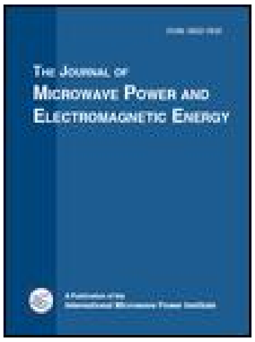

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Numerical Modeling of Continuous Flow Microwave Heating: A Critical Comparison of COMSOL and ANSYS

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ABSTRACT

Numerical models were developed to simulate temperature profiles in Newtonian fluids during continuous flow microwave heating by one way coupling electromagnetism, fluid flow, and heat transport in ANSYS 8.0 and COMSOL Multiphysics v3.4. Comparison of the results from the COMSOL model with the results from a pre-developed and validated ANSYS model ensured accuracy of the COMSOL model. Prediction of power loss by both models was in close agreement (5-13% variation) and the predicted temperature profiles were similar. COMSOL provided a flexible model setup whereas ANSYS required coupling incompatible elements to transfer load between electromagnetic, fluid flow, and heat transport modules. Overall, both software packages provided the ability to solve multiphysics phenomena accurately.

KEYWORDS: Microwave processing, numerical modeling, COMSOL Multiphysics, ANSYS Multiphysics, resonant cavity

INTRODUCTION

In continuous flow microwave heating of liquids, volumetric heat generated as a function of electric field distribution and dielectric properties of the fluid is transferred in the flowing fluid by conduction and convection. Comprehensive 3-D numerical modeling of the process requires coupling of energy and momentum equations to Maxwell's electromagnetic equations. [Le Bail et al. 2000] predicted temperature profiles in fluids under continuous microwave heating assuming uniform volumetric power in the core of the flow. [Ratanadecho et al. 2002] used a 2-D finite difference time domain (FDTD) formulation to solve Maxwell's equations within a finite control volume based on the SIMPLE algorithm to solve heat transport and fluid flow equations in rectangular duct geometry; an iterative computational scheme was used to couple Maxwell's equations with momentum and heat transfer equations. [Zhu et al. 2007a, 2007b, and 2007c] used a similar algorithm for numerical modeling of continuous flow microwave heating in cylindrical and rectangular ducts.

The above mentioned studies [Le Bail et al., 2000; Ratanadecho et al., 2002; Zhu et al., 2007a, 2007b, and 2007c] used complex alliances of FDTD algorithms and finite volume methods using independent codes. In depth knowledge of programming and numerical analysis is required for development of such codes; in addition, authentication of independent codes with benchmark problems is necessary. Engineers not trained in the associated programming languages have the alternative of using commercial multiphysics software packages to create a generic model. These software packages, in general, allow coupling of a variety of fundamental equations each describing different physical phenomena, provide multiple options for geometry and mesh generation, and offer various solvers and post-processing alternatives.

Multiphysics software packages such as ANSYS and COMSOL have been used for modeling of microwave heating in the past. For example, coupling of electromagnetism and heat transfer with mass transfer was accomplished by [Zhou et al., 1995] in ANSYS. Numerical modeling and validation of continuous flow microwave heating of liquids was also completed in ANSYS by [Sabliov et al., 2007] and [Salvi et al., 2008]. Researchers have also used an alternative software, COMSOL, for modeling of microwave heating of solids [Komarov and Yakovlev, 2001; Hu and Mallikarjunan, 2002; Mirabito, et al., 2005; Curet et al., 2006; Hansson, 2006; Feldman et al., 2007], while others [Knoerzer et al., 2006] have used COMSOL to couple electromagnetism with heat transfer from the available EM simulator Quickwave-3D via MATLAB interface. Simulated results were observed to be in agreement with measured values [Hu and Mallikarjunan, 2002; Knoerzer et al., 2006; Hansson, 2006; Curet et al., 2006] and with results from other EM simulators [Mirabito et al., 2005; Komarov and Yakovlev, 2001]. However, no studies are available on relative comparison of coupled models in ANSYS and COMSOL based on electromagnetism, fluid flow, and heat transfer. This information could be critical in consolidating the understanding of the microwave heating process, and could be used as a tool in software selection.

The goal of the present paper was to develop a complete 3-D model based on coupling of Maxwell's equation with heat and momentum transport equations in COMSOL Multiphysics (COMSOL, Inc., MA, USA) and to compare the results with a similar, pre-developed model in ANSYS Multiphysics (Canonsburg, PA). The objectives of the study were:

1. To numerically simulate temperature in Newtonian fluids with different dielectric and physical properties heated at different flow rates in a continuous flow microwave system by coupling electromagnetism, fluid flow and heat transport in COMSOL and ANSYS with model fluids of freshwater and 1.5 % saltwater at flow rates of 1 lit/min and 1.6 lit/min.

2. To verify the results from the developed COMSOL model by comparing the results with a similar ANSYS multiphysics model developed previously. For verification, the modeling parameters were ensured to be consistent in both software packages including microwave cavity geometry, applicator tube (3.81 cm diameter), incident power (4.5 kW), frequency (915 MHz), and material properties.

