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“Computational Modelling of Microwave Tumour Ablations”

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Introduction

Thermal ablation technology is a rapidly emerging alternative to surgical resection for many benign and malignant tumors of the liver, lung, kidney and bone (1–5). Ablation is also being investigated for the treatment of other solid tumors in organs such as the breast, prostate, adrenal glands, pancreas and uterus (6–12). Non-oncologic applications include treatment of cardiac arrhythmia, as well as a means for hemostasis during surgical resection (13–15). Ablation may also be combined with adjuvant therapies such as radiation, chemotherapy and even nanoparticles to improve treatment efficacy (16–22).

Methods of inducing thermal ablation include lasers, high-intensity focused ultrasound, radiofrequency electrical current and microwaves. The applied energy heats the target tissue to cytotoxic temperatures, usually above 50–60 °C, although microwave can heat tissue to over 150°C (23). Due to its minimally-invasive nature, thermal ablation is characterized by quicker recoveries and fewer complications compared to surgical resection (24). Microwave ablation is gaining attention as an alternative to the more widely disseminated radiofrequency ablation, due to several advantages in tissue-heating physics. Microwave energy is capable of propagating through desiccated and charred tissue, which allows for continuous and rapid volumetric heating, potentially leading to a larger ablation zone compared to radiofrequency ablation (23). The high heating rate produced by some microwave systems can overcome heat-sink effects from nearby vessels, creating more uniform ablation zones (25). Microwave antennas can also be tuned to deliver energy more efficiently to specific organ systems such as the liver or lung (26,27).

Computational modeling of microwave ablation procedures plays a critical role in the development and implementation of clinical systems. Numerical simulations can rapidly predict the propagation of electromagnetic (EM) waves from antennas of arbitrary geometry and evaluate antenna performance metrics (28). Energy deposition from the applied electromagnetic fields, heat generation, as well as the subsequent water and vapor mass transfer in tissue can then be used to predict the thermal dose or surviving fraction of cells (29–32). Together, coupled electromagnetic-thermal solutions may improve predictions of how ablation zones form inside patients.

The in-silico nature of computational modeling of thermal ablations provides a highly-controlled environment to investigate and understand the effects of changing input variables (33). Such specific insights can potentially lead to more focused experimental studies, fewer animal studies, decreased developmental costs and greater research efficiency. Faster and more powerful computational techniques can help predict and improve microwave heating

in patient-specific models. Analysis of antenna geometry and materials can also be used to optimize device design and implementation.

This paper will reflect upon the current methods and state of computational modeling for microwave tissue ablation. We will briefly review the relevant physics and basic numerical models. We will then address complexities unique to microwave tissue heating, such as the effects of high temperature on tissue properties and how resulting changes in energy delivery can be incorporated into a computational model. Lastly, we will discuss the current trends and challenges in translating simulation results into practical application.

Theory

Microwave ablation is produced by EM fields radiating from an antenna inserted into the tissue. The EM field is described most generally by the source-free, time-harmonic form of Maxwell's equation in lossy media such as tissue:

$$\nabla \times \mathbf{E} = -j\omega\mu\mathbf{H} \quad (1)$$

$$\nabla \times \mathbf{H} = \mathbf{J} + j\omega\epsilon\mathbf{E} \quad (2)$$

$$\nabla \cdot \mathbf{D} = 0 \quad (3)$$

$$\nabla \cdot \mathbf{B} = 0 \quad (4)$$

where $\mathbf{E}$ is the electric field intensity (V/m), $\mathbf{H}$ is the magnetic field intensity (A/m), ω is the angular frequency, μ is the permeability (H/m) and ϵ is the complex permittivity or dielectric constant (F/m), $\mathbf{B}$ is the magnetic flux density (Wb/m²), $\mathbf{D}$ is the electric flux density (C/m²). And $\mathbf{J}$ is the current density (A/m²). In the case of coaxial microwave antennas in an approximately homogenous, isotropic medium, an axially-symmetric cylindrical coordinate system can often be used to reduce the three-dimensional problem to a two-dimensional domain, accelerating the solution computation.

