CHAPTER 5

A THEORITICAL MODEL TO PREDICT THE PROPERTIES OF THE REINFORCED CEMENT-BASED MATERIALS WHEN SUBJECTED TO MICROWAVE ENERGY

5.1 Electromagnetic theory

The electromagnetic (microwave) fields include electric and magnetic fields that move simultaneously with each other through space. This movement can be represented simplifically by plane waves, as in Fig. 5.1. The relationship between time-varying electric and magnetic fields can be described macroscopically by using Maxwell's equations. The important observations are (a) the displacement current density is simply the rate at which the electric flux density $\bar{D}$ varies with time, (b) a time-varying electric field creates a time-varying magnetic field due to the action of $(\partial\bar{D}/\partial t)$ as a source of the magnetic field, and (c) the time-varying magnetic and electric fields are interdependent. With the help of boundary characteristics, the propagation conditions of plane waves are assumed to be as follows: (a) the component of the field quantities $\bar{E}$ and $\bar{H}$ lying in the transverse plane, a plane perpendicular to the direction of the propagation of the wave; and (b) the amplitude attenuation of the wave is reduced by the familiar factor of e^{-1} (0.368) in a dielectric medium (a type of material, such as concrete, brick, or paper, that can absorb microwave energy and then can be converted partially into other form of energy) by means of creating ion oscillations and continuing dipole relaxation.

The electromagnetic (microwave) waves propagate in free space at the speed of light ($c = 2.9979x10^8\ m/s$). Further information on the form of these waves can be obtained by noting that the $\bar{E}$ - and $\bar{B}$ - fields must also satisfy Maxwell's equations. To consider a specific type of wave, although the results derived are general: This wave is said to be an unbounded plane indicating that there are existing planes (or wave fronts) perpendicular to the direction of propagation, over which all quantities of the wave are constant, as shown in the plain wave in Fig. 5.1.

One of the major achievements of Maxwell's equations is their ability to correctly predict electromagnetic waves from considerations of the compacted forms of the four equations. The equations' validity is based on their consistency with all the existing experiments concerning electromagnetic phenomena. The physical meanings of these equations are listed identically in identical differential forms below:

(a) Gauss's law is a mathematical expression of the experimental fact that electric charges repel or attract one another with a force proportionally inverse to the square of the right distance between them (Eq.(5.1)):

$$\nabla.\vec{D} = q \tag{5.1}$$

(b) Faraday's law is based on time-varying the magnetic flux inducement of electromotive force (Eq.(5.2)):

$$\nabla x\vec{E} = -\frac{\partial \vec{B}}{\partial t} \tag{5.2}$$

(c) Ampère's law states that the line integral of the magnetic field over any close contour must equal the total current enclosed by that contour (Eq. (5.3))

$$\nabla x\vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t} \tag{5.3}$$

(d) The last of Maxwell's four equations relies on the fact that there are no magnetic charges or magnetic monopoles and that magnetic field lines always close on themselves (Eq.(5.4)):

$$\nabla.\vec{B} = 0 \tag{5.4}$$

where $\vec{E}$ is the electric field intensity (V/m), $\vec{H}$ is the magnetic field intensity (A/m), $\vec{D}$ is the electric flux density (C/m), $\vec{B}$ is the magnetic flux density (Wb/m^2), t is the time, and q is the electric charge density (C/m^3).

The constitutive relations that relate $\vec{H}$ and $\vec{B}$, $\vec{E}$ and $\vec{D}$, and $\vec{E}$ and $\vec{J}$ are shown in Eqs.(5.5) – (5.7) respectively. Then, substituting (Eq.(5.5) – (5.7)) into (Eqs.(5.1) – (5.4)) results in (Eqs.(5.8) – (5.10):

$$\bar{B} = \mu \bar{H} \tag{5.5}$$

$$\bar{D} = \varepsilon \bar{E} \tag{5.6}$$

$$\bar{J} = \sigma \bar{E} \tag{5.7}$$

where μ is the magnetic permeability (H/m), σ is the electric conductivity (1/Ohm), and ε is the dielectric constant (F/m).

