

Thermo-mechanical Behavior of Confined Granular Systems

Gülşad Küçük, Marcial Gonzalez and Alberto M. Cuitiño

Abstract We present a mathematical formulation that integrates thermal contact and Hertzian deformation models to understand the thermo-mechanical behavior of consolidated granular systems. The model assumes quasi-static equilibrium and quasi-steady heat conduction conditions that are appropriate for many thermally-assisted manufacturing processes. We perform a parametric study that explores the effect of applied thermal and mechanical loads, and of particles' thermal expansion. The nonlinearity of the multi-physics problem reveals that thermo-mechanical coupling enhances the effective thermal conductivity and mechanical stiffness by directly impacting the interrelation between contact conductance and overlapping between the particles. Alterations in temperature profiles and displacements of particles are significant for materials with higher thermal expansion coefficients. In this regards, it is worth noting that the results of the proposed thermo-mechanical model depart from those of conventional compaction models based on a continuum mechanics description.

1 Introduction

Understanding the fundamental multi-physics behind the thermo-mechanically coupled deformation of granular systems and its projections in macroscopic scale provides the essentials to fabricate particulate assemblies with specific functionalities.

G. Küçük (✉) · A.M. Cuitiño
Department of Mechanical and Aerospace Engineering, Rutgers University,
Piscataway, NJ 08854, USA
e-mail: gulsad@gmail.com

A.M. Cuitiño
e-mail: alberto.cuitino@rutgers.edu

M. Gonzalez
School of Mechanical Engineering, Purdue University, 585 Purdue Mall,
West Lafayette, IN 47907-2088, USA
e-mail: marcial-gonzalez@purdue.edu

A proper estimate of the mechanical strength, and of the thermal and electrical conductivity of a compacted solid is contingent upon the knowledge of microstructure formation during the deformation stage of the compression. Since thermally assisted compaction of granular matter is of great importance for a wide set of manufacturing processes, theoretical modeling and numerical simulations serve as significant tools to forecast the macroscopic behavior of materials, essentially when experimental techniques are also unfeasible.

At present, one of the most implemented methodologies to elucidate the collective behavior of particulate materials is the continuum mechanics approach, in which the granular material is assumed to be statistically homogenous [1]. This is achieved by treating the system as units of ordered groups, simulating disordered arrangements by statistical correlation functions or using empirical correlations. The statistical averaging technique provides homogenized solutions of the highly heterogeneous granular media at the cost of imposing two assumptions: (i) affine motion approximation, namely the motion of each grain follows the macroscopic strain, and (ii) well-bonded structure, contact number and positioning do not change under the applied load. Despite the fact that the effective medium theory particularly estimates the effective elastic moduli of packed bed of spherical particles to a large extent, the discrepancy between numerical and experimental results is remarkable. Makse and co-workers questioned the relevance of force laws defined at single contact level, where they pointed out that the simplification done in effective medium theory is the misleading element in the formulation [2, 3]. Affine motion assumption demolishes the ability of the approach to account for the relaxation and rearrangement of particles that are under shear deformation. Moreover concerning the variety of boundary conditions and geometrical effects, experimentation techniques become insufficient in providing sufficient information about the microstructure to feed empirical correlations.

The second most adopted approach treats the particles as individual bodies. Originating from particle-particle interactions based on constitutive relations of contact mechanics [4–6], the discrete element method has been widely used in the field of particle scale research [7]. Pioneers of this approach, Cundall and Strack introduced an explicit numerical scheme to practice the granular dynamics by defining particles' interactions over the contact networks and solving for particles' motion under the state of force balance equilibrium [8]. The integration of particle motion and energy to the macroscopic behavior of the assembly, provides the required understanding of overall behavior of the confined material [9]. The main advantage of this methodology is the capability of presenting broad information about the micro-structural arrangement of the granular media. Although there exists computational challenges to model a large number of particles system with discrete elements methods, advances in simulation techniques enhance the implementation of this approach into the field of multi-physics problems of granular systems.

Recently researchers also focus on multi-scale approaches to describe the macroscopic behavior of granular systems. Zheng and Cuitino implemented a quasi-continuum approach to bridge the gap between micro and meso scale description by using a discrete-continuum formulation of elastic-inelastic deformations occur-

ring in the post-rearrangement regime of consolidation of inhomogeneous granular beds [10]. Since this approach provides the flexibility of storing individual particle interactions in a FEM scheme, it provides the overall behavior of the entire body without losing critical information specific to microstructure. Koynov et al. presented a notable adaptation of this approach on the topic of powder compactions for pharmaceutical purposes [11]. In this study we present a new methodology to explore the family of multi-physics problems such as thermo-mechanical coupling. The method is an extension of discrete element method that accounts for the effective modeling of heat conduction, and similar in spirit to early studies of Vargas and McCarthy [12] and Feng et al. [9].

Current study incorporates early mathematical models that are developed for conforming thermal contact of elastic, spherical surfaces [13–15]. These theoretical models are validated through experimental studies [16–18]. Also there exist studies that aim to relax some of the assumptions by focusing on elasto-plastic contacts [19], or rough surfaces of non-conforming contact [20–22]. Recently the field of granular matter gained importance in the light of understanding the correlation between geometry, loading conditions and anisotropic microstructural arrangements that determine the macroscopic behavior of compacted particulate system [23]. Gonzalez and Cuitino introduced a new formulation that accounts for the interplay of nonlocal mesoscopic deformations characteristic of confined granular systems. In the absence of the classical restriction of independent contacts of Hertz law, the extended theory of nonlocal contact formulation provides predictive models at moderate levels of deformation and high confinement [24]. In their study on effects of packing grains by thermal cycling, Chen et al. [25] showed that thermal expansion, due to the imposed thermal gradient, has significant effect on the rearrangement of particle bed. Vargas and McCarthy focused on the problem of how the forces supporting the grains are distributed under the effect of thermal expansion [26].

