Coupled Simulation of an Electromagnetic Heating Process Using the Finite Difference Time Domain Method

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Due to the complexity of interactions between microwaves and food products, a reliable and efficient simulation model can be a very useful tool to guide the design of microwave heating systems and processes. This research developed a model to simulate coupled phenomena of electromagnetic heating and conventional heat transfer by combining commercial electromagnetic software with a customer built heat transfer model. Simulation results were presented and compared with experimental results for hot water and microwave heating in a single mode microwave system at 915 MHz. Good agreement was achieved, showing that this model was able to provide insight into industrial electromagnetic heating processes.

INTRODUCTION

Electromagnetic (EM) heating has attracted much attention for food application research because, unlike conventional heating, it generates heat within food packages leading to higher heating rates and reduced heating processes [Osepchuck, 1984]. Several studies with pilot-scale systems have demonstrated the possibilities for short time microwave sterilization processes to produce safe and high quality low-acid shelf-stable packaged foods [Guan *et al.*, 2002; Guan *et al.*, 2003]. The main focus of most recent research activities related to the development of novel thermal processing technologies based on microwave energy was to improve heating uniformity

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and to develop processes with stable heating performance for industrial implementation. But EM fields inside a microwave cavity, governed by Maxwell's equations, are not uniform. Interactions between the cavity and load produce "hot spots" and "cold spots" within the heated object. If not given adequate time, these hot and cold spots cause severe temperature non-uniformity, which adversely affects product quality [Ma and Paul, 1995]. It is desirable to develop an effective numeric model to reliably simulate EM heating processes so that temperature distributions, especially the location of hot and cold spots, could be identified within commercial industrial heating systems as the first step in continuing efforts to improve heating uniformity. The numeric model should include solutions for two separate sets of partial differential equations that govern, respectively, propagation of EM waves and transfer of thermal

energy generated by EM heating. These two sets of equations are in reality coupled with the heating processes because heat transfer due to the gradients generated by localized EM heating alters the dielectric properties of food, which in turn affect the EM field distribution.

Solving these coupled equations for a three-dimensional (3-D) transient EM heating process in an industrial system for foods with temperature-dependent dielectric properties is a challenging task that has not been addressed in literature. Early research used analytical models to describe EM fields inside domestic microwave ovens [Shou-Zheng and Han-Kui, 1988; Watanabe and Ohkawa, 1978], but these were suitable only for oversimplified cases that did not represent real-world systems. Numeric models were developed for EM field distribution calculations in more complicated cases [Paoloni, 1989; Webb et al., 1983]. Coupled EM and heat transfer models were used for simple 1-D [Smyth, 1990] or 2-D cases [Clemens and Saltiel, 1995; Barratt and Simons, 1992]. Detailed 3-D treatment of numeric models for coupled equations had not been explored until recently [Burfoot et al., 1996; Bows et al., 1997; Clemens and Saltiel, 1995; Dibben and Metaxas, 1994; Harms et al., 1996].

Several numerical techniques have been used to solve coupled Maxwell and heat transfer equations using the Finite Difference Time Domain (FDTD) method [Ma and Paul, 1995; Torres and Jecko, 1997], Finite Element Method [Webb et al., 1983; Dibben and Metaxas, 1994;] and Transmission Line Method [Leo et al., 1991]. In [Spiegel, 1984], Spiegel reviewed numeric methods for medical applications and commented that the FDTD method is best suited for coupled EM and thermal processes because it does not require matrix computation, and thus saves computer memory and simulation time. However, a major limitation of the FDTD method is the use of rectangular meshes that are not applicable for irregular geometries such as curvature surfaces. The Finite Element Method (FEM) can handle more complex geometries. In [Zhang and Datta, 2000], two commercial software employing FEM were used together to simulate coupled EM and thermal processes in a domestic oven. But FEM involves computation to inverse matrices that contain information for all elements of the discrete grids within the considered domain. This requires large computer memory and lengthy computation time, making it unsuitable for complicated systems.