Governing Equations

Numerical modeling of continuous flow microwave heating in ANSYS and COMSOL includes coupling of three physics phenomena (electromagnetism, fluid flow and heat transfer), which can be accomplished by solving the following governing equations.
Maxwell's equations are solved to determine electric field distribution in a microwave cavity as follows,

$$\nabla \times \left(\frac{1}{\mu'} \nabla \times \vec{E} \right) - \frac{\omega^2}{c} \left(\varepsilon' - i\varepsilon'' \right) \vec{E} = 0 \qquad (1)$$

where $\vec{E}$ is electric field intensity (V/m), ε′ is relative permittivity or dielectric constant of a material, ε″ is relative dielectric loss of a material, ω is angular wave frequency (2π*f*, rad/sec), μ′ is relative permeability of the material and c is speed of light in free space (3×10^8, m/s).

The electric field intensity obtained from above equation and material properties are required to calculate the volumetric power generation due to microwave exposure by using the following equation,

$$Q = \sigma \mid \vec{E} \mid^2 = 2\pi\varepsilon_0\varepsilon'' f \mid \vec{E} \mid^2 \qquad (2)$$

where, σ is electrical conductivity of the material (S/m), ε_o is free space permittivity (8.854×10^{-12}, F/m) and f is frequency (Hz). This volumetric power generation term calculated above is used as the energy source term in solving Fourier's energy balance equation (Equation 3) to calculate the temperature distribution due to conduction and convection,

$$\frac{\partial T}{\partial t} + \vec{v}\nabla T = \frac{k}{\rho Cp}\nabla^2 T + \frac{Q}{\rho Cp} \qquad (3)$$

where, ρ is material density (kg/m^3), Cp is specific heat (J/kg K), k is thermal conductivity (W/mK), T is temperature, (K), is velocity vector (m/s) and Q is the volumetric heat generation due to the incident microwave energy (W/m^3).

Velocity profiles in the heated liquid are obtained by solving the Navier-Stokes equation (describing the momentum balance and continuity) below,

$$\rho\frac{\partial \vec{v}}{\partial t} = -\nabla P + \mu\nabla^2\vec{v} + \rho g \qquad (4)$$

$$\nabla \cdot \vec{v} = 0 \qquad (5)$$

where, ∇P is the pressure force on element per unit volume (N/m^2), g is the acceleration due to gravity (m/s^2), and μ is viscosity (Pa.s) for Newtonian fluids.

Algorithm Development

The algorithm for coupling electromagnetism with fluid flow and heat transfer was developed in ANSYS as well as COMSOL (Figure 1). First, the wave equation (Equation 1) was solved to calculate the electric field distribution and heat generation (Equation 2) taking dielectric properties of the liquids into account. The heat generation term was used as source term in solving the energy balance equation (Equation 3) based on the physical and thermal properties of the liquids. The energy, momentum and continuity equations (Equations 3-5) were solved simultaneously to obtain velocity and temperature profiles. While developing the algorithm, fluid flow was assumed to be incompressible and the PTFE tube was considered completely transparent to microwaves.

Model Development in ANSYS and COMSOL

The model was developed by one way coupling considering temperature independent physical and dielectric properties of the liquids heated in the continuous microwave system. The geometry representing the resonant cavity setup (Figure 2) was created including the waveguide, elliptical cavity, and applicator tube in both software packages. The computational domain was meshed using a tetrahedral grid. For electromagnetic problems, the element size S_{max} requirement was decided based on the Nyquist criterion (Mirabito et al., 2005)

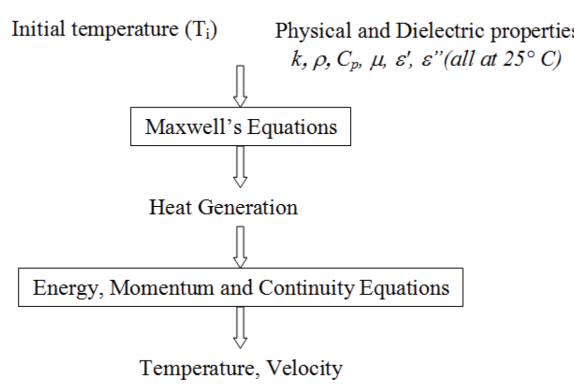


Figure 1. Algorithm for coupling of electromagnetism and heat and mass transfer.

