Multiscale method for the calculation of effective dielectric properties

Ricardo Mimoso
ricardo.mimoso@tecnico.ulisboa.pt

Instituto Superior Técnico, Lisboa, Portugal

May 2014

Abstract

This work presents a new computational method for the calculation of the effective complex dielectric properties of a heterogeneous material using its microscopic properties and structure. This method aims to guarantee that the electric energy stored and dissipated by the heterogeneous material is the same with the use of the calculated effective properties. The use of periodic boundary conditions with a periodic cubic sample was tested to check the homogenization of the material. An iterative procedure that corrects the initial obtained permittivity gives a good electric field distribution to the effective material in comparison with the electric field of the real mixture.

Keywords: Effective dielectric properties, Complex permittivity, Microwave heating, Heterogeneous material, Homogenization

1. Introduction

In microwave heating, a very important parameter is skin depth because it measures the penetration of electromagnetic waves inside a material, i.e., the distance from the surface that waves penetrate before the amplitude of the fields decay to an amount of $1/e$. The skin depth decreases with increasing frequency of the wave inside any lossy material [1], so when using microwaves, for most materials, this distance is very small (e.g., in the micrometer scale for most metals [2]). Due to the fact that microwaves have a high frequency and that microwave heating is a volumetric phenomenon, for a block of bulk material, heating will be very slow because dissipation only occurs within the distance of skin depth from the surface.

Industrial microwave heating applications require very often transformation of the material to powder. In this way, for the same volume of the mentioned block filled with powder of the same material, it will promote microwaves to penetrate the complete volume and dissipation will occur in the entire volume. This is of interest to several industries and particularly for glass, ceramic and cement that are energy intensive processes [3].

The use of powders instead of bulk materials changes the macroscopic properties of the material being heated. This calls for the modelling of the materials’ electromagnetic properties. Microscopic properties are intrinsic to the material and are independent of the size of the material. On the other hand, macroscopic properties are also related to geometrical structures and sizes. Such properties are extrinsic and describe the performance of the material. The development of a multiscale method that calculates electromagnetic macroscopic properties using microscopic properties will allow for the modelling of a wide range of materials for microwave heating.

The most challenging and investigated property is the effective complex permittivity due to its vast range of applications. Initially only theoretical models existed for the prediction of the effective permittivity, the resulting mixing-laws were improved over time with the aid of experimental results and new models. Nevertheless, their use and generality were always very limited. In the mid 90’s, computational electromagnetics approaches started being used for this purpose, which allowed a greater development in the field and the development of models that are able to follow larger ranges of experimental values. In [4], [5] and [6], Finite Element Method (FEM) and Boundary Integral Equations (BIE) were used with a quasi-static simulation of a parallel-plate capacitor, in which the real permittivity, $\epsilon'$, was extracted from the electrostatic energy of the entire composite and the imaginary part of the permittivity, $\epsilon''$, from the dielectric losses. Boudida et al. [7] provided comparisons with the percolation theory using the same methods. The capacitor simulation can also be done with an harmonically os-
cillating potential difference as showed in [8]. With the method of the mentioned article, the generation of the random medium was improved using the Monte Carlo (MC) method in [9]. A comparison of the two above mentioned articles with theoretical models is done in [10] and [11]. Also through the electrostatic field energy, the static effective permittivity was determined [12] using a Finite Difference Method (FDM) in an 3-D dielectric mixture and periodic boundary conditions were used to simulate an infinitely long mixture. The simulation of composites with high concentration of inclusions, which involves interconnected inclusions, is performed with FEM using the commercial software ANSYS [13] and COMSOL Multiphysics [14, 15]. Studies of crossed dielectric cylinders in contact immersed in a dielectric host medium [16] as well as particle-gas mixtures with particle clusters [17] were also performed using the last referred software. All the above mentioned articles [4–17] used what is called an energy based approach to extract the effective dielectric properties. The other types of approaches are internal field and scattering based approach [18].

