



RADIO SCIENCE FOR HUMANITY

Statistical 3-D models for electromagnetic characterization of materials

Modèles statistiques tridimensionnels pour la caractérisation électromagnétique de matériaux

Sébastien Lalléchère¹, Pierre Bonnet¹, and Françoise Paladian¹

¹ Université Clermont Auvergne, UBP, Institut Pascal, UMR 6602 CNRS, sebastien.lallechere@univ-bpclermont.fr

Keywords: Composite materials, Numerical simulation, Statistics, Complex media

Mots-clefs: Matériaux composites, Simulation numérique, Statistiques, Milieux complexes

Abstract:

For the past years, a constant interest has been experienced for macroscopic analysis of the electromagnetic properties of composite materials; it is mainly because of their heavy use in various industrial fields, such as transport (including aerospace and automotive for instance). The work proposed in this abstract aims to demonstrate the ability of a three dimensional statistical modeling tool for the characterization of these heterogeneous materials (micro-scales). Target applications cover areas ranging from metrology to antennas and propagation (AP) through electromagnetic compatibility (EMC).

Résumé:

L'analyse macroscopique des propriétés électromagnétiques de matériaux composites connaît un intérêt constant ces dernières années en raison de leur forte utilisation dans différents domaines incluant les transports (notamment aérospatiaux et automobiles). Les travaux proposés dans cette contribution vise à démontrer l'intérêt du développement d'un outil de modélisation statistique tridimensionnel pour la prise en compte des hétérogénéités (micrométriques) de ces matériaux. Les applications visées couvrent les domaines allant de la métrologie aux antennes en passant par la compatibilité électromagnétique des systèmes.

1 Introduction and motivations

Homogenization procedures are nowadays actively used for the macroscopic characterization of materials (i.e. at macroscopic scale); for instance regarding shielding effectiveness (SE) in the framework of electromagnetic compatibility (EMC) studies [1]. Various works were proposed to extract the properties of composite materials mixing gas, liquid, and solid phases with solid matrix, respectively for metrological control [2], geoscience remote sensing [3], and electromagnetic compatibility (EMC) [1]. In this context, different methods are based upon Effective Medium Theory (EMT, e.g. Maxwell-Garnett, MG, formulation) although the limit of validity of formalisms is often a tricky issue [4]. The motivation of this communication is to propose an automated process to generate tridimensional (3D) models of realistic composite materials including conducting spherical inclusions and dielectric matrix medium. The proposed methodology is based upon use of CST® time domain solver since it is well-fitted regarding the expectation of this work to extract the electromagnetic (EM) attenuation over a large frequency bandwidth. The random generation of the locations of inclusions (here conducting and non-intercepting spheres) is ensured from Monte Carlo (MC) formalism; the works from Zhang and Yi in [5] relied on this technique to compute the conductivity of composite material made of conducting fibers with random orientation with Finite Element Method (FEM) in frequency domain.

The contribution is divided into five parts: following first introductory section, section 2 is devoted to the theoretical and numerical bases used in this work, numerical results are provided in section 3 relying on the statistics of the EM attenuation, and concluding remarks jointly with prospects are given in section 4; final section is dedicated to bibliography.

2 Material and methods

2.1 Fundamentals

Mixing equations such as ones based upon EMTs (e.g. Maxwell-Garnett [1], MG) have been extensively used to avoid costly 3D numerical modelling. Nevertheless, classical mixing formulas may reveal inappropriate (e.g. when increasing volumetric rate of inclusion, frequency range, and/or conductivity of inclusions), and advanced mixing procedures were proposed (for instance Dynamic Homogenization Method, DHM, in [1]). Thus, a crucial issue relies on the ability to realistically model statistical variability of constitutive parameters (e.g. locations of inclusions). In this framework, we propose an automated procedure aiming at: generating random location of inclusions, launching electromagnetic simulations, and extracting shielding strength (attenuation in the following) of materials. A useful synthesis is proposed in [6] regarding classical EMTs such as MG, Bruggeman-Rule (BR), or coherent potential. As expressed in [1], the specific case of biphasic composites (i.e. with two phases 1 and 2) will perfectly suit the expectations of this work. In this framework, we will consider phase 1 as composite matrix (e.g. lossless dielectric medium; but, without any loss of generality, the following procedure may be applied to lossy dielectric media) with volumetric rate η , and phase 2 as conducting spherical inclusions of volumetric fraction ν (obviously, this involves $\nu = 1 - \eta$). By considering ϵ_m as the complex effective permittivity of the composite material, whereas ϵ_1 and ϵ_2 are the complex permittivity, respectively of phases 1 and 2, MG formula provides the relation between complex permittivities and volumetric rate ν (of phase 2, i.e. inclusions) as follows:

$$\epsilon_m = \epsilon_1 \frac{\epsilon_2(1 + 2\nu) - \epsilon_1(2\nu - 2)}{\epsilon_1(2 + \nu) + \epsilon_2(1 - \nu)}. \quad (1)$$

