1 Coupled electromagnetic - heat transfer model

The microwave heating process proposed in this paper involves raising the temperature of PAN fibres using electromagnetic waves, via a lossy dielectric susceptor coating. The electromagnetic waves are generated by a $P = 1\,kW$ magnetron operating with an assumed efficiency of $\eta_{mag} = 60 - 70\%$. A TE_{10} waveguide then passes the electromagnetic waves into the microwave cavity with a volume of $0.32\,m(height) \times 0.45\,m(width) \times 0.28\,m(depth)$. The electromagnetic fields alternate with a frequency of $f = 2.45\,GHz$, which in turn excite the polar molecules in the susceptor material as their poles try to align with those of the waves. This process raises the kinetic energy of molecules in a substance, with the average described by temperature. The susceptor material is made of XXX, which has a high dielectric loss that means the temperature increases rapidly upon exposure to electromagnetic waves. As the temperature of the susceptor increases, heat conducts to the lower temperature PAN precursor material located at the core of the fibre. In order to model the transient temperature distribution on the PAN core, it is necessary to couple the electromagnetic and heat transfer domains.

1.1 Heat transfer domain

First, the heat transfer model will be described for the PAN and susceptor materials (fibre domain). The heat diffusion equation for three dimensional transient heat conduction in cylindrical coordinates is described by the following;

$$\frac{1}{r}\frac{\partial}{\partial r}\left(kr\frac{\partial T}{\partial r}\right) + \frac{1}{r^2}\frac{\partial}{\partial \phi}\left(k\frac{\partial T}{\partial \phi}\right) + \frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right) + \dot{Q} = \rho C_p \frac{\partial T}{\partial t} \tag{1}$$

Where r, ϕ, z describe the radial, circumferential, and axial coordinates, T is the temperature (K), k is the thermal conductivity (W/mK), $\dot{Q}$ represents volumetric heat generation that results from dielectric heating of the fibre (W/m^3), ρ is the density (kg/m^3), C_p is the specific heat capacity (J/kgK), and t represents time (s). Recognising the symmetry that exists in heating of the fibre, and the size of the geometry in comparison to the wavelength of the electromagnetic field, Equation 1 may be reduced to a one dimensional problem by assuming symmetry with respect to the circumferential and axial coordinates $\left(\frac{\partial T}{\partial r}, \cancel{\frac{\partial T}{\partial \phi}}, \cancel{\frac{\partial T}{\partial z}}\right)$. This simplification may be afforded as the cross section of the fibre will not experience a significant variation in electric field strength (E_{rms}), due to the size of the fibre diameter relative to the electromagnetic field wavelength $(10^{-1}\,\mu m$ vs $10^{-1}\,m)$. For simplicity, the fibre is assumed as suspended in the electromagnetic field, with temperatures and heat losses to the environment uniform around the circumference and along the length; embedded in this assumption is the omission of the effects of neighbouring fibres in a bundle, and that conditions are representative of a fibre at the outer surface of a bundle. As the model must be able to describe the transient temperature response of the fibre material as heat is conducted radially through the fibre via the dielectrically heated susceptor material, the temporal and volumetric heat generation terms are retained in the formulation of the one dimensional model;

$$\frac{1}{r}\frac{\partial}{\partial r}\left(kr\frac{\partial T}{\partial r}\right) + \dot{Q} = \rho C_p \frac{\partial T}{\partial t} \tag{2}$$

Mathematical models have been developed for linear and non-linear schemes, both of which are described below using implicit finite difference methods.

1.1.1 Linear model

If constant material properties are assumed, then the model can be linearised, and Equation 2 reduces to the following;

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)+\frac{\dot{Q}}{k}=\frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{3}$$

Where α represents thermal diffusivity $\left(\alpha=\frac{k}{\rho C_p},\, m^2/s\right)$. Equation 3 can be re-written as follows;

$$\frac{1}{r}\frac{\partial T}{\partial r}+\frac{\partial^2 T}{\partial r^2}+\frac{\dot{Q}}{k}=\frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{4}$$

