R\mathrm{d}Z \tag{17}$$

and **PM** is called "mass matrix" whose terms take the form

$$\mathbf{PM}_{ij}=\int_e\!\!\int RN_iN_j\mathrm{d}R\mathrm{d}Z \tag{18}$$

The "Crank-Nicolson" scheme is adopted to deal with the time term in Eq. (16).

Assembling individual element equations into a large system of linear equations, and then solving the resultant equations, we can obtain all the temperature values at all nodal points.

3. Results and discussion

A FORTRAN computer code is developed based on the preceding description. The code must be verified before being applied to calculate the heat transfer between colliding particles. Consider a cylinder with a radius of 0.3 m and a length of 1.0 m. Initially, it is uniformly at the temperature of 30 °C. From time $t>0$, it is subjected to convective cooling at all surfaces. The thermal properties of the cylinder are as follows: density

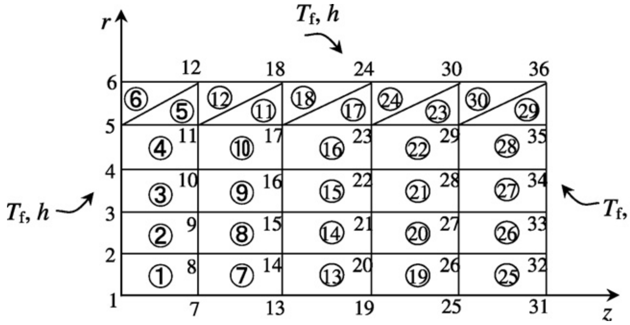

Fig. 2. The cylindrical coordinate system and the mesh arrangement adopted for the case for validity test.

$\rho = 9257.0\,\mathrm{kg/m^3}$, thermal conductivity $k = 40.5\,\mathrm{W/(m\,K)}$, specific heat $c = 70.5\,\mathrm{J/(kg\,K)}$. The convection coefficient and the fluid temperature at the cylinder surfaces are $h = 232\,\mathrm{W/(m^2\,K)}$ and $T_f = 1300\,°\mathrm{C}$, respectively. Fig. 2 shows the cylindrical coordinate system and the mesh arrangement adopted in the calculation. In this figure, the numbers ①, ②, ... indicate the finite elements, and the numbers 1, 2, . . . represent the nodes. To test the robustness of the FEM computer code, the solution region is intentionally discretized into quadrilateral and triangular elements. Fig. 3 shows the calculated temperature as a function of time at the cylinder center. For comparison, the analytical solution for the above-mentioned test problem is also plotted in this figure. It can be seen that the calculated results agree very well with the analytical solution given in [18].

In the following, the FEM model proposed will be used to study the transient heat conduction between colliding particles. Unless otherwise stated, simulation parameters used are as follows: particle density $\rho_1 = \rho_2 = 1451.7\,\mathrm{kg/m^3}$, Young's modulus $E_1 = E_2 = 193\,\mathrm{GPa}$, Poisson ratio $\nu_1 = \nu_2 = 0.29$, particle radii $r_1 = 2\,\mathrm{mm}$ and $r_2 = 3\,\mathrm{mm}$, normal relative velocity $V = 0.5\,\mathrm{m/s}$, initial temperatures $T_{i1} = 20\,°\mathrm{C}$, $T_{i2} = 90\,°\mathrm{C}$. Different temperatures can be used, but they will not affect the final outcomes of this study because all the physical quantities are non-dimensionalized.

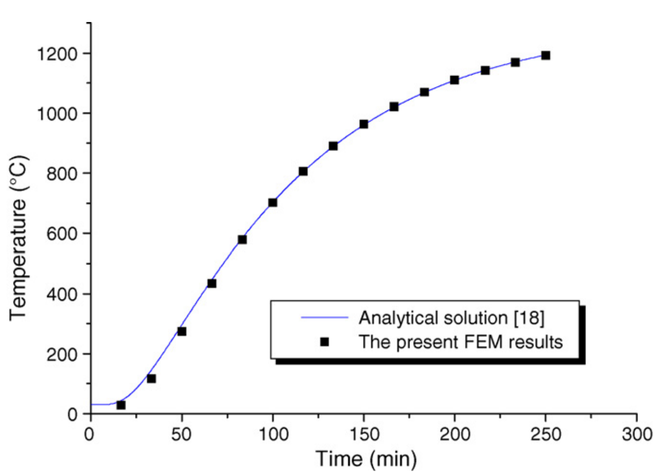

Fig. 3. Comparison of the temperature transients at the cylinder center between the FEM numerical results and the analytical solution [18].