A major development in FDTD applications with EM field simulation is the use of a conformal FDTD algorithm. This algorithm incorporates finite boundary grids that conform to geometry surfaces to accurately match detailed irregularities in a 3-D domain, while also including regular grids identical to those in the original FDTD algorithm for the other parts of the 3-D domain. References [Holland, 1993] and [Harms et al., 1992] provide a detailed description of a conformal FDTD algorithm and its application to some simple cases. In brief, instead of Yee's original algorithm that uses differential forms of Maxwell's equations, the conformal FDTD algorithm uses integral forms of Maxwell's equations for the finite grids conformed to the edge or surface of the geometry, thus avoiding the need to approximate the curved and oblique surface using staircase grid. As a result, complex geometry can be modeled without sacrificing the speed of an FDTD algorithm. This method also saves computer memory and simulation time compared to the original FDTD algorithm when applied to complex geometries. The conformal FDTD algorithm can be used to model arbitrary shape structures and inhomogeneous, nonlinear, dispersive and loss mediums. Since the FDTD method does not require computation of inverse matrices which takes extensive computer memory for fine element grids, the conformal FDTD algorithm is much more efficient compared to the FEM. For example, in [Zhang and Datta, 2000], it took six and half hours for an HP workstation to run a model consisting of 15,000 nodes for a single



Figure 1. Pilot-scale EM heating system (front view).

time step, while the conformal FDTD used in the study reported here took only three hours to complete a coupled simulation that included 720 time steps for a complicated industrial system with 500,000 cells in a 3-D domain.

This paper presents a model that used conformal FDTD algorithms for EM field simulation and the regular FDTD method for heat transfer to simulate coupled processes in an EM heating system for industrial sterilization and pasteurization applications.

EXPERIMENTAL METHODS

Experimental Set-up

Validation is a critical step in developing a new and reliable numeric model. In this study, this was achieved with a single-mode microwave sterilization system developed at Washington State University. The system consisted of a rectangular cavity with one horn-shaped applicator on the top and another identical applicator on the bottom (Figures 1 and 2). Figure 1 shows a front view of the system with an exposed interior cut and vertical central plane, while Figure 2 shows the top view for the central section of the cavity. Microwave energy was provided by a 5 kW generator operating at 915 MHz through a standard waveguide that supported only TE_{10} mode (Figure 3). Figure 3 provides detailed information for the top and bottom rectangular waveguide sections having a length of 128 mm and width of 124 mm. After passing through a circulator, the microwave energy was equally divided at a T-junction and fed to the two horn applicators through two standard waveguides shown in Figure 3. The length of each leg of the waveguide after the T-junction could be adjusted to control the phase difference between the microwaves at the entry port of the two horn applicators, which meant the phase shift between the two waves interacting inside the cavity could be controlled to achieve the desired field distribution. In this study, for simplification, a 0 phase shift was used between the entry ports of the top and bottom horn applicators. That was, microwaves coming to the top and the bottom entry ports of the horn applicators were in the same phase at any moment. The model, however, was able to simulate more complex cases with arbitrary



Figure 2. Pilot-scale microwave heating system (top view).



Figure 3. Rotate view of rectangular waveguide in Figure 1.

phase differences.

The pilot scale system combined surface heating by circulating hot water and volumetric EM heating to improve heating uniformity and reduce heating time. Because microwave sterilization for low-acid foods (pH > 4.5) [Guan et al., 2003] requires that food temperatures at cold spots be processed higher than 121°C, the temperature of the circulation water in the cavity was set at 125°C. The water was pressurized at 41 psia by compressed air through a buffer tank in the water-circulating system (not shown) to prevent boiling. To maintain the steam inside the cavity, two windows made of microwave transparent material were secured at the mouth of both horn waveguides. During thermal processing, the packaged food was positioned at the central line of the cavity. Though it was possible to simulate a heating process with moving packages, only a simple stationary case was considered to better focus on the development and validation of the numeric model.

Temperature History and Heating Pattern Determination

During the experiment, three fiber optic sensors (FOT-L, FISO, Québec, CANADA) were placed at three different points (within the cold and hot spots) to monitor the temperature changes with time. In addition to monitoring temperature changes at selected locations in the packaged foods, heating patterns were measured with the computer vision software IMAQ (National Instruments, TX, USA) using a chemical marker method [Pandit et al., 2005]. This method measures color changes as a result of the formation of a chemical compound commonly referred to as M-2, a product of a Millard reaction between protein amino acids and a reduced sugar (ribose). The color changes depend upon heat intensity at temperatures beyond 100°C and, therefore, served as an indicator of temperature distribution after heating. Detailed information about the kinetics of M-2 formation with temperature can be found

Temperature [°C]	Dielectric constant $\varepsilon_r = '/\varepsilon_0$	Dielectric loss $\varepsilon_r^{"} = "/\varepsilon_0$
20	58.5	24.25
40	57.55	30.25
60	56.36	36.79
80	54.36	45.21
100	52.81	53.89
121	51.14	63.38

Table 1. Dielectric properties of whey protein gels.

Table 2. Thermal properties of whey protein gels.