In order to solve the above equation to deliver a transient temperature profile over the radial coordinate ($0 \leq r \leq r_o$), it is necessary to define initial and boundary conditions. Upon introduction of the electromagnetic field to the heat transfer domain, it is assumed that the temperature of the PAN fibre is equal to the ambient ($T_\infty = 20°C$);

$$T\left|_{t=0}\right. = T_\infty \quad 0 \leq r \leq r_o \tag{5}$$

Due to symmetry, a zero temperature gradient exists at the core of the fibre ($r = 0$);

$$\left.\frac{\partial T}{\partial r}\right|_{r=0} = 0 \quad t > 0 \tag{6}$$

At the surface of the susceptor ($r = r_o$), heat losses through radiation and convection are assumed;

$$-k\left.\frac{\partial T}{\partial r}\right|_{r=r_o} = \epsilon\sigma\left(T^4 - T_\infty^4\right) + h_\infty\left(T - T_\infty\right) \quad t > 0 \tag{7}$$

Where ϵ represents the emissivity of the susceptor coating, σ is the Stefan-Boltzmann constant ($5.68 \times 10^{-8}\, W/m^2K^4$), and h_∞ is the convective heat transfer coefficient. The presence of fourth power terms in the above equation (T^4) makes it highly non-linear, introducing further complication when resolving for temperatures at the boundary node. The radiative heat loss term can be linearised by formulating an expression using the radiation heat transfer coefficient (h_r);

$$\epsilon\sigma\left(T^4 - T_\infty^4\right) = h_r\left(T - T_\infty\right) \tag{8}$$

Where;

$$h_r = \epsilon\sigma\left(T + T_\infty\right)\left(T^2 + T_\infty^2\right) \tag{9}$$

The radiation heat transfer coefficient, with units of W/m^2K, is updated at every point in time during simulation due to its surface temperature dependency. The convection heat transfer coefficient is assumed as $h_\infty = 10\, W/m^2K$. The overall heat transfer coefficient can then be computed by summing the contributions of radiation and convection ($h = h_r + h_\infty$), and Equation 7 transforms to the following;

$$-k\left.\frac{\partial T}{\partial r}\right|_{r=r_o} = h\left(T - T_\infty\right) \quad t > 0 \tag{10}$$

In effect, the $\dot{Q}$ term in Equation 4 represents volumetric heat generation in the susceptor coating only ($\dot{Q}_{sus}$), as the PAN fibre has a negligible dielectric loss ($\dot{Q}_{PAN} \sim 0\, W/m^3$). The susceptor coating is on the order of $10 - 100\, nm$ in thickness. At such scales, the conventional 'bulk' heat diffusion model (Equation 1) no longer holds, as the thickness is likely smaller than the mean free paths of the electrons and phonons that transport heat through the material. Even if the mean free path is smaller than discrete spatial steps (Δr) used in a heat transfer model, the limit imposed on the temporal step (Δt) for stability ($\frac{\Delta r^2}{2\alpha}$ for an explicit finite difference model) and accuracy is prohibitive for transient modelling over $10^1\, s$. In order to circumvent this difficulty in modelling the PAN fibre, the volumetric heat generation term is transformed to a heat flux on the PAN surface. In this manner, the macro-scale Fourier law model can be applied as the susceptor coating is removed from the model, and the PAN fibre is $\sim 10 \mu m$ in diameter. Utilising a $1 \mu m$ spatial step permits a time step of $\Delta t = 10^{-6}\, s$ for stability and accuracy, which is over $10^6 \times$ larger than the limiting temporal increment for modelling at $10 - 100\, nm$ [1]). When the heat generation term is converted to an incident heat flux on the PAN surface, an energy balance dictates the state of thermal equilibrium of the fibre;

$$-k \frac{\partial T}{\partial r}\bigg|_{r=r_o} = h\left(T - T_\infty\right) - Q"_{sus} \quad t > 0 \tag{11}$$

Where $Q"_{sus}$ is the incident heat flux on the PAN surface from the dielectrically heated susceptor, calculated using;

$$Q"_{sus} = \dot{Q}_{sus} L_{sus} \tag{12}$$

Where L_{sus} is the half-thickness of the susceptor coating on the PAN surface. Inherent in the application of Equation 12 is an assumption of uniform temperature across the susceptor material. Assuming a negligible dielectric loss in the PAN fibre, Equation 4 reduces to the following;

$$\frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial r^2} = \frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{13}$$