$$\nabla . \bar{E} = \frac{q}{\varepsilon} \tag{5.8}$$

$$\nabla x \bar{E} = -\mu \frac{\partial \bar{H}}{\partial t} \tag{5.9}$$

$$\nabla x \bar{H} = \sigma \bar{E} + \varepsilon \frac{\partial \bar{E}}{\partial t} \tag{5.10}$$

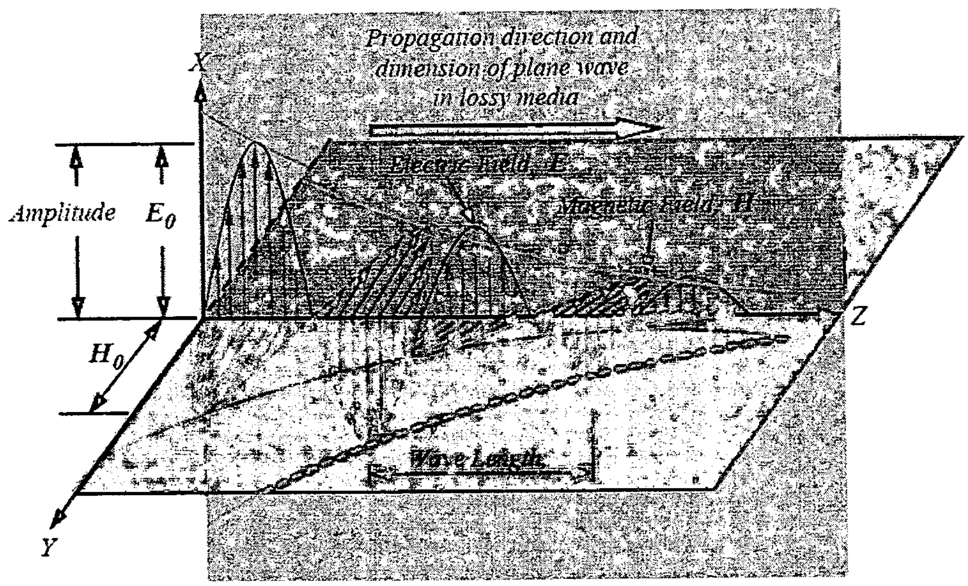

Fig. 5.1 Electromagnetic wave propagation.

5.2 Numerical analysis

Our research concept is to use microwave energy to improve the quality of concrete [61,62,63]. Microwave energy generates heat within a material through rapid changes in polarization as indicated in Equation (5.11) (Rattanadecho P., [27]).

$$Q=\sigma\left|\bar{E}\right|^2=2\pi f\varepsilon_0\varepsilon_r'\left(tan\sigma\right)E^2 \quad (5.11)$$

where Q is the microwave energy, σ is the effective conductivity, f is the frequency (Hz), ε_0 is the permittivity of free space (8.8514×10^{-12} farads/meter), ε_r' is the relative dielectric constant, $tan\ \delta$ is the loss tangent coefficient, and $\bar{E}$ is the electric field intensity (volts/meter).

Equation (5.11) describes the relationship between the intensity of the electric field, the microwave frequency, and the dielectric properties of the material and their effect on volumetric heat generation. Another factor is the penetration depth (*Dp*), which is the depth to which the radiation penetrates the material and still retains 37% (*1/e*) of the energy at the surface, calculated using Equation (5.12) and figure 5.2 (Rattanadecho, [46]). If the penetration depth is less than the thickness of the material, resonance phenomena occur and the electric field distribution does not conform to Lambert's law, resulting in local increases in the intensity of the electromagnetic field.

Equation (5.12) is applicable to materials that are sufficiently thick to be considered infinite. Microwaves rapidly generate heat through the large fields developed in a standing wave created by the forward propagating waves and the waves reflected from the air-solid interface. When such a phenomenon occurs, it can not use these rules to predict wave reflection, so the variation in small pieces to use Maxwell's equations into the analysis (Rattanadecho et al. [46]. The distribution of temperature, velocity and absorbability of microwave energy are described. It's however not considered to be porous material.

$$D_p=\frac{1}{\frac{2\pi f}{\upsilon}\sqrt{\frac{\varepsilon_r'\left(\sqrt{1+\left(\tan\delta\right)^2}-1\right)}{2}}} \quad (5.12)$$

where D_p is the penetration depth, ε_r'' is the relative dielectric loss factor, and υ is the microwave propagation velocity in the dielectric material determined from the relation $c/\sqrt{\varepsilon_r'}$.

