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Discrete element method for effective thermal conductivity of packed pebbles accounting for the Smoluchowski effect

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ABSTRACT

In this paper, a Discrete Element Method (DEM) for the evaluation of the effective thermal conductivity of pebble beds in fusion blankets is presented. Pebble beds are multiphase materials in which both the solid and the gas phase filling the voids between particles coexist. The effective thermal conductivity of a pebble bed depends on the thermal properties of the two phases as well as on the system properties (e.g. gas pressure, temperature etc.). In particular, the pressure of the system is a key parameter for the heat transfer in a packed granular assembly since the thermal conductivity of a confined gas decreases with decreasing pressure (known as Smoluchowski effect). In this work, the influence of the gas pressure on the effective thermal conductivity in the Knudsen domain was implemented, to our knowledge, for the first time in a DEM code. The heat transfer mechanisms implemented are: when two particles touch each other the conduction through the contact area between them and, in any case, the conduction through the gas phase in the gap between neighbouring solid particles, may they be touching or not. These mechanisms are expected to dominate the heat transfer in a fusion breeder packed bed. Parametric studies were carried out to investigate the influence of the solid and gas materials, temperature, pressure and compression state. Numerical results were compared with existing experimental literature data and recent experiments carried out at Karlsruhe Institute of Technology (KIT).

1. Introduction

The breeder blanket is a key component of fusion reactors in which both tritium and heat are generated. In order to ensure tritium release and heat recovery adequate thermal properties of the breeder zone are required [1,2]. In the solid breeder blanket concept the breeder and the neutron multiplier are both in form of packed-pebble beds. Therefore, the thermal properties of the breeder zone are strictly related to the thermal properties of the packed pebbles. Due to their discrete nature, pebble beds show a complex fully coupled thermomechanical behaviour. In a constrained bed, the thermal expansion and the irradiation-induced swelling of each single particle generate stresses that in turn have an impact on the packed state, on the heat exchange between pebbles and thus on the effective thermal conductivity of the bed. Pebble beds are multiphase materials consisting of a solid phase (pebbles) and a gas phase (interstitial purge gas for tritium extraction). The solid phase forms the skeleton of the bed while the gas phase constitutes the filling matrix between pebbles. A variation of the skeleton or matrix material as well as the system conditions (e.g. temperature and gas pressure) can strongly influences the effective thermal conductivity.

The aim of this work is the evaluation of the effective thermal conductivity of packed granular assemblies for different skeleton-matrix combinations, system conditions and compression states. To this end an in-house thermal-DEM code was developed. A 3D network model was implemented to determine the heat exchange in packed systems under an imposed thermal gradient. The particle interconnection is defined by thermal resistors to simulate the resistance to the heat transfer between two contacting particles in function of the thermal contact type. In particular, by implementing the theory developed by Batchelor and O'Brien [3] two main types of contact are defined: particles touching each other or with a separation gap. In order to simulate the influence of the gas pressure on the heat transfer in a packed bed, the Smoluchowski effect [4] was further introduced in the present thermal contact conductance model. The Smoluchowski effect accounts for the reduction of the gas thermal conductivity with its pressure when the gas is confined in small gaps as in a packed bed. In literature, several studies about the influence of the gas pressure on the effective thermal conductivity in packed granular system exist [5–7]. The typical S-shaped curve, characteristic of the Smoluchowski effect, was successfully reproduced by both experiments [5,7] and phenomenological

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models [6,7]. To explicitly model Smoluchowski effect at the scale of contacting pebbles, the pressure-dependent gap conduction has been recently modelled using the finite element method [8]. Nevertheless, this work represents an innovative step in the DEM community being the first investigation in which the influence of the gas pressure on the heat transfer was implemented in a DEM code.

In a packed bed, several heat transfer mechanisms take place: conduction within the solid material, conduction through the contact area between touching particles, conduction in the gas phase, gas convection and radiation between particles. In this work the first three mechanisms were considered, which are expected to dominate the heat transfer in a fusion breeder packed bed. The heat radiation contribution increases with the particle temperature and size [9], while it reduces with the increase of the bed density [10]. A high packing factor increases the absorption of radiation in the packed structure reducing the radiative bed density [10]. It has been reported that the thermal radiation in packed beds is negligible for particles with a diameter less than 1 mm in the temperature range of 0–1440 °C [9]. In the same study, the contribution of thermal radiation was found to be appreciable above 400 and 150 °C for particles with a diameter of 10 and 100 mm, respectively. In [11] the contribution of the thermal radiation was found to be negligible below 130 °C for graphite spheres of 60 mm in diameter with an average PF of 61%. Thus, neglecting thermal radiation is justified here due to the small particle size and the high packing factor of the studied assemblies.

The code was validated by comparison with existing experimental literature data and recent experiments carried out in KIT [12]. Parametric studies were carried out to investigate the influence of both skeleton and matrix materials, temperature, the compressive state of the bed as well as the interstitial pressure.

