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A novel approach to calculate radiative thermal exchange in coupled particle simulations

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ABSTRACT

We present a novel algorithm to calculate radiative energy transfer rates in Discrete Element Method (DEM)-based simulations of mono-disperse spheres. To verify our algorithm we use the Finite Volume Method (FVM) which enables us to picture relevant radiation phenomena in a dense bed of particles. These phenomena include (i) shadowing, (ii) emission and (iii) adsorption by a constant gray medium. After careful verification, we embed our algorithm in `LIGGGHTS`, a solver for the DEM. A combination of `LIGGGHTS` and a solver for intra-particle temperature gradients, i.e., `ParScale`, is then used to quantify the relevance of radiative heat transfer rates in sheared particles beds. Specifically, we evaluate the relative contributions of conductive, convective and radiative thermal fluxes in granular shear flows of frictional inelastic spheres. We find that the radiative flux can be collapsed onto single curve if it is related to an appropriate dimensionless group. Our analysis establishes a rationale on when radiative heat transfer in dense granular flows should be considered or not. Also, our results can be used to close continuum-based granular dynamics model that aim on predicting the particle temperature distribution under extreme temperature scenarios.

1. Introduction

Radiative thermal heat exchange in particulate systems is of major importance in a variety of industrial applications, ranging from chemical reactors, thermal insulation, powder metallurgy, solar-thermal receivers, laser sintering, combustion processes and many other domains. Various experimental studies (see i.e. Chen et al. [1], Baillis et al. [2], Glicksman et al. [3,4], Goshayeshi et al. [5]) outline, that thermal transport through radiation becomes of outmost importance and the leading heat transfer mechanism at high temperatures, i.e., above 750 °C. These temperatures are easily found in fluidized beds used for coal combustion and catalytic reactors (Tien [6]). In fact, Tien [6] provides a comprehensive review on radiation modelling in particle laden flows with focus on packed and fluidized beds. Another topic is the strong local heating: Dayal [7] pointed out that thermal radiation is of particular importance if the heat input is local, as, e.g., found in laser melting applications.

With interactions between particles and their influence on multiple length scales, radiation is an active research area. Approaches to model thermal transfer rates in particle beds are split into (i) discrete models, with focus on single particle properties, and (ii) continuum approaches, where effective properties of the bed are obtained from experiments and closed with an appropriate model (Kaviany [8]). Multiple research groups have focussed on continuum models, e.g. Chen et al. [9] who evaluated the influence of heat transfer mechanisms, including conduction and radiation, on effective packed bed properties. In analogy to that, Yagi et al. [10] calculated the effective thermal conductivity considering heat conduction and radiation. A number of other researchers used similar approaches (see Cheng et al. [11], Fillion et al. [12], Jagota el al. [13], Kunii et al. [14], Dixon [15]). Clearly, continuum approaches are not limited to the prior shown applications, but can also be applied to model radiation inside a single particle. More recent studies (i.e. Di Blasi [16]) outline possibilities to account for a large number of phenomena including the influence of radiation on combustion or wood conversion (Ragland et al. [17], Bryden et al. [18], Lockwood et al. [19]). In fact, continuum models are also frequently applied to study radiative transport in the fluid phase via finite volume Discrete Ordinate Methods (fvDOM). These methods solve the radiative transport equation (RTE) for a finite number of discrete angles. Discrete ordinate methods rely on a simultaneous evaluation of partial differential equations. Therefore, they are similar to the Navier-Stokes equation, and hence a coupling to existing finite volume codes seems natural. Continuum approaches accounting for the radiative thermal flux are also used in flame and combustion simulations including radiative turbulence influences (Bryden et al. [18], Hostikka et al. [20]).

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Drawing back to particle laden flows, and according to Kaviany [8], the theory of independent scattering and adsorption of radiation (Cartigny et al. [21], Howell et al. [22]) is only valid if the gas phase volume fraction is > 0.95. Unfortunately, most of industrial applications, e.g., reacting particle beds, involve solid volume fractions much higher than this critical value. Furthermore, the assumption of independent scattering is weakened since the particle size is usually small. This clearly limits the application of simple stochastic models for particle-particle radiation. For high volume fractions and increasing particle diameter, emission coefficients tend to be as high as 0.7 and 1.0, as found in the experiments of Ozkaynak et al. [23]. With increasing computational resources, also DEM-based models can be applied to relatively large domain problems, simulating the trajectory of $O(10^7)$ particles simultaneously (Kloss et al. [24]). A number of methods, e.g., the Discrete Transfer Radiation Model (DTRM) as described by Toschkoff et al. [25] proved useful in connection with these DEM-based models. DTRMs track a representative number of rays from the point of origin (i.e., the emitting surface), and predict the rays' propagation through the simulation domain. With DTRM-based methods it is possible to account for all optical thicknesses, and take (isotropic) reflections into account. On the downside, with increasing number of rays, the computational time becomes excessively high. Clearly, ray tracing is computationally expensive if applied to a large number of moving particles: While Amberger et al. [26] already applied ray tracing in the DEM solver `LIGGGHTS`, performance problems limited his study to a small number of particles.

