Predicting Temperature-Dependent Dielectric Properties Of Granular Composite Mixtures

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Abstract

Accurately determining the effective dielectric properties (complex permittivity and permeability) of granular mixtures is essential for optimizing microwave-based processes, including materials synthesis and catalytic reactions. Conventional mixing laws often fail to capture the complex interactions between heterogeneous particles, making accurate dielectric constant predictions challenging.

In this study, we utilize COMSOL Multiphysics with the RF Module to create a finite element model that replicates a two-port coaxial transmission line (7 mm, 50 Ω Airline Calibration Standard) [1]. A discrete element method (DEM) was used to generate the initial geometry of a packed bed of granular particles situated within the dielectric region of the transmission line. Each particle was assigned complex permittivity and permeability values based on fully dense, temperature-dependent dielectric properties. The temperature was assumed constant across the granular packed bed. The RF Module was then used to predict the scattering parameters at a specific temperature for the granular composite. Realistic microstructural features, such as varying particle size, porosity, polydispersity, thin dielectric coatings, and temperature-dependent material properties, were explicitly incorporated into the simulation. Electromagnetic simulations were performed over a frequency range of 0.915 to 10 GHz, with 2.45 GHz being of primary interest. The model leverages symmetry conditions (PEC and PMC boundaries) to minimize computational complexity. The transition boundary condition was also used to investigate thin dielectric coatings on particles. A Python-based post-processing algorithm was employed, utilizing the Nicolson-Ross-Weir (NRW) method [2,3] to convert the COMSOL-derived scattering parameters into effective dielectric properties of the granular composite.

Results reveal that larger particle sizes, lower porosities, and polydisperse particle distributions enhance both the real and imaginary components of effective permittivity due to increased interfacial polarization and improved field localization. Additionally, thin dielectric coatings significantly influence interfacial polarization, further enhancing the dielectric response at elevated temperatures. The developed model was validated against experimental data and showed good agreement, providing confidence in the model's ability to capture temperature-dependent dielectric behavior.

Overall, this COMSOL-based approach provides fundamental insight into the important role of particle surface characteristics and specifically interfacial polarization on effective dielectric properties. Ultimately, the model is an important tool for predicting and optimizing dielectric properties of granular mixtures as a function of temperature, facilitating their effective application in microwave-driven industrial processes.

Reference

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2. A. M. Nicolson et al., “Measurement of the intrinsic properties of materials by time-domain,” IEEE Trans. Instrum. Meas., vol. IM-19, no. 4, pp. 377–382, Nov. 1970.
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Figures used in the abstract

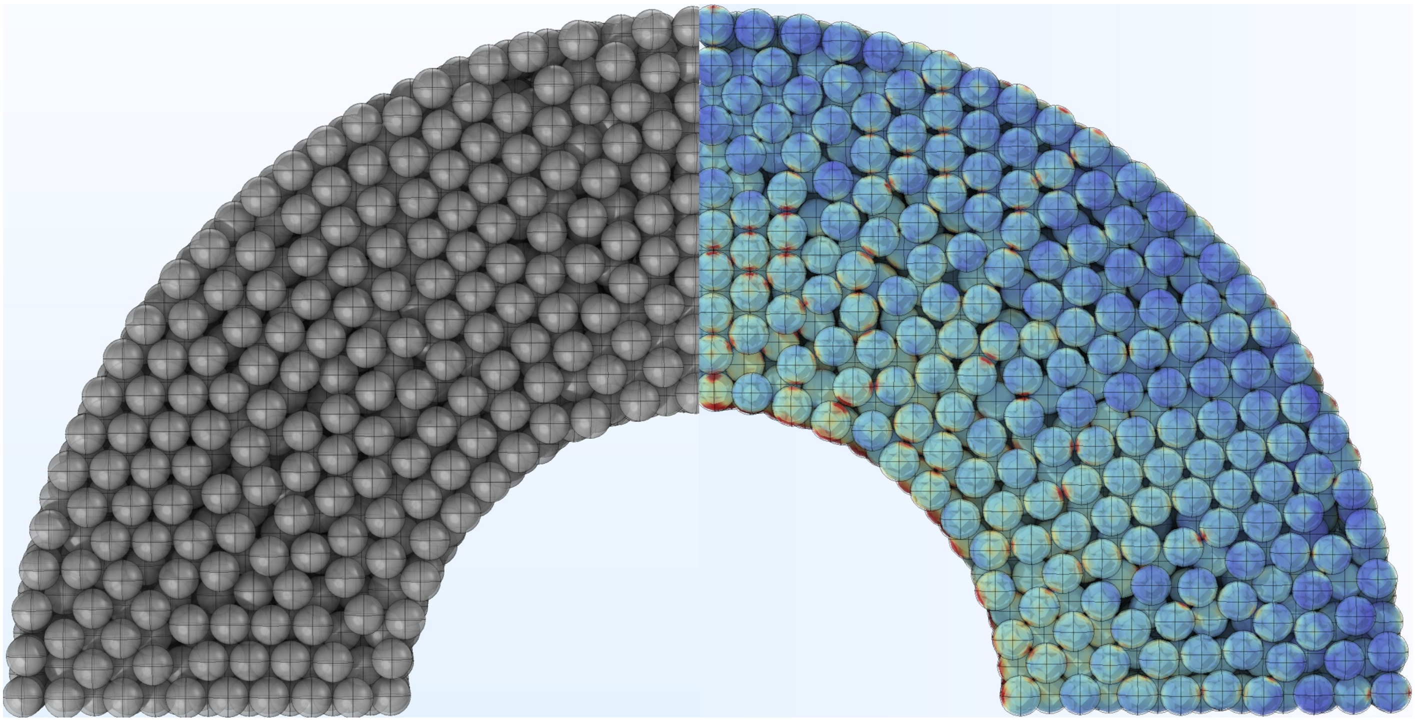

Figure 1 : Finite element model of a packed bed of granular particles and the resulting electric field distribution. (Left) Packed bed geometry generated by discrete element method (DEM), showing randomly arranged granular particles within the coaxial transmission l