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# Discrete element method for high-temperature spread in compacted powder systems

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ABSTRACT

The discrete element method is applied to investigate high-temperature spread in compacted metallic particle systems formed by high-velocity compaction. Assuming that heat transfer only occurs at contact zone between particles, a discrete equation based on continuum mechanics is proposed to investigate the heat flux. Heat generated internally by friction between moving particles is determined by kinetic equations. For the proposed model, numerical results are obtained by a particle-flow-code-based program. Temperature profiles are determined at different locations and times. At a fixed location, the increase in temperature shows a logarithmic relationship with time. Investigation of three different systems indicates that the geometric distribution of the particulate material is one of the main influencing factors for the heat conduction process. Higher temperature is generated for denser packing, and vice versa. For smaller uniform particles, heat transfers more rapidly.



## Introduction

Many studies have modeled heat transfer in powder media. For systems with small particles, such as nanoparticles, numerical methods based on the continuous medium hypothesis are well established (Rahimi-Gorji, Pourmehran, Hatami, & Ganji, 2015). The Galerkin method, least square method (LSM), and computational fluid dynamics (CFD) are used to calculate the temperature distributions of nanofluids and porous media, and they provide accurate results (Pourmehran, Rahimi-Gorji, Hatami, Sahebi, & Domairry, 2015; Pourmehran, Rahimi-Gorji, Gorji-Bandpy, & Gorji, 2015). However, modeling heat transfer in systems that contain millimeter-sized solid particles remains a challenge. In some applications, such as packed beds, interactions between particles are more complicated, the positions of particles instantaneously change, and the influences of the friction of particles and surface roughness cannot be ignored (Chaudhuri, Muzzio, & Tomassone, 2006; Guo & Dai, 2010). High-velocity compaction (HVC) is a new technique for metal powder formation proposed by Hoaganas AB Company (Skoglund, 2001). In HVC, metal powders are compressed by high-energy impact from a hammer at speeds of 2–30 m/s. Because of the high energies involved in dynamic compaction, the process inherently induces adiabatic heating with thermal softening of the powder and even melting at particle contacts, giving good pressed compact properties, such as high and homogenous density, and low elastic after-work (Sethi, Hauck, & German, 2006). High temperature affects compacted powder systems in various ways. At high-energy loading, heat can be generated in shear bands because of friction between particles. Temperature increase in a sample reduces the maximum tensile stress, thereby effectively suppressing brittle failure (Zhou, Rosakis, & Ravichandran, 1996). Therefore, knowing the thermal conductivity of powder materials is essential to provide theoretical evidence for further investigation, experiments, and production. The irregular arrangement and heat dissipation in particles significantly affect the heat transfer process in powder materials. Only a few good simulation methods have been developed to investigate the effect of high temperature on compacted powder systems. Although the temperature can be obtained by continuum models, the complexity of powder materials leads to difficulties in the calculations.

The discrete element method (DEM) is an effective numerical approach to simulate the physical behavior of noncontinuous materials. The method considers interaction of a number of discrete semirigid spherical or polyhedral shaped particles through contact or noncontact forces, and tracks the movement of each particle using Newton's equations. The interactions between particles are described by specific contact constitutive relations. A new equilibrium state of the granular system is then obtained by

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**Nomenclature**

| | |
|---|---|
| $C_V$ | specific heat at constant volume (J/(kg K)) |
| $E$ | elastic modulus |
| $F_n$,$F_t$ | normal force and shear force (N) |
| $I$ | principal moment of inertia (kg m$^2$) |
| $k_s$,$k_f$ | thermal conductivity (W/(m K)) |
| $M$ | resultant moment (N m) |
| $\mathbf{q}$ | heat flux vector (W/m$^2$) |
| $T$ | temperature (°C) |
| $R$ | radius (m) |
| $u_n$ | normal expansion amount or overlap (m) |
| $\rho$ | mass density (kg/m$^3$) |
| $\alpha$ | thermal expansion coefficient (K$^{-1}$) |
| $\mu$ | friction coefficient |
| $\nu$ | Poisson's ratio |

updating the spatial position of each particle by solving the state equation using the finite difference method. DEM has established itself as an important simulation technique for engineering applications involving large granular deformable systems (Cundall, 2002; Iordanoff, Richard, & Tcherniaieff, 2008). Although thermal and mechanical systems are completely different, they are regarded as equivalent systems because of the interchangeable nature of force (mechanical system) and heat (thermal system) in their diffusional forms (Hahn, Schwarz, Kröplin, & Wallmersperger, 2011).