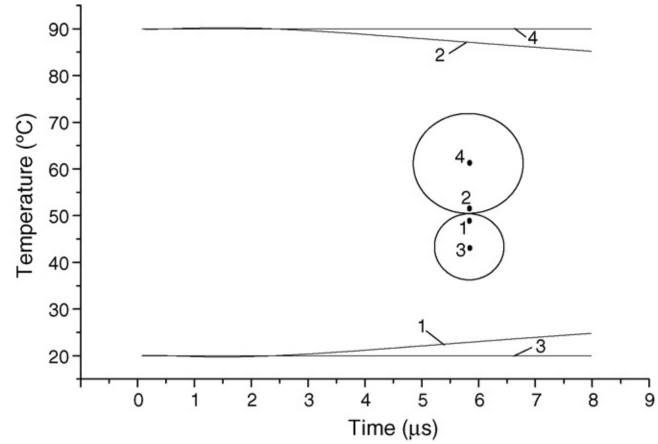

Fig. 4. Variation of temperature with time at four typical locations. The maximum contact radius is 41.30 μm, and the total contact time is 8.36 μs for this case.

Fig. 4 shows the temperature variations with time at four typical positions. Positions 1 and 2 are near the contact area (the distance between position 1 (or position 2) and the contact surface is 12 μm) whereas positions 3 and 4 are located at the centers of the two particles. It can be seen that temperature variation is confined in a small region around the contact area. This is further confirmed by Fig. 5 which shows the temperature distribution at the half time during one collision. Only the temperature distribution in the vicinity of the contact area is shown since the temperatures at the particle centers are almost unchanged after one collision. This is expected since the heat exchange after one single collision is very small (in the order of 10^{-6} J).

Sun and Chen [5] derived an analytical equation to calculate the heat exchange (e) between colliding spheres based on the well established "semi-infinite-media assumption". Their equation is given by

$$e = Ce_0 \tag{19a}$$

and

$$e_0 = \frac{0.87(T_2 - T_1)\pi r_c^2 t_c^{1/2}}{(\rho_1 c_1 k_1)^{-1/2} + (\rho_2 c_2 k_2)^{-1/2}} \tag{19b}$$

where parameter C can be determined graphically as given by Sun and Chen [5].

Fig. 6 shows the comparison of the calculated heat exchange obtained by the present FEM simulation. It can be seen that the results obtained by the present FEM simulation agree well with those obtained by Sun and Chen for the cases of small Fourier number Fo. However, when the Fourier number is high, the analytical model proposed by Sun and Chen will overestimate the heat exchange. Clearly, the reason for this stems from their semi-infinite-media assumption. Another deficiency of their approach is that graphic solution has to be used for C, which is not convenient for numerical calculation for a particle system which often involves many simultaneous collisions between particles and various heat transfer mechanisms [2,6,13,19]. The conduction due to the collision between particles is one of the heat transfer mechanisms that should also be considered properly in

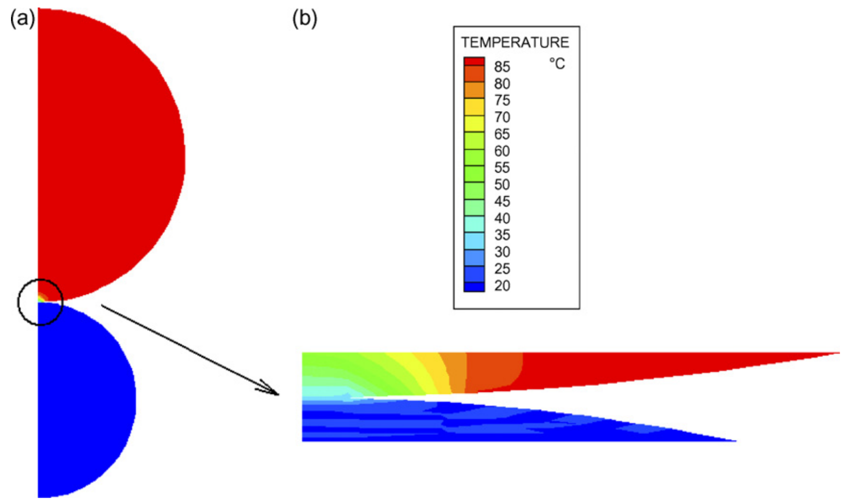

Fig. 5. Temperature distribution in the vicinity of contact area at the half time during one collision: (a) in the whole region and (b) in the vicinity of the contact area.

order to describe the heat transfer comprehensively. Therefore, there is a need to modify their equation. This can be achieved based on the present FEM results.