The internal field based approach consists in calculating the averaged electric flux density (displacement) and electric field in the sample and then using the respective constitutive law to obtain the effective permittivity. Using this technique, Calame et al. [19] obtained the electrostatic field solution with FDM and describing porous ceramics with fractal-geometry boundaries. A comparison of this approach with porous alumina experimental results was done in [20]. The simulations done within this approach usually use as well a parallel plate capacitor to obtain the fields. The connection of the potential onto the boundaries of the unit cell using periodic Born-Von Karman condition was tested by Peón-Fernández et al. [21]. In a quasi-static approximation, frequency variations of the computed effective complex permittivity are discussed and compared with experimental data in [22]. These authors performed the numerical simulations using both FEM and Finite-Volume Method (FVM). The computation cost of solving the electrostatic problem using a FE code can be decreased by the use of an averaging method where the same simulated sample is solved three times with orthogonal field directions. This helps to minimize the artificial anisotropy that results from the pseudo-randomness inherent in the limited computational domains and was used in [23] and [24]. A numerical investigation reporting the effective permittivity of two-phase graded composite materials [25] and heterostructures made of multilayered particles [26] was performed also using the internal field approach with the FE COMSOL Multiphysics software. A different homogenization approach shows that an integral representation establishes that the microscopic electric field can be written in terms of the induced microscopic currents and of the macroscopic electric field. This integral equation is then discretized and numerically solved using the Method of Moments (MoM) [27] and using Finite-Difference-Time-Domain (FDTD) method [28]. The calculated current density and electric fields were then used to extract the effective properties of metamaterials. Instead of using a capacitor model for generating the fields, Wu et al. [18] used a propagating signal with an incidence angle with the composite material surrounded by perfect matched layer boundary condition to truncate the simulation domain in one direction and with periodic boundary condition on the other direction using the FDTD method.

The scattering based approach determines the effective permittivity of a mixture by calculating the reflection or transmission of a wave passing through a sample. Using the reflection, Karkkainen et al. [29] put the sample in a TEM waveguide and solved the fields by the FDTD method. Being this a time-domain method, the reflected voltage is obtained as a function of time. The resulting time series is Fourier transformed to frequency domain and only the lowest frequency points of the transformation were used to determine effective permittivity, obtaining in this way a quasi-static solution. Metamaterials is one of the areas were the calculation of effective permittivity is of major importance. Weiland et al. [30] calculated it with the transmission and reflection coefficients, or S-parameters, using the commercial code CST Microwave Studio, which is based on a finite integration technique with perfect boundary approximation. Originally developed independently as a frequency domain approach, this technique can be regarded as a generalization of the FDTD method. Using the same software and approach, Galek et al. [31] extracted the effective permittivity and permeability of a metallic powder using periodically arranged spherical particles in a cubic close packed (CCP) structure. The commercial FEM software High Frequency Structure Simulator 8 was used in [32] to compute the complex transmission coefficient resulting from a plane wave illuminating a planar composite with conductive fibers to obtain the complex effective permittivity. A comparison with other numerical schemes can also be found in the mentioned article. An inversion process using a rectification algorithm was employed [33] to correctly obtain the effective permittivity from the scattering parameters of a mixture using the FDTD software EMPIRE XCell. This article used cubes instead of spheres in order to increase the volume fraction of a mixture without having interconnected inclusions, which allows
higher permittivity values closer to that of metallic particles permittivities. A comparison between the unit cell free space approach (TEM mode) and the waveguide approach (TE10 mode) as well as a comparison between CST Microwave Studio and Ansys HFSS can be found in [34].

In [35], images were implemented into a FE code as checkerboards structures composed of two media to estimate various material and system parameters. The advantage of this approach is that one can just use optical, scanning and transmission images as well as computer tomography structures to describe a mixture and obtain the effective properties of materials.

The successive modelling of material properties would be an important tool in microwave heating. It would allow: optimization of the material structure for the fastest heating possible; study of the introduction of other high loss materials (susceptors) in the material to be heated; optimization of a cavity for a specific material once it is modelled.

