CALCULATION OF EFFECTIVE THERMAL CONDUCTIVITY OF POWDER BED SYSTEMS USING SMOOTHED PARTICLE HYDRODYNAMICS METHOD

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ABSTRACT
A method to solve thermal transport problems while taking into account the thermal contact conductance at interfaces between individual powder particles and between particles and an ambient medium is developed based on the Smoothed Particle Hydrodynamics approach. The developed method is applied to study the effective thermal conductivity of two-dimensional powder bed systems with parameters typical for powder bed fusion additive manufacturing of metallic parts. The simulations show that the effective thermal conductivity of loose powder bed systems is limited by the thermal contact conductance at interfaces between individual powder particles.

NOMENCLATURE

\[ B_{w} \] \quad thickness of heat bath, m

\[ B_{i} \] \quad Biot number

\[ H \] \quad domain height, m

\[ L \] \quad domain width, m

\[ R \] \quad powder radius, m

\text{SPH} \quad \text{Smoothed Particle Hydrodynamics}

\[ T \] \quad temperature, K

\[ T_{L} \] \quad temperature of left heat bath, K

\[ T_{R} \] \quad temperature of right heat bath, K

\[ W \] \quad kernel function, m^{-3}

\[ c \] \quad heat capacity per unit mass, Jkg^{-1}K^{-1}

\[ f \] \quad volume fraction

\[ h \] \quad smoothing length, m

\[ k \] \quad thermal conductivity, Wm^{-1}K^{-1}

\[ k_{e} \] \quad effective thermal conductivity, Wm^{-1}K^{-1}

\[ m \] \quad mass, kg

\[ r \] \quad position vector, m

\[ \Delta x \] \quad spatial distance between two SPH particles in x and y-direction, m

Greek symbols

\[ \delta \] \quad parameter controlling the degree of overlap between powder particles

\[ \rho \] \quad density, kgm^{-3}

\[ \sigma \] \quad contact conductance coefficient, Wm^{-2}K^{-1}

Subscripts

\[ i \] \quad index of SPH particle

\[ j \] \quad index of neighbor SPH particle

\[ l \] \quad index of interface particle

\( (m) \) \quad properties of background medium

\( (p) \) \quad properties of powder material

\( (s) \) \quad properties of either powder material \((s = p)\) or background medium \((s = m)\)

INTRODUCTION
Selective Laser Melting (SLM) and Selective Laser Sintering (SLS) are amongst the primary approaches for additive manufacturing of metal parts by successive deposition of layers of metallic powders and their heating by a laser beam for melting in SLM and sintering in SLS. Computational modelling of the temperature field in the powder bed and tuning of the process parameters require accurate calculations of the effective thermal conductivity of the powder bed.

In powder bed fusion, the size of powder particles ranges from microns to hundreds of microns [1]. Powder particles have small areas of contact with each other, which serve as “bottlenecks,” limiting thermal transport in the powder bed. As a result, the effective thermal conductivity across the powder bed is significantly reduced compared to thermal conductivity of the bulk material. Another reducing factor is the thermal contact resistance at the inter-particle and particle-medium interfaces. The thermal contact resistance at interfaces is especially important for loose powder systems and powders composed of particles with rough surfaces or small, sub-micron particles.

The main purpose of the present work is to develop a numerical method which is capable of predicting the effective thermal conductivity of powder bed systems in vacuum or in the presence of a background medium based on the Smoothed
Particle Hydrodynamics (SPH) approach. The SPH is a general-purpose Lagrangian meshless, particle-based numerical approach for solving continuum equations of fluid and solid mechanics, and heat transfer [2–4]. In this approach, the material is represented by a set of particles (SPH particles) interacting with each other via some “force field,” which is derived directly from the equations of continuum mechanics and describes the mass, momentum, and energy exchange between SPH particles. As a meshless approach, the SPH method is especially useful for systems with topologically complex interfaces like interfaces in powder systems or porous media. Although, it has been used to predict the thermal conductivity of powder systems [5], the effect of finite thermal contact conductance has not been taken into account so far in SPH calculations of thermal transport.

In the present paper, a special form of the SPH force field is developed in order to describe the exchange of thermal energy through heat conduction inside particles and ambient medium, and to explicitly account for the finite thermal contact conductance at the interfaces. The developed method is then applied for simulations of thermal transport and calculations of the effective thermal conductivity in two-dimensional static powder systems with random distributions of particles.