Based upon the relation 1 and numerical bidimensional (2D) simulations, some complementary works were proposed by Preault et al. [1] in order to take into account the influence of the size of inclusions (Dynamic Homogenization Method, DHM). Extending previous works in 3D would be of great interest and is nowadays in progress; in the following, MG analytical results will rely on classical MG equation (relation (1)). Indeed, a particular interest will be given in next part (section 3) to the computation of electric field transmitted through a composite material (see numerical setup) both using analytical formulation given in [7] and CST® 3D models including conducting spheres at μm -scale for microwave frequency bandwidth. In the following, the statistics of the EM attenuation obtained from MC simulations with 3D realistic CST® models will be considered as reference data and will be compared to analytical data given by relation (1) and [7].

2.2 Methodology

Relying on a similar methodology than works in [6], the four major steps of the automated process are summarized here:

- initializing randomly located spherical inclusions with Matlab® given radii, and non-intersecting rules,
- automatically generating FIT models (source, probes, matrix basis and conducting inclusions, meshing) with CST® and Matlab®,
- launching required time simulations (CST® and Matlab®),
- extracting the EM attenuation of composite materials (Matlab®).

The proposed methodology is entirely controlled with Matlab® and enables statistical extraction relying on numerical setup depicted in next subsection 3.1. An example of automated mesh generation (two samples, including dielectric matrix and conducting inclusions) is given in Fig. 1 with volumetric rate of inclusions $\nu = 0.10$.

3 Statistics of the EM attenuation at microwave frequency

This section is devoted to the presentation of numerical setup and results extracted from automated CST® procedure previously described in subsection 2.2.

3.1 Numerical setup

Figure 2 details numerical setup developed with CST® MWS and transient solver (Finite Integration Technique, FIT).

Similarly to previous works proposed by Preault et al. [1] and achieved for 2D circular inclusions, this numerical test case is proposed in order to extend the computation of EM attenuation (SE in [1]) in 3D with FIT time

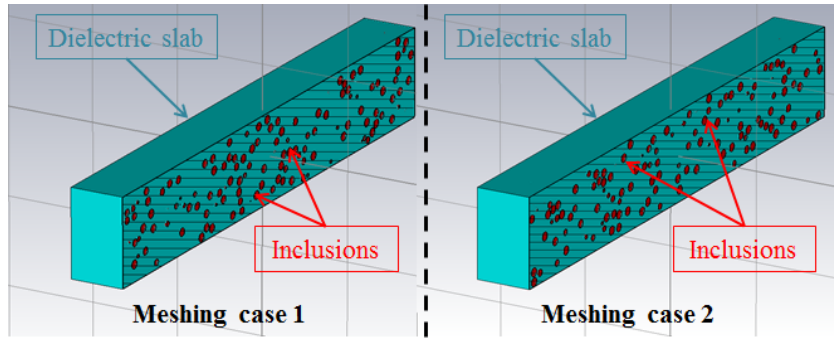


Figure 1 – Sectional views of two different samples of composite material (with volumetric rate of inclusions $\nu = 0.1$).

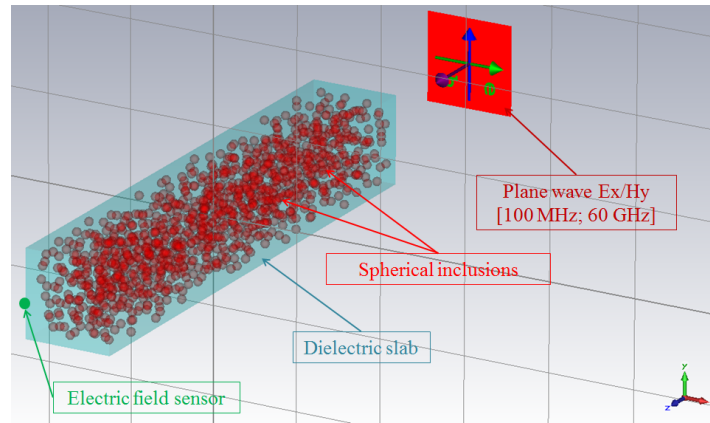


Figure 2 – Mockup of numerical setup based upon 3-D CST® model of the material (transient FIT solver).

domain solver. The two-phases mixture is characterized by the properties of media 1 and 2 as follows (ϵ_0 is the air-permittivity):

- $\epsilon_1 = 5\epsilon_0$ and $\sigma_1 = 0$ S/m,
- $\epsilon_2 = \epsilon_0$ and $\sigma_2 = 1000$ S/m,
- and volumetric rates $\nu = 1 - \eta \in [0.01, 0.05, 0.10]$ ($\nu = 0.10$ in Fig. 2).