It is the purpose of this study to suggest that insight into the nature of thermo-mechanical behavior of confined granular materials. We aim to discover the effects of thermal and mechanical coupling at the particle level and implement the required amendments to continuum level models. We present the system of governing equations, which define prescribed state of the assembly under steady state conditions, in terms of heat and force transfer between the contacting particle pairs. Owing to the fact that the nature of the problem leads to highly non-linear coupled equations, regular packing simplifies the problem and makes it mathematically traceable. Moreover we consider the analogous problem from the perspective of the conventional continuum mechanics approach. Practicing a thermo-elastic continuum model to simulate the system, we focus on the effective mechanical and transport properties to account for the unique characteristics of granular materials.

2 Particle Mechanics Approach

Our point of departure for the particle-scale description of thermo-elastic contact of spherical smooth particles is to integrate the well-known theory of Hertzian deformation, [4], and heat conduction through the common interface of deformed particles in contact, [13, 14]. Under steady state conditions, the total heat transferred to individual particle m from neighboring particles n and the total of forces acting on particle m are zero,

$$Q^m = \sum_{n \in \mathcal{N}_m} Q^{mn} = 0 \quad (1)$$

$$\mathbf{F}^m = \sum_{n \in \mathcal{N}_m} F^{mn} \mathbf{n}^{mn} = 0 \quad (2)$$

$$\mathbf{n}^{mn} = \frac{\mathbf{x}^m - \mathbf{x}^n}{\|\mathbf{x}^m - \mathbf{x}^n\|}. \quad (3)$$

where \mathbf{n}^{mn} is the unit normal vector defined from centers of particle n to particle m . \mathbf{x}^m and \mathbf{x}^n are the position of the particles.

Johnson identifies the elastic deformation of locally spherical particles that are subject to a compression load by contact mechanics considerations in his book [27]. Small-strain deformation of conforming surfaces results in a flat circle of contact area. Collinear contact force at this elastic contact of the particles m and n is defined through Young's moduli, E^m and E^n ; Poisson's ratios, ν^m and ν^n ; particle radii, R^m and R^n of particle m and n ; and overlap, γ^{mn} , between these particles,

$$F^{mn} = \frac{4}{3} E^{mn} (R^{mn})^{1/2} (\gamma^{mn})^{3/2} \quad (4)$$

where

$$R^{mn} = \left[\frac{1}{R^m} + \frac{1}{R^n} \right]^{-1} \quad (5)$$

$$E^{mn} = \left[\frac{1 - (\nu^m)^2}{E_m} + \frac{1 - (\nu^n)^2}{E_n} \right]^{-1} \quad (6)$$

$$\gamma^{mn} = R^m + R^n - \|\mathbf{x}^m - \mathbf{x}^n\|. \quad (7)$$

One particular effect of applied thermal load on the system of particles is the change in radii due to thermal expansion. Similar to previous studies in the literature [26, 28], in the present study, linear thermal expansion formulation is taken into consideration.

$$R^m = R_{ref}^m [1 + \alpha^m (T^m - T_{ref}^m)] \quad (8)$$

Here α^m is the thermal expansion coefficient, T_{ref} is the reference temperature and R_{ref}^m is the radius of particle at the reference temperature. Due to the dependence of contact geometry on the nature of thermo-mechanically coupled problem, it is expected to capture a distribution of contact area formation throughout the compacted medium.

There has been considerable research on thermal-contact models. The major heat transfer mechanisms in compacted particle beds consist of conduction through solid, conduction through the contact area between two touching particles, conduction to/from interstitial fluid, heat transfer via convection, radiation between particle surfaces, radiation between neighboring voids [12]. For a system of granular media where the thermal conductivity of the solid particles is much larger than the interstitial medium, the driving mechanisms for the heat transfer are the first two. Concerning the problem of thermally-assisted compaction of spherical particles in vacuum, we focus on the thermal contact models that consider the conduction through solid particle and through the contact area between two touching particles.

Analytical solution of the heat conduction through the solid phase of ordered spherical particles has been proposed by Chan and Tien [14] and Kaganer [15]. Moreover the problem of heat transfer regarding the compaction of particles that are in or nearly in contact is deeply investigated by Batchelor and O'Brien [13]. In an attempt to find the approximate effective thermal conductivity of ordered and randomly packed granular beds, Batchelor and O'Brien discussed the heat flux across the flat circle of contact between smooth, conforming, and elastic particles. In this study we adopt Batchelor and O'Brien's model for predicting the heat conductance, which is the ability of two touching surfaces to transmit heat through their mutual interface. Heat flux across the contact area of two spherical smooth particles is given as

$$\dot{Q}^{mn} = 2a^{mn}k^{mn}(T^m - T^n) \quad (9)$$

where k^{mn} is the arithmetic mean of the thermal conductivities of two conforming particles, and a^{mn} is the Hertzian contact area.