**COMPUTATIONAL MODEL OF TWO-DIMENSIONAL THERMAL TRANSPORT IN POWDER SYSTEMS**

Two-dimensional random distributions of circular particles of radius $R$ are generated by an acceptance-rejection algorithm (Figure 1). Individual particles are added to the computational sample on a one-by-one basis until the desired value of the powder volume fraction $f$ is achieved. For every new particle $i$, the position vector of its center $\mathbf{r}_i$ is first generated at random inside a rectangular domain of width $L$ and height $H$. Next, it is checked that the new powder particle center lies sufficiently far from center of all existed particles. Namely, if the condition $|\mathbf{r}_i - \mathbf{r}_j| > 2R(1 - \delta)$ (here $\delta$ is a small parameter controlling the degree of overlap of particle volumes) is satisfied for every existing particle $j$, then particle $i$ is added to the sample, otherwise particle $i$ is rejected and a new random position vector is generated. Periodic boundary conditions in the $y$-direction are used during sample generation and calculations of thermal transport. The space between generated particles is assumed to be a vacuum or filled with a background medium.

In order to calculate an effective thermal conductivity for the generated sample, the sample is first placed between two heat baths of thickness $B_w$ with fixed temperature $T_L$ and $T_R$. A steady-state temperature field inside the powder and background medium is then calculated. Heat energy flow between the heat baths is governed by thermal conduction within the powder and background medium and by thermal contact conductance between powder particles in contact and between powder particles and medium. The thermal conduction within the powder material or the ambient medium is described by the heat conduction equation

$$\rho(s)c(s) \frac{dT}{dt} = \nabla \cdot (k(s) \nabla T) \quad (1)$$

where $T$ is temperature, $t$ is time, $c(s)$ is the heat capacity per unit mass, $\rho(s)$ is the density, $k(s)$ is the thermal conductivity, and subscript “(s)” marks the properties of either powder material ($s = p$) or background medium ($s = m$).

The heat flux through the contact between two powder particle or particle-medium interface is equal to [8]

$$q = \sigma \Delta T \quad (2)$$

where $\sigma$ is the contact thermal conductance and $\Delta T$ is the temperature jump across the interface. In the present paper, Equation (2) was applied only at particle-particle interfaces, while no temperature jumps and zero contact resistance are assumed at powder-medium interfaces. In the case of simulation of a powder system in vacuum, the heat flux at particle-vacuum interfaces is assumed to be zero.

![Figure 1. Sketch of the computational domain for simulations of thermal transport in two-dimensional powder systems.](image)

Once the steady-state temperature distribution is found, the total heat flux $Q$ through any cross-section of the sample is constant. Then the effective thermal conductivity $k_e$ of the system is calculated based on the Fourier law

$$Q/H = -k_e \langle \nabla T_a \rangle \quad (3)$$

where $\langle \nabla T_a \rangle$ is the gradient of average temperature. In order to calculate $\langle \nabla T_a \rangle$, the domain is divided into a number of one-dimensional columnar cells along the $x$-direction. The average temperature of each cell is calculated by taking the average of the temperatures of all SPH particles belonging to it. Assuming that the distribution of average temperature $T_a(x)$ is linear in a central part of the sample between $x = x_*$ and $x = L - x_*$, the gradient is then calculated as $\langle \nabla T_a \rangle = [T_a(x_*) - T_a(L - x_*)] / L$. 

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The effective thermal conductivity $k_e$ is related to the thermal conductivity $k$ of the powder material by

$$k_e = \frac{k}{f} \quad (4)$$

where $f$ is the powder volume fraction.

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The resulting thermal conductivity is then calculated by

$$k_e = \frac{k}{f} \quad (4)$$

where $f$ is the powder volume fraction.
The preliminary simulations showed that for the conditions considered in the present paper and $B_0/L \leq 0.1$, the choice of $x_s/L = 0.15$ ensures accurate calculation of $\nabla T_0$.