5.2.1 Analysis of dielectric properties

The dielectric properties can be represented in Table 5.1.

Table 5.1 Dielectric permittivity of 1CW/S_0.38 paste.

Water-to-solid ratio (w/s) = 0.38		
Time after mixing (at hours)	ε'	ε''
0	15.1288	4.8219
0.5	**15.0861**	**4.4458**
1	14.8792	4.2154
3	14.5707	4.1633
6	12.4870	3.2410
9	5.6590	0.9733
12	4.4850	0.4793
15	3.7910	0.5140
18	3.1623	0.3777
21	4.0093	0.5853
24	4.2740	0.7100

5.2.2 Analysis of heating problem: Conduction mode of heat transfer

A schematic diagram of the physical model is shown in Fig. 5.2. The temperature of the material introduced to the incident wave is obtained by solving the conventional heat transport equation with the microwave power included as a local electromagnetic heat-generation term.

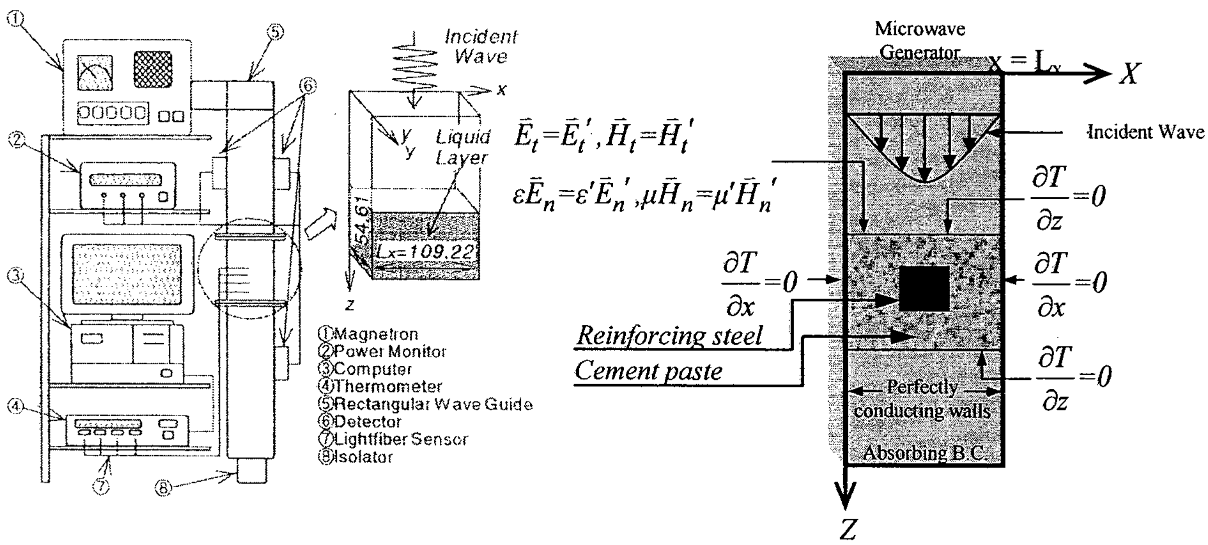

Fig 5.2 The distribution of microwave radiation in the XZ plane.

5.2.2.1 Assumptions

The materials considered were cement pastes at a w/s equal to 0.38, which consist of Portland cement Type I, water, and air. They are, therefore, homogeneous and isotropic in terms of structure. In order to analyze the process of heat transport due to microwave heating of dielectric materials, the following assumptions were made:

- The local thermodynamic equilibrium is achieved.
- The liquid phase is not compressible $\rho_l = constant$.
- No chemical reactions within the material are taken into account.
- Radiation modes are negligible.
- The effect of the natural and induced convections can be neglected.
- In this task, from a macro-level point of view, the pore structure within the microwave-cured paste is assumed to be homogeneous and isotropic. Therefore, a heating model for a homogeneous and isotropic is used in this analysis.

