Modeling Microwave Heating During Batch Processing of Liquid Sample in a Single Mode Cavity

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Abstract: In this study, the objective is to model the microwave heating process of a liquid sample (water) in the fundamental mode, denoted TE_{10}, operating at a frequency of 2.45 GHz.
The model considers the coupling between the fluid flow (natural convection in laminar flow from the CFD module), electromagnetic field (frequency domain with RF module) and thermal kinetics during the process (heat transfer module). For all of the transient state simulations, thermophysical and dielectric properties of water are considered as temperature dependant.
As a whole, the study highlights both the complexity of physical phenomena and a high computational demand in order to model microwave interaction within a liquid sample in a batch configuration. This study will also help to prevent the hot and cold spots that occur during the microwave processing of liquids.

Keywords: microwave heating, modeling, liquid, natural convection

1. Introduction

The use of microwaves for heating purposes of dielectric materials is encountered in many industrial applications (food processing, chemistry, material engineering and medical applications). The main problem related to microwave heating processes lies in the non uniform temperature distribution within the processed material (Vadivambal and Jayas 2010). This non uniformity highly depends on the physical and geometrical properties of the product and also on its dielectric properties (Salazar-González, San Martín-González et al. 2012, Sturm, Verweij et al. 2012).
Nowadays, in order to help preventing such non uniformity of heating, modeling of the microwave heating process remains one affordable solution. The numerical modeling enables to predict the temperature evolution within the processed material in order to optimize the treatment. In the literature, numerous studies are devoted to the modeling of microwave processes dedicated to liquid samples (Datta, Prosetya et al. 1992, Zhang, Jackson et al. 2000, Ratanadecho, Aoki et al. 2002, Chatterjee, Basak et al. 2007, Sturm, Verweij et al. 2012, Cherbanski and Rudniak 2013). All of these studies investigated the microwave induced natural convection or forced convection of liquids in various geometrical configurations (single mode or microwave resonant cavity) and by using different numerical methods (Finite Volume and Finite Difference Time Domain).
Based on those previous publications, the current study is dedicated to the microwave heating simulation of pure water in a single mode applicator. In contrast to earlier publications which mostly deal with cylindrical geometries, the current study considers smaller rectangular sized water sample (8.5 mL) placed within a waveguide applicator. COMSOL®5.1 is used to model the microwave processing of liquid from the finite element method. The study also takes into account the variation of thermophysical and dielectric properties as a function of temperature.

2. Governing equations

In this work, the objective is to model the microwave heating process of a liquid sample in the fundamental mode, denoted TE_{10}, operating at a frequency of 2.45 GHz.
A dielectric material, consisting of pure water, is placed within a single mode applicator at a location where the electric field strength is set at its maximum amplitude. The bottom ended of the rectangular waveguide consists in a water load which absorbs the transmitted microwave power throughout the waveguide.
The sample is inserted within a Teflon® mold (PTFE) and settled on a Teflon® support plate which fills the cross section of the rectangular waveguide. The support is located between the inlet and the absorbing water load (figure 1).

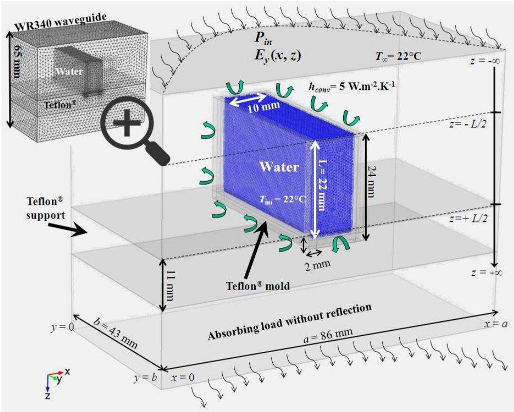

Figure 1. Model design

2.1 Electromagnetic modeling

The numerical modeling of microwave interactions with dielectric materials is governed by the classical Maxwell's equations. In this model, the equations are solved within the air, water & PTFE materials by considering a harmonic propagation with sinusoidal time-varying fields at $f = 2.45$ GHz.