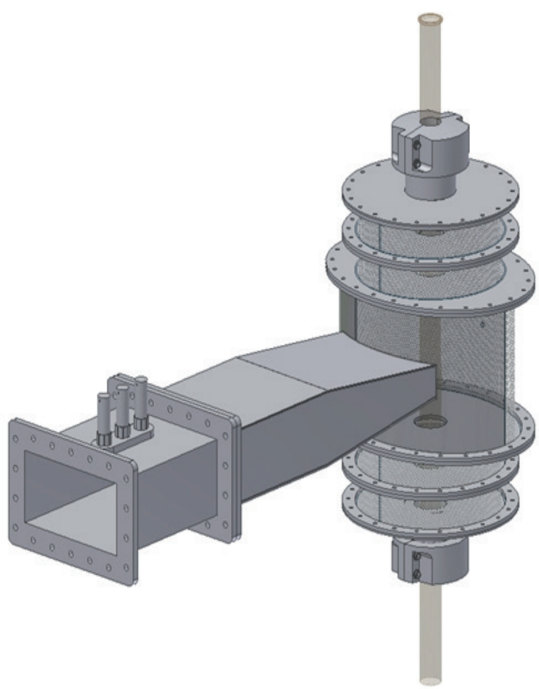


Figure 2. Continuous flow microwave system (IMS) with temperature measurement locations.

$$S_{\max} < \frac{\lambda}{2} = \frac{c}{2f\sqrt{\varepsilon'\mu'}} \qquad (6)$$

where, λ is the wavelength (m), f is the frequency of the wave (Hz), c is the speed of light in a vacuum (m/s), ε' is the dielectric constant, and μ' is the relative permeability.

Based on material properties and the Nyquist criterion the mesh size used in this model was 0.03 m in the waveguide and cavity, and 0.005 m in the applicator tube. In ANSYS, the tetrahedral elements HF119 were used in the electromagnetic module (for solving Maxwell's equations) and tetrahedral elements FLUID142 (size 0.005) were applied in the FLOTRAN module (for solving fluid flow and heat transfer). In contrast to ANSYS, the same mesh can be used for the RF module (for solving electromagnetism) and in the Fluid Dynamics module and Heat Transfer module in COMSOL and as such the transfer of the generated heat is simplified.

The applicator tube (diameter 3.81 cm) was considered transparent to microwaves. Boundary conditions for electromagnetism included the TE_{10} mode specific to WR975 rectangular waveguide, perfect electric conductor walls in the waveguide and cavity, 915 MHz frequency, and 4.5 kW input power.

For the energy and momentum balance equation, average initial velocities (0.021 m/s at 1 lpm and 0.034 m/s at 1.6 lpm) were used. The zero velocity condition was applied along the wall of the applicator tube, inlet temperature was chosen to have an initial value of 25°C, and the outlet pressure was set to atmospheric pressure. Adiabatic conditions were applied at the applicator wall (no heat was assumed exchanged between the dielectric and the air in the elliptical cavity). The heat generation obtained from the wave equations was used as the source term in solving energy, momentum, and continuity equations. Phase change and latent heat were not included in either model. Material properties for freshwater and 1.5 % saltwater were obtained from literature (Table I).

The Sparse Direct Solver was used to solve Maxwell's equation to obtain heat generation in the ANSYS model. Energy, momentum, and continuity equations were solved using a tri-diagonal matrix algorithm (TDMA) in the FLOTRAN Module to obtain temperature profiles in the fluid. As ANSYS used dissimilar meshes in the electromagnetic module and FLOTRAN modules, the ANSYS Multifield Solver was used to transfer the heat generation term between these modules. The ANSYS model was validated for ballast water applications in the past (Salvi et al., 2008), and compared against COMSOL results in the present paper.

In COMSOL, the wave equation (Equation 1) was solved in the RF module using generalized minimum residual solver (GMRES) to calculate the heat generation (Equation 2). The energy and momentum equations (Equations 3-5) were solved in the Fluid Dynamics and Heat Transfer modules using the parallel direct linear solver (PARDISO) by using the heat generation term from the RF

Table I. Physical properties of fluids.

Fluid	Thermal conductivity (k), W/m K [Choi and Okos, 1986]	Material density (ρ), kg/m^3 [Choi and Okos, 1986]	Specific heat (Cp), J/kg K [Choi and Okos, 1986]	Viscosity (μ), Pa·s [Geankoplis et al., 1993]	Dielectric Constant (ε′) [Komarov and Tang, 2004]	Dielectric Loss(ε″) [Ikediala et al., 2002]
Freshwater	0.6110	994.9	4177.3	0.8937×10^{-3}	84.89	4.08
1.5 % Saltwater	0.6035	1037.6	4086.2	0.8629×10^{-3}	76.5	52.08

module to solve for velocity and temperature profiles.

All the simulations were run on Dell Precision PC (Windows 32 bit operating system installed) with a single 3 GHz Xeon processor with 3GB RAM. ANSYS Multiphysics version 9 and COMSOL Multiphysics 3.4 were used for this particular study.

RESULTS

The COMSOL and ANSYS models were compared at two different salinities (0 and 1.5 %) and two different flow rates (1 lit/m and 1.6 lit/m) in terms of electromagnetic power density and temperature profiles.

Electromagnetic Power Generation Density

Total volumetric power generation was calculated based on material properties and the electric field distribution was obtained by solving Maxwell's equations (Equation 2).