$$k^{mn} = \frac{1}{2} \left[\frac{1}{k^m} + \frac{1}{k^n} \right]^{-1} \quad (10)$$

$$a^{mn} = \sqrt{\gamma^{mn} R^{mn}} \quad (11)$$

The total heat flow to an individual particle, Eq. (1), is calculated by adding the heat flow at each contact of the particle between its neighboring particles Eq. 9. As discussed by the thermal contact models introduced in the literature [13, 14], Eq. (1) requires that at each contact of the individual particle, the temperature is equal to the temperature calculated at the center of the particle. In other words, the temperature does not vary significantly within the particle, which also imposes that the contact conductance at the interface of conforming particles is relatively smaller than the heat conductance within the particle.

$$\frac{2k^{mn}a^{mn}}{k^{mn}A/R^m} \ll 1 \quad (12)$$

where A is the cross sectional area, $A = \pi(R^m)^2$ and Eq. (12) defines the state of Biot number much less than 1. This assertion is applied by several authors in earlier studies [12, 29]. The condition of $a^{mn} \ll R^m$ is also enforced by the assumption of small-strain deformation of elastic bodies in contact.

2.1 Simulation Configuration

Referring to the previous experimental studies on regular and random packings of granular media, Walton points out that although the regular packing models are founded on extreme assumptions, they are capable of capturing vast majority of the characteristics of a real granular media [30]. In the present study we consider a simple cubic packing of identical elastic spheres, which are constrained between parallel planes of infinite extent. Compression load, temperature gradient are applied along the major and finite direction. Stress and heat flux are defined to only depend on externally applied thermal and mechanical loads, and weight of the particles is neglected. For such regular packings each layer of arrangement is isothermal normal to the direction of applied load. Also, since these transversely oriented particles are, at most, point contact, for each individual particle there is only one pair of contact area aligned with the direction of applied thermal and mechanical load. Due to the symmetry of the problem, it is sufficient to consider a single column of square cross-section containing the longitudinally compressed spheres together. This concept is similar, in spirit, to the work of Chan and Tien [14], who proposed the effective thermal resistance, and to the work of Walton [30] who presented a method to calculate the effective elastic moduli of such packings. The above description for the specified granular media, which is under thermally-assisted compaction, can be modeled as a chain of elastic particles, seen in Fig. 1.

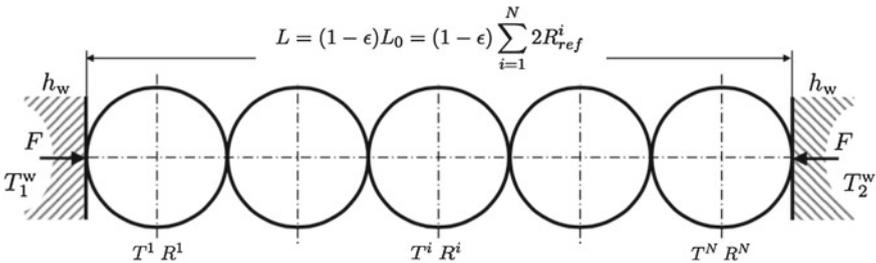


Fig. 1 Sketch of initial configuration

2.2 Wall-Particle Interaction

Given such a setting that the chain of particles is compressed between two parallel walls, which are maintained at different temperatures, the wall-particle interaction is one of the important factors of this problem. In this study, analogous to ghost-cell method, the contact between boundary particle and adjacent wall is simulated as the contact between a boundary particle and a ghost particle. Based on the rigid wall assumption, ghost particle and boundary particle are set to have the same material properties and radius. The temperature difference between the ghost particle and the wall surface is the same as the temperature deviation between the wall surface and the boundary particle. The boundary wall is assumed to be located in the midst of these symmetrically deformed particles. The temperature difference, overlap and contact area are formulated in Eqs. (13)–(15), where T^{ws} and T^w refer to the temperature at the wall surface and wall temperature, respectively. Subscript g is used to indicate the ghost particle.

$$\Delta T^{mg} = 2(T^m - T^{ws}) \quad (13)$$

$$\gamma^{mg} = 2(R^m - \|\mathbf{x}^m - \mathbf{x}^{ws}\|) \quad (14)$$

$$a^{mg} = (\gamma^{mg} \frac{R^m}{2})^{1/2} \quad (15)$$

At the boundary surfaces, heat transfer between the boundary particle to the wall can be expressed by two main heat transfer mechanisms, (i) heat is conducted over flat circle of contact between the particle and adjacent wall surface; (ii) convective heat transfer, which is dependent on walls' convection coefficient of h_w , takes place between the wall surface and the wall.

$$Q^{m-ws} = k^m a^{mg} \Delta T^{mg} \quad (16)$$

$$Q^{ws-w} = -h_w \pi (a^{mg})^2 (T^{ws} - T^w) \quad (17)$$

The temperature at the wall surface can be obtained for the equilibrium of Eqs. (16) and (17). The final set of equations, which define the wall-particle interaction, are the following:

$$Q = 4ka^{mg} \left(T^m - \frac{4k^m T^m + h_w \pi a^{mg} T^w}{4k + h_w \pi a^{mg}} \right) \quad (18)$$

$$F = \frac{E^m}{3(1 - (\nu^m)^2)} R^m \gamma^{mg} . \quad (19)$$

3 Conventional Continuum Mechanics Approach

While the particle mechanics approach aims to elucidate the formation and the evolution of the microstructure of the granular media at particle-level, there has been considerable research directed towards understanding macroscopic behavior of compacted materials. Some of the early work on theoretical modeling of transport properties are devoted to the estimation of thermal, and electrical conductivity, elastic, plastic mechanical properties of ordered and disordered arrangements. Originating from the pair interactions between particles, the macroscopic properties are obtained using various homogenization techniques and postulating continuum constitutive laws [31]. In this study, we consider a continuum system that mimics the particle level description for small strain thermoelasticity, which incorporates the proposed effective mechanical and thermal properties for granular beds under compaction. Governing field equations of motion and energy are the following

$$\operatorname{div}(\boldsymbol{\sigma}) = \mathbf{0} \quad (20)$$

$$\operatorname{div}[k \operatorname{grad}(T)] = 0 \quad (21)$$

where the Cauchy's stress, $\boldsymbol{\sigma}$, is formulated as combination of classical linear elasticity theory and simple linear thermal expansion.