**SPH FORMULATION OF THE THERMAL TRANSPORT PROBLEM**

Following the SPH approach, every powder particle or space filled with the ambient medium is divided into a number of SPH particles. In the present work, the SPH particles are placed in nodes of a square mesh with the cell size $\Delta x$. The standard SPH kernel function $W(r, h)$ in the form of cubic splines [6]

$$W(r, h) = a_d \begin{cases} \frac{2}{3} - \hat{r}^2 + \frac{1}{2} \hat{r}^3, & 0 \leq \hat{r} < 1 \\ \frac{1}{6} (2 - \hat{r})^3, & 1 \leq \hat{r} < 2 \\ 0, & \hat{r} \geq 2 \end{cases}$$

is used in calculations, where $r$ is the distance between two SPH particles, $h = \sqrt{2}\Delta x$ is the smoothing length, $\hat{r} = r/h$, and value of $a_d = 15/7\pi h^2$ is given by the normalization condition for the kernel function [4]. With this implementation of $W$, a SPH particle $i$ can interact with other SPH particles that lie within a circle of radius $2h$, with the center in point $r_i$. This circle is known as the support domain of particle $i$ [2–4].

The SPH particles carry properties of the representing material, thus every SPH particle $i$ has its own density $\rho_i$, mass $m_i$, and thermal conductivity $k_i$. Then, for homogeneous material, the SPH approximation for the right-hand-side term in Equation (1) can be written as follows [7]

$$\nabla \cdot (k_i \nabla T) \big|_i = \frac{2}{V_i} \sum_j \left( \frac{m_j}{\rho_j} k_j |r_{ij}|^2 \nabla W_{ij} \right) \left( T_i - T_j \right)$$

where $j$ is the index of SPH particles belonging to the support domain of particle $i$, $r_{ij} = r_i - r_j$, $W_{ij} = W(|r_{ij}|, h)$, and $\nabla W_{ij}$ is the gradient of the kernel function with respect to coordinates of particle $i$. The efficient $2k_j/(k_i + k_j)$ allows one to apply Equation (5) to materials with a strong dependence of thermal conductivity on temperature or for multi-material systems.

Equation (5) can be applied only if the temperature field $T(x, y, z)$ in the support domain of particle $i$ is the doubly differentiable function of coordinates. This equation cannot be used if an interface with finite thermal contact conductance crosses the support domain since the temperature field is discontinuous at such an interface in accordance with Equation (2). For SPH particles lying in the vicinity of the interface, Equation (5) should be replaced with a more general equation that explicitly accounts for the boundary condition at the interface given by Equation (2).

In the present work, the SPH approximation of the right-hand-side term in Equation (1) is obtained based on the integral representation of the $\nabla \cdot (k_i \nabla T)$, the approach that was initially used to derive Equation (5) [7]. In order to find temperature jumps at interfaces, special interface particles are introduced as illustrated in Figure 2. Contrary to “regular” SPH particles, the interface particles do not carry mass and their properties are calculated by the SPH interpolation of parameters of surrounding SPH particles. The SPH approximation for the right-hand side in Equation (1) now takes the form

$$\nabla \cdot (k_i \nabla T) \big|_i = \frac{2}{V_i} \left( \sum_j \left( \frac{m_j}{\rho_j} k_j |r_{ij}|^2 \nabla W_{ij} \right) \left( T_i - T_j \right) \right)$$

where $V_i$ is the integral of the SPH kernel function $W_{ij}(r) = W(|r_i - r_j|, h)$ over the part of the support domain belonging to the same powder particle, $l$ is the index of interface particles in the support domain, $T_{i(l)}$ is the temperature of interface particle $l$ at the side of SPH particle $i$, $T_{i(\ell)}$ is the temperature of interface particle $l$ at the another side of the interface, $W_l = W(|r_i - R_l|, h)$, $R_l$ is the position vector of interface particle $l$, and $\Delta s_l$ is the length of the part of the interface corresponding to particle $l$. The temperatures $T_{i(l)}$ and $T_{i(\ell)}$ are calculated by means of a one-side SPH interpolation of temperatures of “regular” SPH particles around interface particle $l$. Unlike atomistic simulations, the interface is treated as a temperature discontinuity rather than very thin layer with high temperature gradient, and the contact conductance $\sigma$ in Equation (2) is assumed to be a known constant.

Equation (6) can be used for all SPH particles, including particles placed far from any interfaces. If the support domain of particle $i$ is not crossed by any interface, then $V_i = 1$ and $W_l = 0$, so that for any such particle Equation (6) reduces to Equation (5). Equation (6) has been validated with two test cases with finite contact conductance at interface including one-dimensional heat transfer between two straight bars in contact and two-dimensional heat transfer across a system containing a cylinder tightly fitted inside a cylindrical shell. In

![Figure 2](image-url)
both cases, the numerical results are found to be in very good agreement with the respective exact solutions of test problems.