5.2.2.2 Basic equations

The governing equations describing the temperature rise in the paste to be processed by microwave energy are:

Electromagnetic wave:

$$\nabla \times \left(\mu_r^{-1} \nabla \times \vec{E} \right) - k_0^2 \left(\varepsilon_r - j \frac{\sigma}{\omega \varepsilon_0} \right) \vec{E} = 0, \varepsilon_r = n^2 \tag{5.13}$$

Heat transfer (conduction mode):

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \times \left(-k \nabla T \right) = Q \tag{5.14}$$

where μ_r is the relative permeability, $\vec{E}$ is the electric field intensity (volts per metre (V m^{-1})), k_0 is the free space wave number, ε_r is the relative permittivity, σ is the electric conductivity (siemens per metre (S·m^{-1})), ω is the angular frequency (radians per second), and n^2 is the relative permittivity.

k is the thermal conductivity (W/(m·K)), T is the absolute temperature (K), Q contains heat sources other than viscous heating (W/m^3), ρ is the density (kg/m^3), and Cp is the specific heat capacity at constant pressure (J/(kg·K)).

5.2.2.3 Boundary conditions

(a) Adiabatic boundary condition

Assuming that the surroundings of the paste are insulated (no heat and moisture transfer between the system and surroundings):

$$\left.\frac{\partial T}{\partial n}\right|_{sample\,surface} = \left.\frac{\partial T}{\partial t}\right|_{sample\,surface} = 0 \tag{5.15}$$

(b) Continuity boundary condition

For the microwave heating of the cement paste, the temperature and heat flux at the interface of sample and air within the microwave cavity to be continuity:

$$T = T', \quad \lambda_{eff}\left.\frac{\partial T}{\partial n}\right|_{boundary} = \lambda'_{eff}\left.\frac{\partial T}{\partial n}\right|_{boundary} \tag{5.16}$$

(c) Electromagnetic boundary condition

$$n \times \vec{E} = 0 \tag{5.17}$$

where n is the normal vector.

(d) The initial condition of the microwave-cured cement reinforced paste sample defined as:

$$T = T_0 = 298.15K \quad at\ t = 0 \tag{5.18}$$

5.2.2.4 Numerical solution program

The COMSOL Multiphysics is excellent, state-of-the-art software for the solution of many types of partial differential equations (PDEs), both stationary and time-dependent, by numerical techniques based on the finite element method for the spatial discretization. It also provides step-by-step instructions regarding how to solve a simple PDE using the COMSOL Multiphysics' graphical user interface (GUI). This example should be useful to get an initial idea regarding how COMSOL's GUI works, and it can also be used by users (or system administrators) to test whether a given installation of COMSOL works properly. Radio

Frequency (RF) Module 3.4 is an optional package that extends the COMSOL Multiphysics® modeling environment with customized user interfaces and functionality optimized for the analysis of electromagnetic waves. Like all modules in the COMSOL Multiphysics family, it provides a library of prewritten ready-to-run models that make it quicker and easier to analyze discipline-specific problems. This particular module solves problems in the general field of electromagnetic waves, such as RF and microwave applications, optics, and photonics. The application modes (modeling interfaces) included here are fully multiphysics enabled, making it possible to couple them to any other physics application mode in COMSOL Multiphysics or the other modules.

The RF Module contains a set of application modes adapted to a broad category of electromagnetic simulations. Those who are not familiar with computational techniques but have a solid background in electromagnetics should find this module extremely beneficial. It can serve equally well as an excellent tool for educational purposes. Because the RF Module is smoothly integrated with all the COMSOL Multiphysics functionality, a simulation in this module can be coupled with an arbitrary simulation defined in any of the COMSOL Multiphysics application modes. This forms a powerful multiphysics model that solves all the equations simultaneously.

A guide to the COMSOL setting for this problem is shown in Fig. 5.3. By using 3D Electro-Thermal Interaction mode, Fig. 5.3, this mode predefines combinations of application modes and couplings for electro-thermal interaction.