In this work, we propose an homogenization approach using a periodic sample of a mixture. With this sample we may extract the effective properties of any material with a complex microscale structure. When considering the propagation of a microwave in heterogeneous media, in order for the material to appear homogeneous to the probing wave, the wave must not resolve the individual scatterers of its inhomogeneities [4]. For that reason, we use a sample much smaller than the wavelength, nonetheless we are not necessarily using the quasi-static approximation. This could be seen as an advantage of the homogenization used in this article because, when using the quasi-static approximation, the polarisabilities and local fields are calculated from the properties of the Laplace equation and this neglects the coupling effects of time-variation of the electric and magnetic fields. This means that the wave-propagation properties of the fields are excluded from the treatment when using the quasi-static approach [36]. For the calculation of complex permittivity, an iterative method using a energy based approach was built up. This method may be called an inverse engineering exercise because we use the electromagnetic fields of the real mixture obtained from a computer simulation to get the effective properties by comparing the fields of the real mixture with the fields of the effective material where, in an direct method, properties are extracted directly from the simulation of the real mixture. The computer simulations were performed with COMSOL Multiphysics software with the aid of the Matlab environment. COMSOL was the chosen software to make the electromagnetic simulations due to its vast documentation which allowed the development of this method, and to its capability to deal with coupled problems which allowed the comparison of different samples heating rate.

The content of this manuscript is organized as follows. Section 2 will be devoted to the introduction of the fundamental equations and concepts essential to our computational procedure. Next, Sec. 3 presents the created method and used model. Sec. 4 shows the obtained results using this method, some of its perks and limitations and a comparison between different models. In the concluding remarks, Sec. 5, we suggest future directions for continuing the development and understanding of this method.

2. Background

2.1. Maxwell’s equations

The electromagnetic theory is based in the four Maxwell equations. The electric and magnetic Gauss’s law, Faraday’s law of induction and Maxwell-Ampère’s law which can be found ordered below:

\[
\begin{align*}
\nabla \cdot \mathbf{\bar{D}} &= \rho \\
\nabla \cdot \mathbf{\bar{B}} &= 0 \\
\nabla \times \mathbf{\bar{E}} &= -\frac{\partial \mathbf{\bar{B}}}{\partial t} \\
\nabla \times \mathbf{\bar{H}} &= \mathbf{\bar{J}} + \frac{\partial \mathbf{\bar{D}}}{\partial t}
\end{align*}
\]

where \(\mathbf{\bar{D}}\) is the electric displacement or electric flux density (C/m²), \(\rho\) is the charge density (C/m³), \(\mathbf{\bar{B}}\) is the magnetic flux density (T or Wh/m²), \(\mathbf{\bar{E}}\) is the electric field (V/m), \(\mathbf{\bar{H}}\) is the magnetic field (A/m) and \(\mathbf{\bar{J}}\) is the electric current density (A/m²).

The above equations are valid for an arbitrary time dependence, but this work will involve vectorial fields having harmonic time dependence. In this case, phasor notation is very convenient and so all field quantities will be assumed to be complex vectors with an implied \(e^{j\omega t}\) time dependence. Therefore, temporal variation of an arbitrary complex vector field \(\mathbf{\bar{U}}\) can be written as

\[
\frac{\partial \mathbf{\bar{U}}}{\partial t} = \frac{\partial (U_0 e^{j\omega t})}{\partial t} = U_0 \frac{\partial (e^{j\omega t})}{\partial t} = j\omega U_0 e^{j\omega t} = j\omega \mathbf{\bar{U}}
\]

where \(U_0\) is a time independent vector, \(j\) is the imaginary number and \(\omega\) is the wave angular frequency.