The COMSOL® software solves the governing equation for the electric field propagation in free space for a general lossy medium, as follows:

$$\nabla \times \mu_r^{-1}(\nabla \times E) - k_0^2\left(\varepsilon'_r - \frac{j\sigma}{\omega\varepsilon_0}\right)E = 0$$

$$with\ \ k_0 = \omega\sqrt{\varepsilon_0\mu_0}$$

The complex propagation constant which governs the electric field distribution is defined as follows:

$$\gamma^2 = k_0^2\left(\varepsilon'_r - \frac{j\sigma}{\omega\varepsilon_0}\right)$$

Where ε_0 is the permittivity of a vacuum, ε_r' is the relative dielectric constant. σ represents the electrical conductivity for a lossy material.
σ is linked to the pulsation ω of the wave from the following expression:

$$\sigma = \omega\varepsilon_0\varepsilon_r''$$

where ε_r'' is the relative dielectric loss factor.

The permeability μ may be represented by $\mu_0 = 4\pi\times10^{-7}$ H.m^{-1}, the permeability of a vacuum.

In this study, the walls of the waveguide consist in a brass material. In COMSOL®, the impedance boundary condition is used on external walls in order to represent the surface of a lossy domain (the tangential electric field is small but non zero at the boundary walls). The electrical conductivity of brass is fixed at 1.57×10^7 S/m (http://www.diehl.com).

The main initial and boundary conditions are summarized as follows:

$$\begin{cases} E = 0 & at\ \ t = 0, \forall x\, y\, z \\ E_{in} = E_0 \cos\left(\dfrac{\pi x}{a}\right) with\ E_0 = 4Z_{TE}\dfrac{P_{in}}{ab} & at\ z = -\infty, \forall x \\ n \times \left(\mathbf{H}_{air} - \mathbf{H}_{sample}\right) = 0 & at\ z = -L/2,\ z = L/2, \forall x \\ \sqrt{\dfrac{\mu_0\mu_r}{\varepsilon_0\varepsilon_r - j\sigma/\omega}}\, n \times \mathbf{H} + E - (n.E)n = 0 & at \begin{cases} x = 0 \\ x = a \\ y = 0 \\ y = b \end{cases}, \forall z \end{cases}$$

E_0 represents the amplitude of the incident electric field. This value is linked to the wave impedance Z_{TE} (Ω) of the electromagnetic wave within the TE_{10} rectangular waveguide.

At the end of the rectangular waveguide, the resulting wave exits the system without any reflection.

2.2 Heat Transfer modeling

According to figure 1, heat transfer is only solved within the PTFE support and the water sample (conduction and convection). The temperature evolution within the water sample is described from the general heat equation which depends on thermophysical properties of the sample:

$$\rho C_p \frac{\partial T}{\partial t} = div.(k\nabla T) + Q_{abs}$$

Where ρ is the density, C_p the heat capacity and k the thermal conductivity of the different materials under consideration.
The heat generation Q_{abs} due to microwaves is determined from the local electric field computation at any point of the domain.

$$Q_{abs} = \frac{1}{2}\omega.\varepsilon_0.\varepsilon_r''|E_{local}|^2$$

The initial and boundary conditions for the thermal problem are defined as follows:

$$\begin{cases} T = T_0 & at\ t = 0, \forall x\ \forall y\ \forall z \\ k\nabla T = h(T - T_\infty) & at\ external\ boundary\ walls \end{cases}$$

with $\begin{cases} T_0 = 22°C \\ h = 5\ W.m^{-2}.K^{-1} \quad (free - convection) \end{cases}$

2.3 Fluid Flow modeling

The velocity field *U (u, v* and *w* components for *x, y* and *z* directions, respectively*)* issued from microwave induced natural convection within water is computed from the resolution of the Navier Stokes equations (Newtonian fluid with incompressible flow):

$$\begin{cases} \dfrac{\partial u}{\partial x} + \dfrac{\partial v}{\partial y} + \dfrac{\partial w}{\partial z} = 0 & (continuity) \\ \rho \dfrac{d\vec{U}}{dt} = \rho \vec{g} - \nabla P + \mu \Delta \vec{U} & (momentum) \end{cases}$$

with $\dfrac{d\vec{U}}{dt} = \dfrac{\partial \vec{U}}{\partial t} + (\vec{U}\nabla)\vec{U}$

The initial and boundary conditions are defined with the following mathematical expressions:

$$\begin{cases} U_0 = 0\ and\ P_0 = \rho g L \quad at\ \ t = 0, \forall x\ \forall y\ \forall z\ with\ 0 < L < 22mm \\ U = 0 \quad at\ the\ \text{liquid - container interfaces} \end{cases}$$

3. Simulation strategies with COMSOL®

The user-defined total mesh consists in 811988 tetrahedral elements (440581 elements for modeling the water sample). In order to insure the best numerical precision, the maximum element sizes of each tetrahedral element are limited to 2 % of the free space wavelength at 2.45 GHz (0.122 m).