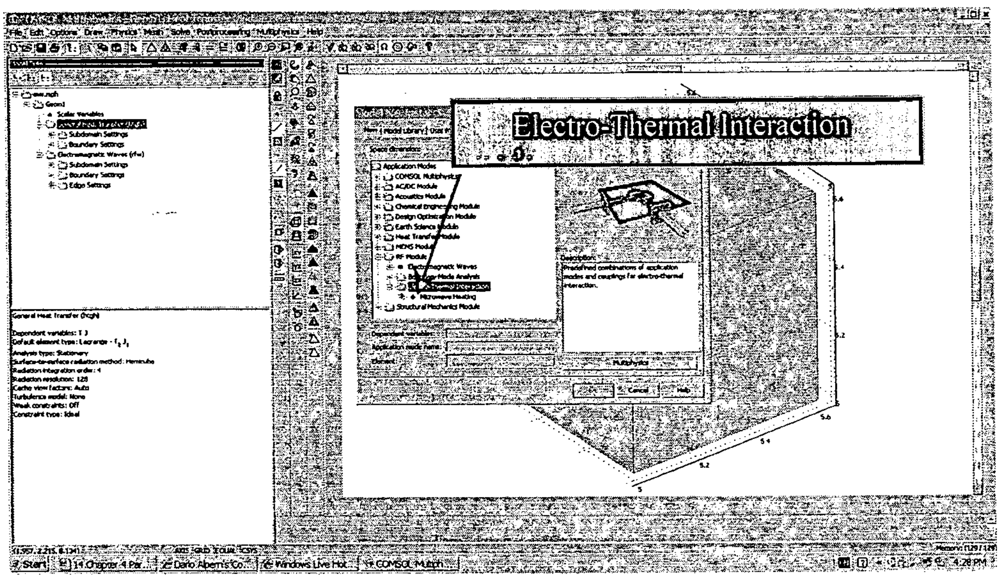

Fig. 5.3 Mode predefines combinations of application modes and couplings for electro-thermal interaction.

5.2.2.5 Parameters used to calculate

The parameters used in this calculation are shown in the Table 5.2.

Table 5.2 Variables used for calculation.

Variables	Values	Unit	Remark
Scalar			
Sigma_htgh (Stefan-Boltmann constant)	5.67e-0.08	$W.m^{-2}.deg^{-4}$	Data bases
Rg_htgh (Universal gas constant)	8.31451	$J.mol^{-1}.K^{-1}$	Data bases
Epsilon0_rfw (Permittivity of vacuum)	8.854187817e-12	$F.m^{-1}$	Data bases
Nu_rfw (Frequency)	2.45e9	Hz	Data bases
General Heat Transfer (htgh)			
Subdomains: air, 1 atm			
k (isotropic)	0.0257	$W.m^{-1}.K^{-1}$	Data bases
ρ (density)	1.205	$kg.\ m^{-3}$	Data bases
C_p (heat capacity at constant pressure)	1.005	$J.kg^{-1}.K^{-1}$	Data bases
$T(t_0)$ Initial temperature	293.15	K	Test result
k (isotropic)	155	$W.m^{-1}.K^{-1}$	Data bases
ρ (density)	2730	$kg.\ m^{-3}$	Data bases
C_p (heat capacity at constant pressure)	893	$J.kg^{-1}.K^{-1}$	Data bases
$T(t_0)$ Initial temperature	293.15	K	Test result
Subdomains: Cement paste			
k (isotropic)	1.005-0.0025×T	$W.m^{-1}.K^{-1}$	Kim, 2003
ρ (density)	1915	$kg.\ m^{-3}$	Test result
C_p (heat capacity at constant pressure)	$0.75+3.43\times M_f^{water}$ $M_f^{water} = 0.38/1.38$	$J.kg^{-1}.K^{-1}$	Hansen, 1982
Q (heat source)	421.0559	$W.m^{-3}$	Test result
$T(t_0)$ Initial temperature	295.35	K	Test result
Boundary condition			
$T = T_0$	298.15	K	Test result
Electromagnetic Wave (rfw)			
Subdomains: air, 1 atm			
n (refractive index)	1.0008		Data bases
Subdomains: Aluminium 3003-H18			Data bases
relative permittivity	1		Data bases
electrical conductivity	2.326e7	$S.m^{-1}$	Data bases
Relative permeability	1		Data bases
Subdomains: Cement paste			Data bases
relative permittivity	15.0861-*j**4.4458		At 30 min delay time
electrical conductivity	1.042	$S.m^{-1}$	Test result
Relative permeability	1		Data bases

Table 5.2 (Cont.) Variables used for calculation.