According to this, Maxwell’s equations can be rewritten as

\[
\begin{align*}
\nabla \cdot \mathbf{\bar{D}} &= \rho \\
\nabla \cdot \mathbf{\bar{B}} &= 0 \\
\nabla \times \mathbf{\bar{E}} &= -j\omega \mathbf{\bar{B}} \\
\nabla \times \mathbf{\bar{H}} &= \mathbf{\bar{J}} + j\omega \mathbf{\bar{D}}
\end{align*}
\]
When electromagnetic fields exist in a material medium, the field vectors relate to each other by the following constitutive laws,

\[ \vec{D} = \varepsilon_0 \vec{E} + \vec{P} \]  
\[ \vec{B} = \mu \vec{H} \]  
\[ \vec{J} = \sigma \vec{E} \]  

where \( \varepsilon_0 \) is the permittivity in vacuum, \( \vec{P} \) is the polarization (C/m\(^2\)), \( \mu \) is the permeability (H/m), and \( \sigma \) is the electrical conductivity (S/m). Equation (12) is Ohm’s law in vectorial form.

### 2.2. Complex permittivity

Over certain frequency ranges, due to atomic and molecular processes involved in the macroscopic response of a medium to an electromagnetic field, there appears relatively strong damping forces that give rise to a delay between \( \vec{P} \) and \( \vec{E} \) (a phase shift between \( \vec{P} \) and \( \vec{E} \)), and consequently between \( \vec{E} \) and \( \vec{D} \), and to a loss of electromagnetic energy as heat in overcoming damping forces [37]. At macroscopic level this effect is analytically expressed by means of a complex permittivity, \( \varepsilon \), as

\[ \varepsilon = \varepsilon' - j\varepsilon'' = \varepsilon_0 (\varepsilon' - j\varepsilon'') \]  

The electric field interacts with the material in two ways: storing energy and dissipating energy. The ability of a material to store electric energy from the electric field is described by the real part of the permittivity \( \varepsilon' \). It is called dielectric constant and it is responsible for the phase shift in the electric field. The ability of a material to dissipate electric energy from the electric field is described by the imaginary part of the permittivity \( \varepsilon'' \). It is called loss factor and it is responsible for losses of electric energy which is transformed into heat [38]. Both \( \varepsilon' \) and \( \varepsilon'' \) are dimensionless parameters. An analogous demonstration can be made for the permeability.

### 2.3. Poynting theorem

For a better understanding of the physics of electromagnetism it is convenient to express the Maxwell equations under an energy form. From Faraday’s law, (8), and Maxwell-Ampre’s law, (9), in its complex conjugate form, we have

\[ \nabla \times \vec{E} = -j\omega \mu \vec{H} \]  
\[ \nabla \times \vec{H}^* = -j\omega \varepsilon \vec{E}^* + \sigma \vec{E}^* \]  

Performing a scalar multiplication of the Eq. (14) by \( \vec{H}^* \) and of Eq. (15) by \( \vec{E} \), and subtracting the results, we get

\[ \vec{H}^* \cdot \nabla \times \vec{E} - \vec{E} \cdot \nabla \times \vec{H}^* = -j\omega (\mu H_0^2 - \varepsilon E_0^2) - \sigma E_0^2 \]  

where it has been taken into account that \( \vec{H} \cdot \vec{H}^* = H_0^2 \) and \( \vec{E} \cdot \vec{E}^* = E_0^2 \), with \( H_0 \) and \( E_0 \) being the amplitude of the two harmonic fields. The left side of Eq. (16) is equal to \( \nabla \times (\vec{E} \times \vec{H}^*) \), which represents the flux of power associated with electromagnetic waves, i.e., waves entering and exiting an infinitesimal control volume. Dividing the previous equation by 2 and using the complex form of permittivity and permeability, we get

\[ -2j\omega (W_m - W_e) = \nabla \cdot \left( \frac{1}{2} \vec{E} \times \vec{H}^* \right) \]
\[ + \frac{1}{2} (\sigma - \omega \varepsilon'') E_0^2 + \frac{1}{2} \omega \mu'' H_0^2 \]