CST® modelling is summarized as follows:

- Transient solver,
- Total duration $T_{end} = 400$ ps,
- Boundary conditions are periodical ones,
- Source = Plane Wave (PW) excitation from 100 MHz to 60 GHz,
- Composite material is modelled as a $1 \times 1 \times 6$ mm³ parallelepiped (dielectric slab),
- Mean value Δ of elementary cells required for solving the problem with transient solver has been assessed (here, $\Delta = \lambda/40$, where λ is the minimum excitation wavelength; data not shown in this article).

3.2 Impact of the size of inclusions

First of all, Figure 3 shows that the size of inclusions is of great importance especially for spheres' radius greater than $50 \mu\text{m}$. Since it is not classically taken into account by mixing formulas (e.g. MG relation), Figure 3 provides the statistics (here from 10 simulations) of EM attenuation with mean trend (curves) and error bars (extrema) from CST® time simulations.

Then, the influence of the radii of spherical inclusions is taken into account; as expected, by increasing the size of the inclusions, the statistical dispersion (i.e. standard deviation) is enhanced. Actually, the results obtained respectively for $r_2 = 0.050$ mm and $r_3 = 0.025$ mm are in a great accordance since the extrema of the EM attenuation are close to mean values extracted from 10 simulations.

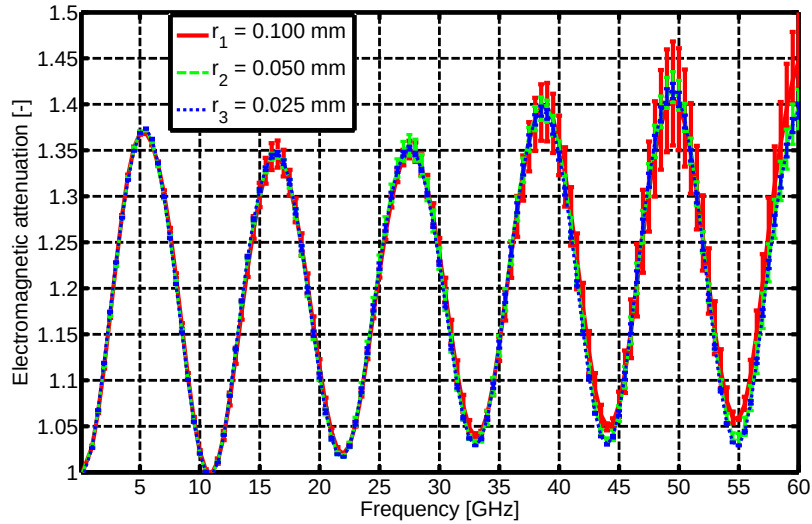


Figure 3 – Effect of the size of inclusions on EM attenuation (here similar to EMC shielding effectiveness and standing for the linear rate between electric field in absence/presence of composite material). Variations are proposed regarding three distinct radii of spheres (respectively r_1 , r_2 , and r_3) with a constant volumetric rate $\nu = 0.01$.

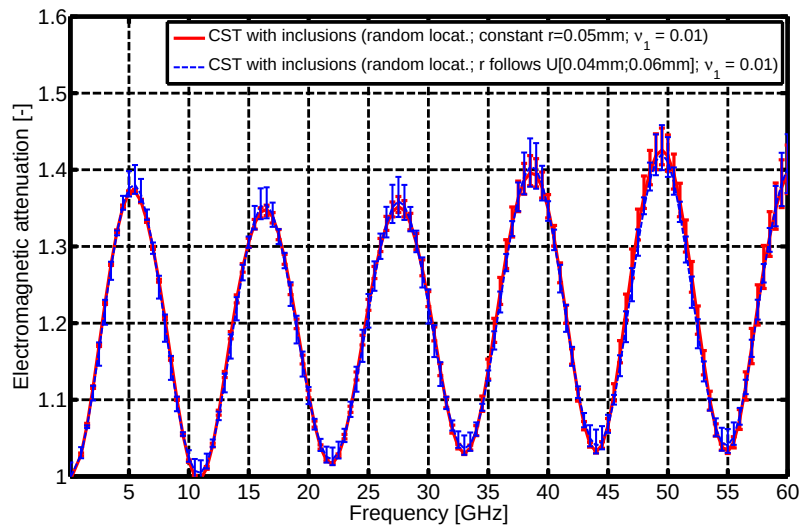


Figure 4 – Effect of the statistical distribution of the sizes of inclusions regarding constant radius of spheres $r = 0.05$ mm (i.e. deterministic case) and uniformly distributed between 0.04 and 0.06 mm (constant volumetric rate $\nu_1 = 0.01$).

