Preserving Tangencies in Postprocessed DEM Results: Enabling FEM Electromagnetic Simulation

Carlos González Niño[1], and Miguel Ángel Castán Lascorz[1]
[1]Fundación CIRCE, Avenida Ranillas, Edificio Dinamiza 3D, 50018 Zaragoza, Spain

Microwave heating has gained prominence as a versatile and efficient technique with the potential to significantly contribute to the decarbonization efforts in various industrial and scientific sectors, particularly in Europe. Among the commonly employed equipment in these industries, packed-bed reactors stand out as widely utilized units. Expanding on the versatility of microwave heating, the particles of catalyst within these reactors can serve a dual purpose by not only facilitating catalytic reactions but also potentially acting as effective heating agents for the fluid, depending on their dielectric properties.

However, a distinctive characteristic of such configurations is that, when subjected to a varying electromagnetic field, the concentration of electric field and the resulting electromagnetic losses, which drive the heating process, tend to occur predominantly at the tangent points between the particles [1], and so preserving these is of the outmost importance for microwave heating process simulation.

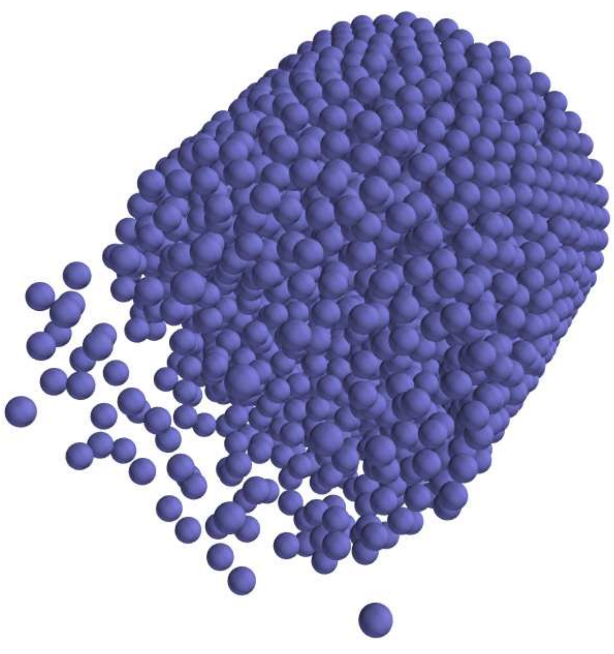

Fig. 1. Packed-bed distribution of spheres generated by DEM simulation.

In our study, we depart from the conventional approach of utilizing an artificially ideal arrangement of particles, such as the commonly referenced FCC packing found in the literature [2]. Instead, we employ Discrete Element Method (DEM) simulations to model a realistic packing within a fixed-bed reactor. However, this approach presents a challenge as the DEM simulations result in small interpenetrations between the particles, hindering the import of the geometry into Finite Element Method (FEM) software for MW heating simulation.

To overcome these challenges, we have devised an algorithm that facilitates minor repositioning and size adjustments for each sphere, resulting in tangent geometries. These modified geometries can be seamlessly imported and meshed using FEM software, enabling us to conduct precise simulations of microwave heating in the packed bed system. Our iterative algorithm utilizes a combination of trigonometric calculations and equation-solving to come up with the tangent geometry.

The algorithm we have developed incorporates a partition scheme that divides the space into cells, enabling efficient checks for tangencies between spheres within the current cell and its surrounding cells. This partitioning strategy avoids the need for unnecessary distance checks between separate spheres, resulting in a significant computational time reduction.

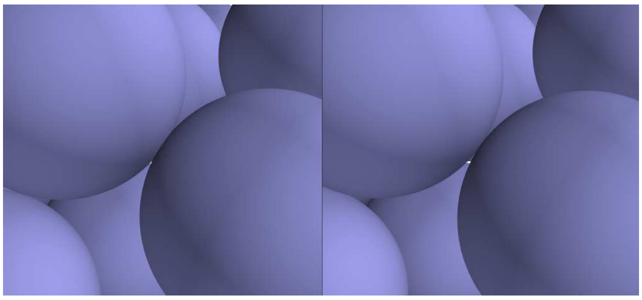

Fig. 2. Details of the initial (left) and final (right) particle arrangements. The algorithm provides a tangency point in a previously interpenetrating position.

Given the high density of spheres present in the real-world applications, the relocation of spheres is a process that must be carried out in iterative stages, as the movement of one sphere can affect those around it. Due to the high computational cost of the calculation process, which grows exponentially with the number of spheres, it is necessary to parallelize the separation algorithm so it can be performed within a reasonable time frame. The proposed methodology includes this parallelization, which involves generating sets of spheres that can be processed independently and are based on unsupervised clustering algorithms. This approach allows for the distribution of the separation algorithm, leading to computational time savings that are almost proportional to the number of clusters.

[1] N. Haneishi, S. Tsubaki, E. Abe *et al.*, *Enhancement of Fixed-bed Flow Reactions under Microwave Irradiation by Local Heating at the Vicinal Contact Points of Catalyst Particles.*, Sci. Rep. **9**, 222 (2019).

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