The terms \( W_m \) and \( W_e \) represent, respectively, the mean density of the magnetic and electric energy (J/m\(^3\)), and are equal to

\[ W_m = \mu' H_0^2 \frac{1}{4} \]  
\[ W_e = \varepsilon_0 E_0^2 \frac{1}{4} \]

while the term \( (\sigma + \omega \varepsilon'') E_0^2 + \omega \mu'' H_0^2 \) is the mean power transformed into heat (W/m\(^3\)), since the mean value of the square of a sine or cosine function is 1/2. Equation (17) is known as the complex Poynting theorem in its differential form. This equation allows us to quantify each energy term. However, because of the complex nature of this equation, care must be taken to interpret results derived within this notation [39]. For instance, the signs in this equation are not consistent with signs derived within this notation.

### 2.4. The heat equation

The heat transfer phenomenon, existent in microwave heating, is given by the heat equation

\[ \rho c_p \frac{\partial T}{\partial t} - \nabla \cdot \kappa \nabla T = Q_{em} \]

where \( \rho \) is the density (kg/m\(^3\)), \( c_p \) is the specific heat capacity (J/(kg · K)), \( T \) is the temperature (K or °C), \( \kappa \) is the thermal conductivity (W/(m · K)) and \( Q_{em} \) is the heat generation term (W/m\(^3\)).
our case, it represents the power dissipated by Joule effect and electromagnetic power dissipated per unit volume. This term is equal to the mean power transformed into heat obtained in Eq. (17) with the correct signs

\[ Q_{em} = (\sigma + \omega \epsilon''') \frac{E_0^2}{2} + \omega \mu'' H_0^2 \] (22)

and represents the coupling of Maxwell’s equations with the heat equation. Another way to represent the heat generation term is

\[ Q_{em} = Q_{rh} + Q_{ml} = \frac{1}{2} \text{Re}(\vec{J} \cdot \vec{E}^*) + \frac{1}{2} \text{Re}(j\omega \vec{B} \cdot \vec{H}^*) \] (23)

where \( \vec{J} = \sigma_{eff} \vec{E} \), with \( \sigma_{eff} = \sigma + \omega \epsilon''' \).

2.5. Numerical simulations with COMSOL

The numerical simulations done in this work were all performed with COMSOL Multiphysics v4.4. This finite element software solves coupled systems of partial differential equations in domains with complex geometries using unstructured meshes. Helmholtz equation in the frequency domain is used to obtain the electromagnetic (EM) field using time harmonic sources.

\[ \nabla \times \mu^{-1}_r (\nabla \times \vec{E}) - k_0^2 \epsilon_r' \vec{E} + k_0^2 j(\epsilon_r'' + \frac{\sigma}{\omega \epsilon_0}) \vec{E} = 0 \] (24)

where the wave number in free space is defined as

\[ k_0 = \omega \sqrt{\epsilon_0 \mu_0} \] (25)

In order to describe microwave heating, Eq. (24) has to be coupled with Eq. (21).

3. Model

For the effective properties of an inhomogeneous material to be obtained it is necessary that an homogenization approach is established. For that, we use a periodic cubic sample that must be considered representative of the material being studied. Because electromagnetic properties are being calculated, in order to the inhomogeneities of the material to be considered, it is necessary that they are smaller than the wavelength of the field under operation [12]. Considering that the sample is being irradiated by microwaves at a frequency of 2.45 GHz, which corresponds to a wavelength of 12.24 cm, the sample will have less than 1 cm in each characteristic dimension.

3.1. Effective properties

The relevant effective properties that must be calculated in order to completely characterize a material’s electromagnetic and thermal behaviour are the electric conductivity, \( \sigma_{eff} \), complex permittivity, \( \epsilon_{eff} \), permeability, \( \mu_{eff} \), density, \( \rho_{eff} \), specific heat capacity, \( c_{p,eff} \) and thermal conductivity, \( k_{eff} \).

