An Artificial Neural Network Technique for Determining the Volume Fraction of Solids in Particulate Materials

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Characterization of materials is a critical part of modeling high temperature microwave processing, including sintering. In this paper, an original modeling-based microwave imaging technique for determining solids volume fraction of dielectric powders or particulate materials is described. The desired characteristic is determined by analyzing S-parameter measurements in a waveguide containing the sample material with the help of an artificial neural network trained by data generated by full-wave 3D FDTD simulation. Computational tests with SiC and ZrO_2 powders show that excellent accuracy can be achieved with minimal computational resources.

Keywords: Artificial neural network, electromagnetic modeling, microwave imaging, particulate materials, solids volume fraction.

INTRODUCTION

High-temperature microwave processing methods, including sintering, are known to be promising technologies that, when carried out in properly designed systems, could facilitate energy savings and high quality processing of powders and particulate materials [1-2]. There is a growing effort to develop corresponding multiphysics models and computational tools capable of assisting engineers in designing systems for efficient high temperature microwave processing (see, e.g., [3-5]). Characterization of materials involved in the process is an integral part of the modeling process, but reliable experimental data on electromagnetic and thermal parameters of the processed material are not always available.

Thermal conductivity is a critically important input parameter in the computation of microwave-induced temperature fields. For many powders, it can be relatively accurately estimated using advanced physical models for thermal conductivity of porous materials [6]. However, this approach requires the solids volume fraction ϕ (or porosity $\psi = 1 - \phi$) of the powder to be known. For many materials the data provided by the manufacturers or in handbooks is available in only a certain range, so the resulting value of thermal conductivity is necessarily uncertain [7]. This, in turn, may impact the results of computer simulation.

In this paper, an original modeling-based microwave imaging technique for determining solids volume fraction of dielectric particulate materials is described. The

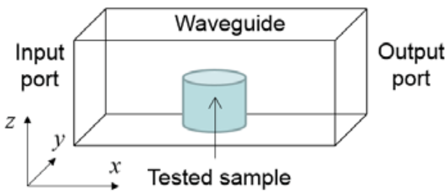


Figure 1. Microwave system with the sample.

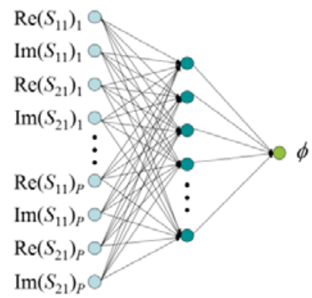


Figure 2. The ANN structure.

proposed approach further develops the authors' earlier artificial neural network (ANN) inversion technique for finding the position and size of an object inside a dielectric sample in a waveguide system [8]. The ANN is trained with data from full-wave numerical simulations. The technique is tested with of silicon carbide (SiC) and zirconium dioxide (ZrO_2) (zirconia) powders in a rectangular waveguide. The solids fraction of the powders with ϕ = 60-80% is reconstructed with less than 5% errors.

TECHNIQUE AND MATERIAL

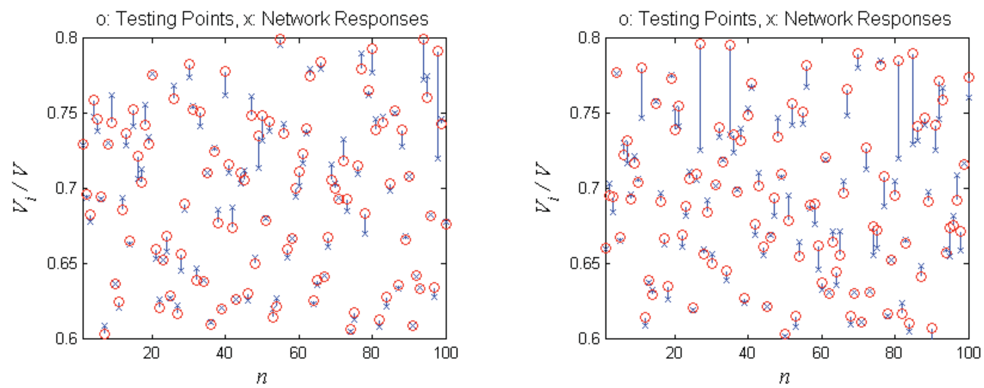
The approach to determining the solids volume fraction in particulate materials is based on measurement of *S*-parameters of a simple microwave system containing a sample of the tested material and an ANN inversion procedure, backed by data on the S-parameters in a finite-difference time-domain (FDTD) simulation of this system. The complex reflection and transmission coefficients are considered, as shown in Figure 1. Consistent with the Cheng-Hsu model for thermal conductivity [9], the tested particulate material is treated as an air-filled sample with solid inclusions of randomly distributed sizes and positions.