The total electromagnetic power generation for freshwater was 826 W as predicted by the model developed in COMSOL, as compared to 729 W as predicted by ANSYS, whereas for 1.5 % saltwater these values were 2883 W by COMSOL and 2511 W by ANSYS. Prediction of total power loss in the two fluids by ANSYS and COMSOL was in close agreement (5-13% variation). Cross axial power density profiles for both models exhibited Mathieu function distribution with highest electromagnetic power density at the center of the tube and lower around the walls (Figure 3). The discrepancy in the power densities values in the center between the ANSYS and COMSOL models was 6 % for

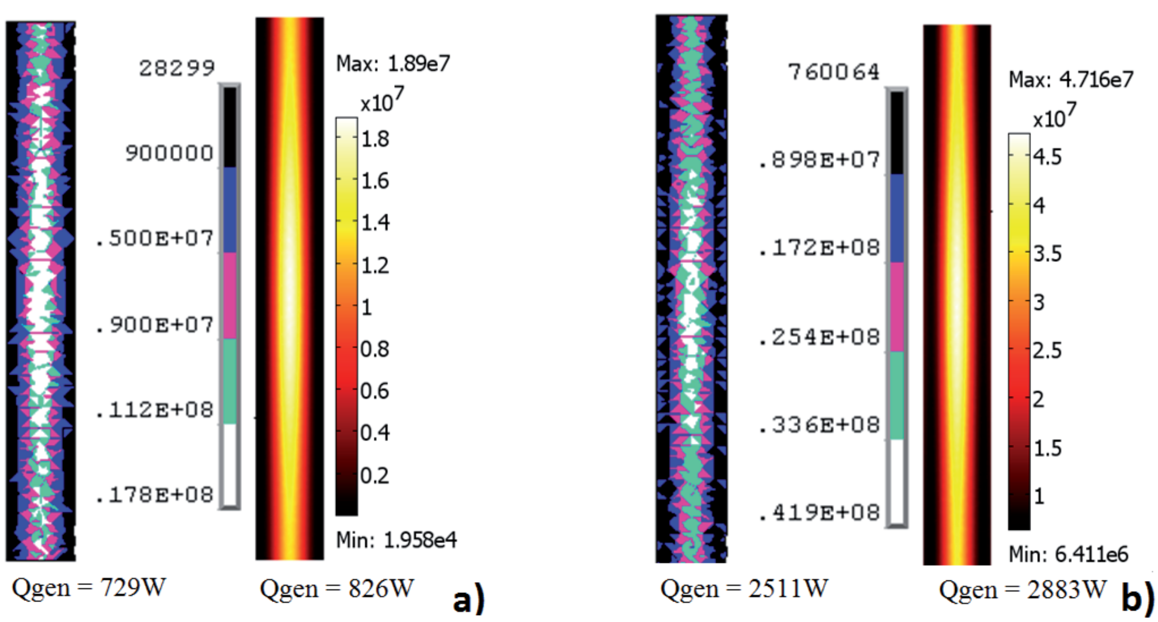


Figure 3. Cross-axial (x-y) plane view of electromagnetic power density (W/m^3) by ANSYS (left) and COMSOL (right) for a. freshwater and b. saltwater (1.5 %) Note: The scale is inverse in the COMSOL model.