In this method it is assumed that: (i) The sample is representative of the material; (ii) The material is isotropic; (iii) The microscopic properties of the materials inside the sample are known; (iv) The relative permeability is equal to 1 (\( \mu_{eff} = \mu_0 \)); (v) The structure of the mixture is known. To calculate \( \rho_{eff} \) and \( c_{p,eff} \) it was used the law of conservation of mass and energy, respectively. To obtain \( \sigma_{eff} \) and \( k_{eff} \), a computer simulation with a prescribed electric potential difference and temperature difference was used to calculate the electric current density, \( J \) (A/m²), and the heat flux, \( q \) (W/m²), so that throughout Ohm’s law and Fourier’s law, respectively, the effective electric and thermal conductivity could be obtained.

3.2. Effective Complex Permittivity

The behaviour of the EM fields created by the interaction with the mixture should be similar to the fields of a sample (with the same size) of a bulk material with the effective properties of the mixture. Based on this idea, a method was developed to calculate the effective complex permittivity of a mixture using an iterative rectification algorithm. A diagram explaining the iterative procedure can be found in Fig. 1.

The FE simulation of the mixture and of the bulk material is done, for example, using a model geometry similar to Fig. 2, and the methodology consists in exciting the periodic sample with a plane wave with the direction of propagation along the z-axis,
the electric field polarized in the $y$-direction and with the magnetic field polarized in the $x$-direction. This model structure represents a plane wave passing through a material with an infinite extent in the $x$- and $y$-directions, the space outside the material represents free space. To emit the wave, a port boundary condition is applied in the $-z$ limit of the domain and, on the other side, another port is used which is turned off. This results in a face with non-reflecting properties. To simulate the infinite extent of the material, periodic boundary conditions are used in $x$- and $y$-limits and the cell is repeated at least 3 times in the $z$-direction.

In order to retrieve an estimate of the dielectric constant, $\epsilon_r'$, and the loss factor, $\epsilon_r''$, two parameters that contain the mentioned properties need to be calculated from the EM field solution inside the samples. The two parameters that contain this property are the mean density of the electric energy, $W_e$, and the mean power transformed into heat, $Q_{em}$, respectively. The chosen parameters are related to the definition of $\epsilon_r'$ and $\epsilon_r''$ presented in Sec. 2.2, and this gives a physical character to this approach. So calculating $W_e$, $Q_{em}$ and the electric field norm, $|\vec{E}|$, inside the cells and using Eq. (19) and (22), the estimates of $\epsilon_r'$ and $\epsilon_r''$ are obtained.

After this, a new FE simulation is done substituting the cells containing the mixture with bulk cells containing the obtained effective properties and estimates. From the solution fields, new parameters ($W_e$, $Q_{em}$ and $|\vec{E}|$) for the bulk cells are obtained which are different from the ones obtained with the mixture. Using the difference between $W_e$ and $Q_{em}$, to calculate the increments of $\epsilon_r'$ and $\epsilon_r''$, new estimates can be obtained (Fig. 1). Repeating the last FE simulation with the new estimates until they converge results in an effective complex permittivity that guaranties that the same electric energy will be stored and electromagnetic energy will be dissipated in the effective material as in the real mixture. This iterative procedure was automated using a Matlab code linked with COMSOL. An example of the convergence of the permittivity can be found in Fig. 3.

For the FE simulations, COMSOL Multiphysics was used with tetrahedral elements in a mesh automatically generated by the software. The solution of the real mixture converged for 102,024 elements and with the effective material for 6,656 elements, taking 3 min 31 s and 32 s, respectively, to achieve the solution in a computer with 8 CPUs of 3GHz and 12GB RAM. If more complex structures are used, the number of elements will increase and, for instance, if the number of elements goes to 500,000 elements, COMSOL will require around 200GB RAM and around 3 hours. This rapid increase is due to the fact that periodic boundary conditions require the use of a direct solver in COMSOL.

