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The dependence of mantle thermal conductivity on particle shape and size

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Abstract

Recent spacecraft observations suggest that ice can be present in cometary nuclei even within the first few decimetres below the surface [e.g 1,2]. Together with the observation that cometary surfaces tend to be hot and dry, this implies a low thermal conductivity and a strong thermal gradient in the upper layers. Traditional modelling approaches typically use either a fixed or a temperature dependent value for thermal conductivity of bulk porous material which is more or less independent of the particle shape and size. The validity of this approximation is explored here and a discrete element approach is used to evaluate the thermal conductivity for a variety of particle shapes and sizes.

1. Introduction

Thermal conductivity is an important input parameter to all global comet models since the thickness and conductivity of the dust mantle effectively determine whether or not a given region will be active. In a dry porous material heat can be transported conductively via particle contacts or radiatively (neglecting for the moment the influence of gas flow).

The work reported here concentrates in the first instance on conductive heat flow through a complex network of particle-particle contacts generated by packing of polydisperse spheres and ballistic aggregates.

2. The DEM approach

Various modelling approaches exist to describe heat transfer through a porous medium. The approach taken here is to use the Discrete Element Method [3] since it allows a completely self-consistent description of the microphysics of interacting particles and aggregates and provides a framework for connecting microscopic thermo-physical properties with macroscopic ones. In the context of the Rosetta mission, which will provide data with a length scale spanning many orders of magnitude, this will become increasingly important to build a coherent picture of cometary behaviour.

By treating pair-wise interactions of individual particles and integrating their subsequent equations of motion, a porous particle packing can be produced. Both mono-disperse materials and those with a Gaussian distribution of monomer sizes are investigated. In each case the particles are allowed to settle under appropriately low gravity, and the effect of cohesion can be included if desired. The resulting packing can then be studied to yield, for example, the average coordination number (the average number of contacts per particle), and the average contact area through which heat can be conducted (which is a function of the material properties). As well as deriving the bulk porosity for a given particle packing, Voronoi tessellation techniques can calculate the local porosity.

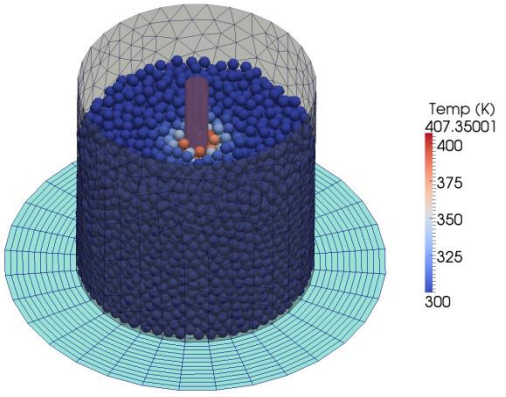

Figure 1: A typical simulation domain with co-axial central “heater”.

Thermal conductivity simulations are performed using an analogue of the coaxial cylinder experimental setup, as shown in Figure 1. In this

simulation, particles are packed into a volume between two cylinders. These are kept at two constant temperatures and the temperature evolution is tracked until equilibrium is achieved. The effective thermal conductivity can then be derived using the heat flux through one of the boundaries and the geometry of the system. The software used for performing these simulations is the open source DEM code LIGGGHTS (http://www.liggghts.com).

3. Aggregates

As well as simple spherical particles, the effect of particle shape has been investigated by building aggregates themselves comprising spherical monomers. A ballistic aggregation approach has been followed. Figure 2 shows such an aggregate, built from 128 monomers of 0.1 micron diameter. The previous simulations can then be performed by packing aggregates into the simulation volume and following the same procedure.

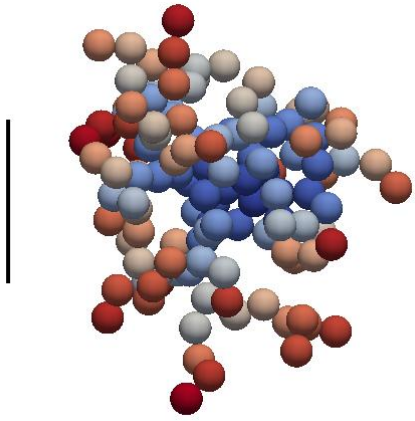

Figure 2: An example 128 particle aggregate and 1 micron scale bar

The results of these simulations are reviewed in the context of the upcoming Rosetta mission, with particular reference to the MUPUS thermal sensor [4] and the MIDAS atomic force microscope [5].

4. Strengths and weaknesses

The DEM technique described here has the advantage of being highly flexible. Additional short range (nearest neighbor) forces - for example the van der Waals attraction between particles - can be readily implemented. Although thermal conductivity is primarily discussed here, the model is more general and can also be used to investigate the physical properties of aggregate mantle material, for example. Finally, particle sizes and contact points ("necks") can be modified to account for annealing processes.

The drawback of the DEM technique is that it can lead to long computational run times, and that evaluation of forces that are longer ranging than the neighboring particle cause extreme performance degradation. Finally, in the context of thermal conductivity, radiative heat transfer is not included; it is known that at high temperature this becomes important and must be included to derive an accurate value of thermal conductivity. If the thermal simulations are performed with a static particle network, however (i.e. if the particle deposition and thermal modelling are separated) it may be possible to include an approximate radiative transfer model, although this has not yet been attempted.

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