Temperature [℃]	Volumetric specific heat $\rho_{c_p[MJ/m^3K]}$	Thermal conductivity K[W/mK]
0	3.839	0.513
20	3.973	0.537
35	3.901	0.550
50	3.814	0.561
65	3.883	0.578
80	3.766	0.588

elsewhere [Lau *et al.*, 2003; Pandit *et al.*, 2006]. In brief, with increasing temperature during the heating process, the density of M-2 also increased following an Arrhenius relationship with temperature and first order kinetics with time. The density of M-2 was then transferred to pixel density, which was further mapped into red, green, and blue (RGB) values, where red indicates the hottest area and blue the coldest.

Experimental Procedures

Whey protein gels (78% water, 20% protein, 1.7% salt, 0.3% D-ribose) were used as the model food because they have uniform properties and are easily formed. They also maintain a stable shape during the process. Dielectric properties of the whey protein gels were measured with an open coaxial cable from a HP8491B dielectric

probe kit connected to an HP8491B network analyzer (Hewlett-Packard, CA, USA; Table 1). Thermal properties were measured with a KD2 device (Decagon, WA, USA) using the double needle method [Campbell *et al.*, 1991] (Table 2). Table 1 shows dielectric property data at temperatures up to 121°C to allow for sterilization [Guan *et al.*, 2004]. Table 2 shows thermal property data only at temperatures up to 80°C because of measurement difficulties beyond this temperature. For temperatures over 80°C, thermal properties were assumed constant.

The whey protein gels were sealed in a 7 oz polymeric tray to maintain the food shape during EM heating. Prior to the experiment, six identical food trays containing whey gel slabs (95 mm x 140 mm x 16 mm) were removed from a refrigerator where they had been stored

at 9°C overnight. Fiber optic sensors were inserted carefully to the locations shown in Figure 4 with seals at the tray wall entry ports to prevent leakage of water. All six trays were secured in the center plane of the cavity with equal distance from the top and bottom windows of the cavity (Figure 1). Hot water at 125°C was filled at a speed of 40 lit/min into the cavity prior to microwave heating of the food. A uniform surrounding water temperature (125° C) was assumed during the heating process. The thermal properties and dielectric properties were measured using the same methods as for whey protein gel.

In experiments and simulation, the gel samples were preheated with circulating pressurized water at 125°C. When the temperature at the cold spots (spot 1 or 2 measured in the experiment in Figure 4) of the gel reached 60°C, microwave heating continued until the cold spot temperatures reached 121°C. Microwave power was then stopped, and cold tap water at 12°C was pumped in to cool the gel packages. Temperature histories at the cold and hot spots were recorded via a data acquisition system; the heating pattern in the middle layer of the gel samples was determined using a chemical marker/computer imaging system to highlight the influence of the microwave fields. After each heating process, the gels were carefully sliced into upper and lower halves and color images were taken of the middle layers. The intensity of the brown color was correlated with the heating intensity. The heating pattern was then obtained by mapping the pixel color intensity into an RGB values. Detailed procedures for capturing color image are provided in Pandit, et al. [2007].

FUNDAMENTALS FOR NUMERIC MODELING

Conformal FDTD Method

The conformal FDTD algorithm used the timedomain integral form of Maxwell's equations for



Figure 4. Top view of the middle layer of a whey protein gel inside a 7 oz tray with three fiber optic sensors at hot (3) and cold spots (1 and 2).

the EM field calculation [Balanis, 1989; Jurgens *et al.*, 1992]:

$$\int_{C} \overrightarrow{E} \cdot \overrightarrow{dl} = \frac{\partial}{\partial t} \int_{S} \overrightarrow{B} \cdot \overrightarrow{ds}$$
(1)

$$\int_{C} \overrightarrow{H} \cdot \overrightarrow{dl} \quad \frac{\partial}{\partial t} \int_{S} \overrightarrow{D} \cdot \overrightarrow{ds} \quad \oint_{S} (\overrightarrow{J}_{i} + \overrightarrow{J}_{c}) \quad \overrightarrow{ds} \quad (2)$$

$$\int_{S} \overrightarrow{D} \cdot d \overrightarrow{s} \quad \mathcal{Q}^{e} \tag{3}$$

$$\int \vec{B} d\vec{s} \quad \Theta \tag{4}$$

where \vec{E} is the electric field, \vec{H} is the magnetic field, $D = \varepsilon E$ is the electric flux density, $\vec{B} = \mu H$ is the magnetic flux density, Q^e is the electric charge surrounded by surface S, and μ and ε are permeability and permittivity, respectively. Permeability μ is assumed equal to the μ_0 constant in free space. The dielectric permittivity $\varepsilon = \varepsilon_0 \varepsilon_r = \varepsilon_0 (\varepsilon'_r - j \varepsilon''_r)$. *C* is a contour path surrounding the surface *S*, while J_i and J_c are source current density and conduction current density, respectively.