4. Presentation and discussion of results

The simulations were conducted for a fused quartz powder that consists of periodically arranged spherical particles of 6 mm in a CCP structure with an interparticle distance of 1 mm. This material was chosen for being a dielectric ($\sigma \approx 0$), for not responding to the magnetic field ($\mu = \mu_0$) and for having a complex permittivity at room temperature $\epsilon_{r}(25{\circ}C) = 3.78 - j2.27$ [40], constituting a simple case study. The host material in the mixture is air.

To assure a converged solution of the FE simulations, the electric field norm was observed in a line that crosses the middle of the cells. The number of elements inside the cells was increased until the curve of the electric field tended to a solution.

As showed in Fig. 1, a convergence criteria has to be defined for both $\Delta \epsilon_r'$ and $\Delta \epsilon_r''$. Considering that the precision of the material permittivity went up to the second decimal value, the increments have to be lower then 0.001 for the permittivity value to be
Figure 4: Effect of the evolution of permittivity on the electric, Fig. 4(a), and magnetic, Fig. 4(b), fields of the effective material in a line that passes through the middle of the cells with the $z$-direction. The arrows represent the tendency of the evolution throughout the iterative process. The dashed dark blue lines represent the fields of the mixture.

considered converged. The number of iterations for both $\epsilon'_r$ and $\epsilon''_r$ to converge for this case study was 12 iterations, as can be seen in Fig. 3.

The effective complex permittivity obtained for this case was $\epsilon_r = 2.00 - j0.47$. Taking into account that the simulated mixture is a pure dielectric, which means that the waves penetrate the entire material, and that the host of the mixture has a $\epsilon_r = 1$, the value obtained is an expected value. The same can be said for the results from the simulation of the same structure with spheres of 2 mm and an interparticle distance of 0.33 mm where the obtained effective permittivity was $\epsilon_r = 1.99 - j0.46$. The results are so close to each other because the volume fraction of inclusions was kept constant. The improvement of the effective permittivity throughout the iterative process is clearly showed in Fig. 4, where the electric and magnetic fields of the effective materials tend to shape of the fields of the mixture. The existing oscillations in the mixture fields relative to effective fields are due to the interfaces between two media inside the mixture. After the microwave, generated in $z = 0$ mm, passes through the cells, the field norm takes a constant value. This is due to the non-reflective boundary in the end of the domain, so no reflections exist after the wave passes through the cells and the constant fields represent a plane wave travelling through space.

To test the quality of the effective permittivity, a series of runs were made to see if a good homogenization was performed with the selected sample. Considering that, in fact, the chosen periodic cubic sample is representative of a material, the obtained effective permittivity should not vary when the size of the sample is increased. Indeed, when the number of cells in the direction of the propagation of the wave was increased, a maximum variation of 1.5% in $\epsilon'_r$ and 6.5% in $\epsilon''_r$ was found. If the cells are collocated in different positions relative to the wave, the exact same values are obtained. To check if the periodic boundary conditions were describing well the material, an increase of the number of cells in the $x$- and $y$- directions was tested, resulting in the same value of the effective permittivity. In all the above mentioned results, $W_e$ and $Q_{em}$ were measured in all the existing cells in the domain. If we only measure in one cell and study the effect of increasing number of neighbour cells, effects of relative positioning of the cell to the wave inside the cells (the wavelength inside a material is different from outside the material) will make the permittivity values oscillate up to 26%. For this reason, this last approach is not recommended.