Fig. 7 shows the plot of the ratio between the heat exchange e' obtained by the present FEM simulation and e_0 given by Eq. (19). It can be seen that e'/e_0 increases with the increase of Fo number or ρ_1c_1/ρ_2c_2 ratio. By fitting the FEM results, a modified equation has been formulated to calculate the heat exchange during particle collision, given by

$$e' = \frac{C'(T_2 - T_1)\pi r_c^2 t_c^{1/2}}{(\rho_1 c_1 k_1)^{-1/2} + (\rho_2 c_2 k_2)^{-1/2}} \tag{20}$$

where coefficient C' is computed by

$$C' = \frac{0.435\left(\sqrt{C_2^2 - 4C_1(C_3 - Fo)} - C_2\right)}{C_1} \tag{21}$$

and

$$C_1 = -2.300\left(\frac{\rho_1 c_1}{\rho_2 c_2}\right)^2 + 8.909\left(\frac{\rho_1 c_1}{\rho_2 c_2}\right) - 4.235 \tag{22a}$$

$$C_2 = 8.169\left(\frac{\rho_1 c_1}{\rho_2 c_2}\right)^2 - 33.770\left(\frac{\rho_1 c_1}{\rho_2 c_2}\right) + 24.885 \tag{22b}$$

$$C_3 = -5.758\left(\frac{\rho_1 c_1}{\rho_2 c_2}\right)^2 + 24.464\left(\frac{\rho_1 c_1}{\rho_2 c_2}\right) - 20.511 \tag{22c}$$

Fig. 8 shows the comparison between the FEM results and those obtained by the modified equation. It is evident that the error arising from the semi-infinite-media assumption, as observed in Fig. 4, can be eliminated with this modified equation.

Eq. (20) is formulated for the case $k_1 = k_2$. Strictly speaking, it is only applicable to the conditions specified. On the other hand, it is noticed that this equation is just a modified equation derived from the semi-infinite-media theory which has taken into account the effects of variables such as particle density, thermal capacity and conductivity, and temperature difference between colliding particles. Moreover, the collision mechanics, which may involve particles of different mechanical properties, can be taken into account with the Hertz theory. Therefore, Eq. (20) may be used more generally, e.g. for smooth spherical par-

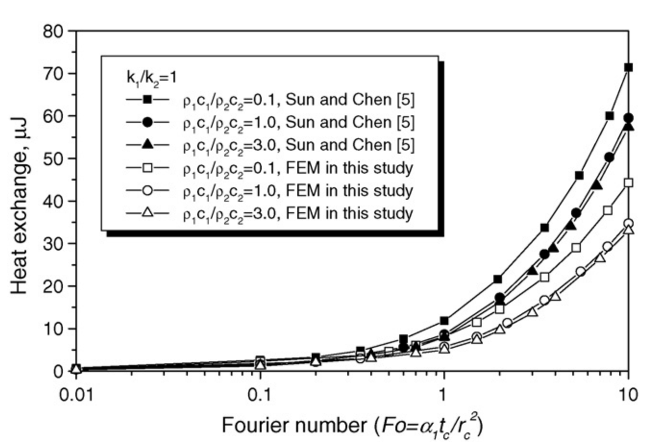

Fig. 6. Heat exchange as a function of Fourier number Fo for different ρ_1c_1/ρ_2c_2 ratios.

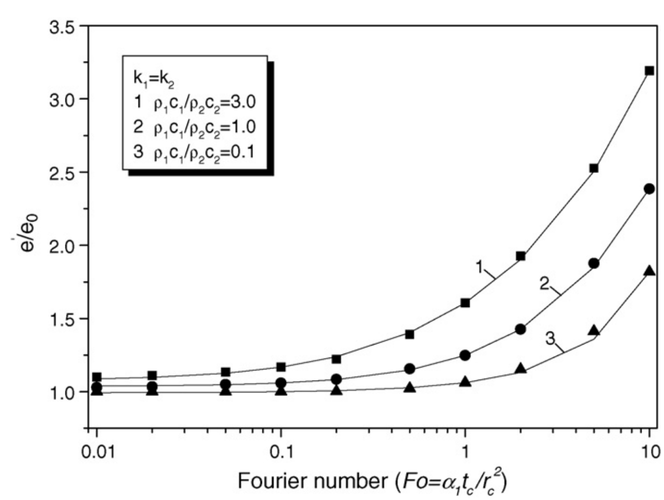

Fig. 7. Heat exchange ratio e'/e_0 as a function of Fourier number and ρ_1c_1/ρ_2c_2 ratio.

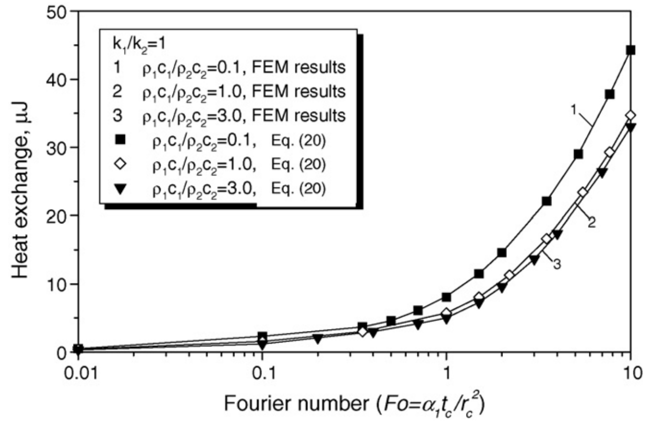

Fig. 8. Comparison between the results by Eq. (20) and the FEM results for $k_1 = k_2$.