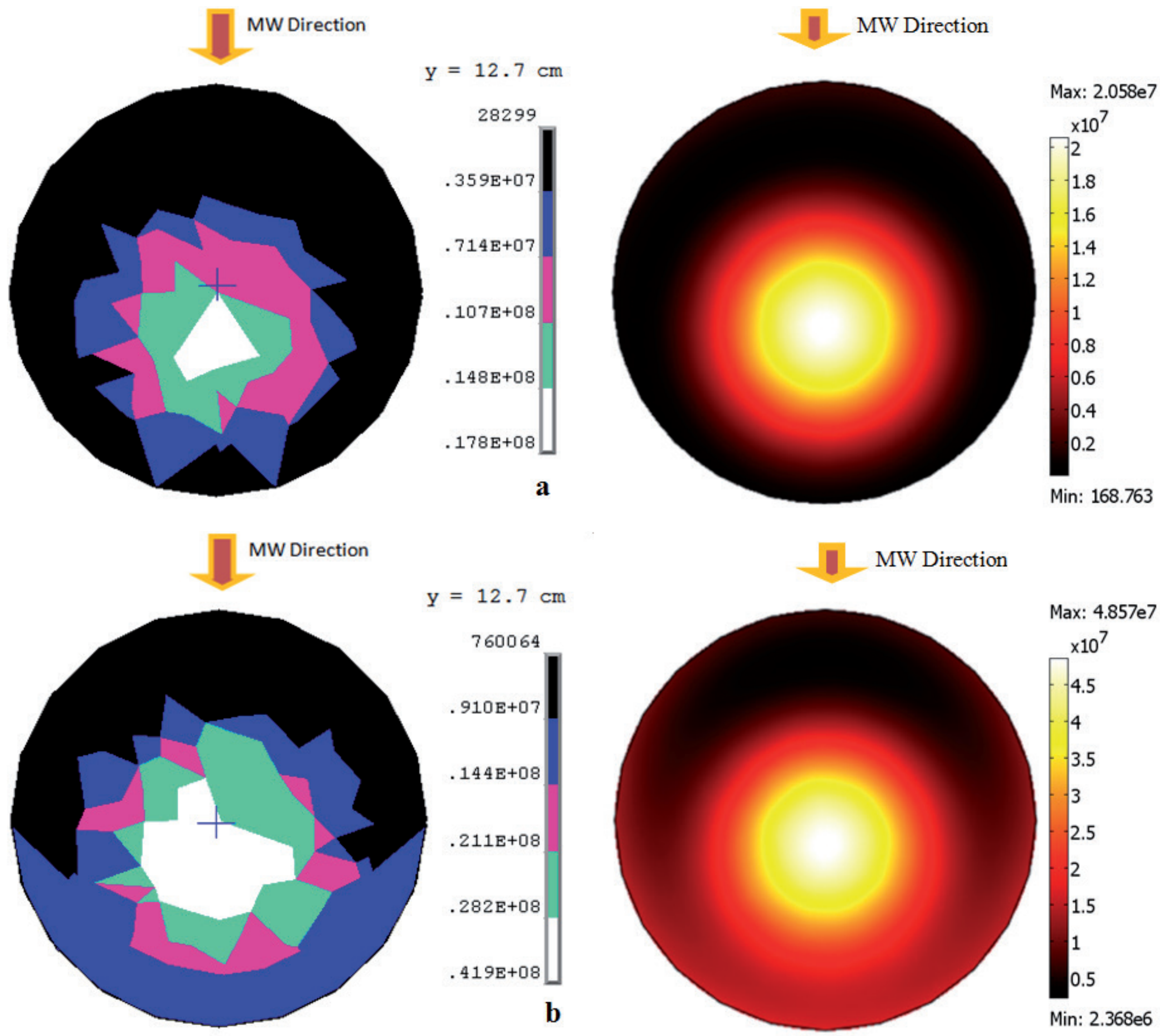


Figure 4. Cross-section spatial view (x-z plane) electromagnetic power density (W/m^3) for a freshwater, and b saltwater (1.5%) at the center of the tube (y= 12.7 cm). ANSYS left, COMSOL right.

freshwater and 12 % for saltwater.

The cross-axial electromagnetic power density (Figure 4) also demonstrated that the two models displayed high power density regions located slightly off center and lower density regions at the edges with different gradients from the exterior surface of the applicator tube to the center. For freshwater, ANSYS achieved a power density range of 2.8299 x 10^4 to 1.78 x 10^7. COMSOL, in comparison, had a much larger gradient, with a minimum density of 1.958 x 10^4 and maximum density of 1.89 x 10^7. This represents a 30% decrease in minimum density and 6% increase in maximum. As previously discussed, the total heat generation in the COMSOL model was approximately 12% higher than the ANSYS model, indicating a larger region of higher electromagnetic power density in the COMSOL model. Solutions for 1.5% saltwater produced a similar discrepancy in power density. COMSOL results indicated a 16% decrease in the minimum density and a 12% increase in maximum. Total heat generation in saltwater was approximately 15% greater in the COMSOL model, again leading to a larger region of higher power density with less pronounced effect in comparison to that of the freshwater case. In general, however, the generated values agreed quite closely for each fluid, with the higher loss factor of saltwater accounting for the differences in heat generation between each result.

Cross-section Spatial Temperature Distribution (x-z plane)

Cross sectional temperature profiles obtained from the models developed in ANSYS and COMSOL for both flow rates (1 and 1.6 lit/min) for freshwater and 1.5 % saltwater are presented in Figures 5 and 6. For freshwater, the temperature values ranged from 26-42°C in ANSYS and 25-47°C in COMSOL at 1 lit/min (Figure 5a) where as at 1.6 lit/min the temperatures were 25-37°C in ANSYS and 24-39°C in COMSOL (Figure 5b). The spatial temperature distribution profiles from both models were nearly identical with the hot spot slightly off-center opposite to the direction of incident microwaves for both models in freshwater. It should be noted that the temperature gradients for each result are similar as well, with differences in maximum temperature accounted for by flow