A description of heat transfer in tissues can be realized using Pennes' formulation of the non-stationary heat equation (34):

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k_t \nabla T) + Q_h - Q_p + Q_m \quad \left[\text{W/m}^3 \right] \quad (6)$$

where c_p is the specific heat capacity of the tissue (J/kg·K), k_t is the thermal conductivity (W/m·K), T is the temperature (K). Q_m is the metabolic heat generated from the tissue (W/m³) but usually ignored due to its minimal impact compared to the other heat terms. Q_p represents heat loss through blood perfusion,

$$Q_p = \omega_{bl} c_{bl} (T - T_{bl}) \quad \left[\text{W/m}^3 \right] \quad (7)$$

where ω_{bl} is the blood perfusion velocity (kg/m³·s), c_{bl} is the specific heat capacity of blood (J/kg·K) and T_{bl} is the blood temperature (K). The remaining term of equation (6) is the heat absorbed by the electromagnetic field into the tissue,

$$Q_h = \frac{\sigma}{2} \|\mathbf{E}\|^2 \quad \left[\text{W/m}^3 \right] \quad (8)$$

where $\mathbf{E}$ is the electric field (V/m) solution found previously through solving Maxwell's equations, and σ is the tissue conductivity (S/m) (23,35). Solving this set of equations provides a visual representation for how tissue temperature changes during a microwave ablation procedure (**Figure 1A and 1B**). The equations can also be solved simultaneously or iteratively to account for changing tissue properties; for example, those that are dependent on temperature or water content.

Although tissue damage is composed of many complex biological processes, there are two widely-accepted models that predict thermal damage as a single simplified process: the thermal iso-effective model and the Arrhenius damage model (36,37). The thermal iso-effective model describes how cellular damage is related to cumulative thermal dose; that is, the relationship between temperature and exposure time. The cumulative equivalent minutes at 43°C (CEM43) is a common metric that equates the likelihood of cellular death to that of cells exposed to 43°C for a specified number of minutes (38,39). The Arrhenius damage model, using similar assumptions as the CEM model, expresses the percentage of cells in a given volume that will survive at a given temperature and exposure time. However, there are limits in quantifying thermal damage, especially at the higher temperatures seen in thermal ablations compared to mild or moderate hyperthermia (36,40). Models that describe thermal damage due to cellular or metabolic disruption have also been described but have not been as widely-utilized to date due to complex inputs and high computational costs (41,42).

Analytical solutions to equations 1-8 are available for only certain antenna geometries and assumptions about the medium, such as a homogenous tissue environment. For more general models, numerical methods are required. The most commonly-used techniques include the finite element method (FEM), the finite difference time domain method (FDTD) and the method of moments (MOM). The finite-element method has been used extensively due to its availability in commercial software such as COMSOL and ANSYS, which are capable of coupling electromagnetic field solutions to other physics models such as heat transfer and diffusion.

Uses of Computational Modeling in Microwave Ablation

Antenna Evaluation

Common microwave ablation antenna performance metrics include those that describe how efficiently an antenna can deliver power into the tissue and the resulting heating pattern. Antenna efficiency can be described by the ratio of power output to power input, or reflection coefficient Γ ,

$$\Gamma(f)_{dB} = 10 \cdot \log \left(\frac{P_r(f)}{P_{in}} \right) \quad (9)$$

where $P_r(f)$ is the reflected power and P_{in} is the input power (W). More efficient power delivery is characterized by lower reflection coefficients. Specific absorption rate (SAR), which represents the rate of power deposition in tissue, is given as

$$SAR = \frac{\sigma}{2\rho} \|\mathbf{E}\|^2 \quad [\text{W/kg}] \quad (10)$$

where $\mathbf{E}$ is the electric field (V/m), σ is the tissue conductivity (S/m) and ρ is the liver tissue density (kg/m³) (35,25). SAR can roughly estimate potential shape of an ablation zone created by a given antenna (**Figure 1C**).

With transient analysis of coupled EM-thermal problems, it is also possible to observe the changes in reflection coefficient and SAR occurring during the ablation process. Using these metrics, automated optimization techniques can be employed to find microwave antenna geometries that suit a specific clinical need. Due to the multiple factors involved in antenna design, the final design is usually the result of a trade-off between the objective heating pattern and reflection coefficient (43–45). Improving ablation antenna design remains an area of active research (46–49).

Power Delivery Frequencies

In addition to facilitating computer-aided antenna design, computational modeling can also be used to evaluate the effect of the applied frequency during power delivery. Current microwave ablation generators provide continuous power, from 30–180 W at 915 MHz or 2.45 GHz, although higher and lower frequencies have been described (50–54). While some previous studies suggested that lower frequencies are associated with greater penetration depth and larger ablation zones, power output was not normalized to offset cable losses at each frequency (55,56). When modeling the dipole antennas used in those studies, and controlling for applied power, we found virtually no difference in ablation SAR diameter between 915 MHz and 2.45 GHz (**Figure 2A and 2B**). This result confirmed the conclusions of an earlier microwave hyperthermia antenna study (57). When comparing antenna designs in a controlled environment with varying powers, computational modeling can play a critical role.

