Enhancing Multi-Physics Microwave Heating Simulation of a Packed Bed of Spheres: Insights from Tangency-Preserving DEM Simulations

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Microwave heating offers a promising avenue for renewable and efficient heating processes by directly transferring heat into the core of matter. However, certain materials may be transparent to the electromagnetic waves due to their low permittivity values. In such cases, the utilization of a susceptor material such as silicon carbide (SiC) becomes necessary, which absorbs the power of the waves and subsequently transfers the generated heat to the surrounding material. This work delves into the investigation of microwave heating in a packed bed of SiC spheres where emphasis is placed on accounting for the concentration of the electromagnetic field at the tangent points between spheres, a well-known characteristic of such systems.

In the present study, the position of the SiC spheres was obtained by using the open-source DEM software LIGGGHTS, with the aim of exporting the resulting packed bed geometry and importing it into COMSOL Multiphysics to carry out a radio-frequency simulation of the MW heating. However, this approach proved unsuccessful due to the presence of small interpenetrations in the DEM simulation results, rendering the construction of the COMSOL geometry unfeasible.

To overcome these limitation, an algorithm was developed in Python to modify the DEM-generated geometry, allowing for slight repositioning and small changes in the sizes of the spheres to achieve a fully tangent geometry. The algorithm employs a grid-based technique to partition the space and takes into account the number of spheres surrounding each given sphere, imposing constraints to determine its new position and radius. Python automatically generates the necessary Java code for the fully tangent geometry generation, which can be executed through COMSOL's built-in application builder.

This algorithm is useful when setting up MW simulations of packed beds with a reduced number of spheres. However, this approach becomes impractical when simulating tens of thousands of spheres, leading to computationally unfeasible simulations. To address this limitation, we developed a novel method based on existing literature [1] to calculate the permittivity of a bulk material with dielectric properties equivalent to those of a real unit cell. Initially, the permittivity for a unit cell was calculated using the constitutive relation $\mathbf{D} = \epsilon\mathbf{E}$ and obtaining an average permittivity in the unit cell by integrating volumetrically $\mathbf{D}$ and $\mathbf{E}$ over it before division [2]. Unlike previous cases examined in the literature, the packing configuration considered in our study was not isotropic, but a realistic arrangement of particles. As a result, the calculated permittivity obtained in this manner takes the form of a tensor of phasors.

Based on the permittivity value obtained through detailed simulations (Fig. 1) using the equation mentioned earlier, a parametric study of a bulk material is conducted in which both the real (ϵ') and imaginary (ϵ'') parts of the permittivity are varied in a range around the obtained permittivity ϵ_0. The objective is to determine the combination of ϵ' and ϵ'' that minimizes errors by calculating electromagnetic losses and the time-averaged electrical energy in the material. Thus, the problem is reduced to a multi-objective optimization that can be automated.

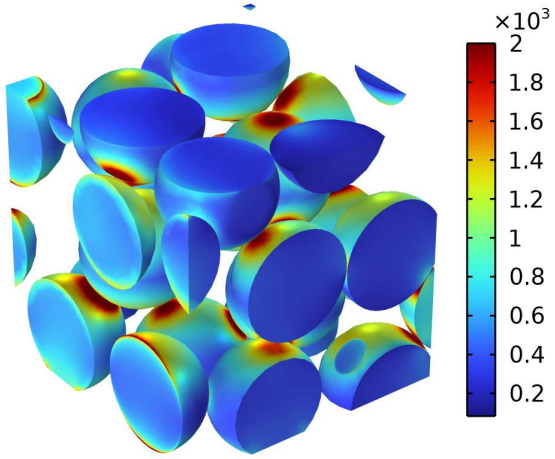

Fig. 1. Electric field distribution in the unit cell [V/m].

The procedure was repeated for a wide range of temperatures to account for the temperature dependency of the permittivity of the SiC. This enables the calculation of a time-dependent permittivity for the bulk material, which can then be utilized in radio-frequency simulations and even coupled with turbulent flow simulations in a porous material.

Furthermore, it becomes possible to accurately model chemical reactions in a flowing phase within a microwave-heated packed bed of susceptor spheres. In this way, there is no longer a need to mesh the detailed packed bed geometry, which for a great number of spheres results in unfeasible meshes and memory errors.

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[2] H. Goyal, and D.G. Vlachos, *Multiscale modeling of microwave-heated multiphase systems*, Chem. Eng. J. **397**, 125262 (2020).