By reducing the heat diffusion equation to a one-dimensional radial conduction problem, the transient temperature profile can be solved numerically using implicit finite difference methods with appropriate initial and boundary conditions. This method is unconditionally stable, meaning a solution can be obtained using any temporal step size (Δt), and is resolved iteratively with a set of linear algebraic equations. However, the chosen time increment does influence solution accuracy, so caution must be exercised in this regard. The equations needed to build the finite difference model are essentially discrete approximations of the differential terms present in the heat equation, and are formulated using the second-order accurate central difference scheme;

$$\frac{\partial T}{\partial t} \approx \frac{T_i^{n+1} - T_i^n}{\Delta t} \tag{14}$$

$$\frac{\partial T}{\partial r} \approx \frac{T_{i+1}^{n+1} - T_{i-1}^{n+1}}{2\Delta r} \tag{15}$$

[1] In formulating a non-linear finite difference model, stability limits associated with explicit modelling are used as a guide for approximate temporal steps in the implicit schema.

$$\frac{\partial^2 T}{\partial r^2} \approx \frac{T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}}{\Delta r^2} \tag{16}$$

In the above equations, the n superscript represents discrete time steps of size Δt, whilst the i subscript represents discrete spatial steps of size Δr. A temporal position can therefore be located with $t^n = n\Delta t$, whilst spatial positions are located by $r = (i-1)\Delta r$. When the partial derivative approximations are recombined, Equation 13 is described in the implicit finite difference schema by the following;

$$\frac{1}{r}\frac{T_{i+1}^{n+1} - T_{i-1}^{n+1}}{2\Delta r} + \frac{T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}}{\Delta r^2} = \frac{1}{\alpha}\frac{T_i^{n+1} - T_i^n}{\Delta t} \tag{17}$$

In order to solve the transient heat conduction problem using the finite difference scheme, temperatures are evaluated at a *new* time $(n+1)$, rather than in a previous (n) time, as is the case using conditionally stable explicit solution methods. The Gauss-Seidel iteration technique is employed here to resolve temperatures in the finite difference stencil at *new* times. This method is robust, efficient, and involves solving a linear set of finite difference equations describing nodal temperatures at *new* times (T_i^{n+1}) simultaneously by iterating towards converged solutions, then *marching* the solution at each time step by setting the outputs at time n as the inputs for time $n+1$. Considering a system of N finite difference equations with N unknowns that correspond to the number of discrete nodes in the finite difference stencil, the linear algebraic equations are reordered according to the following;

$$\begin{aligned} a_{11}T_1^{n+1} + a_{12}T_2^{n+1} + a_{13}T_3^{n+1} + ... + a_{1N}T_N^{n+1} &= C_1 \\ a_{21}T_1^{n+1} + a_{22}T_2^{n+1} + a_{23}T_3^{n+1} + ... + a_{2N}T_N^{n+1} &= C_2 \\ &\vdots \\ a_{N1}T_1^{n+1} + a_{N2}T_2^{n+1} + a_{N3}T_3^{n+1} + ... + a_{NN}T_N^{n+1} &= C_N \end{aligned} \tag{18}$$

Where a_{ii} is the coefficient for the temperature at node i (T_i^{n+1}), a_{ij} represents coefficients for temperatures at neighbouring nodes in the stencil, and C_i is a coefficient comprised of the remaining terms in the diffusion equation for T_i^{n+1}. For ease of convergence, the equations should be re-ordered in order to ensure that the diagonal coefficients (a_{ii}) are the largest elements in each row; in this problem, and indeed most heat transfer problems, the diagonal coefficients prove to be the largest in each unknown equation. A satisfactory convergence condition is as follows;

$$|a_{ii}| > \sum_{j=1}^{i-1} |a_{ij}| + \sum_{j=i+1}^{N} |a_{ij}| \tag{19}$$

With the coefficients for each node determined and appropriately sequenced, the iteration procedure can commence using a general description of the form;

$$T_i^{n+1(k)} = \frac{1}{a_{ii}}\left\{C_i - \sum_{j=1}^{i-1} a_{ij}T_j^{n+1(k)} - \sum_{j=i+1}^{N} a_{ij}T_j^{n+1(k-1)}\right\} \tag{20}$$