Methods developed with the application to radiation are also used in related fields. In fact Toschkoff et al. [25] showed the application of ray-tracing for wet tablet coating. Thereby every ray represents a fixed amount of liquid based on the injection rate and the number of rays. Zohdi [27] used ray tracing in order to rapidly simulate the effect of acoustical pulses on an agglomeration composed of a collection of discrete particles. In summary, along with Monte-Carlo approaches, discrete models have proven to be a powerful tool in combination with DEM-based simulations.

At this point we see a gap in modelling approaches that we want to close: efficient methods for predicting radiative heat transfer in DEM-based simulations of dense granular flows do not exist. In fact, we will present a discrete algorithm to account for surface radiative exchange in particle laden flows which we embed in the DEM solver `LIGGGHTS`. We generate verification cases for particle assemblies based on the continuum discrete ordinate method, compare them to analytic expressions and use that verification setup to evaluate our model implemented in `LIGGGHTS`. In fact, we take the idea to calculate view factors, as done in DTRM methods, and compute them in a fast and efficient way. We take an existing setup, i.e., a sheared particle bed that we considered already in our earlier work (Forgber et al. [28,29]), and extend the analysis by radiative thermal transport. For further background information on sheared particle beds, the reader is referred to the work of Forgber et al. [28,29], Rognon et al. [30], Chiavlo et al. [31] and Mohan et al. [32] who discussed various effects and regimes of sheared granular materials in great detail.

At the beginning of our manuscript (see Section 2) we explain our simulation method for the verification setup and present an overview of all relevant equations solved in the continuous model, including known and unknown simulation parameters. Furthermore, we introduce a novel approach to determine view factors and calculate the radiative flux between mono-disperse particles. Also, we introduce the calculations of thermal fluxes in this section. Section 3 summarizes our verification studies, limiting cases and shows an application to a fixed bed at different volume fractions. In Section 5 we apply our novel approach to a fully periodic, sheared particle bed and evaluate the radiative flux over a wide range of dimensionless parameters. Section 6 summarizes the presented work and outlines ideas for further studies. Note that we included Nomenclature at the end of our manuscript where all symbols are defined.

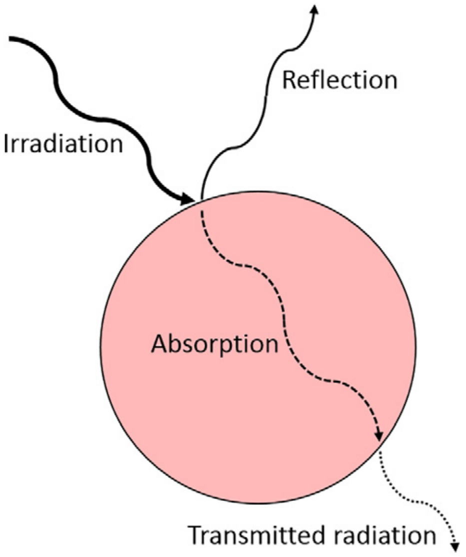

Fig. 1. Thermal radiation mechanisms acting on a particle.

2. Radiation modelling

To predict the radiative thermal fluxes in particle laden flows, the energy exchange rate between all relevant surface elements of the involved particles has to be determined. The energy exchange of two surface elements is, besides the temperatures, a function of their surface distance, their relative orientation and individual size. All these geometrical factors can be described with a single variable, which is called the view factor in our present contribution. In literature, this factor is also referred to as diffuse view factor, configuration factor, angle factor or shape factor. The surface radiation transport approach relies on the assumption of a non-participating media in between exchanging elements. This is valid for vacuum conditions, as well as most of di- and mono-atomic gases (including air) at moderate temperatures. The principally occurring radiation processes are shown in Fig. 1. While transmitted radiation can typically be neglected for most industrial applications, absorption and reflection need to be accounted for. Especially reflection remains a delicate phenomena to balance for the entire enclosure. Fig. 2 shows a general enclosure where all visible parts contribute energy towards the enclosed surface (i.e., the particle). This makes radiative thermal transfer in a fluid-particle suspension a long distance interaction, especially if the ambient fluid is treated as a "gray media". Thus, photons are allowed to travel freely through the fluid without having interactions with the molecules that constitute the fluid. Consequently, the entire enclosure of the system of interest needs to be accounted for. This is in contrast to other thermal transport phenomena such as conduction or thermal transfer to an ambient fluid which can be described on a particle or contact level.

In order to limit the complexity of our surface radiation model to a manageable extent, some assumptions on relevant surface properties are made. A key simplification arises if all surfaces are treated as black, i.e., reflected thermal radiation is not accounted for. We will adopt this simplification for the bulk of our simulations. Furthermore, radiation leaving the point of origin is assumed to be diffusive, i.e., the intensity of radiation is independent of the wave length. Finally, accounting for an enclosure constituted of complex surfaces is often done by introducing a sufficiently large number of isothermal flat surfaces (e.g., triangles) as illustrated in Fig. 2.