The temperature variation of each particle can be tracked by constructing partial differential equations and then solving them by Fourier transformation. In addition, the heat flux surface at the boundary of particles can be described by specific contact relations (Sun & Chen, 1988; Vafai & Tien, 1981). Many researchers have used this local modeling method to simulate and determine the thermal conductivity within a granular material flow containing solid fractions from 0.015 to 0.68 (Argento & Bouvard, 1996; Hunt, 1997). DEM has also been used to obtain dynamic temperature distributions of particle systems that are similar to colliding particles in vacuum, where the heat transfer by convection within the packed-bed particles can be ignored (Sridhar & Yovanovich, 1994; Vargas & McCarthy, 2001). Because the fundamental research has already been performed, some applications have recently been reported for simulation of transient heat conduction in fluidized particulate beds, rotary kilns, and sintering processes (Li & Mason, 2000). DEM–CFD models have been developed for particle phases and particle–fluid interactions to predict the effective thermal conductivity of particulate beds under compression, and a CFD simulation has been performed to investigate the complex interior structure of a packed bed (Guo & Dai, 2010; Tsory, Ben-Jacob, Brosh, & Levy, 2013). However, few studies have focused on application of high-temperature spread in compacted particle systems.

We have previously developed DEM models to account for the momentum and press force of the particle flow process in HVC (Wang, Zheng, & Zhou, 2011; Zheng, Wang, Zheng, & Qu, 2010). In this study, the heat transfer model is coupled into our DEM formulation. A two-dimensional cylindrical bed packed with metallic particles is simulated. The contact forces between particles are calculated by Hertz's kinetic theorem (Matuttis, Luding, & Herrmann, 2000).

## Mathematical models

### *Basic hypothesis*

Each particle is considered to be a dense disk element. The density is considered to be uniform. The heat transfer process is an irreversible process, in which thermal conduction is expected to dominate and occur through contact areas between particles. According to Vargas and McCarthy (2001), this assumption is valid as long as $k_s a/k_f r \gg 1$, where $k_s$ is the thermal conductivity of the powder material, $k_f$ is the thermal conductivity of the interstitial medium, $a$ is the contact area between metal particles, which is given in Eq. (8), and $r$ is the radius of the spherical particles. The interstitial medium is air, whose thermal conductivity is 0.023 W/(m K) under steady-state conditions, and the thermal conductivity of iron-based metallic particles is 80 W/(m K). In this study, the ratio of $k_s$ to $k_f$ is always greater than 1.

### *Governing equations for the heat conduction process*

Assuming that changes in strain do not affect the temperature, the heat conduction equation for a continuum particle is given by

$$\rho C_V \frac{dT}{dt} = -\nabla \cdot \mathbf{q} + \gamma, \tag{1}$$

where $\rho$ is the mass density (kg/m$^3$), $C_V$ is the specific heat at constant volume (J/(kg K)), $T$ is the temperature (K), $\mathbf{q}$ is the heat flux vector (W/m$^2$), and $\gamma$ represents the additional heat source (W/m$^3$). Integrating Eq. (1) over the target volume element gives

$$V\rho C_V \frac{dT}{dt} = -\int_V \nabla \cdot \mathbf{q}\ dV + \int_V \gamma\, dV. \tag{2}$$

According to the Gauss divergence theorem, for a closed surface surrounding the target particle, the volume integral is converted to the surface integral:

$$\int_V \nabla \cdot \mathbf{q}\ dV = \int_S \mathbf{q} \cdot \mathbf{n}\ dS, \tag{3}$$

where $\mathbf{n}$ is the unit normal vector with respect to the surface. If the particles are closely compacted, heat will flow mainly through the contact areas between particles. Therefore, the surface integral can be replaced by a summation. Suppose that the number of particles in contact within the target volume element is $N$ and subscript $i$ representing the physical quantity of the target particle is omitted, then

$$\int_S \mathbf{q} \cdot \mathbf{n}\ dS = \sum_{j=1}^{N} q_{ij} n_j\ \Delta S_{ij} = \sum_{j=1}^{N} Q_{ij}, \tag{4}$$

where $n_j$ is the unit normal vector of contact surface $S_{ij}$ and $Q_{ij}$ is the heat intensity flowing from the center-line of particle $i$ to particle $j$.

Letting $Q_{Vi} = \int_V \gamma\, dV$ and $m = V\rho$ in Eq. (2) gives the following heat conduction equations for the discrete system:

$$m_i C_V \frac{dT_i}{dt} = -\sum_{j=1}^{N} Q_{ij} + Q_{Vi}. \tag{5}$$

The time derivative is approximated by up-forward differences. According to Eq. (5), the temperature of the target element at time $t + \Delta t$ can be obtained by

$$T_i(t + \Delta t) = T_i(t) + \frac{-\sum_{j=1}^{N} Q_{ij} + Q_{Vi}}{m_i C_V} \Delta t, \tag{6}$$

where $\Delta t$ is the time step. By repeating the operation for all of the particles, the temperatures are updated for successive $\Delta t$.

### *Heat exchange relationship for two adjacent particles*

The heat intensity at the boundary of particles can be described by specific contact relations, which account for both granular heat

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