The numerical study is performed following two main steps. Firstly, the simulation of the electromagnetic field with the PTFE mold and support plate is performed. A stationary study is thus set up where the electromagnetic field is solved within the empty cavity without the water sample. This study enables to characterize the influence of the PTFE material on the electric field distribution within the single mode cavity.

Then a transient study is considered where the water is filled within the PTFE mold. The microwave heating process is simulated during 160 seconds with a microwave input power fixed at 50 W. The transient simulations are solved by using strong couplings between equations from the Radio frequency, Heat Transfer and CFD modules (electromagnetism, heat transport and fluid flow, respectively). During the transient state simulations, thermophysical and dielectric properties of water are considered as temperature dependant.

In order to simulate 160 s of the process, the total CPU time is approximately 1 day and 11h on a Dell® *Precision*™ Workstation, equipped with 2×Intel® *Xeon* processors (8 cores), at 2.8 GHz, with 256 GB of RAM, running on Windows®8 Professional, 64 bits.

The table 1 depicts the material properties of the PTFE support plate. These properties are considered as constant during the process.

Table 1: Material properties of Teflon® (PTFE) (From *du Pont de Nemours)*

	PTFE
Density (kg.m^{-3})	2180
Heat capacity (J.kg^{-1}.K^{-1})	1300
Thermal conductivity (W.m^{-1}.K^{-1})	0.25
Dielectric constant	2.1
Dielectric loss factor	3.15×10^{-4}

The figure 2 displays the variations of thermophysical and dielectric properties of pure water as a function of temperature (Zhang, Jackson et al. 2000). These properties are directly implemented in the COMSOL® model by using interpolation functions.

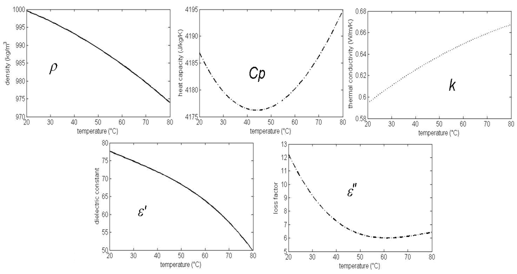

Figure 2. Thermophysical properties (ρ, *Cp*, *k*) and dielectric properties (ε'_r, ε''_r) for pure water within the range [20; 80 °C].

4. Electromagnetic field distribution within the empty cavity

The electric field strength following the microwave propagation direction *z* is thoroughly analyzed in order to quantify the influence of the PTFE mold and support plate. The numerical results are presented in term of absolute value of

the electric field component propagating within the waveguide structure (norm of E_y component). For convenience, the E_y component is normalized following the maximum electric field strength at any location of the computational domain, so that numerical values lie between 0 and 1.
The figure 3 depicts the electric field distribution within the waveguide filled with the PTFE support plate.

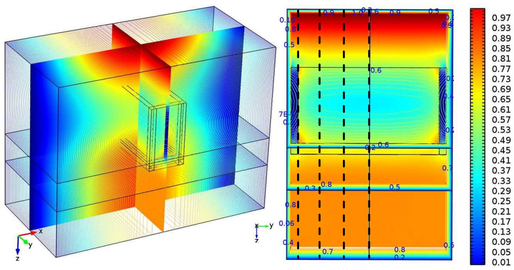

Figure 3. Electric field distribution (normalized) within the waveguide filled with the PTFE support: 3D distribution map (left), 2D cross section in y, z plan (right)

Overall the electric field strength near the top surface is attenuated when passing through the PTFE support plate (magnitude reduced from 90% to approximately 30%). The figure 3 (left) demonstrates that microwave propagates following a fundamental TE_{10} mode until they reach the top surface of the PTFE support. Especially, the E_y component remains almost constant following the small side of the rectangular waveguide (figure 3, right)
Then, low electric field gradients from 60% to approximately 10% are encountered near the large side walls due to the thickness of the PTFE support plate (figure 3, right).
Below the PTFE support plate, the electric field shape depicts a kind of travelling wave propagation regime before exiting the waveguide within the air surrounding medium (figure 3, left and right).

