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► **To cite this version:**

L. Estel, Claire Lafossas, Martine Poux, Junwu Tao. Materials thermal properties investigation by inverse modeling technique. 18th International Conference on Microwave and High Frequency Applications (AMPERE 2021), Sep 2021, On line, Sweden. pp.170-174. hal-03822163

HAL Id: hal-03822163

<https://hal.science/hal-03822163>

Submitted on 20 Oct 2022

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MATERIALS THERMAL PROPERTIES INVESTIGATION BY INVERSE MODELING TECHNIQUE

L. Estel¹, C. Lafossas², M. Poux², J. Tao³

¹Normandie University, INSA Rouen, UNIROUEN, LSPC, 76000 Rouen, France

²Laboratoire de Génie Chimique, Université de Toulouse, CNRS, INPT, UPS, France

³Toulouse University, INP-ENSEEIH, LAPLACE, France

tao@laplace.univ-tlse.fr

Keywords: Microwave heating, Measurement applications, Inverse modelling

New materials play very important role in industrial, scientific and medical sectors. Accurate knowledge of their mechanical, electrical and thermal properties is a prerequisite for the development of novel and original applications. Many techniques were developed for the determination of these parameters, often under conditions of use of these materials [1-2]. In applications involving the use of microwave energy, the strong interaction between electromagnetic waves and materials provided a new means of investigation in addition to conventional techniques. The use of multiphysics simulation software based on the numerical resolution of coupled partial differential equations offers the possibility of simulating the dynamic system more or less close to real conditions [3-4]. Combining well-controlled and mastered experimental means, simulation tools allow us to go back to the physical properties of the system studied, including the thermal properties of the materials under test.

In this article we propose to characterize the thermal properties of new materials by an inverse modeling technique. It consists in minimizing an objective function built from experimental measurements and multi-physical simulations and then in extracting the desired thermal parameters.

1. Principe

In our study we are interested in candidate materials for microwave chemistry or microwave materials processing applications. As a result, these materials will first play the role of receptor of microwave energy, transforming it into thermal energy, before returning it to a "load", the final destination of this energy. The important thermal properties for this kind of application are the *thermal conductivity* and the *specific heat* of the material to be characterized.

We design an experiment setup using a microwave generator. For a chosen microwave power, a target temperature is given for the material to be heated. The generator is stopped when the target temperature is reached. The cooling phase begins until thermal equilibrium. The temperature evolution in specific point inside the material will be recorded using optical temperature probes for the heating and the cooling steps. The modeling of the entire experimental system with a commercial software COMSOL Multiphysics coupling the heat equation to Maxwell's equations provides an estimate of this same evolution as a function of the trial values of thermal conductivity and specific heat, on the two phases of the process: heating and cooling.

The use of an optimization algorithm allows the extraction of thermal properties as a function of temperature.

2. Direct analysis

2.1 Physical laws



The physics laws which govern the thermal exchanges between a microwave source and a thermal system are the Maxwell equations and the heat transfer equation:

$$\nabla \times \mu_r^{-1} (\nabla \times \vec{E}) - k_0^2 \varepsilon_r \vec{E} = 0 \quad (1)$$

$$Q + \nabla \cdot (k \nabla T) = \rho C_p \frac{\partial T}{\partial t} \quad (2)$$

with E the local electric field, μ_r the relative permeability, ε_r the relative permittivity, $k_0^2 = (\omega/c)^2 \mu_r \varepsilon_r$, $\omega = 2\pi f$ the angular frequency, f the working frequency, and c the light velocity in free space.

For the thermal study, the heat source Q results from absorbed electromagnetic power by material under test and locally proportional to $|E|^2$. ρ , C_p , and k correspond respectively to the density, specific heat under constant pressure and thermal conductivity of material. T is the local temperature. At a convective boundary the convective heat condition is determined locally by using T_{ext} the external ambient temperature and h the thermal exchange coefficient.

The axisymmetric 2D approximation will allow a simplification in the formulation as in the numerical simulation for a geometry presenting symmetry of revolution as shown in Fig. 1. For microwave feeding system only the TEM mode will propagate for the given working frequency. Therefore, a small disturbance of the symmetry does not fundamentally change the distribution of electromagnetic fields, and subsequently the absorption of electromagnetic energy by the material. On the thermal side, insofar as the radial variation is predominant, the error introduced by the assumption of symmetry of revolution will remain negligible. This is especially true if the whole structure can be considered thin thermally.

By choosing cylindrical coordinates (Fig.1) all physical quantities vary with r , z and t , respectively the radial and axial coordinates, as well as the time for a transient study.

Note that equation (1) is in sinusoidal steady state. This is not really contradictory because the microwave time constant is quite negligible compared to that of the heat transfer of the system studied.