Finally, Figure 4 gives an overview of the impact of randomly choosing the size of the inclusions. Indeed, results from 0.05 mm-conducting spheres are compared to those extracted with statistical assumptions about the distribution of spheres' radii (uniform law from 0.04 to 0.06 mm). The proposed automated process enables assessing the effect of random locations and sizes of inclusions. According to errorbars in Fig. 4, the statistical dispersion of the computed EM attenuation is greater for uniformly distributed test case (thin dashed (blue) line in Fig. 4) than for constant size (thick (red) curve in Fig. 4), especially about resonances (below 40 GHz).

3.3 Influence of the volumetric rate

Figure 5 gives an overview of the EM attenuation simulated from three different volumetric fractions: respectively $\nu_1 = 0.01$, $\nu_2 = 0.05$, and $\nu_3 = 0.10$. Each of the previous test cases were simulated with ten CST® simulations. Numerical FIT results were compared to theoretical value given by analytical approach for the

propagation of field inside an homogeneous dielectric medium extracted from MF formalism (equation (1)).

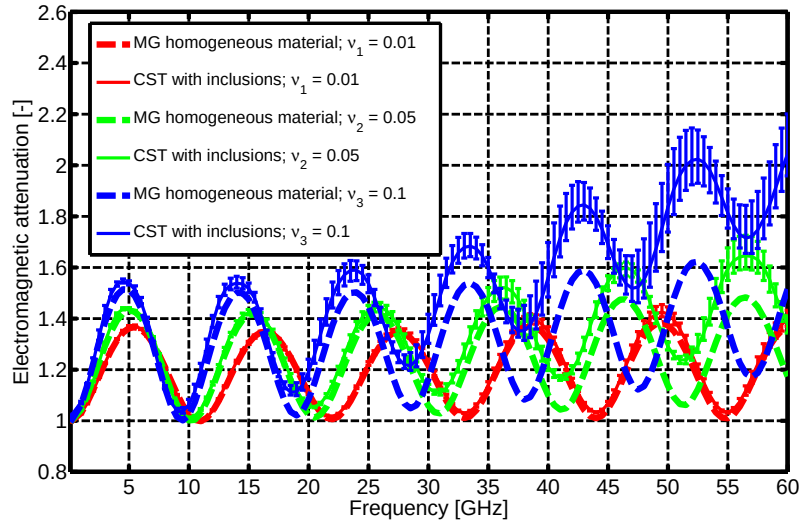


Figure 5 – Effect of the volumetric rate on EM attenuation regarding constant radius of inclusions $r = 0.050$ mm and two distinct rates $\nu_1 = 0.01$ and $\nu_2 = 0.1$.

The numerical model is faced with theoretical expectations in Figure 5. Indeed, the validity of homogenization formalism is checked with regards to volumetric rate of inclusions and frequency of interest. MG formulation is almost accepted over the entire frequency bandwidth for $\nu_1 = 0.01$, whereas increasing ten times the volumetric rate ($\nu_3 = 0.1$) leads to restricting the domain of validity below 10 GHz (Figure 5, dashed blue curve). In between volumetric rate $\nu_2 = 0.05$ leads to an intermediate domain of validity for MG formalism. Consequently, the analytical mixed approach is accepted from 0.1 to about 25 GHz.