In this study, a commercial EM solver Quick-Wave 3D (QW3D) was used to solve the set of Maxwell's equations in (1)-(4). First, the computational domain was specified and the Maxwell's equations were discretized to setup the conformal FDTD algorithm. Then, the required conformal mesh with its appropriate boundary condition was constructed by a built-in mesh generator of QW3D [Gwarek *et al.*, 1999]. At last, the EM field components on each mesh grid were calculated until the steady state was established.

In the development of the model, the conformal FDTD algorithm was chosen to handle more complex geometry compared with classic Yee algorithm. The conformal FDTD method keeps all the traits introduced by standard FDTD approach, including mathematical manipulation, short simulation time and small memory usage. It also simulate curvature surface accurately by deforming the cells intersected by surface instead of using staircase grids in standard FDTD approach. Since the deformation only happens on the surfaces while the grid layer inside the simulated geometry is still same as that in standard FDTD approach, it does not introduce too much computational overhead compared with the standard one. In Figure 5 and Figure 6, a remarkable improvement was observed on 3-D and 2-D modeling of a sphere [Gwarke et al., 1992].

Finite Difference Equations for EM Fields

Discretization of Maxwell's equations in the integral form was obtained by computing the field components (E, H) at discrete nodes [Ta-

flove, 1998]:

$$H_{z}^{n+\frac{1}{2}}(i+\frac{1}{2},j+\frac{1}{2},k) = H_{z}^{n-\frac{1}{2}}(i-\frac{1}{2},j+\frac{1}{2},k)$$
$$-\frac{\Delta t}{\mu} \left[\frac{1}{\Delta y_{j}} \left(E_{x}^{n}(i+\frac{1}{2},j-4,k) - E_{x}^{n}(i-\frac{1}{2},j,k) \right) \right]$$
$$\left[-\frac{1}{\Delta x_{i}} \left(E_{y}^{n}(i-4,j+\frac{1}{2},k) - E_{y}^{n}(i,j+\frac{1}{2},k) \right) \right]$$
(5)

$$\Delta t \leq \sqrt{\frac{\mu \varepsilon}{1/(\Delta x)_{\min}^{2} + 1/(\Delta x)_{\min}^{2} + 1/(\Delta x)_{\min}^{2}}$$
(6)

where Δx_i and Δy_i denote the cell size in x and y directions and i, j, and k denote the index numbers for numeric computation in x, y, and z directions, respectively. Δt denotes the time step in simulation. The 1/2 appeared in the equations because of the leapfrog structure for the FDTD mesh. The $J_{iz}^{n+1/2}(i, j, k+1/2)$ in (6) was the z component of source current J_z at node $(i, j, k+\frac{1}{2})$, which is only involved in the computation where the input source was specified. Equations (5) and (6) only gave part of Maxwell's equations in their integral forms. The updated equations for other field components could be obtained similarly by shifting *i*, j, and k clockwise in (5) and (6) to get the components in x, y, and z directions, respectively [Taflove, 1998].

The presentation of Δx_i , Δy_j , and Δz_k (in different equations for other field components not presented here) provides the possibility for using non-uniform mesh so that the grids can conform to the curvature surface. For the leapfrog arrangement, the h_{x_i} , h_{y_j} and h_{z_k} were defined as in [Taflove, 1998]:

$$\begin{aligned} h_{x_i} &= (\Delta x_i \quad \Delta t_{i-1}) / 2, \\ h_{y_j} &= (\Delta y_j \quad \Delta t_{j-1}) / 2, \\ h_{z_k} &= (\Delta z_k + \Delta z_{k-1}) / 2 \end{aligned}$$
(7)



Figure 5. (a) Sphere modeled by standard FDTD approach. (b) Sphere modeled by conformal FDTD approach. [Gwarek, 1999]



Figure 6. (a) Circle modeled by standard FDTD approach. (b) Circle modeled by conformal FDTD approach [Gwarek,1999].

By numerically solving the above equations, the *E* and *H* fields were obtained so that the dissipated power per unit volume q(r,T) inside the food could be easily determined. Here *r* denotes that the dissipated power per unit volume is a spatial dependent variable. In fact, q(r,T) was determined from the root mean square value of the electrical field E_{rms} :

$$E_{rms}^2 = \frac{\int (\vec{E}^* \cdot \vec{E}) dV}{2V}$$
(8)

$$q(r,T) = 2\pi \, \mathop{\mathrm{gf}}\nolimits E^2_{rms} \mathcal{E}^{"}_r(r,T) \tag{9}$$

Finite Difference Equations for Thermal Fields

One important unique feature in EM heating is that the dielectric properties change with temperature. Therefore, after calculating E and H by solving the integral form of Maxwell's equations numerically, temperature responses to the EM fields must be calculated by solving the heat transfer equation.