The k superscript refers to the level of the Gauss-Seidel iteration. In establishing T_i^{n+1}, rational estimates of nodal temperatures at $k=0$ can be obtained using the converged solution at T_i^n. At subsequent Gauss-Seidel iterations ($k > 0$), new values of $T_i^{n+1(k)}$ are calculated using current values of $T^{n+1(k)}$ at $1 \leq j \leq i-1$, and values of $T^{n+1(k-1)}$ at $i+1 \leq j \leq N$. The iteration continues until an appropriate convergence criterion is reached. In this study, the following must be satisfied for each node in the stencil;

$$\left| T_i^{n+1(k)} - T_i^{n+1(k-1)} \right| < E \tag{21}$$

Where Err is an acceptable error in temperature; $0.001\,K$ is applied here. Due to the cylindrical fibre geometry and imposed boundary conditions, different coefficients exist for modes at the root, the interior, and at the surface. For interior nodes ($0 < r < r_o$, $1 < i < N$), the coefficients extracted from Equation 17 are as follows;

$$a_{ii} = -\frac{2}{\Delta r^2} - \frac{1}{\alpha \Delta t} \tag{22a}$$

$$a_{i(i+1)} = \frac{1}{\Delta r^2} + \frac{1}{2r\Delta r} \tag{22b}$$

$$a_{i(i-1)} = \frac{1}{\Delta r^2} - \frac{1}{2r\Delta r} \tag{22c}$$

$$C_i = -\left(\frac{T_i^n}{\alpha \Delta t} \right) \tag{22d}$$

For the core node ($r = 0$, $i = 1$), symmetry is assumed, with Equation 17 reducing to the following when T_{i-1}^{n+1} is replaced with T_{i+1}^{n+1};

$$\frac{2T_{i+1}^{n+1} - 2T_i^{n+1}}{\Delta r^2} = \frac{1}{\alpha} \frac{T_i^{n+1} - T_i^n}{\Delta t} \tag{23}$$

With the following coefficients extracted;

$$a_{ii} = -\frac{2}{\Delta r^2} - \frac{1}{\alpha \Delta t} \tag{24a}$$

$$a_{i(i+1)} = \frac{2}{\Delta r^2} \tag{24b}$$

$$a_{i(i-1)} = 0 \tag{24c}$$

$$C_i = -\left(\frac{T_i^n}{\alpha \Delta t} \right) \tag{24d}$$

The fictitious node concept is leveraged to define an appropriate equation for the outer surface ($r = r_o$, $i = N$), as node $i+1$ is beyond the confines of the nodal stencil. The finite difference representation of the surface boundary condition (Equation 11) is as follows;

$$-k \left(\frac{T_{i+1}^{n+1} - T_{i-1}^{n+1}}{2\Delta r} \right) = h \left(T_i^{n+1} - T_\infty \right) - Q" \tag{25}$$

When rearranged for T_{i+1}^{n+1};

$$T_{i+1}^{n+1} = \frac{2\Delta r \left(Q" - h \left(T_i^{n+1} - T_\infty \right) + \frac{T_{i-1}^{n+1} k}{2\Delta r} \right)}{k} \tag{26}$$

Equation 26 is then substituted into Equation 17, yielding the following coefficients;

$$a_{ii} = -\frac{\left(\frac{2\Delta rh}{k}\right) + 2}{\Delta r^2} - \frac{1}{\alpha \Delta t} - \frac{h}{kr} \tag{27a}$$

$$a_{i(i+1)} = 0 \tag{27b}$$

$$a_{i(i-1)} = \frac{2}{\Delta r^2} \tag{27c}$$

$$C_i = -\left(\frac{T_i^n}{\alpha \Delta t} + \frac{2\left(Q" + hT_\infty\right)}{k\Delta r} + \frac{\left(Q" + hT_\infty\right)}{kr}\right) \tag{27d}$$