Multiple Antenna Optimizations

Modeling has also been utilized to analyze and optimize antenna arrays for microwave tissue heating. Such arrays can produce larger, more homogenous ablation zones than with a single antenna (58–62). As with single antennas, computational models can predict the electromagnetic interactions between antennas and resulting heating pattern in tissue. Zones of constructive and destructive wave interference that can affect relative heating rates have been of particular interest. Computational modeling can help optimize the input wave amplitude and phase to produce deeper tissue penetration and improved local control of the tumor ablation zone (63–65). Temporal modulation of the amplitude and phase of each antenna has also been analyzed during computational modeling (66,67). Placement of phased antennas in non-parallel fashion while maintaining the same homogenous ablation zone has also been explored (68). Array optimization with modeling has led to increased efficacy in treating more irregularly-shaped tumors that are deep within the body and provide more options in the number of antennas placed and their insertion points (35,69–72).

Tissue Property Changes during Thermal Ablation

Dielectric properties of various tissues are strongly influenced by temperatures and tissue water content (73). The dielectric properties of tissue include relative permittivity ϵ_r , which describes the tissue's ability to hold electrical charge, and effective conductivity σ , a measure of how well the tissue absorbs electromagnetic energy. The dielectric properties of biological tissue can be described across a wide frequency domain by the multi-pole Cole-Cole dispersion model:

$$\epsilon_r(\omega) = \epsilon_\infty + \sum_n \frac{\Delta\epsilon_n}{1 + (j\omega\tau_n)^{1-\alpha_n}} + \frac{\sigma_s}{j\omega\epsilon_0} \quad (11)$$

where τ_n is a time constant to characterize the polarization in a relaxation region, ϵ_∞ is the permittivity at field frequencies where $\omega \gg 1/\tau_n$, $\Delta\epsilon_n$ is the magnitude of dispersion, α_n is a measure of the broadening of the dispersion and σ_s is the static conductivity (74).

The temperature-dependence of dielectric permittivity and conductivity in tissue has been documented in multiple studies. Within a narrow range around physiological temperatures (20-45°C), temperature-dependence can be reasonably described as a linear function (75,76). Parabolic temperature-dependent models have also been described in the range of 20-60°C (77). Microwave ablation systems, however, are capable of heating tissue to temperatures well over 100°C (27,78). At these higher temperatures, tissues undergo structural changes and water loss, which affect tissue properties substantially (38,79,80). By lumping physical phenomena such as water vaporization and tissue dehydration into a temperature-dependent model and using coupled EM-thermal simulations, more accurate temperature profiles can be predicted, even at temperatures over 100°C. One study compiled a table of dielectric properties of tissue which were measured at the end of a microwave ablation with various sets of power and time (81). The results were fitted to a Cole-Cole model and suggested significant changes in the amount of dispersion, time constant and static conductivity values during heating (82). Two other studies monitored the dielectric property values during high temperature microwave heating of *ex vivo* bovine liver, revealing a sigmoidal relationship between permittivity and conductivity with temperature (83,84). These curves were then applied to the computer simulations and found to be more accurate in predicting experimental temperatures when compared to existing models (83). The temperature-dependent model also more accurately described changes in antenna reflection coefficient and heating pattern caused by non-uniform changes in the tissue dielectric property during ablation. Establishing the relationship between dielectric properties and heating physics is an ongoing topic of research that holds promise for even more accurate simulations.

Trends in Microwave Ablation Modeling

Microwave ablation technology development has undergone rapid growth in the last decade and there are multiple areas of active research that leverage the benefits of numerical modeling. The effect of individual parameters on the entire ablation process can be predicted prior to experimental work, saving time and resources for more focused study (85). But despite the advantages of working with simulations and leveraging nearly a century of research in electromagnetic theory, there is much work needed with regards to the inputs and the validation of existing numerical models.

Water Vaporization and Tissue Contraction in Tissue

Intense heating during microwave ablation leads to physical changes such as water vaporization, vapor mass diffusion and re-condensation. This is evident during experimental studies with microwave antennas in tissue, where vapor formation can be observed with imaging during longer and more powerful ablations. The center of the ablation zone typically becomes dehydrated first, and the water is driven outwards from the antenna. Vapor formation and transport leads to dehydration of the tissue around the ablation zone (3,38,78–80,86). Two separate groups tried improving matching between modeling and experimental results by incorporating a latent heat of vaporization term to account for the energy needed to change water from its liquid to gas phase within tissue (78,87). However, there was an unaccounted decrease in heating rate after 100°C and a high temperature SAR correction term was required to match the model to the experiments. One possible explanation for this model mismatch is a change in the EM field profile secondary to changes in permittivity and conductivity as noted in other works (79,83). Incorporating the dielectric changes due to tissue dehydration in the ablation treatment may yield a more accurate model to predict the physical changes occurring during an ablation treatment.