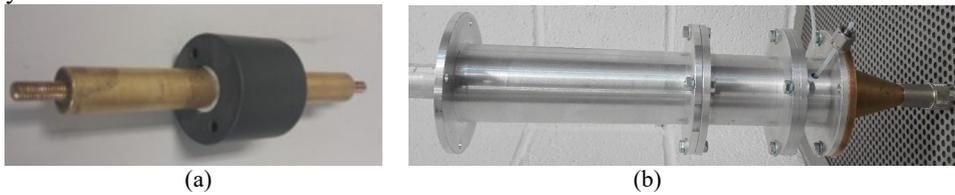


Fig. 1. Photos of axisymmetric system. (a) Ceramic tube around a bronze rod. (b) Coaxial structure with material under test inside.

2.2 Numerical modeling

To start the description of the geometry (Fig. 1) was in axisymmetric 2D version as shown in Fig. 2 (a). The sample material was made in a cylindrical ring shape, inserted into a coaxial structure that also serves as feeding component for microwave TEM waves. Between the central conductor of the coaxial structure and the inner wall of the ring there is a distance of 1mm filled with thermal insulation fiber material. The outer conductor of the coaxial structure is a stainless steel of 5mm thick and has an internal diameter of 40mm. For the purpose of limiting the simulation volume, convective boundary conditions are applied at the external of stainless steel cylinder. For the electromagnetic simulation the electrical conductors were considered perfect. This assumption remains valid as the dielectric losses in the material under test dominate other losses for a heating application. The finite element method is used here to effectuate transient study of the coupled electromagnetic / heat transfer problem. For an axisymmetric 2D model like that of Fig. 2

the triangular elements were chosen, followed by an automatic mesh refinement leading to convergent results.

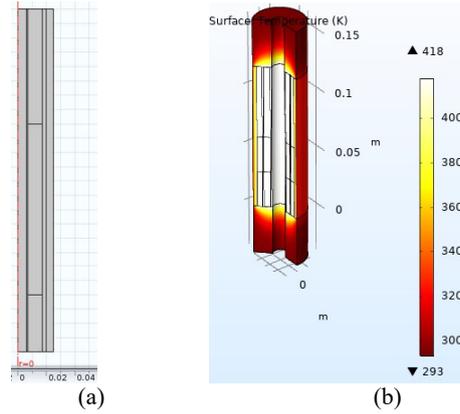


Fig. 2. (a) Cutter view of structured under study. (b) Reconstituted 3D view.

2.3 Analytical modeling for effective approximate structure

A one-dimensional theoretical model is developed, leading to a quasi-analytical solution of the effective thermal parameters.

When only one space variable l is needed to describe space temperature variation, the heat transfer equation is reduced in the following form

$$Q + \frac{\partial}{\partial l} \left(k \frac{\partial T}{\partial l} \right) = \rho C_p \frac{\partial T}{\partial t} \quad (3)$$

If the radiation losses can be neglected, a more compact equation can be obtained

$$\frac{\partial T}{\partial t} = -\frac{p}{\rho C_p} + \frac{\partial}{\partial l} \left(D \frac{\partial T}{\partial l} \right) \quad (4)$$

D being the thermal diffusivity and p the heat source. A dimensionless equation is deduced for zero heat source case

$$\frac{\partial \bar{T}}{\partial \bar{t}} = \frac{Dt_c}{L^2} \frac{\partial^2 \bar{T}}{\partial \bar{l}^2} = F_0 \frac{\partial^2 \bar{T}}{\partial \bar{l}^2} \quad (5)$$

$$\bar{T} = \frac{T - T_{\text{inf}}}{T_{\text{inf}}}, \bar{l} = \frac{l}{L}, \bar{t} = \frac{t}{t_c}$$

with time, temperature and length normalized by corresponding reference quantities (structure time constant t_c , infinite location temperature T_{inf} and maximum structure size L). The advantage of this model is the negligible computation time compared to the use of a three-dimensional or 2D axisymmetric computational code based on the finite element method.

Numerical studies were carried out on a structure similar to the experimental model. It is a solid copper cylinder (4cm diameter and 20cm height). The temperature was raised to 200°C before the power was turned off. With a heat exchange coefficient of 10W/m².K, the analytical solution of (5) is plotted in Fig. 3, compared to the numerical results. In Fig. 3 (b) the entire surface of the cylinder participates in the heat exchange while in Fig. 3 (a) the ends are considered as thermally insulated. In both cases one notes a very good agreement between the analytical solution (blue line) and the numerical results ('+').

It should be noted that the temperature gradient is not taken into account in the analytical solution, whereas it is present in the digital simulation. The good agreement between the two results confirms the hypothesis of a thermally thin structure.