1.1.2 Non-linear model

The heat diffusion problem becomes non-linear when material properties are assigned a temperature dependency. A number of approaches have been developed for solving non-linear problems, such as lagging the evaluation of temperature dependent properties by one time step, a three-time-level implicit scheme, and linearisation procedures [1]. For the current model, the three-time-level implicit scheme developed by Dupont et al. [2] is used (known as the Dupont-II scheme [1]). In this method, linear algebraic finite difference equations are solved simultaneously for time $n+1$ using results at times n and $n-1$. This approach is deemed to be more accurate than simply lagging temperature dependent properties by one time step, can be readily implemented once the time marching procedure is started, and is stable across large time steps [1]. As this method requires the results of two previous time levels to solve for $n+1$, a two-time-level scheme is necessary to start the model. The implicit finite difference model described in Section 1.1.1 can be used to start the time marching procedure, passing results for $n = 1$ to the three-time-level model for the evaluation of results at $n \geq 2$. Hogge [3] found the Dupont-II model with a weight parameter of $w = \frac{1}{4}$ to produce excellent results to non-linear diffusion problems after critically examining a number of methods [1]. This parameter dictates the proportional time-averaging weight for times $n+1$ and $n-1$. For interior nodes, the three-time-level finite difference equation in the Dupont-II scheme is as follows;

$$\frac{1}{r_i}\frac{1}{\Delta r^2}\left[\frac{3}{4}F_i^{n+1} + \frac{1}{4}F_i^{n-1}\right] = \rho_i^* C_{p_i}^* \frac{T_i^{n+1} - T_i^n}{\Delta t} \tag{28}$$

Where F_i^{n+1} and F_i^{n+1} are as follows;

$$F_i^{n+1} = r_{i+\frac{1}{2}} k_{i+\frac{1}{2}}^* \left(T_{i+1}^{n+1} - T_i^{n+1}\right) - r_{i-\frac{1}{2}} k_{i-\frac{1}{2}}^* \left(T_i^{n+1} - T_{i-1}^{n+1}\right) \tag{29a}$$

$$F_i^{n-1} = r_{i+\frac{1}{2}} k_{i+\frac{1}{2}}^* \left(T_{i+1}^{n-1} - T_i^{n-1}\right) - r_{i-\frac{1}{2}} k_{i-\frac{1}{2}}^* \left(T_i^{n-1} - T_{i-1}^{n-1}\right) \tag{29b}$$

Localised radial and thermal conductivity parameters between neighbouring nodes are evaluated as follows;

$$r_{i\pm\frac{1}{2}} = \frac{r_i + r_{i\pm 1}}{2} \tag{30}$$

$$k_{i\pm\frac{1}{2}}^* = \frac{k_i^* + k_{i\pm 1}^*}{2} \tag{31}$$

Material properties k_i^*, ρ_i^*, and $C_{p_i}^*$ are time-averaged over the two most recent time steps;

$$k_i^* = \frac{3}{2}k_i^n - \frac{1}{2}k_i^{n-1} \tag{32}$$

$$\rho_i^* = \frac{3}{2}\rho_i^n - \frac{1}{2}\rho_i^{n-1} \tag{33}$$

$$C_{p_i}^* = \frac{3}{2}C_{p_i}^n - \frac{1}{2}C_{p_i}^{n-1} \tag{34}$$

Empirical models for material properties as a function of temperature have been developed and incorporated into the model. For the core node ($r = 0$, $i = 1$), the following application of l'Hôpital's rule to treat the singularity at $r = 0$ yields the following finite difference equation [1];

$$k_i^* \frac{2}{\Delta r^2}\left[\frac{3}{4}F_i^{n+1} + \frac{1}{4}F_i^{n-1}\right] = \rho_i^* C_{p_i}^* \frac{T_i^{n+1} - T_i^n}{\Delta t} \tag{35}$$

Where F_i^{n+1} and F_i^{n+1} are as follows;

$$F_i^{n+1} = 2\left(T_{i+1}^{n+1} - T_i^{n+1}\right) \tag{36a}$$
$$F_i^{n-1} = 2\left(T_{i+1}^{n-1} - T_i^{n-1}\right) \tag{36b}$$