$$\boldsymbol{\sigma} = -\lambda \operatorname{tr}(\boldsymbol{\varepsilon})\mathbf{I} - 2\mu\boldsymbol{\varepsilon} + (3\lambda + 2\mu)\alpha(T - T_{ref})\mathbf{I} \quad (22)$$

For the basic problem of one dimensional steady state thermoelasticity of continuum media, where the body forces are neglected, the solution depends linearly on elastic constants (λ , μ), thermal expansion and conduction coefficients, compaction strain and thermal gradient. Since $\varepsilon_{22} = \varepsilon_{33} = 0$ holds, ε_{11} is referred as ε . Equations of motion and energy Eqs. (20) and (21) can be rewritten as

$$\sigma = -(\lambda + \mu)\varepsilon + \alpha(3\lambda + 2\mu)(T - T_{ref}), \quad (23)$$

$$q = k \frac{\partial T}{\partial x}. \quad (24)$$

Effective mechanical properties of granular beds are of heavy interest in many theoretical studies. Some of these include: calculation of the principal elastic modulus of vertical compression of spherical particles without any lateral extension [30]; derivation of the finite and incremental elasticity of random packing of identical particles using energy methods [32]; enhancement of the derived formulas based on the pressure dependence of the elastic moduli of granular packings [2, 3].

In this study we extend the effective medium theory with the thermal contact model principles by incorporating the particle interactions to account for the local field effects. We re-formulate the effective elastic properties and effective thermal conductivity accordingly, and implement these parameters in continuum mechanics

model. The effective mechanical properties can be expressed in terms of the applied stress, σ , and bulk material properties [32],

$$C_n = 4 \frac{\mu}{1-\nu} = 4 \frac{E}{2(1+\nu)} \frac{1}{1-\nu} = \frac{2E}{1-\nu^2} \quad (25)$$

$$\tilde{\lambda} + 2\tilde{\mu} = \frac{3}{20\pi} C_n (\phi_s Z)^{2/3} \left(\frac{6\pi\sigma}{C_n} \right)^{1/3} \quad (26)$$

$$3\tilde{\lambda} + 2\tilde{\mu} = \frac{1}{4\pi} C_n (\phi_s Z)^{2/3} \left(\frac{6\pi\sigma}{C_n} \right)^{1/3} \quad (27)$$

where C_n is named as stiffness of the system, ϕ_s is the packing fraction, and Z is the coordination number. Effective mechanical properties, $\tilde{\lambda}$, $\tilde{\mu}$, and effective thermal conductivity, \tilde{k} , are implemented in continuum mechanics model and listed as conventional continuum solution. As a simple application of this theory, we consider a case of particles' chain that is compacted by a ratio of ε , under the effect of a thermal gradient of $T_2^w - T_1^w$. The expression that defines the stress evaluation through the chain is found as

$$\sigma = \phi_s Z C_n \left(\frac{3}{32\pi^2} \right)^{1/2} \left(1 - \varepsilon \frac{3}{5} - \alpha \left(\frac{T_2^w + T_1^w}{2} - T_{ref} \right) \right)^{3/2}. \quad (28)$$

Effective thermal conductivity, \tilde{k} , of the granular bed is substantially sensitive to the thermal and the elastic properties of individual particle. Regarding ordered cubic packing configuration, it is known that thermal contact models provide accurate results in estimating steady and average temperature profiles [33]. Three major analytical solutions in literature, by Batchelor and O'Brien [13], Chan and Tien [14], Kaganer [15] and Siu and Lee [34], are proposed to determine the effective thermal conductivity. Since Batchelor and O'Brien's [13] solution stays in remarkable agreement with the particle mechanics results in terms of heat transferred through the chain, we adopted this solution for effective thermal conductivity coefficient in our continuum mechanics approach. This comparison is shown in Fig. 2, where PMA and CMA refer to particle mechanics approach, and conventional continuum mechanics approach, respectively.