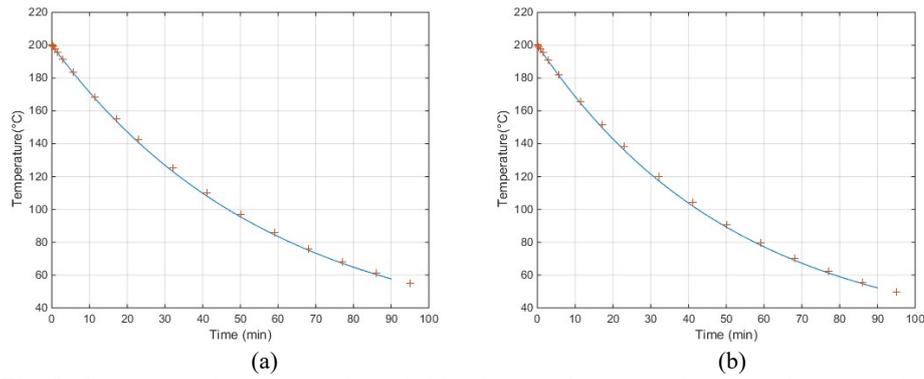


Fig. 3. Comparison between analytical (blue line) and numerical (+) coupling procedure.
 (a) Extremity disks isolated. (b) Convective condition at all sides.

3. Inverse modeling

3.1 Comparison between experimental data and numerical results

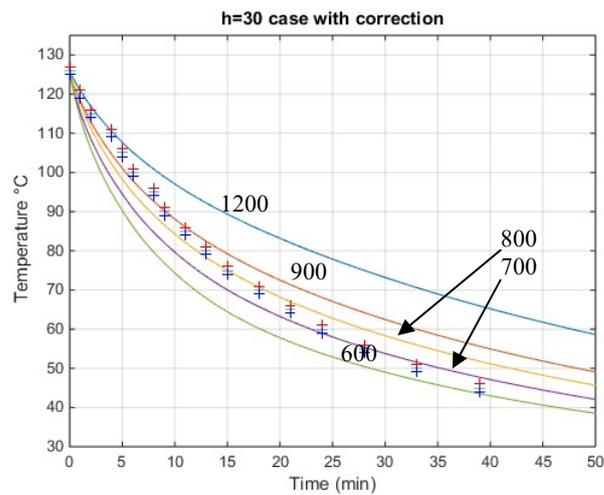


Fig. 4. Simulated coupling phase with specific heat varying from 600 to 1200 J/kg.K.
 Comparison with measured data with error crosses ('+')

We will focus on the cooling phase. Different couples of trial values allow the simulation of transient temperature variation. Fig. 4 plots these different temperature variations with the assumption of a constant exchange coefficient and constant specific heat compared to the measurement data.

It can be seen that the assumption of a constant specific heat value is not valid. The extraction by inverse modeling must be done for each moment of measurement, corresponding to different temperatures.

3.2 Extraction of specific heat of material under test

From the simulation results, we have extracted the specific heat value by comparing it with the measured data by considering $\pm 0.8^\circ\text{C}$ uncertainty of our thermal probe. Fig. 5 shows the estimation of these parameters as a function of temperature.

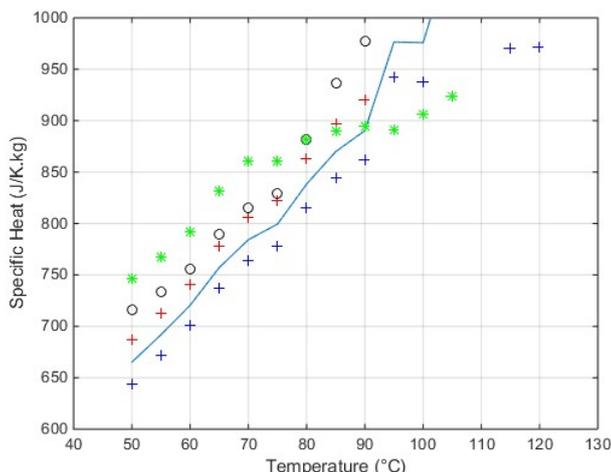


Fig. 5. Extracted specific heat of material under test with different scenarios.

Several situations give different results. When using the 7mm nominal internal radius of the ceramic tube, the highest specific heat curve is obtained (* green'); if we consider the slight offset of the ceramic tube by using a small 0.1mm reduction of this radius, lower curve (o' black) is obtained but divergent results appear above 80°C. By further reducing this radius by 0.15mm the specific heat curve becomes the blue line. Now adding the temperature uncertainty to the measured temperatures the extracted specific heat will be limited for each temperature by red and blue crosses.

The variation trend corresponds to that expected for this type of material. However, the strong influence of both the mechanical precision of the sample and the uncertainty of the probe, which is of good quality, can be observed.

4. Conclusion

A method of extraction of thermal properties of a material used for microwave heating is presented by inverse modeling based on numerical simulation and temperature measurement in the material cooling phase. The results obtained show a great sensibility to both geometry accuracy of the experiment setup and the uncertainty of used thermal probe.

An analytical solution is presented for a simplified scenario and verified by numerical investigation. This solution will be of great utility to the future sensitivity study of proposed inverse modeling method.

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