For the outer surface node ($r = r_o$, $i = N$), a Taylor series expansion is used to derive a finite difference equation for the energy balance over the fibre boundary, yielding the following in the Dupont-II scheme [1];

$$-\frac{2}{\Delta r}\frac{1}{\Delta r}\left[\frac{3}{4}F_i^{n+1} + \frac{1}{4}F_i^{n-1}\right] + \left(\frac{2}{\Delta r} + \frac{1}{r_i}\right)Q"^* = \rho_i^* C_{p_i}^* \frac{T_i^{n+1} - T_i^n}{\Delta t} \tag{37}$$

Where F_i^{n+1} and F_i^{n+1} are as follows;

$$F_i^{n+1} = k_{i-\frac{1}{2}}^*\left(T_i^{n+1} - T_{i-1}^{n+1}\right) \tag{38a}$$
$$F_i^{n-1} = k_{i-\frac{1}{2}}^*\left(T_i^{n-1} - T_{i-1}^{n-1}\right) \tag{38b}$$

The incident heat flux term is established through an energy balance on the surface;

$$Q"^* = \frac{3}{2}Q"^n - \frac{1}{2}Q"^{n-1} \tag{39}$$

Where;

$$Q"^n = Q"_{sus} - h^n\left(T_N^n - T_\infty\right) \tag{40}$$

The $Q"_{sus}$ term is assumed as constant in this analysis, with its calculation described in Section 1.2. Initiation of the three-time-step model necessitates the use of a two-time step model for time $i = 1$. After the fully implicit two-time-stepping model is used to initialize the three-time-stepping Dupont-II scheme, the Gauss-Seidel procedure is again used to solve the linear algebraic equations simultaneously for $n \geq 2$ (see Equations 18-21). Coefficients are extracted from the finite difference representation of each node as before, however they are listed here for completeness. For interior nodes ($0 < r < r_o$, $1 < i < N$), the coefficients extracted from Equation 28 are as follows;

$$a_{ii} = -\frac{\rho_i^* C_{p_i}^*}{\Delta t} - \frac{\left(3k_{i+\frac{1}{2}}^* r_{i+\frac{1}{2}}\right)/4 + \left(3k_{i-\frac{1}{2}}^* r_{i-\frac{1}{2}}\right)/4}{\Delta r^2 r_i} \tag{41a}$$

$$a_{i(i+1)} = \left(3k_{i+\frac{1}{2}}^* r_{i+\frac{1}{2}}\right)/\left(4\Delta r^2 r_i\right) \tag{41b}$$

$$a_{i(i-1)} = \left(3k_{i-\frac{1}{2}}^* r_{i-\frac{1}{2}}\right)/\left(4\Delta r^2 r_i\right) \tag{41c}$$

$$C_i = \frac{\left(k_{i+\frac{1}{2}}^* r_{i+\frac{1}{2}}\left(T_{i+1}^{n-1} - T_i^{n-1}\right)\right)/4 + \left(k_{i-\frac{1}{2}}^* r_{i-\frac{1}{2}}\left(T_{i-1}^{n-1} - T_i^{n-1}\right)\right)/4}{\Delta r^2 r_i + \frac{T_i^n * \rho_i^* C_{p_i}^*}{\Delta t}} \tag{41d}$$

For the core node ($r = 0$, $i = 1$), the coefficients extracted from Equation 35 are as follows;

$$a_{ii} = \frac{1}{\Delta t} + \frac{3k_i^*}{\left(\Delta r^2 \rho_i^* C_{p_i}^*\right)} \tag{42a}$$

$$a_{i(i+1)} = -\frac{3k_i^*}{\left(\Delta r^2 \rho_i^* C_{p_i}^*\right)} \tag{42b}$$

$$a_{i(i-1)} = 0 \tag{42c}$$

$$C_i = -\left(\frac{-T_i^n}{\Delta t} - \frac{2k_i^*\left(T_{i+1}^{n-1}/2 - T_i^{n-1}/2\right)}{\Delta r^2 \rho_i^* C_{p_i}^*}\right) \tag{42d}$$