In this paper, the developed 3D thermal network model is presented in Section 2. Parametric sensitivity studies and the comparisons with existing experimental results are discussed in Section 3. Finally, in Section 4, the conclusions are reported.

2. 3D thermal network model

In this work the 3D thermal network model based on the theory proposed in [3] and later used in [13,14] was implemented to evaluate the effective thermal conductivity of a packed granular system. The model was further extended to include the influence of the interstitial gas pressure and temperature, by including the Knudsen number in the thermal contact conductance model. This decisive step allows to study, for the first time by means of DEM code, the influence of the interstitial gas pressure on the heat transfer and thus on the effective thermal conductivity in the gas flow transition region named Knudsen domain.

2.1. Global thermal model

To investigate the heat transfer in a granular system, with the main aim to determine the effective thermal conductivity of the assembly, an in-house thermal-DEM code was developed.

A 3D thermal resistor network model was implemented to determine the heat exchange in packed systems under an imposed thermal gradient. Monosized and polydispersed packed granular systems were generated by means of a modified version of the Random Close Packing (RCP) algorithm described in [15,16]. The RCP presented in [15,16] generates assemblies of packed spheres in periodic configuration. With the implementation of periodic boundary conditions (PBCs), the generated assemblies represent the bulk region of the pebble beds. In order to apply a thermal gradient along the height of the assemblies, the RCP was slightly modified [17]. The PBCs in the upper and bottom boundaries were replaced by rigid walls. As thoroughly explained in [17], during the iterations the desired packing factor is approached reducing the radius of the spheres. The diameter of the particles is equal to the desired value only if the objective packing factor is reached. Otherwise if a slight variation between the objective and the obtained PF occurs, the radius of the particles is scaled to match the objective PF with the desired particle size. In a granular system two phases coexist. Pebbles as a whole identify the solid phase composing the skeleton of the system, while the interstitial gas represents the matrix of the system. In the proposed thermal contact conductance model the pebbles are interconnected by thermal resistors defined by the different type of thermal contact. The heat q_{ij} transferred between the two particles i and j is

$$q_{ij} = C_{ij}^{eff}(T_i - T_j). \tag{1}$$

Here, T_i and T_j are the temperatures of particle i and j, respectively. An individual temperature is assigned to each particle. C_{ij}^{eff} [W/K] is the local effective conductance, which is related to the type of the thermal contact as thoroughly described in Section 2.2. Then, q_{ij} [W] is evaluated at each time step for each contact in the whole assembly. The rate of temperature change $\dot{T}_i$ of the i-th pebble is updated as

$$\dot{T}_i = \sum_j \frac{q_{ij}}{m_i c_p}, \tag{2}$$

where m_i [Kg] and c_p [J/Kg K] are the mass and the heat capacity of the solid material, respectively. For an imposed thermal gradient, the calculation ends when the assembly reaches the steady state configuration according to

$$\frac{\sum_i m_i c_p T_i^n - \sum_i m_i c_p T_i^{n-1}}{\sum_i m_i c_p T_i^{n-1}} < \text{TOL}, \tag{3}$$

where TOL is set to 10^{-10} in the present work for a typical time steps of ~0.01–1 s. Eq. (3) represents the variation of the thermal energy in the assembly between two consecutive iterations. The thermal diffusion time defined as

$$\delta t = \frac{\rho c_p R_{min}^2 \tau^2}{k_s} \tag{4}$$

determines the time step required to achieve the solution for the explicit scheme used in the simulation [18]. Here, the ratio $\left(\frac{\rho c_p}{k_s}\right)^{-1}$ [m^2/s] represents the thermal diffusivity of the solid material, which determines the heat transfer rate in the particles. ρ [kg/m^3]and k_s [W/mK] are the density and the thermal conductivity of the solid material, respectively. The minimum thermal diffusion time in the assembly is defined by dividing the square of the minimum radius in the assembly R_{min}^2 [m^2] by the thermal diffusivity of the solid material. The parameter τ [/] is introduced to ensure stability of the calculation for several conditions (e.g. different gas pressure, gas type, solid materials, radius of the particles etc.). A value of $\tau = 0.5$ ensured the stability and the convergence of the simulations in every condition. However, under certain conditions such as low gas pressure or small pebble diameters $\tau = 0.5$ turned out to be too restrictive resulting in a high computational time. In these circumstances τ can be increased (e.g. to 1, 2, 4) until the convergence is assured to reduce the computational time. If the convergence is achieved, the variation of this parameter does not affect the results of the simulation. Once that the steady state configuration is reached, the effective thermal conductivity of the assembly is evaluated as

$$k_{eff} = \frac{\sum_i q_{i,bw} H}{A(T_{top} - T_{bottom})}, \tag{5}$$

where $\sum_i q_{i,bw}$ [W] is the total heat transferred between pebbles and the bottom wall. H [m] and A [m^2] are the height and the cross sectional area of the assembly, respectively. $T_{top} - T_{bottom}$ is the imposed thermal gradient between the top and the bottom wall, set to 1K in this work.