The figure 4 shows the normalized electric field strength as a function of the propagation direction z for various crossing lines in the (y, z) plan. These positions are illustrated in figure 3 (right) with the vertical black dashed lines in the (y, z) plan.

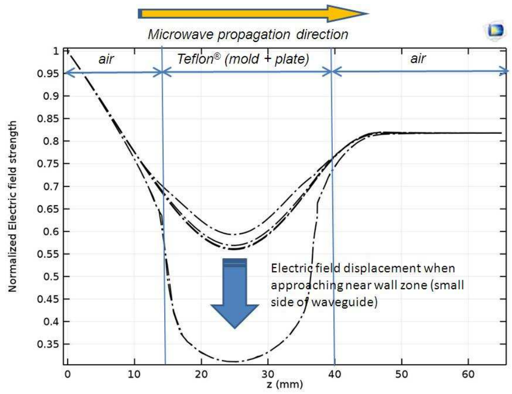

Figure 4. Electric field distribution (normalized) within the waveguide filled with the PTFE support as a function of microwave propagation direction.

Under those operating conditions, the reflection coefficient (ratio of reflected power over microwave input power) is fixed at 14 %. This result indicates that the PTFE support does not act as a perfectly matched layer with low reflection. Due to slightly different dielectric constant of PTFE comparing to air (2 vs. 1), the electric field polarization occurs within the waveguide resulting in the presence of non negligible microwave reflected power from the load.

5. Microwave heating simulations with distilled water

8.5 mL of distilled water is then poured within the PTFE mold (the container is completely filled). The microwave input power is fixed at 50W and the thermal treatment is started during 160 seconds.

The figure 5 depicts the temperature distribution for the water sample and the PTFE container at the external surfaces and at the end of microwave processing (t=160s).

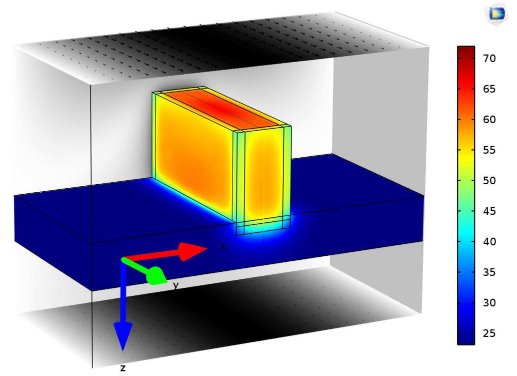

Figure 5. Temperature distribution (°C) within water and PTFE support plate at *t*= 160s

As the PTFE support does not dissipate any heat due to low loss factor; the plate is only heated by conduction from the water sample. At the end of microwave processing, the surface of the water is close to 70 °C while the external temperatures of the walls range from 55 to 60 °C.

In figure 6, the microwave induced natural convection of liquid is illustrated at the end of processing.

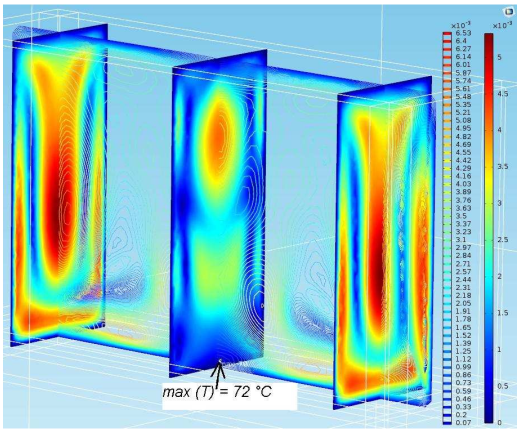

Figure 6. Cross sections areas of velocity fields (m/s) at *t* = 160s (local maximum of temperature is located at the bottom side of the water sample)

The gravitationally driven flow of water occurs mainly due to the coupling between the fluid flow and the heat transfer equation. The temperature evolution within the computational domain creates density variation of water which induces free convection with relatively small magnitude (max velocity gradients are limited to ≈ 6 mm/s).

In the presence of a microwave source term, the free convection due to the motion of fluid is characterized by a height-based modified Grashof number (Gartling 1982).

$$Gr^* = \frac{\rho^2 g \beta L^5 Q_{abs}}{\mu^2 k}$$

In COMSOL®, this modified Grashof number is computed as a function of time by using an average coupling operator (thermophysical properties and microwave heat source term are volume-averaged within the computational domain associated to water). The volume thermal expansion coefficient of water, β, is equal to 5.344×10^{-4} K^{-1} (Zhang, Jackson et al. 2000).