RESULT AND DISCUSSION

The calculations of the effective thermal conductivity were performed for SHKH15 steel powder with \( \rho(p) = 7780 \text{ kgm}^{-3}, \ c(p) = 500 \text{ Jkg}^{-1}\text{K}^{-1}, \text{ and } k(p) = 40 \text{ Wm}^{-1}\text{K}^{-1}. \) The background gas was assumed to be air with \( \rho(m) = 1.225 \text{ kgm}^{-3}, \ c(m) = 1000 \text{ Jkg}^{-1}\text{K}^{-1}, \text{ and } k(m) = 0.0258 \text{ Wm}^{-1}\text{K}^{-1}. \) and volume fraction of particles \( f = 0.717. \) The thermal contact conductance \( \sigma \) at the inter-particle interfaces was varied in all simulations. The numerical parameters took the following values: \( H/R = L/R = 32, \ T_L = 300 \text{ K}, \ T_R = 280 \text{ K}, \ B_{\text{max}}/L = 0.075, \ \delta = 0.15, \ L/\Delta x = 200, \text{ and } h = \sqrt{2}\Delta x. \) The sample shown in Figures 3-5 consisted of 243 powder particles, which are discretized into 28691 SPH particles. For the case of powder in air (Figure 3), the ambient gas is represented by 11309 SPH particles.

Figure 3 shows the temperature field in the powder bed in the presence of a background gas, while Figure 4 shows the temperature field in the same powder system in a vacuum. These results are obtained at zero thermal contact resistance, i.e. assuming no temperature jumps at interfaces and using Equation (5). The values of the effective thermal conductivity \( k_e \) obtained in these two simulations correspond to the solid and dash lines in Figure 6. The contribution of the background gas to the total conductivity of the system is small since \( k(m)/k(p) \sim 5 \cdot 10^{-4}. \)

The effect of the finite thermal contact conductance on the overall conductivity of the sample can be characterized by the Biot number for an individual particle, which is the ratio of the contact conductance to the conductance of the bulk material \[ Bi = \frac{\sigma L_c}{k(p)} \] (7)

where \( L_c \) is the characteristic length that is defined by the ratio of volume to surface area of the body, and for circular particles of radius \( R \) it is equal to \( R/2. \) The case of \( Bi = 0 \) corresponds to the thermally insulating interfaces between particles, when, in the absence of the background medium and \( H > R, k_e \) is equal to zero. The case of \( Bi \to \infty \) corresponds to the zero contact thermal resistance.

Figure 5 demonstrates the temperature field for the powder system in vacuum obtained at \( Bi = 0.1. \) At this Biot number, the
finite thermal conductance at inter-particle interfaces results in a pronounced difference in the temperature when compared to the field in the same sample obtained at $Bi \to \infty$ as shown in Figure 4. At the adopted value of powder volume fraction $f$, the connectivity in the random samples is poor, so that the powder sample shown in Figures 4 and 5 contains multiple particles or clusters of particles, which are not connected to the percolating part of the sample. In numerical simulations, the temperature field in such particles is determined by the adopted initial condition, when the temperature distribution in the $x$-direction is assumed to be linear, between $T_L$ and $T_R$.

Values of the effective thermal conductivity calculated in the range of Biot numbers from 0.01 to 1 are shown in Figure 6 by square symbols. With increasing $Bi$, these values approach the dashed line that corresponds to the case of $Bi \to \infty$. The dependence of $k_e/(fk_{(m)})$ exhibits a power scaling with $Bi$ in the considered range of Biot numbers. The effective thermal conductivity in reduced units is the function of $f$ and $Bi$ only, so that the obtained results can be re-scaled for arbitrary particles size.

CONCLUSION

The developed SPH-based numerical method is found to be an effective tool for computational prediction of the effective thermal conductivity of powder bed systems, when finite thermal conductance at the inter-particle interfaces is taken into account. The simulations of two-dimensional powder systems showed that when the Biot number, based on the radius of individual powder particle, is less than 1, the contact thermal conductance dominates the thermal transport. Such conditions are specific for loose systems of micron-size particles or for powders composed of nanoparticles. The developed approach can be generalized for three-dimensional powder systems as well as arbitrary porous materials.

ACKNOWLEDGEMENTS

This work is supported by the NSF CAREER award CMMI-1554589. The computational support is provided by the Alabama Supercomputer Center.

REFERENCES