$$\tilde{k}^{B\&O} = k \left(\frac{6\sigma}{C_n} \right)^{1/3}$$

$$\tilde{k}^{C\&T} = 0.9454k \left(\frac{6\sigma}{C_n} \right)^{1/3}$$

$$\tilde{k}^{S\&L} = 0.8278k \left(\frac{6\sigma}{C_n} \right)^{1/3}$$

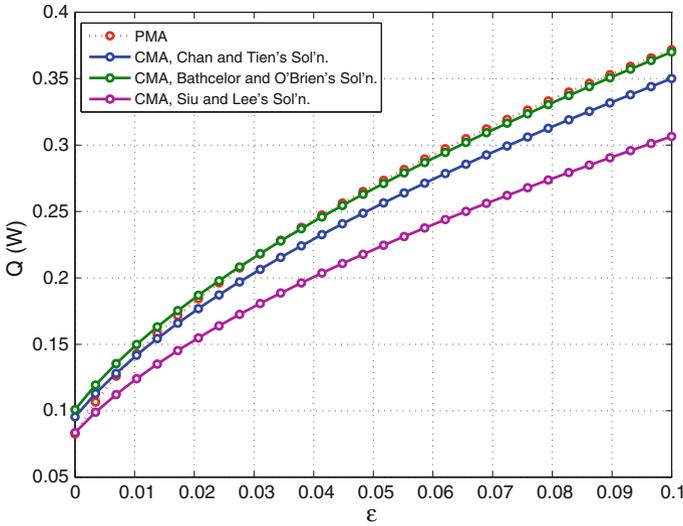


Fig. 2 Comparison of continuum solutions adopting different thermal contact models with respect to particle mechanics solution. Heat versus compaction strain, ε , is evaluated at $T_2^w - T_1^w = 600$ K

4 Results

According to the Hertz theory [35], the collinear contact force between the elastically compressed particles is a nonlinear function of the overlap, which is generated under the effect of the external load, between the particles. For the case of thermally-assisted compaction of granular system of particles, this dependency is altered under the effect of applied thermal gradient. Figure 3 shows the ratio of force, needed to compress the system, in particle mechanics approach to the force in conventional continuum mechanics approach. CMA significantly overestimates the thermal stress within the chains system, particularly for the range of high thermal gradient and low mechanical load. Moreover concerning the highly compacted systems CMA underestimates PMA solution for the system of particles by 10 %.

Similar to compaction force comparison, conventional continuum solution predicts higher heat transferred values for analogous particles system. It is also shown in Fig. 4 that as the packing density of the deformed particles system is increased, conventional continuum mechanics solution becomes more effective in estimating the particle-level solution.

Under three difference compaction strains, 2.5, 5, 10 %, the effect of wall-particle interaction is examined through the chain of particles by imposing a thermal gradient of 300 K between the two boundary walls of the system. For each case, wall heat transfer coefficient, h_w , is ranged from 1 to 10^7 W/m² K. Figure 5 indicates the two limiting cases of perfect insulating and perfect conducting walls.

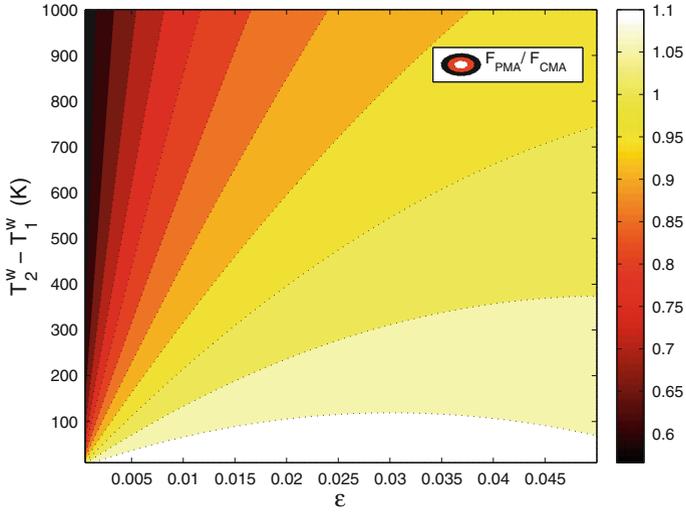


Fig. 3 Comparison of force calculated in PMA and CMA under varying thermal and mechanical loading conditions

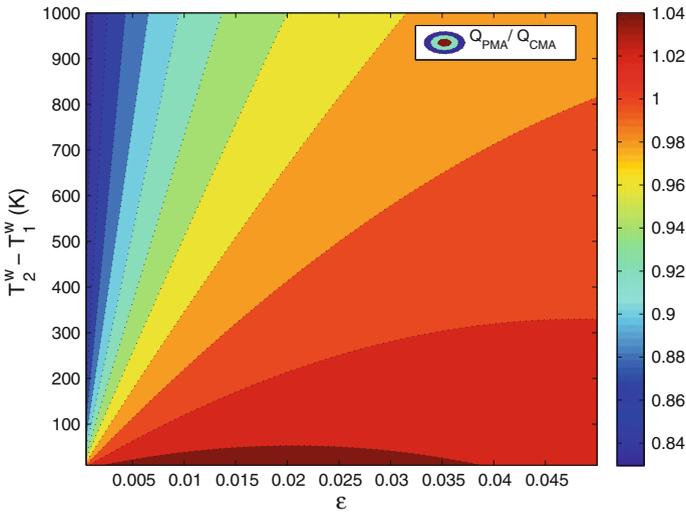


Fig. 4 Comparison of heat calculated in PMA and CMA under varying thermal and mechanical loading conditions

4.1 Role of Thermal Expansion

Systems of granular materials with different thermal expansion properties respond in various re-arrangements to a particular thermal and mechanical load. The following