The figure 7 indicates the temperature map over 3 cross sections areas at the mid processing time (t = 80s).

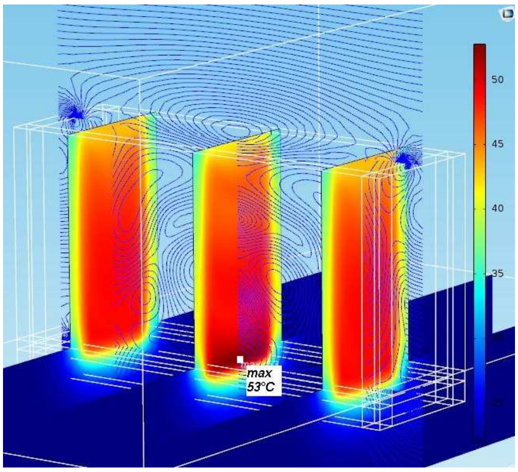

Figure 7. Cross sections areas of temperatures (°C) and electric field shape (blue contours) at *t* = 80 s (local maximum of temperature is located at the bottom side of the water sample)

The hot spot (53°C) is still located at the same position as in figure 6 for *t*=160s. Overall the temperature seems to be quite homogeneous within the water sample. Nevertheless, hot spots locations are depicted at the near bottom zone of the liquid-container interface.

The temperature evolution at three locations T_1, T_2 and T_3 (respectively 2 mm, 5 mm and 10 mm below the upper water surface) are presented in figure 8. Experimentally, the three temperature probes within water are all located at the centre of the (x, y) plan; only the depth position from the upper surface of water is modified following the z direction.

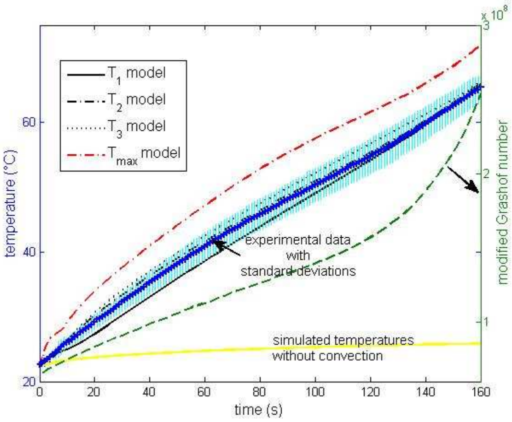

Figure 8. Simulated temperatures from T_1 to T_3 (black) and max temperature (red) vs. experimental measurements (blue) with standard deviations (cyan) as a function of processing time (left *y*-axis), modified Grashof number (right *y*-axis)

Simulated temperature evolutions for T_1, T_2 and T_3 are quite similar which is in agreement with the 3D temperature map reported in figure 7. Experimentally, the temperature measurement uncertainties illustrated by the standard deviations plots shows that it is particularly difficult to obtain good repeatability when measuring temperature evolution within a liquid medium subjected to microwave heating and natural convection. Nevertheless, the comparison between numerical results and experimental measurements gives a fairly good agreement, especially near the central zone.

The maximum temperature is located numerically near the bottom wall of the water sample (figure 6 and 7). Its evolution is directly illustrated as a function of time in figure 8. The position of this max value depends on the electric field interaction with the water sample and the spatial evolution of dielectric properties. This could not be directly predicted experimentally. At the end of microwave processing, the maximum temperature reaches approximately 70°C while temperature at the centre remains close to 65°C (figure 8). This result illustrates that small volumes of interest may be submitted to higher electric field strength than other resulting in a non homogeneous thermal treatment even with a small volume of liquid. This result is in agreement with a previous study under different operating conditions with cylindrical water sample (Cherbanski and Rudniak 2013).

During the heating process, the modified Grashof number increases from approximately 5×10^7 to more than 2.5×10^8 (figure 8). This result is significantly higher than in a previous study (Zhang, Jackson et al. 2000). It indicates that microwave induced natural convection increases as a function of processing time. The large magnitude of the Grashof number in comparison to previous study is also due to the small volume (8.5 mL) of the water sample placed within the PTFE container.