Heat conduction took place inside food package while on the boundary a convective boundary condition was applied to take into account the effect of circulating water in the system. QW3D contains a built-in Basic Heating Module (BHM) that can be used to calculate temperature response of heat conduction. But it only allows adiabatic boundary condition on the surface between two different mediums, which, apparently, does not satisfy our needs. Therefore, a thermal model was developed to consider convective heat transfer boundary conditions.

The heat transfer equation and its boundary condition are presented in the following equations [Incropera and DeWitt, 2001]:

$$\rho(T)c_p(T)\frac{\partial T}{\partial t} = \cdot \left[\mathbf{W}(T) \ \mathbf{\nabla}\right] + q(r,T) \quad (10)$$

$$q = hA(T_s \quad T) \tag{11}$$

where K(T) is thermal conductivity at temperature T, $\rho(T)$ is mass density at temperature T, $c_p(T)$ is specific heat at temperature T, q is thermal energy exchanged between food and water on the boundary, h is the heat transfer coefficient of 220 Wm⁻²k⁻¹, A is the boundary surface area, and T_s is surrounding temperature [Incropera and DeWitt, 2001]. Here we assume that is isotropic so that its subscript for spatial variable was dropped in (10).

To use the same mesh generated for the EM field calculation, the heat transfer equation was also solved numerically with the FDTD method. Away from the surface, since only heat conduction took place, its finite difference form is:

$$T^{n+1}(i, j, k) = (1 \quad 12F_0)T^n(i, j, k) + F_0[T^n(i \quad 4, j, k) + T^n(i \quad 4, j, k) + T^n(i, j \quad 4, k) + T^n(i, j \quad 4, k) + 4T^n(i, j, k \quad 4) + 4T^n(i, j, k \quad 4)] + \frac{q(i, j, k)\Delta t}{\rho c_p}$$
(12)

where $F_0 = \alpha \Delta t / \Delta x^2$ and *i*, *j*, and *k* have the same meaning as the finite difference form of the EM field. For simplification, $\Delta x = \Delta y = 2\Delta z$ was used for all the finite difference equations for illustration purpose.

At the food surface, both heat conduction between interior nodes and convection between food and water happened at the same time, hence the finite difference form of the heat transfer equation was slightly modified on the surface nodes by replacing the conduct terms in (12) with the corresponding convective terms. For example, for the nodes on the surface plane vertical to the z-plane, the boundary condition from (11) can be written:

$$q = h\Delta x \, \Delta [T_s \quad T(i, j, k, n)] \tag{13}$$

The conduction term:

 $[T(i, j, k+1, n) - T(i, j, k, n)] * K * \Delta x$ was replaced by (13) for the corresponding surface nodes.

Numeric Model

An EM solver QW3D was used to compute the field components using finite difference equations such as those in (5) and (6). Before computer simulation was conducted, the desired microwave propagation mode was set up, which included specifying the excitation type, input power and boundary condition that represented the simulated physical system. Since gel movement was not considered, the whole industrial EM heating system was treated as a metal box with a Perfect Electrical Conductor (PEC) boundary condition on the surface. Because it worked at 915 MHz, the only propagation wave in TE₁₀ mode propagated through a rectangular waveguide on the top and bottom via an electrical field with E_{y} as its only component [Balanis, 1989]. A 915 MHz sine wave was used as an excitation, with its amplitude determined from the input power. Front and top views of the numeric model are shown in Figures 7 and 8.

In QW3D, it was possible to define physical geometry in a user defined object as a parameterized macro. The macro defined the physical geometry and settings for the EM field discussed in the last paragraph and formed the basis of the EM model. A heat transfer model using explicit finite difference equations such as (12) and (13)was also required to calculate the temperature response to the EM field. The mesh for EM field calculation in QW3D was kept in an external file for use in the heat transfer model, which saved computer memory and computation time because the numeric model did not need extra adaptation to the computational grids for temperature calculation. The EM model was then coupled with a customized thermal model by defining a script to communicate QW3D with an external heat transfer program and exchange



Figure 7. Geometry of the EM heating system with five identical trays (front view, middle layer).

data between them. The dissipated power per unit volume was thus calculated by QW3D and then used in the heat transfer model to calculate the temperature information.