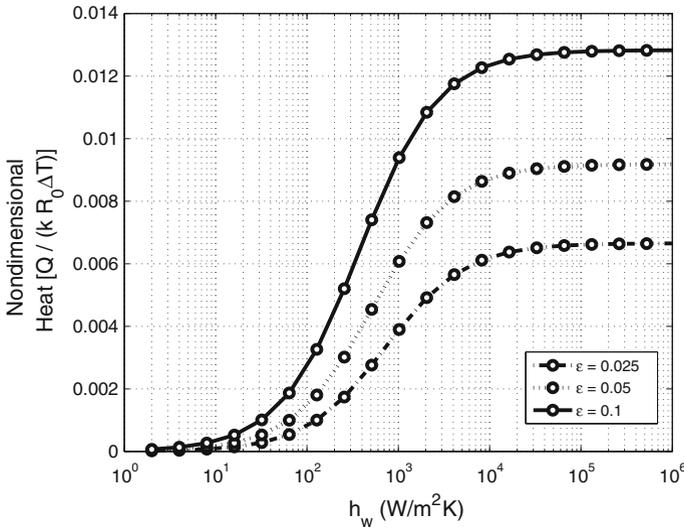


Fig. 5 Correlation between heat and wall conductance at different compaction strains

numerical experiment compiles the results of three different homogeneous system of particles: SS304, Aluminum, and Teflon with different thermal expansion values, $17.3 \cdot 10^{-6} \text{ 1/K}$, $23.6 \cdot 10^{-6} \text{ 1/K}$, $250 \cdot 10^{-6} \text{ 1/K}$, respectively. In the above-mentioned cases of comparison, the chain is compacted to 2.5 % of the initial length and a total thermal gradient of 300 K is applied between the two boundary walls. Alterations in displacement of each particle due to increase of thermal stress can be traced to unveil the effect of thermal expansion coefficient on the system of particles under thermally-assisted compaction. In Fig. 6 the displacement of each particle is divided by the total mechanical deformation applied on the system. The non-dimensional displacement of the particle in contact with the fixed boundary is listed as 0, whereas the one in contact with the heated moving boundary wall is 1.

While reaching to equilibrium the two dominant mechanisms, thermal and mechanical stresses, induce a nonlinear distribution of displacements, which is a unique characteristic of particulate systems. This deviation from linear continuum solution is enhanced for systems with high thermal expansion property.

4.2 Role of Applied Mechanical Load

Under the effect of a modest thermal gradient of 300 K, three different mechanical loading conditions, 1, 2, 5–10%, are compared in Fig. 7. In order to compare the coupled effect of thermal gradient and mechanical deformation, two extreme cases for wall-particle interactions are also considered. In case of perfect insulating walls, h_w is

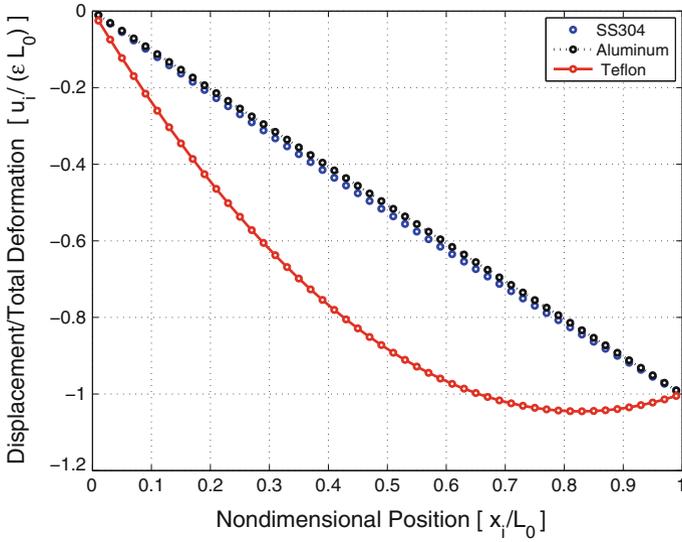


Fig. 6 Relative displacement of each particle within the chain at $\epsilon = 0.025$ and $T_2^w - T_1^w = 300$ K

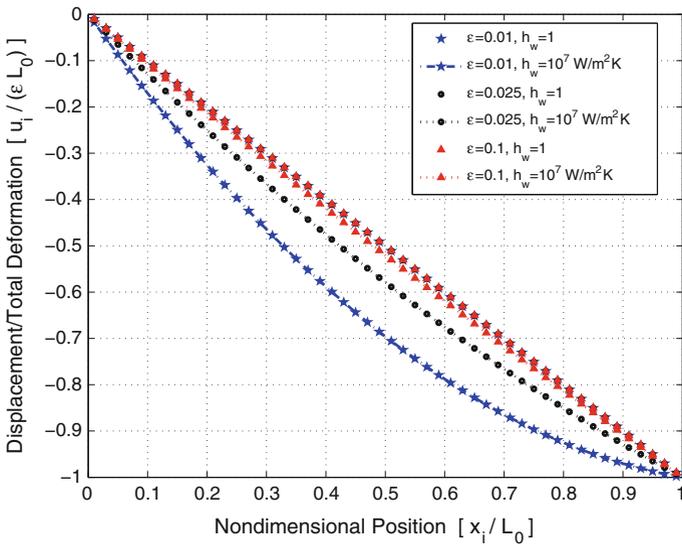


Fig. 7 Non-dimensional displacement versus initial position of the particles under different mechanical loads, with varying heat convection coefficients of the boundary walls

assumed to be $1 \text{ W/m}^2 \text{ K}$. This particular condition is a simulation of pure mechanical loading where we expect to have linear distribution of non-dimensionalized positions of particles within the chain system. On the other hand the case of $h_w = 10^7 \text{ W/m}^2 \text{ K}$ simulates the condition of perfectly conducting walls.

Regarding the system of SS304 spherical particles' chain Fig. 7 indicates that nonlinearity in distribution of displacements is more dominant for low mechanical loading cases.