4.1. Comparison between different models
Microwave heating of the characterized samples were simulated in the single mode ($TE_{10}$) cavity in order to compare the heating profiles of the mixture with the effective material. The cavity boundaries consist of one port, in the $z$ limit, and perfect electric conductors in the rest of the walls and the
sample was positioned in the peak of the electric field as can be seen in Fig. 5. Despite the fact that the boundary conditions around the sample inside the cavity do not represent the infinite extent of the material, which makes this model unsuitable for an homogenization procedure, the developed method can still be performed with this model and a permittivity can be obtained. The advantage of using this model instead of the plane wave model is that it is closer to the case of a real sample being heated inside a microwave oven and using our method can guarantee that the mixture will have the same \( W_e \) and \( Q_{em} \) as the effective mixture. To compare the electromagnetic and heating behaviour of the mixture with the sample with the effective properties, simulations were performed using the cavity of Fig. 5 and a sample of 1 cm\(^3\) with: the mixture with 2 mm spheres; the bulk material with effective properties obtained with the plane wave model; the bulk material with effective properties obtained with the cavity model. In Tab. 1, it can be verified that the cavity model gives closer \( W_e \) and \( Q_{em} \) to the mixture; however, the rest of the parameters have very proximate values. If one looks at the electric fields inside the cavity and the samples an interesting result can be found. The electric field norm curve near and inside the sample of the plane wave model follows the mixture curve much better than the cavity model. Such result can be observed in Fig. 6. This shows the quality of the homogenization performed with the plane wave model.

<table>
<thead>
<tr>
<th>Model</th>
<th>Mixture</th>
<th>Plane wave</th>
<th>Cavity</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \epsilon_r )</td>
<td>-</td>
<td>1.99</td>
<td>1.88</td>
</tr>
<tr>
<td>( F_r )</td>
<td>-</td>
<td>0.46</td>
<td>0.45</td>
</tr>
<tr>
<td>( W_e [J/m^3] )</td>
<td>2.0827e-3</td>
<td>2.1065e-3</td>
<td>2.0818e-3</td>
</tr>
<tr>
<td>( Q_e [W/m^3] )</td>
<td>1.5257e7</td>
<td>1.4859e7</td>
<td>1.5250e7</td>
</tr>
<tr>
<td>HR [C/s]</td>
<td>15.2</td>
<td>15.4</td>
<td>15.8</td>
</tr>
<tr>
<td>( S_{11} [\text{dB}] )</td>
<td>0.0668</td>
<td>0.0650</td>
<td>0.0667</td>
</tr>
</tbody>
</table>

Table 1: Results of the electromagnetic and heating response of the different models. HR stands for Heating Rate.

5. Conclusions

This article presents a new energy based method for characterization of the effective dielectric properties of a heterogeneous material. With the material’s properties and their micro-structure, all the effective macro-properties needed for the modelling of microwave heating can be obtained. The method was demonstrated for a powder consisting of spherical inclusions in a CCP structure.

This method uses an iterative procedure to improve the estimates of the effective complex permittivity based on the stored electric energy and dissipated electromagnetic energy. With a Matlab code, the FE simulations performed in COMSOL were carried out automatically in order to make the iterative process faster and less wearing. The FE simulations needed to extract the permittivity only include the electromagnetic waves physics. The simulations done to compare the different model geometries also used the heat transfer physics. Simulations with multiphysics are more computationally expensive.

On the modelling side, a periodic cubic sample being irradiated by microwaves surrounded of periodic boundary conditions allows the extraction of a consistent effective permittivity. The improvement of the effective permittivity throughout the iterative procedure results in electromagnetic fields closer to the ones of the heterogeneous material. The permittivity obtained using this model enables the effective material to get a smooth electric field very close to the one of the real mixture, while respecting the thermal response and the ability of the material to store and dissipate electric energy.

Although the present results seem promising, it is clear that new tests in inhomogeneous materials should be carried out with the present methodology. Comparison with existing theoretical models and available experimental results will allow a greater understanding of the method. Adapting the method to also obtain the effective permeability of magnetic sensitive materials in an analogous way to
the permittivity, will allow the increase of the range of applications. Special interest lays in the use of this method to study the introduction of susceptors in materials for microwave heating applications.

Acknowledgements
The author would like to acknowledge Prof. Afonso Barbosa, Prof. António Topa and Prof. Carlos Fernandes for comments and explanations made during the work. This work was partially supported by DAPhNE EC FP7 project contract N° NMP2 LA 2012 314636.

References