The electromagnetic field intensity was calculated in the order of nanoseconds while the thermal response in the order of seconds. At a specific heat transfer time step, EM field was obtained by QW3D, the corresponding dissipated power was then used as the heating source for heat transfer calculation. Between each heat transfer time step, the dissipated power in each cell was assumed to be constant. Because of the temperature-dependent dielectric properties of food, after every heat transfer time step, new dielectric properties were calculated from Table 1 and then fed back to QW3D for the EM calculation of the next heat transfer time step. This coupled calculation loop did not end until the required heating time was reached. Figure 9 summarizes the above simulation schema for the coupled model. The node transformation process shown in Figure 9 was used to exchange the data between computational nodes for power and computational nodes for temperature, which will be discussed in detail in the next section.

COMMUNICATION ALGORITHM

QW3D allowed the whole computed domain to be discarded and the dissipated power extracted at the place occupied by the gel. This dramatically decreased the size of the data set handled by the heat transfer model and therefore greatly reduced the simulation time. After obtaining the temperature distribution during the period when the EM power dissipated inside the gel, new dielectric properties were calculated with a linear



Figure 8. Geometry of the EM heating system with five identical trays (top view).



Figure 9. Numeric schema for coupled simulation of the EM heating process.

interpolation technique in QW3D. To facilitate the coupling function, the heat transfer model not only acted as a tool to calculate the temperature response to EM heating, but also served as an interface to communicate with QW3D. Special care was taken during this communication - for each single cell containing dissipated power dumped from QW3D, the power nodes were assumed to be placed in the cell centre. To avoid numeric instability, the temperature nodes needed to be placed on the corners of each cell. Because nodes for EM calculation (cells in QW3D) were different from those for heat transfer calculation, it was necessary to calculate the dissipated power associated with the temperature nodes using the following formula:

$$\begin{split} q_{T}(i,j,k) &= [q(i,j,k)\Delta x_{i} \, \mathbf{A}_{j}\Delta z_{k} + q(i-1,j,k) \\ \Delta x_{i-1}\Delta y_{j} \, \mathbf{A}_{k} + q(i,j-1,k)\Delta x_{i} \, \mathbf{A}_{j-1}\Delta z_{k} + \\ q(i-1,j-1,k)\Delta \mathbf{A}_{i-1} \, \mathbf{A}_{j-1}\Delta z_{k-1} + q(i,j,k-1) \\ \Delta x_{i} \, \mathbf{A}_{j}\Delta z_{k-1} + q(i-1,j,k-1)\Delta x_{i-1} \, \mathbf{A}_{j}\Delta z_{k-1} \\ &+ q(i,j-1,k-1)\Delta x_{i} \, \mathbf{A}_{j-1}\Delta \mathbf{A}_{k-1} + q(i-1,j-1,k-1) \\ \Delta x_{i-1} \, \mathbf{A}_{j-1}\Delta z_{k-1}] / (8h_{x_{i}}h_{y_{j}}h_{z_{k}}) \end{split}$$

$$(14)$$

where $q_T(i, j, k)$ is the dissipated power associated with the temperature node T(i, j, k). Equation (14) was only used to calculate the power associated with the inner temperature node. For the temperature nodes on the boundary, some of the power terms on the right hand side of (14) were replaced by zero if any of their index numbers (i, j, or k) exceeded the specified computation domain.

After the heat transfer calculation, the temperature data were transformed back to the dissipated power nodes so that they could be used in QW3D for updating the EM field. This was done in (15):

$$\begin{split} T_q(i,j,k) &= [T(i,j,k) \quad T(!i-1,j,k) \\ &+ T(i,j \quad 4,k) + T(i-1,j \quad 4,k) \\ T(i,j,k-1) \quad + T(i-1,j,k \quad 4) \\ &+ T(i,j \quad 4,k-1) \quad + T(i-1,j \quad 4,k-1)] / 8 \end{split}$$

(15)

where $T_q(i, j, k)$ is the temperature at the cells (i, j, and k) associated with the dissipated power nodes. The algorithm is shown in the following:

- 1. Obtain dissipated power from QW3D.
- 2. Initialize temperature for computation in the next time step based on previous tem perature distribution.
- 3. Loop through the whole computational grids:

(a). for inner nodes, calculate dissipated power based on (14);

- (b). for boundary nodes, set the corre sponding power terms in (14) to zero; (c). conduct heat transfer calculation.
- 4. Find the temperature distribution based on Eq. (15) and feed back to QW3D.