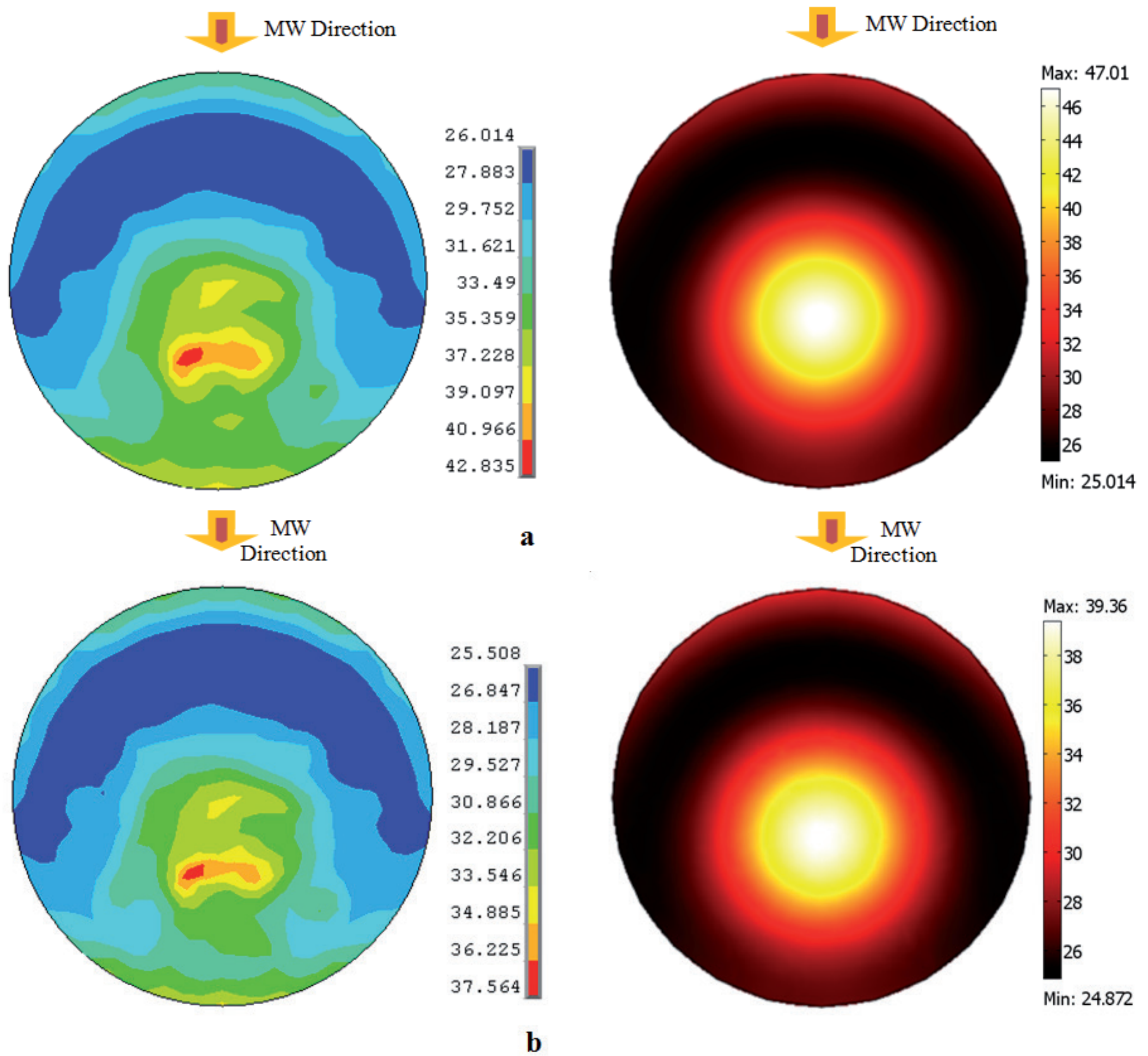


Figure 5. Cross-section spatial temperature distribution (x-z plane) for freshwater heated at 1 lit/min (a) and at 1.6 lit/min (b) at the center of the tube (y= 12.7 cm). ANSYS on left, COMSOL right.

rate. Similarly, for 1.5 % saltwater (Figure 6) the temperature profiles matched well with highest temperature at the edges (away from the direction of microwave) and lowest temperatures near the incident direction at both flow rates. The temperature values ranged from 29-115°C in ANSYS and 27-85°C in COMSOL at 1 lit/min (Figure 6a), respectively 27-91ºC in ANSYS and 26-66°C in COMSOL at 1.6 lit/min (Figure 6b). The cross sectional temperature values for saltwater (1.5 %) (Figure 6) from the COMSOL model at the center of the tube were similar with results from the ANSYS model, but at the edges a higher discrepancy was observed (≈1.35 times higher for COMSOL than ANSYS, at both flow rates). This discrepancy was attributed to the result of load transfer between same versus dis-similar meshes, differences in the meshing algorithms, and the numerical solvers