Another important phenomenon affecting the accuracy of computational modeling is the contraction of tissue exposed to ablative temperatures. One previous study had demonstrated that ablation zones contract up to 15-50% in diameter and 27-75% in volume during

radiofrequency and microwave ablation. The same study implemented an exponential correction term to the computational model to compensate for the 20-25% radial contraction at various distances from the antenna after 5 minutes (88). Greater contraction was noted during microwave ablations than RF ablations, likely due to increased water vaporization and collagen dehydration (**Figure 3**). Contraction can complicate the validation of numerical and experimental results because temperature sensors placed into the tissue will move during contraction, artificially increasing temperatures compared to static points in a computational model. Contraction can also confound imaging-based diagnostic and post-ablation staging efforts by shrinking the original boundaries of the tumor. Accurate comparison of numerical simulations and experimental results is possible only by accounting for such contractions (83).

Model Validation

Experimental validation of computational model predictions is critical to establish broader applicability of the model. Visual inspection and correlation of experimental ablation zone dimensions to numerical predictions is one validation technique. Blanching and desiccation inside the ablation zone are good predictors of cell death in many parenchymal tissues such as the liver (**Figure 4A**). Further histological analysis such as microscopic examination, enzyme histochemistry and transmission electron microscopic analysis can help stratify various regions of ablation (89–91). These techniques compare cell death to the predictors of cytotoxicity calculated during simulation. However, such comparisons rely on the numerical metric of cell death, which can vary widely by method (36).

Alternatively, arrays of thermocouples or fiber-optic temperature probes have been successfully used to map temperatures around the ablation antenna (83,87,92). These temperature probes are structurally robust, exhibit quick response times and provide enough temporal resolution in real-time. Temperature data can be recorded and correlated spatially and temporally with the modeling data. Since contraction can change the location of the temperature probes, it is important to similarly recalibrate the evaluation points in the simulation output or establish a temperature-contraction relationship in the model to accurately compare numerical and experimental results (83,88).

Imaging techniques such as ultrasound, CT or MRI can also be used to validate computational models (93–95). Contrast-enhanced scans delineate boundaries of the coagulation zone compared to perfused tissues and can be used to compare ablation zone size to predicted sizes (94). Non-contrast scans with sufficient temporal resolution can be used to monitor ablation zone growth, but thermal ablation features can still be difficult to discern. One more prominent feature is water vapor formation, which appears as hyper-echoic gas bubbles under ultrasound and hypo-dense regions under CT. The visible gas is not a surrogate for the ablation zone, but can provide an estimate of the most desiccated zone of tissue. The highly visible gas can also be tracked during the ablation to estimate vapor transport (**Figure 4B and 4C**). However, water vapor formation and transport must be calculated in the computational model to use gas as the validation metric. Alternatively, MR thermometry can be used to quantify the temperature change in tissue experimentally for comparison with numerical predictions, but most studies have been targeted toward radiofrequency ablation measurements (96–98). Current microwave devices are not MR compatible so the utility of MR thermometry has been limited (99–101).

Extension to patient-specific planning

Treatment planning is most typically performed by the attending physician and is, therefore, heavily dependent on physician experience. Patient-specific treatment planning based on computational modeling may be able to assist in the physicians' decision-making process.

Ablation precision would theoretically improve as physicians would be able to recognize whether a given antenna placement could achieve the necessary margins, but also potentially avoid critical structures that could lead to procedural complications (102).

While information needed to create patient-specific antenna guidance systems is available, there are still multiple challenges that need to be addressed before being integrated into hospital workflow. Cooling effects from vasculature can disrupt the growth of a thermal ablation zone, decreasing the efficacy of an ablation treatment and increasing the risk for local recurrence. Previous literature investigating the effect of blood vessels on thermal ablations are based primarily on radiofrequency ablation (103–105). Studies relating the effects of blood vessels and vascular trees to radiofrequency ablation zone sizes have revealed additional flow mechanics that influence how a thermal ablation zone may appear (106–109). While the focus of these studies were on radiofrequency ablation, the implications are increasingly relevant for microwave ablations, which are much more efficient at heating tissue and blood vessels. Vessels near microwave ablations have been shown to act as a heat conduit, as opposed to a “heat-sink” for thrombotic events and perivascular damage (110–112). Understanding the effect of vessel flow and nearby vascular beds in thermal ablations is currently an area of active research.