BOUNDARY TREATMENT

Although only a stationary case was considered in this study, the actual physical system had a left and right end open to allow food trays to move in and out of the cavity. Therefore, in the numeric model, the left and right ends of the cavity needed to be terminated with proper boundary conditions to represent the real system as close as possible. A perfect matched layer was used as the absorbing boundary condition to terminate the finite grid. With the perfect matched layer method, the electrical or magnetic field components on the boundary were split into two components, which allowed for the assigning of different losses at different grids [Taflove, 1998]. After choosing the proper loss at each sub-layer, the numeric reflection gradually decreased with the layers further away from the boundary and eventually disappeared as if the wave propagated into a far region. It therefore acted like an open boundary without physical wave reflection. To set up the PML layer, 8 sub-layers parallel to the y-z plane were assigned to complete the numeric grids. The Exponential Time-Stepping algorithm was used to assign the conductivity at each sublayer as: $A^*exp(B^*x)$, where A = 0.02, B = 4, and x = distance from perfect matched layer divided by the layer thickness. The perfect matched layer method accurately modeled the boundary in the presented system, though it also introduced more computational complexity and increased simulation time. However, since the system was single mode and EM waves were concentrated on the central portion of the microwave section, the field intensity was very small near the absorbing boundary. For this reason, the perfect matched layer might be replaced by a simpler perfect electric conductor boundary condition without introducing too much inaccuracy. The maximum difference observed on the left and right ends of the cavity was only 5%, while the minimum difference (< 2%) was observed in the centre of the cavity.

NUMERIC CONVERGENCE

Numeric error always occurs when modeling a process by a finite grid. Since large errors significantly affect final results, a study is necessary to make sure that the model converges to a final value. Because the models used in this study included both EM and heat transfer, these were examined separately. From Table 1 and (9), the dielectric properties did not change much with the temperature and the dielectric properties did not cause many changes in dissipated power at 915 MHz. Therefore, it was assumed that convergence for the coupled model could be achieved once convergences for the EM and heat transfer models were guaranteed separately.

Convergence Study for the EM Model

For an FDTD model to satisfy numeric stability, the maximum time step has to be selected as the following according to [Taflove, 1998]:

$$\Delta t \leq \sqrt{\frac{\mu \varepsilon}{1/(\Delta x)_{\min}^2 + 1/(\Delta x)_{\min}^2 + 1/(\Delta x)_{\min}^2}}$$

(16)

where $(\Delta x)_{\min}$, $(\Delta x)_{\min}$, $(\Delta x)_{\min}$, represent the minimum cell size of non-uniform mesh in each direction, respectively.

In addition, the standard FDTD rule of thumb indicates that at least ten cells need to be used per wavelength [Pathak *et al.*, 2003]:

$$\Delta cell \le \frac{1}{10 f \sqrt{\mu} \epsilon} \tag{17}$$

One result of using a conformal FDTD algorithm is that the mesh in the computational domain is not necessarily uniform. Therefore, maximum cell size was specified in each direction with QW3D. The actual cell size was generated automatically by QW3D. According to (17), the maximum cell size was 10 mm in free space, while 4 mm in water and gel. Therefore the cell size was chosen to be 4 mm in x and y directions. We selected 2 mm in z direction since the food tray dimensions in z direction was much smaller than that in x and y directions. Though the cell size was chosen to be as small as possible to avoid numeric instability, it was still able to affect the propagation velocity of the numeric wave in the finite-difference-grid approximation of the wave equation [Taflove, 1998]. In [Taflove, 1998], the numeric convergence study for a simple 1-D system was analyzed using an eigenvalue method and the concept of numeric dispersion. However, in a very complicated 3-D case such as an industrial EM heating system, there is no closed-form solution for wave equations. In practice, one way to check the convergence of a numeric model is to track the numeric results at different cell sizes and time steps. If the numeric results remain stable as cell sizes are reduced and simulation time increased, the model could be considered to converge. In the model discussed here, the cell size on a vertical plane was chosen to be half the cell size in the horizontal plane, and the change of cell size in the horizontal plane automatically changed the cell size in the vertical plane. Therefore, for this special grid arrangement, model convergence in the horizontal plane led to the convergence of the overall 3-D domain. Figure 10a-b (horizontal plane) shows the convergence in terms of discretization of space.

Usually it is highly possible for singularity to occur at the interface between two different mediums as well as the sharp edge of the geometry. Therefore, model stability was checked on the corners of both the food and Ultem material (A, B in Figure 8) inside the microwave cavity. Figure 11 shows the electrical field converging to a final value as the simulation time proceeded.