Variables	Values	Unit	Remark
Subdomains: Aluminium 3003-H18			Data bases
Boundary condition			
Subdomains: air, 1 atm	Perfect electric conductivity		
Subdomains: Aluminium 3003-H18	Continuity		
Subdomains: Cement paste	Port, Power 390	watt	
Finite element			
Number of subdomains	7		
Depent variavles	Temperature (T)		
Mesh consists of elements.	84258	elements	
Analysis type of heat transfer	Transient		
Tolerance	0.01		
Transient duration	10, 20, and 30	minutes	
Sample	Cement paste		at w/s = 0.38

5.2.3 Results and discussion

Based on the transient analysis (a microwave-cured sample's temperature-change rate is proportional to the difference between its own temperature and the temperature of its surroundings in the microwave cavity); the calculated temperature of the 1CW/S_P0.38 paste under microwave times of 10, 20 and 30 minutes. It illustrates an increase of maximum temperature within the samples as the microwave application times increase, such that temperatures of 61.27, 83.14, and 95.26 ^{0}C were reached at times of 10, 20, and 30 minutes, respectively. In addition, the points at which maximum and minimum temperatures occur are in the middle of the sample and at the edge of an inlet waveguide. The maximum temperature point arises from the interaction between microwave energy and cement paste; the heat generated by the microwave energy works in conjunction with the heat generated by the hydration of the cement, so that at the center the accumulation is high and very little heat dissipates.

The predictions and experimental data of the maximum temperature history within the 1CW/S_0.38 paste when microwave power of 100 watt is applied for up to 30 minutes are compared in Fig. 5.4. The result shows that the prediction data are higher than those of the experimental data. This is mainly due to the fact that the parameter used in this calculation, especially the permittivity value, is kept constant at $\varepsilon_r^* = 15.0861 - \bar{j}4.4458$, while in the real state this value decreases continuously as free water content decreases. That is, free water content is consumed and then transformed to fixed water (Taylor, 1997); as a result, microwave radiation can interact with cement paste and generate a low amount of heat [4,5]. As well as the dielectric value, the heat transfer values also changes according to how long microwave energy is applied and the formation of hydration products decreases heat transfer with time also. Furthermore, it can be seen that heat generation takes place when the free water can move from the center to another location within the paste; therefore, at the middle point, the temperature is then dropped.

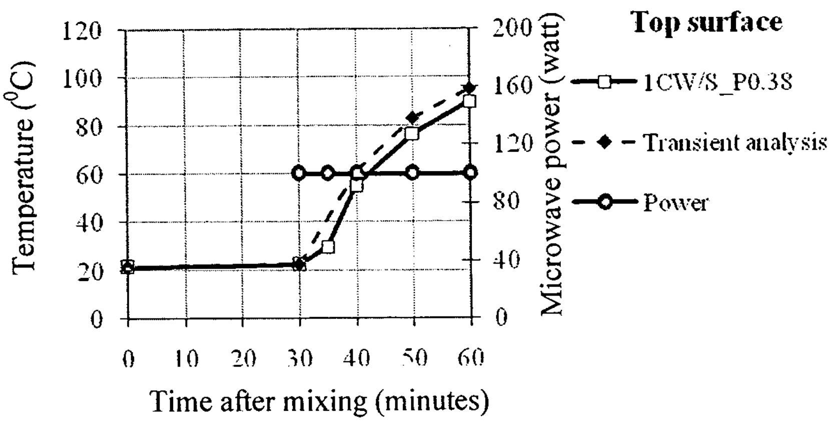

Fig 5.4 Temperature history of the 1CW/S_0.38 paste when applying microwave power 100 watt on a period of 30 minutes.

5.3 Conclusion

In order to predict temperature rise during curing by microwave energy, the model explored the interaction between the microwave (electromagnetic field) and cement paste, the heat dissipation (conduction mode) model by using the Multiphysics Modeling and Simulation: COMSOL. The results showed that the simple model associated with assumptions, and initial and boundary conditions can predict temperature rise higher than those of the experimental data.