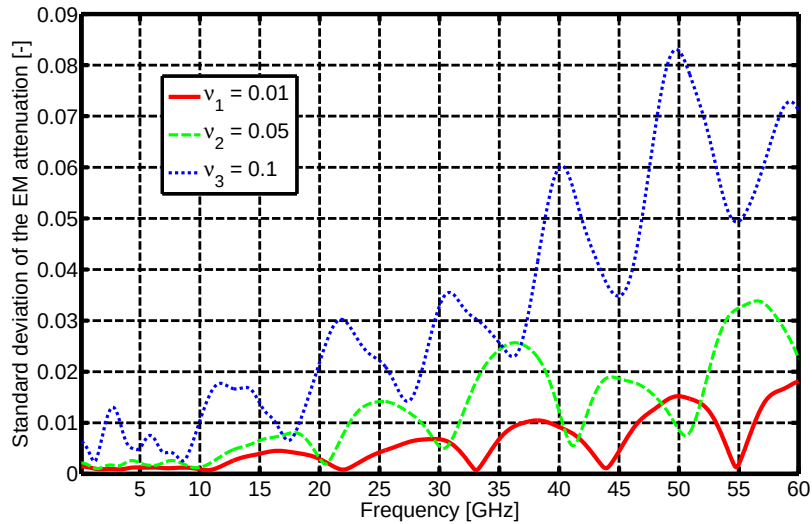


Figure 6 – Standard deviation of the EM attenuation regarding constant radius of inclusions $r = 0.050$ mm and three distinct fractions $\nu_1 = 0.01$, $\nu_2 = 0.05$, and $\nu_3 = 0.10$.

Moreover, the extreme values (minimum and maximum) given in Fig. 5 via errorbars provide interesting information regarding the statistical dispersion of results. Figure 6 supplements the previous results with the standard deviation (std) of the EM attenuation regarding volumetric rates. Obviously, enhancing the rate of inclusions leads to an increase of the std of the EM attenuation. The coefficient of variation (rate of std over mean value) is similar for ν_1 and ν_2 test cases (bounded by 2% at maximum over the whole frequency bandwidth). The results for $\nu_3 = 0.10$ provide maximum CV of 4% which demonstrate the relatively weak sensitivity of data to the different CST® models for this kind of materials. Despite all, this work demonstrates the ability of the

proposed procedure to quantify the effect of micrometer inclusions and to calibrate use of mixing formulas such as MG ones.

4 Conclusion

This article proposes an automated procedure relying on time domain modeling of composite biphasic mixture. It has been validated wrt classical mixing rules (here MG) and offers a statistical overview of the EM attenuation of micro-structured composites. The automation of the entire procedure provides useful information about the statistical dispersion of results, jointly with numerical trustworthy data to calibrate advanced homogenization model, such as DHM.

In this context, some additional works are nowadays in progress to extend current study to: alternative shapes of inclusions, different electrical characteristics (e.g. conductivity, complex permittivity modelling) of particles and multi-physics issues (thermal and mechanical ones for instance). As a consequence, the proposed methodology and tools could be useful in different domains including metrology [2], plasma modeling [7], antennas and propagation [8], and remote sensing [9].

5 References

- [1] V. Préault, R. Corcolle, L. Daniel, and L. Pichon, “Effective permittivity of shielding composite materials for microwave frequencies,” *IEEE Transactions on Electromagnetic Compatibility*, vol. 55, pp. 1178–1186, 2013.
- [2] C. Baer, T. Jaeschke, P. Mertmann, N. Pohl, and T. Musch, “A mmwave measuring procedure for mass flow monitoring of pneumatic conveyed bulk materials,” *IEEE Sensors Journal*, vol. 14, pp. 3201–3209, 2014.
- [3] A. Arslan, H. Wang, J. Pulliainen, and M. Hallikainen, “Effective permittivity of wet snow by using two-phase strong fluctuation theory with non-symmetrical inclusions,” in *International Symposium on Geoscience and Remote Sensing 2000*, pp. 1519–1521, 2000.
- [4] P. Uhd Jepsen, B. Fisher, A. Thoman, H. Helm, J. Suh, R. Lopez, and R. Haglund, “Metal-insulator phase transition in a vo2 thin film observed with terahertz spectroscopy,” *Physical Review B*, vol. 74, pp. 1–9, 2006.
- [5] T. Zhang and Y. Yi, “Monte carlo simulations of effective electrical conductivity in short-fiber composites,” *Journal of Applied Physics*, vol. 103, 2008.
- [6] C. Baer, B. Hattenhorst, C. Shultz, B. Will, and I. Rolfes, “Analysis of composite materials with periodically aligned inclusions using 3d field simulations,” in *GeMiC 2016*, pp. 120–123, 2016.
- [7] P. Andre, G. Faure, A. Mahfouf, and S. Lallechere, “Plasma permittivity and key parameters for electromagnetic wave propagation and emc numerical experiments,” in *18th International Symposium on Electromagnetic Compatibility (CEM 2016)*, 2016.
- [8] C. Njoku, W. Whittow, and J. Vardaxoglou, “Effective permittivity of heterogeneous substrates with cubes in a 3-d lattice,” *IEEE Antennas and Wireless Propagation Letters*, vol. 10, pp. 1480–1483, 2011.
- [9] G. Bailly, J. Rossignol, B. de Fonseca, P. Probetich, and S. Stuerger, “Microwave gas sensing with hematite: Shape effect on ammonia detection using pseudocubic, rhombohedral, and spindlelike particles,” *ACS Sensors*, 2016.