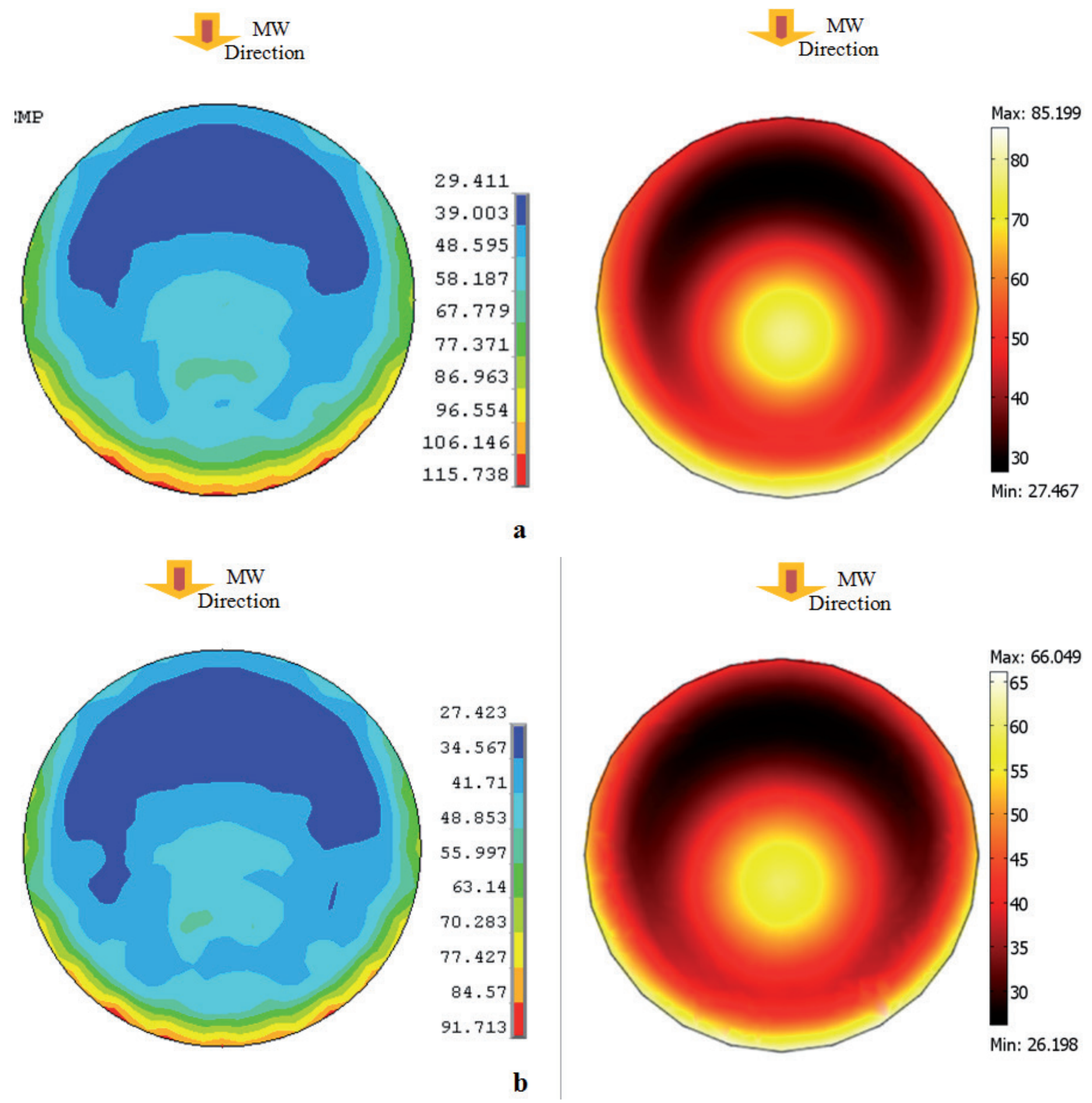
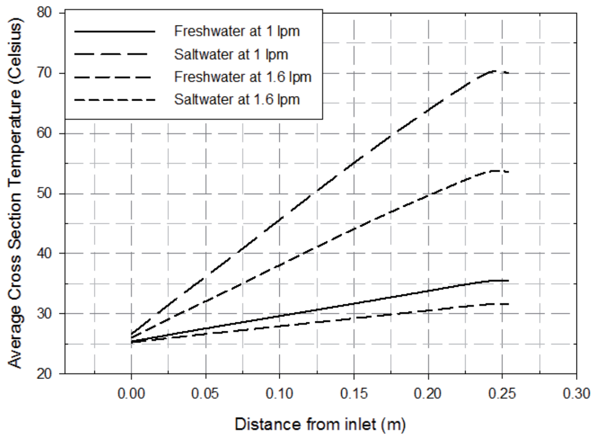


Figure 6. Cross-section spatial temperature distribution (x-z plane) for saltwater (1.5%) heated at 1 lit/min (a) and at 1.6 lit/min (b) at the center of the tube (y= 12.7 cm). ANSYS on left, COMSOL right.



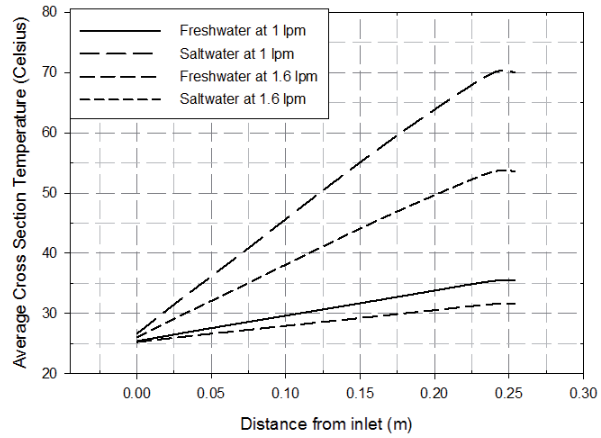


Figure 7. Cross-section average temperature for each fluid and flow rate. ANSYS on left, COMSOL right.

used. The dissimilar meshes in ANSYS might have exacerbated the effects at the wall where the no slip boundary condition imposed a zero velocity and therefore an extremely high residence time in the electric field. Accounting for this effect, the temperature profiles predicted by the COMSOL and the validated ANSYS model were very consistent with one another for the two materials and flowrates tested.