4.3 Role of Thermal Gradient

A recent experimental study on silos of spherical glass particles showed that thermal cycling, and the difference in thermal expansion properties of the granular material with respect to its container, significantly affect the packing fractions of granular materials in the absence of mechanical compaction [25]. In the current study we focus on the active interval where thermal gradient acts as a dominant mechanism compared to mechanical deformation. A chain of spherical particles is gradually consolidated up to a compaction strain of 5% of their initial length, while thermal gradient between the two boundary walls is increased to 1000 K.

The ratio of the displacements calculated in PMA to CMA indicates a discrepancy between these two approaches. In Fig. 8 the maximum difference between particle mechanics approach and conventional continuum mechanics approach is traced. Under the effect of low mechanical deformation, such as $\varepsilon < 0.02$, and high thermal gradient conditions the continuum solution overestimates the actual position of particles up to 40% of the solution provided by particle mechanics approach. The difference between these two solutions diminishes as the packing density of the granular system increases.

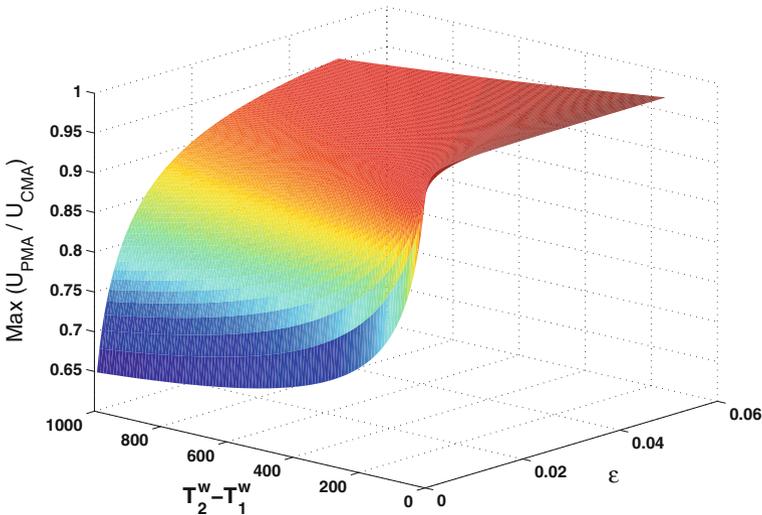


Fig. 8 Maximum difference between the calculated displacements in particle mechanics and in conventional continuum mechanics approaches

5 Conclusion

In this study we present a numerical model to describe the thermo-mechanical behavior of a confined granular system by adopting a detailed description at the particle level. We integrate thermal-contact and Hertzian deformation models to simulate the temperature and displacement of consolidated granular medium. One-dimensional model provides an opportunity to unveil the relation between two dominant mechanisms affecting the thermal and mechanical equilibrium of the particulate systems. In order to capture the actual physical conditions, we consider wall-particle interactions ranging from perfect insulating to perfect conducting walls.

The numerical results indicate that integration of thermal deformation with the elastic contact models induces the incongruity seen in mechanical deformation based compaction models. The coupled phenomena introduce highly nonlinear system of equations, and it imposes variation in contact areas and nonlinear temperature distribution within the particulate material. This effect is enhanced for particles with larger thermal expansion coefficient. It appears that the critical regime, where the nonlinearity due to thermo-mechanical coupling becomes more dominant, is low mechanical load and high thermal gradient conditions.

As a multi-physics problem, thermally-assisted compaction shows a significant dependence on the thermal expansion of the particles. Discrete solution based on the particle mechanics approach that adopts the thermal contact model, carries out this dependence and the nonlinearity enhanced by thermal strains, successively. Despite the fact that effective medium theory improves the continuum solution to a large extent, it fails to capture the characteristics of multi-physics of the problem, particularly for the cases of low thermal gradient coupled with high mechanical load.

Looking toward to future, we are now in a position to address a variety of important questions, such as; (i) what can be a further improvement in effective medium theory that also account for an effective thermal expansion coefficient depending not only on the bulk properties but also loading conditions of the compacted granular assembly? (ii) what is the role of uneven distribution of contact areas and nonlinear temperature distribution on formations of heterogeneous force and heat networks within the concept of the micro-structural arrangement of granular system to macroscopic behavior of the thermally-assisted compacted end product?

Acknowledgments This work has been partially supported by U.S. Army ARDEC grant under the project titled as: Multifunctional Nanomaterials: Processing, Properties, and Applications. The authors would also like to acknowledge the support provided by the National Science Foundation Engineering Research Center for Structured Organic Particle Systems (C-SOPS).