Convergence Study for the Heat Transfer Model

In addition to the numeric convergence of the EM model, accuracy of the heat transfer model was considered. Figure 12 presents a result from the heat transfer model used in coupled simulation in comparison with those from the FEM model and experimental measurement. The FEM thermal model was also developed in our group to validate the FDTD heat transfer model. The experiment measurement was



(a) $\Delta x = \Delta x = 10 = 5$



(b) $\Delta x = A + 4$, = 2Figure 10. Convergence check for EM fields at different cell sizes.

conducted in a water bath where the gel placed in a 7 oz polymetric tray was heated and the temperature profile at its centre point was monitored using a fiber optic sensor ($\pm 0.5^{\circ}$ C). The solid red line is the simulation result calculated using FDTD method; the dashed blue line is the simulation result calculated using the FEM model and the yellow solid-dash line presents the measured temperature profile from experiment. Good agreement was achieved. The difference between the calculated temperature and actual measurement was less than 1°C. It is worth noting that with different heat transfer coefficient the simulated heating curve varies. In this study, the heat transfer coefficient 220Wm⁻²k⁻¹ was chosen based on agreement between simulation and experiment results for hot water heating.

VALIDATION OF THE COUPLED MODEL

This section describes validation of the coupled model by comparing the simulated temperature

distribution and temperature profile with experimental results. Excitation in the model was a sinusoidal source at 915 MHz and amplitude was the square root of the required input microwave power. Figure 13 shows the temperature profiles in two separate runs with the simulated results, respectively. The temperature profile at point 1 (Figure 4) is represented by a solid line, the temperature profile at point 2 (Figure 4) by a dashed line, the temperature profile at point 3 (Figure 4) by a solid-dash line, while the measured results are marked as red and simulated results as blue. It was clear from both experimental and simulated results that the heating rate increased significantly when microwave power was on. The heating rate calculated from the simulation was similar to the experimental measurement. The difference between the simulated final temperature and measured final temperature was less than 5°C, which is generally considered adequate considering the complex nature of the heating process.

Experimentally obtained heating pattern

0.08 0.07 0.06 E/sqrt(377)[v/mm] 0.05 food corner A 0.04 - ultern corner B 0.03 0.02 0.01 0 0 2000 4000 6000 8000 10000 12000 14000 16000 18000 20000 Iteration no.

Electrical field at simulation time from FDTD algorithm

Figure 11. EM model convergence with simulation time.



Figure 12. Validation of the heat transfer model.



Figure 13. Comparison of simulation results for temperature evolution at hot and cold spots with experiment results from two identical experimental runs.

as reflected by color changes in the middle layer on the horizontal plane of the gel, and temperature distribution from simulation after a 5.5min heating process are presented in Fig. 14(a) and Fig. 14(b), respectively. In the experimental heating pattern, deep blue color corresponds to low heating intensity while light yellow indicates high heating intensity. For the simulated temperature distribution, red color corresponds to high temperature while blue indicates low temperature. From Fig.14, the experimental heating pattern correlates well with simulated temperature distribution, especially the locations of cold and hot spots. The good agreement between these results showed that the model correctly represented the real system in consideration. However, there were some mismatches between the simulation and experimental results; for example, the simulated temperature distribution was more symmetric than the heating pattern obtained from experiment. It was very difficult to place the fiber optic sensors at the exact locations as those used in the simulation and to maintain



Figure 14. Heating pattern reflected by color image from chemical marker (left), simulated temperature profile (right) for the middle plane of whey protein gel after 5.5min microwave heating.

the exact geometry of food trays during the thermal processes. Another source of error was introduced by the heat transfer model because the surrounding temperature was assumed to be uniform (125°C), but in reality it might have changed with time and space.

CONCLUSION

A model was developed that enables computer simulation for a 915 MHz pilot-scale microwave sterilization system in which conventional hot water heating and EM heating took place at the same time. Because the hot water heated the product from the outside while the microwave heated it from the inside, the combination of these two heating mechanisms improved heating uniformity and shortened heating time. The model presented in this paper used a commercial EM solver combined with a user-defined heat transfer program to simulate the EM heating process. The combination of using commercial software with a thermal solver in this model was unique compared with other methods reported in the literature - it employed a conformal FDTD

algorithm so that the details of the physical geometry could be modeled accurately without requiring significant computer memory or simulation time. The EM portion was modified automatically as a macro with an external script to quickly construct different geometries for EM field calculation, and then coupled with the customized heat transfer model to simulate a MW heating process at different system configurations. In addition, the external user-defined heat transfer model provided extra flexibility to control the heating process in different ways, which was a big advantage for system optimization of industrial microwave sterilization.

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