In addition to the modeling of local anatomy near the antenna placement location, patient-specific planning requires detailed knowledge of many other parameters such as the thermal and electrical properties of the organ and surrounding tissue that may be affected by underlying disease processes (113,114). Accurately integrating these additional facets into clinically useful information in the hospital workflow in real-time has led to the development of ranking algorithms, image registration and computing reduction techniques. Optimization algorithms have been used to rank the possible insertion points and find the best antenna placement location, maximizing chances of the best clinical outcome and minimizing risks for complications (115–117). To cut down on computing costs, some groups have utilized an objective cost function that optimizes the temperature distribution by avoiding larger vasculatures, creating an optimal trajectory of an RFA applicator (104). Decreasing the computational time of calculating ablation zone behavior near major vasculatures has also been demonstrated using patient-independent lookup tables. These tables utilized previously-calculated cooling rates of blood vessels based on vessel size and distance from an RF applicator. Using these tables to predict ablation zone characteristics was demonstrated to be computationally faster than solving for the electromagnetic and heat transfer solutions independently for a patient-specific anatomy (118). Other efforts to improve computational speed have involved a GPU-driven real-time calculation of the projected ablation zone, while incorporating the cooling effects of nearby liver vasculature (119).

Conclusion

Microwave tumor ablation is a rapidly growing modality already used to treat early-stage tumors and gaining traction in combination therapies. The ability to predict the active heating zone and heating behavior within tissue has led to improved understanding of the basic physics behind microwave ablations. The exquisite control of modeling studies affords in-depth investigation of the effects of single variables, leading to decreased experimental sample sizes and costs. Computational and experimental studies have helped optimize the design of microwave antennas, generators and techniques, facilitating clinical translation and further adoption into clinics worldwide. The concurrent development of modeling and validation will lead to better integration of patient-specific, interactive models that can change how ablation procedures are performed in the future.

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A

B

C

Figure 1.

A) Model of temperature profiles during microwave ablations in liver tissue at various time points. The ablation zone temperature boundary grows more in the first 3 minutes, compared to the last 2 minutes. B) Temperature elevation through the transverse cross section of ablation zone at various time points. Microwave ablation zones can reach temperatures as high as 150°C. C) Specific absorption rate (SAR) mapping of a microwave ablation zone along with corresponding temperature isotherms at 5 minutes.

2.45GHz-Tuned Dipole Antenna

915 MHz-Tuned Dipole Antenna

A

B

Figure 2.

A) Numerical modeling demonstrating nearly equivalent maximum ablation zone diameters between dipole antenna designs emitting power at 2.45 GHz (right) and 915 MHz (left). The color bars represent the heating rate from 0-100000 W/m³. The white line iso-contour gives a visual approximation to the ablation heating zone. B) The heating rate normalized by density, also known as the specific absorption rate (SAR). Microwave antenna performance at the two frequencies shows nearly equivalent SARs at radial distances 7 mm from the antenna.

A)

Initial Marker Positions

Ablation On

1 minute

7 minutes

11 minutes

Figure 3.

A) Ex-vivo tissue contraction is shown by placing pairs of high-density wire markers 10-40 mm away from the antenna shaft. The original marker positions are shown in the top image and begin to move closer together as the microwave ablation begins and continues shrinking until the end of the procedure. B) Graph showing distances between marker pairs decreasing during the ablation. Contraction is most rapid in the first 2-3 minutes.

A)

B)

c)

Figure 4.

A) Microwave ablation created in ex-vivo liver tissue. The charred zone is the darkened area at the center of the ablation zone that highly desiccated from the intense heat and water vaporization ($>100^{\circ}\text{C}$). The coagulation zone is the blanched region of the ablation zone, usually showing pyknotic nuclei on histology ($70\text{-}100^{\circ}\text{C}$). The congestive zone is the red peripheral area of the ablation zone that represents the boundary of the ablation zone and is sometimes called the transition zone ($50\text{-}70^{\circ}\text{C}$). B) Intra-procedural imaging of a monopole antenna during an in-vivo ablation procedure. The central hypo-dense zone identifies water vaporization. C) Gas bubbles resulting from water vaporization are visible on ultrasound imaging and can be used to monitor treatment progress.