A limitation of COMSOL faced in this study and also mentioned by others (Achkar et al., 2008) is the extensive memory requirement for solving models with a large number of grid elements. Regardless of the hurdles associated with each software package, the electromagnetic power density and temperature distribution from the COMSOL model matched well with the previously validated ANSYS model. This verification ensured accuracy of the COMSOL model and provided confidence in using either one of the software packages for simulation of continuous microwave heating of liquids. The similarity in results of the two models is further exemplified by examining the rate of increase of the average temperature throughout the applicator tube (Figure 7).

For each fluid and flow rate, the average temperature and rate of increase of average temperature at any given position is very similar for both models. This similarity allows further comparison of the COMSOL model to the validated model in ANSYS, in that for each fluid, the rate of increase is approximately the same for each model and flow rate, ranging from 2 °C/cm for saltwater at 1 lpm to 0.3 °C/cm for freshwater at 1.6 lpm.

In general, both ANSYS and COMSOL provided an interface for multiphysics coupling electromagnetism with fluid flow and heat transfer (Table II). ANSYS used different mesh elements for different physical phenomenon and the coupling was achieved by transfer of results from one physics to another between dissimilar meshes. However, for such coupling a compatible element was essential and available to facilitate in information transfer between the modules. A new version of the software, ANSYS 12.0, will facilitate such linking, and embedded coupling of modules such as those inherent in this study will now be available. The COMSOL software package, in comparison, offered common elements that can be used to couple all physics providing a more flexible model setup.

Solution times were markedly different for the two programs, with ANSYS required approximately 2.5 hours to complete, whereas COMSOL required approximately 15 minutes for each model tested, however, the COMSOL model required one-way coupling of physics phenomena while

Table II. Comparison of several ANSYS and COMSOL parameters.

	ANSYS	COMSOL
Mesh size	Waveguide and cavity - 0.03 m Applicator tube- 0.005 m	Waveguide and cavity - 0.03 m Applicator tube- 0.005 m
No. of elements	107564	82570
Element type	Tetrahedral (HF119 for electromagnetism, FLUID142 for fluid flow and heat transfer)	Tetrahedral (same for electromagnetism, fluid flow, and heat transfer)
Processing time	2.5 hrs	15 min
Processor	3 GHz Xeon processor	3 GHz Xeon processor
Memory	3GB RAM	3GB RAM
Criterion for convergence	Normalized rate of change of the solution from one global Iteration to the next calculated for each degree of freedom	Maximum iterative difference of 10^{-6} for each solver
Solvers used	EM- Sparse direct solver Fluid and HT- tri-diagonal matrix algorithm (TDMA) Coupling- ANSYS Multifield Solver	EM- Generalized minimum residual solver (GMRES) Fluid and HT- Parallel direct linear solver (PARDISO)
Method of coupling	Iterative – with physical and electromagnetic properties constant with temperature	One way*- First EM was solved and heat generation was transferred to solve fluid flow and heat transfer
Coupling Technique	Via dissimilar meshes	Via same meshes
Learning curve	Difficult	Easy
Ease of use	Difficult	Easy
Post processing	Difficult- using different result files for different physics	Easy- everything is saved in one file
Heat Generation	Freshwater- 729 W 1.5 % saltwater - 2511 W	Freshwater- 826 W 1.5 % saltwater - 2883 W
Temperature values	Freshwater @ 1 lit/min –26-42ºC Freshwater @ 1.6 lit/min – 25-37ºC 1.5 % saltwater @ 1 lit/min – 29-115ºC 1.5 % saltwater @ 1.6 lit/min –27-91ºC	Freshwater @ 1 lit/min - 25-47ºC Freshwater @ 1.6 lit/min – 24-39ºC 1.5 % saltwater @ 1 lit/min – 27-85ºC 1.5 % saltwater @ 1.6 lit/min –26-66ºC

the ANSYS model was capable of iteratively solving for all three physics modules with the same available processing power.

CONCLUSIONS

A numerical model was developed in COMSOL to simulate continuous flow microwave heating of liquids. The COMSOL model was compared with a previously validated ANSYS model and it was found to be in close agreement. Although ANSYS and COMSOL offered an interface for coupling of electromagnetism with fluid flow and heat transfer, COMSOL provided a more flexible model setup as compared to ANSYS, though it required more memory. This study concludes that results from the COMSOL and ANSYS models were comparable and either one can be used to further the understanding of continuous microwave heating processes through numerical modeling.

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