For the outer surface node ($r = r_o$, $i = N$), the coefficients extracted from Equation 37 are as follows;

$$a_{ii} = \frac{2\Delta t\, k_{i-\frac{1}{2}}^*}{\left(\Delta r^2 \rho_i^* C_{p_i}^*\right)} + 1 \tag{43a}$$

$$a_{i(i+1)} = 0 \tag{43b}$$

$$a_{i(i-1)} = -\frac{3\Delta t\, k_{i-\frac{1}{2}}^*}{\left(2\Delta r^2 \rho_i^* C_{p_i}^*\right)} \tag{43c}$$

$$C_i = -\left(\frac{\Delta t\, Q"^* \left(2/\Delta r + 1/r_i\right)}{\rho_i^* C_{p_i}^*} - T_i^n - \frac{\Delta t\, T_{i-1}^{n-1} k_{i-\frac{1}{2}}^*}{2\Delta r^2 \rho_i^* C_{p_i}^*}\right) \tag{43d}$$

1.2 Electromagnetic domain

Maxwell's equations constitute a fundamental model for electromagnetism. These equations are generally represented in integral or differential form to describe the electric and magnetic fields in a three-dimensional space. Numerical techniques such as Finite-difference time-domain (FDTD) and Finite element method (FEM) are commonly used to solve Maxwell's equations in electromagnetic problems. In the present model, the $\dot{Q}$ term necessary to resolve the transient temperature field in the PAN fibre is established using a series of analytical expressions that describe peak electric field strength. This simplification is afforded as the location of 'hot spots' in the commercial microwave oven are first identified in the experimental analysis, with the PAN fibre then positioned appropriately. The volumetric heat generation term is calculated from the following;

$$\dot{Q} = \omega \varepsilon_0 \varepsilon'' E_{rms}^2 \tag{44}$$

Where ω is the angular frequency in rad/s ($\omega = 2\pi f$), ε_0 is the permittivity of free space ($8.85 \times 10^{-12}\, C^2/Nm^2$), ε'' is the dielectric loss constant, and E_{rms} is the root mean square value of the electric field intensity in V/m. Assuming a fixed input power of $P = 0.7\, kW$ from the magnetron, the average microwave strength over the cavity cross section is calculated from the following;

$$I_{avg} = \frac{P}{A} \tag{45}$$

Where I_{avg} is the average intensity in W/m^2, and A is the cross sectional area of the cavity ($0.32\, m \times 0.45\, m$). With the intensity established, the peak electric field strength can then be obtained from the following;

$$I_{avg} = \frac{c\varepsilon_0\, E_{max}^2}{2} \tag{46}$$

$$E_{max} = \sqrt{\frac{2I_{avg}}{c\varepsilon_0}} \tag{47}$$

Where c is the speed of light ($2.99 \times 10^8\, m/s$). The root mean square value is obtained using;

$$E_{rms} = \frac{E_{max}}{\sqrt{2}} \tag{48}$$

1.3 Material properties

This section will describe material properties of PAN and CNT susceptor using graphs and polynomial expressions when available

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Nomenclature

Symbol	
a	diagonal coefficients
A	cross sectional area (m^2)
c	speed of light (m/s)
C	remainder coefficient
C_p	specific heat capacity (J/kgK)
E	electric field strength (V/m)
Err	error criteria
f	frequency ($1/s$)
h	heat transfer coefficient (W/m^2k)
I	electric field intensity (W/m^2)
k	thermal conductivity (m)
L	length (m)
P	power (W)
Q"	heat flux (W/m^2)
$\dot{Q}$	heat generation (W/m^3)
r	radial position (m)
t	time (s)
T	temperature (K)
Greek	
α	thermal diffusivity (m^2/s)
Δr	spatial step (m)
Δt	time step (s)
ϵ	emissivity
ε	dielectric loss constant
ε_0	permittivity of free space (C^2/Nm^2)
η	efficiency
σ	Stefan-Boltzmann constant (W/m^2K^4)
ω	angular frequency (rad/s)
Sub / superscript	
$*$	time-averaged index
∞	ambient
avg	average
i	spatial increment
j	neighbouring spatial nodes
k	Gauss-Seidel iteration level
max	maximum
n	temporal increment
N	total discrete spatial nodes
PAN	PAN fibre material
r, ϕ, z	cylindrical coordinates
rms	root mean square
sus	susceptor material