In figure 8, some additional simulations results are displayed in yellow colors where the Navier Stokes equations were removed from the numerical resolution of the coupled equations. For the 3 temperature probe locations (T_1, T_2 and T_3), simulated temperature evolutions are very similar. In those conditions, the maximum temperature only reaches 25 °C at the end of microwave processing with the same input microwave power. This result clearly illustrates that the fluid flow equations has to be coupled to the heat transfer and the Maxwell's equations in order to describe quantitatively the real microwave process.

In figure 9, the reflection coefficient (ratio between the microwave reflected versus the microwave input powers) is computed.

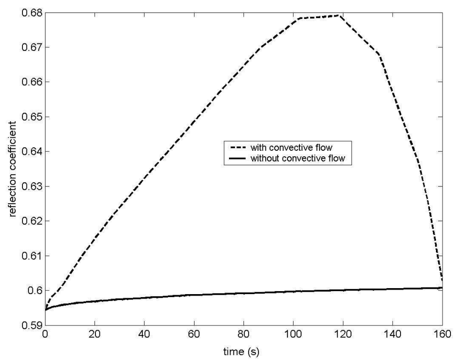

Figure 9. Reflection coefficient as a function of processing time.

The figure 9 clearly shows the differences in reflected power magnitude if convective flow of water is solved or withdrawn within the

COMSOL® solver. If the Navier Stokes equations are coupled to heat transfer and electromagnetism, the variations of the reflection coefficient are due to the temperature dependant dielectric properties of water during microwave processing. These variations are clearly reduced when convective flow is removed from the solver due to lower temperature gradients (see yellow curve in figure 8)

6. Conclusions

Finally, this study enables to give complementary results comparing to the existing literature on the modeling of microwave heating for liquids. Based on our operating conditions, the most important information of this study can be summed up by the following points:

- The PTFE material (Teflon®) which is often considered as transparent to microwaves clearly interacts with the electric field, however the heat dissipation could be considered as negligible (very low loss factor).
- Even with a small volume of interest, the microwave heating of a water sample in a single mode rectangular cavity leads to a non uniform inner temperature distribution. The modeling enables to locate precisely the hot spots.
- When modeling microwave heating of liquids, the Navier Stokes equations must be coupled to the thermal and the Maxwell's equations in order to give realistic results. Nevertheless, this modeling approach needs high computational resources for a strong coupling between the differential equations.

This study could now be extended to other configurations and is considered as a good start point in order to develop specific microwave applicator dedicated to liquid phase processing.

7. References

1. Chatterjee, S., T. Basak and S. K. Das. "Microwave driven convection in a rotating cylindrical cavity: A numerical study." *Journal of Food Engineering* **79**(4): 1269-1279 (2007)
2. Cherbanski, R. and L. Rudniak. "Modelling of microwave heating of water in a monomode applicator - Influence of operating conditions." *International Journal of Thermal Sciences* **74**: 214-229 (2013).
3. Datta, A., H. Prosetya and W. Hu. "Mathematical-modeling of batch heating of liquids in a microwave cavity." *Journal of Microwave Power and Electromagnetic Energy* **27**(1): 38-48 (1992).
4. Gartling, D. K. "A finite element analysis of volumetrically heated fluids in an axisymmetric enclosure." *Finite Elements in Fluids* **4**: 233-250 (1982).
5. Ratanadecho, P., K. Aoki and M. Akahori. "A numerical and experimental investigation of the modeling of microwave heating for liquid layers using a rectangular wave guide (effects of natural convection and dielectric properties)." *Applied Mathematical Modelling* **26**(3): 449-472 (2002).
6. Salazar-González, C., M. San Martín-González, A. López-Malo and M. Sosa-Morales. "Recent studies related to microwave processing of fluid foods." *Food and Bioprocess Technology* **5**(1): 31-46 (2012).
7. Sturm, G. S. J., M. D. Verweij, T. van Gerven, A. I. Stankiewicz and G. D. Stefanidis. "On the effect of resonant microwave fields on temperature distribution in time and space." *International Journal of Heat and Mass Transfer* **55**(13-14): 3800-3811 (2012).
8. Vadivambal, R. and D. S. Jayas. "Non-uniform Temperature Distribution During Microwave Heating of Food Materials-A Review." *Food and Bioprocess Technology* **3**(2): 161-171 (2010).
9. Zhang, Q., T. H. Jackson and A. Ungan. "Numerical modeling of microwave induced natural convection." *International Journal of Heat and Mass Transfer* **43**: 2141-2154 (2000).