References

1. Vargas-Escobar, W. L. (2002). *Discrete modeling of heat conduction in granular media*. Ph.D. thesis, University of Pittsburgh.
2. Makse, H. A., Gland, N., Johnson, D. L., & Schwartz, L. M. (1999). Why effective medium theory fails in granular materials. *Physical Review Letters*, 83(24), 5070–5073.
3. Makse, H. A., Gland, N., Johnson, D. L., & Schwartz, L. (2001). The apparent failure of effective medium theory in granular materials. *Physics and Chemistry of the Earth, Part A: Solid Earth and Geodesy*, 26(1), 107–111.
4. Hertz, H. (1881). On the contact of elastic solids. *Journal für die reine und angewandte Mathematik*, 92(156–171), 110.
5. Mindlin, R. D. (1949). Compliance of elastic bodies in contact. *Journal of Applied Mechanics*, 16.
6. Mindlin, R. D., & Deresiewicz, H. (1953). Elastic spheres in contact under varying oblique forces. *Journal of Applied Mechanics*, 20.
7. Zhu, H. P., Zhou, Z. Y., Yang, R. Y., & Yu, A. B. (2007). Discrete particle simulation of particulate systems: Theoretical developments. *Chemical Engineering Science*, 62(13), 3378–3396.
8. Cundall, P. A., & Strack, O. D. L. (1979). A discrete numerical model for granular assemblies. *Geotechnique*, 29(1), 47–65.
9. Feng, Y. T., Han, K., Li, C. F., & Owen, D. R. J. (2008). Discrete thermal element modelling of heat conduction in particle systems: Basic formulations. *Journal of Computational Physics*, 227(10), 5072–5089.
10. Zheng, S., & Cuitino, A. M. (2002). Consolidation behavior of inhomogeneous granular beds of ductile particles using a mixed discrete-continuum approach. *Kona*, 20, 168–177.
11. Koynov, A., Akseli, I., & Cuitiño, A. M. (2011). Modeling and simulation of compact strength due to particle bonding using a hybrid discrete-continuum approach. *International Journal of Pharmaceutics*, 418(2), 273–285.
12. Vargas, W. L., & McCarthy, J. J. (2001). Heat conduction in granular materials. *AIChE Journal*, 47(5), 1052–1059.
13. Batchelor, G. K., & O'Brien, R. W. (1977). Thermal or electrical conduction through a granular material. *Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences*, 355(1682), 313–333.
14. Chan, C. K., & Tien, C. L. (1973). Conductance of packed spheres in vacuum. *Journal of Heat Transfer (United States)*, 95(3).
15. Kaganer, M. G. (1966). Contact heat transfer in granular material under vacuum. *Journal of Engineering Physics*, 11(1), 19–22.
16. Hadley, G. R. (1986). Thermal conductivity of packed metal powders. *International Journal of Heat and Mass Transfer*, 29(6), 909–920.
17. Nozad, I., Carbonell, R. G., & Whitaker, S. (1985). Heat conduction in multiphase systems—II: Experimental method and results for three-phase systems. *Chemical Engineering Science*, 40(5), 857–863.
18. Shonnard, D. R., & Whitaker, S. (1989). The effective thermal conductivity for a pointcontact porous medium: An experimental study. *International Journal of Heat and Mass Transfer*, 32(3), 503–512.
19. Sridhar, M. R., & Yovanovich, M. M. (1996). Elastoplastic contact conductance model for isotropic conforming rough surfaces and comparison with experiments. *Transactions-American Society of Mechanical Engineers Journal of Heat Transfer*, 118, 3–9.
20. Bahrami, M., Yovanovich, M. M., & Culham J. R., et al. (2005). A compact model for spherical rough contacts. *Transactions-American Society of Mechanical Engineers Journal of Tribology*, 127(4), 884.
21. Fletcher, L. S. (1988). Recent developments in contact conductance heat transfer. *ASME Transactions Journal of Heat Transfer*, 110, 1059–1070.

22. Majumdar, A., & Tien, C. L. (1991). Fractal network model for contact conductance. *Journal of Heat Transfer (Transactions of the ASME (American Society of Mechanical Engineers), Series C;(United States)*, 113(3).
23. Majumdar, T. S., & Behringer, R. P. (2005). Contact force measurements and stress-induced anisotropy in granular materials. *Nature*, 435(7045), 1079–1082.
24. Gonzalez, M., & Cuitiño, A. M. (2012). A nonlocal contact formulation for confined granular systems. *Journal of the Mechanics and Physics of Solids*, 60(2), 333–350.
25. Chen, K., Cole, J., Conger, C., Draskovic, J., Lohr, M., Klein, K., et al. (2006). Granular materials: Packing grains by thermal cycling. *Nature*, 442(7100), 257–257.
26. Vargas, W. L., & McCarthy J. J. (2007). Thermal expansion effects and heat conduction in granular materials. *Physical Review E*, 76(4), 041301.
27. Johnson, K. L. (1987). *Contact mechanics*. Cambridge University press.
28. Lu, Z., Abdou, M., & Ying, A. (2001). 3d micromechanical modeling of packed beds. *Journal of nuclear materials*, 299(2), 101–110.
29. Siu, W. W. M., & Lee, S. H.-K. (2004). Transient temperature computation of spheres in three-dimensional random packings. *International Journal of Heat and Mass Transfer*, 47(5), 887–898.
30. Walton, K. (1975). The effective elastic moduli of model sediments. *Geophysical Journal of the Royal Astronomical Society*, 43(2), 293–306.
31. Markov, K. Z. (2000). Elementary micromechanics of heterogeneous media. In *Heterogeneous media* (pp. 1–162). Springer.
32. Norris, A. N., & Johnson, D. L. (1997). Nonlinear elasticity of granular media. *Transactions-American Society of Mechanical Engineers Journal of Applied Mechanics*, 64, 39–49.
33. Vargas, W. L., & McCarthy, J. J. (2002). Stress effects on the conductivity of particulate beds. *Chemical Engineering Science*, 57(15), 3119–3131.
34. Siu, W. W. M., & Lee, S. H.-K. (2000). Effective conductivity computation of a packed bed using constriction resistance and contact angle effects. *International Journal of Heat and Mass Transfer*, 43(21), 3917–3924.
35. Landau, L. D., & Lifshitz, E. M. (1959). *Theory of elasticity*. Pergamon Press.