ticles for Fourier number up to 10 as used in the present FEM study. To test its applicability, the FEM method has been used to calculate the heat exchange during particle collision when the two particles have different thermal conductivities or other physical properties. Fig. 9 shows the results for different thermal conductivity ratios. They show that the heat exchange increases

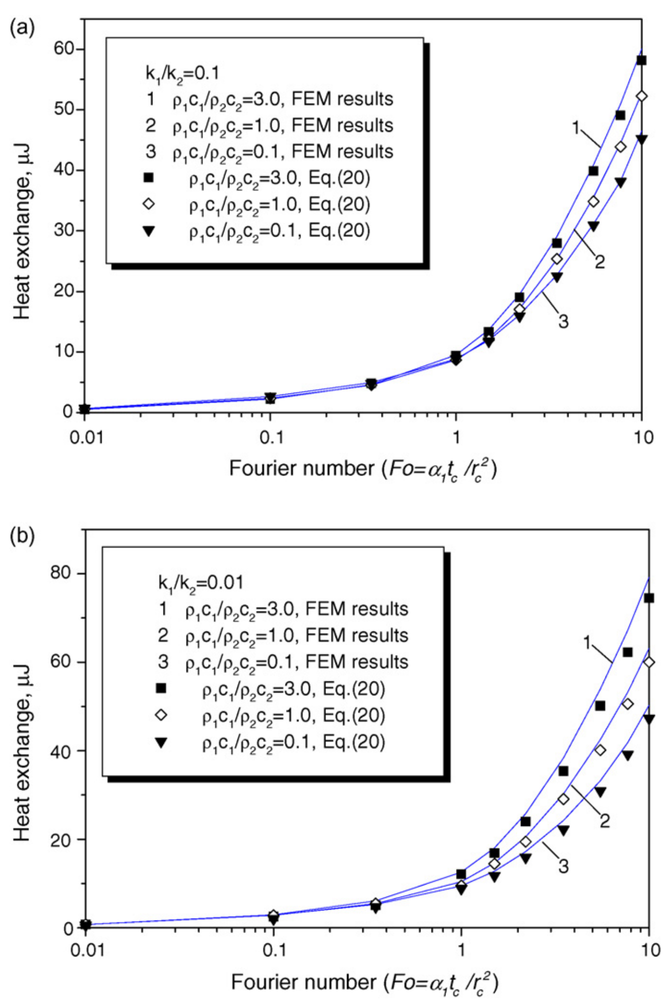

Fig. 9. Comparison between the results by Eq. (20) and the FEM results for $k_1 \neq k_2$: (a) $k_1/k_2 = 0.1$; and (b) $k_1/k_2 = 0.01$.

with the increase of the Fourier number and $\rho_1 c_1/\rho_2 c_2$, but its variation rate decreases as k_1/k_2 decreases. Eq. (20) can describe the behaviour reasonably, although it overestimates the heat flex when the difference in thermal conductivity is very significant, as seen from this figure. Thus, it can be used as a first approximation in engineering application. To be more accurate, Eq. (21) should be reformulated based on the data generated by the FEM approach which is much more general in nature. In this connection, further work has been planned to extend the approach to consider the effects of other variables such as the roughness of particle surface and the existence of gas layer near contact point.

4. Conclusions

Finite element method has been used to simulate the transient heat conduction between colliding spheres of different temperatures. The transient temperature distribution in a particle and the overall heat exchange are obtained. It is confirmed that the variation of temperature is confined in the vicinity of contact area. The results show that the applicability of the semi-infinite-media assumption, as used by Sun and Chen [5], mainly depends on the Fourier number. When the Fourier number is small, the semi-infinite-media model can give satisfactory prediction. But when the Fourier number is high, this model will overestimate the heat exchange. Another deficiency of their approach is that the graphic solution rather than a full analytical equation was provided, which is not suitable for implementation in discrete particle simulation. Based on the FEM results, a modified equation has been proposed to overcome this deficiency. The proposed FEM approach and the modified equation should be useful in the microscopic study of the heat transfer in particle systems involving smooth spherical particles with temperature-independent thermal properties. In fact, in connection with the previous efforts [2,6,10,13], the modified equation, together with other equations to count for other heat transfer mechanisms, has been incorporated in our discrete particle simulation of coupled fluid and heat transfer in fluidized beds [19]. Efforts are currently being made to extend the present model to a nonlinear finite element method such that the heat conduction between two rough particles with temperature-dependent thermal properties can be simulated.

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