An ANN with global cubic radial basis functions for single hidden layer neurons as an inversion mechanism for determining the solids fraction of the sample was used. The network architecture is shown in Figure 2. The ANN inputs are the real and imaginary parts of the *S*-parameters at *P* points in the considered frequency range (4*P* input nodes). The output of the ANN is the solids fraction ϕ of the material.

The ANN is trained using numerical data from an FDTD model of the system. For each simulation, a distribution of particles in the $C_1 \times C_2 \times C_3$ mm sample is generated assuming rectangular cubiod particles with sizes randomly distributed from l_1 to l_2 mm. (It is assumed that $l_i << C_i$ and that $l_i << \lambda_g$, the wavelength in the waveguide.) The *S*-parameters of the system loaded with the sample were computed with the FDTD model and used for ANN training. After sufficient training, the ANN was able to reconstruct ϕ of a tested material from *S*-parameters obtained by physical measurement.

RESULTS

The proposed technique was tested with a sample ($C_1 \times C_2 \times C_3$ = 40×40×40 mm) of powders made of SiC and ZrO_2 in a section of WR340 waveguide of 250 mm length. The size distribution of solid particles was chosen from l_1 = 4 mm to l_2 = 8 mm. The



(a) (b)

Figure 3. ANN performance for SiC power (a) and ZrO_2 powder (b) for n = 100 training points. V_i/V is a relative volume of solid particles in the sample of a particulate material.

dielectric constant ε' and electric conductivity σ of the bulk materials were taken to be ε' = 10.4 and σ = 0.1225 S/m for SiC [1] and ε' = 6.69 and σ = 0.0258 S/m for ZrO_2 [10].

The underlying numerical modeling was performed with the 3D conformal FDTD simulator *QuickWave 2013* [11]. In the model, the domain was discretized with a non-uniform mesh (with max cell sizes of 5 mm in air and 1 mm in the powder) making 178,000 cells. Simulations were run on a Dell T-4700 workstation (64-bit Windows XP) with two quad-core Intel Xeon 3.20 GHz processors; a single simulation took approximately 15 s.

Frequency dependencies of $|S_{11}|$ for different particle sizes l and solids fractions ϕ were computed for both SiC and ZrO_2 powders. It turned out that the curves corresponding to different l are almost identical, whereas the curves corresponding to different ϕ are fairly different. This allows us to expand the results obtained for samples with rather large particles to powders containing particles of micro- and nanometer scales without reproduction of their actual sizes in the FDTD model.

Figure 3 shows ANN performance for the test random-size particle distributions and solids fraction ranging from 60% to 80%. For both powders, the ANN was trained with 800 distributions of particles of the material in air. It is seen that reconstructed positions appear to be very close to the actual positions of the tested points.

Table 1 shows the reconstructed solids fractions of both samples in comparison with their actual values. For powders of lower density (ϕ < 0.75), the reconstruction error does not exceed 1.5%. When the sample appears to be closer to a solid (ϕ ~ 0.8), the reconstruction is less accurate, but the errors are still less than 5%. Since in these examples, the experimental data for S-parameters are simulated using a computer model, it is expected that a practical implementation of this technique sight may suffer somewhat lower accuracy. However, the reconstructed solids volume fraction is still anticipated to be sufficiently accurate for subsequent use in physical models for thermal conductivity, especially in the absence of experimental data.

Table 1. Solids Fractions of the Powders Reconstructed by the Trained ANN

Actual solids fraction ϕ	SiC powder Reconstructed ϕ	SiC powder Relative error (%)	ZrO_2 powder Reconstructed ϕ	ZrO_2 powder Relative error (%)
0.60	0.601	0.1	0.597	0.5
0.65	0.643	1.1	0.643	1.1
0.70	0.690	1.4	0.690	1.4
0.75	0.746	0.5	0.751	0.1
0.80	0.766	4.3	0.777	2.9

CONCLUSIONS

A new modeling-based technique for determining the solids volume fraction of particulate materials has been outlined. The required characteristic was extracted from *S*-parameters of a waveguide system and was independent of the particle size. Functionality of the technique was shown in two computational experiments with silicon carbide and zirconia powders. It was shown that in both cases excellent accuracy (less than 5% error) was achieved with the use of minimal computational resources. In future developments, with an appropriate alteration of the ANN structure, the proposed technique can be transformed for determining the effective complex permittivity of a powder.

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