FDTD analysis to simulate interaction between microwave and chemical reaction

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ABSTRACT

By coupling Maxwell's equations, Fourier equation of heat conduction and chemical reaction together, FDTD method was used to simulate a simplified chemical reaction model under microwave irradiation. Chemical reaction process, temperature distribution and electromagnetic characters of the system can be obtained. This is useful for microwave chemistry applications.

In microwave chemistry and its applications, it is very useful to know the temperature inside the chemical reaction system and microwave reflection of the reaction system. This can not only keep some thermal sensitive products from overheating, but also control the system reflection under the safe standard to the microwave source. So before applying into a real system some tentative numerical simulations are helpful.

A simplified liquid phase chemical reaction is chosen for numerical simulation. In the simulation system, one test tube of 1cm diameter is put in the central of the BJ220 waveguide broadside to accept the microwave irradiation. Microwave frequency is 2450MHz and the amplitude is 10^3V/m. It is well known that in the chemical reaction system the concentration of reactants are time varying, and most of the reactants are dispersing medium. Therefor, $(FD)^2TD$ analysis is chosen to obtain the interaction between chemical reaction system and microwave irradiation.

A chemical reaction A+B→D+E in hydrosolvent, which is supposed to be an Arrhenius type primitive reaction, is carried in a test tube. Reactant A, B, D, and E are with different dielectric constant and conductivity. During reaction, the system dielectric constant and conductivity are time varying. (See Table I) $x(t)$ is the concentration of the product, and c is the initial concentration.

Table I

Concentration		x_A	x_B	x_D	x_E
Time	0	c	c	0	0
	t	c-$x(t)$	c-$x(t)$	$x(t)$	$x(t)$
	∞	0	0	c	c

Each reactant concentration, reaction speed and its thermal relation all can be calculated. Eq. 1 shows the chemical reaction speed calculated from Arrhenius equation.

$$v(t) = k(t)\cdot(c - x(t))^2 = Ae^{-\frac{E_a}{RT}}\cdot(c - x(t))^2 \qquad (1)$$

In each FDTD cell, Osager equation is applied to get the mixed material dielectric constant, which is used in the FDTD calculation formula, while the mixed conductivity can be got from the concentration of each component. The effective dielectric constant is calculated by

$$\varepsilon_{eff} = \varepsilon_{mix} + \sum_{A,B,D,E} \frac{3(\varepsilon_i - \varepsilon_{mix}) \cdot \varepsilon_{eff}}{2\varepsilon_{eff} + \varepsilon_i} \cdot x_i \qquad (2)$$

At the same time, microwave-heating effect is calculated to get the heat absorbed by the reaction system. The steady-state equation of dissipated power is

$$\overline{P_d(\omega)} = \frac{1}{2}\varepsilon_0 \omega \varepsilon''(\omega) \left|\vec{E}\right|^2 \qquad (3)$$

Since the dielectric constant is the time-domain evolution, the dissipated power should be directly calculated form the Poynting equation. It is as Eq. 4 instead of Eq. 3.

$$P = \frac{1}{2}(\vec{E} \cdot \frac{\partial \vec{D}}{\partial t} - \vec{D} \cdot \frac{\partial \vec{E}}{\partial t}) + \sigma \vec{E} \cdot \vec{E} \qquad (4)$$

Then 3-D heat transport equation (HTE) is used to obtain the temperature distribution and evolution in the chemical reaction system.

$$\rho_m C_m \frac{\partial T(x,y,z,t)}{\partial t} = k_t \nabla^2 T(x,y,z,t) + P_d(x,y,z,t) \qquad (5)$$

Thermal isolation boundary condition is applied to the top and bottom surfaces of the test tube, and convection thermal boundary condition is adopted for the other side. This HTE can be solved using explicit deference scheme in the same FDTD grid.

The chemical reaction time and heat transport are always over seconds or minutes, while the FDTD time step is less than 0.1 nanosecond for microwave of frequency 2450MHz. This means that more than 10^{11} FDTD time steps have to be calculated to meet the requirement of chemical reaction. The task is so huge that it can be done only by a workstation in several days. However by using different time scale between FDTD and chemical reaction, only 10^3 to 10^4 steps are necessary to calculate. This method has been proved sensible to calculate some heat transport process in temperature dependent material. Therefor, using this method is more efficient, and makes a general Personal Computer (PC) possible to solve this problem. The time proportion between FDTD and heating is

$$T_{FDTD} = T_{heat} / \alpha \qquad (6)$$

Then the HTE can be written to

$$\frac{\partial T}{\partial \frac{t}{\alpha}} = \frac{\alpha k_t}{\rho_m C_m}\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right) + \frac{\alpha P_d}{\rho_m C_m} \qquad (7)$$

The explicit difference form of Eq. 7 is

$$\begin{aligned} T^{n+1}(i,j,k) = T^n(i,j,k) + \Delta t \frac{\alpha k_t}{\rho_m C_m \Delta S^2}[T^n(i+1,j,k) + T^n(i-1,j,k) \\ + T^n(i,j+1,k) + T^n(i,j-1,k) + T^n(i,j,k+1) \\ + T^n(i,j,k-1) - 6T^n(i,j,k)] + \Delta t \frac{\alpha P_d^n(i,j,k)}{\rho_m C_m} \end{aligned} \qquad (8)$$

In the waveguide, the test tube is very small compare to the waveguide. To consider the chemical reaction and thermal distribution in the test tube 1mm grid has to be chosen. Because the test tube only occupied a small space, subgrid is used to improve the calculation efficiency. In this case 1:3 subgrid is chosen. For this method, traveling wave equation is used to get the connection boundary condition between fine grid and coarse grid. On the top and bottom surfaces of the test tube, symmetry condition is used to get the boundary connection value.

On the two sides surfaces of the waveguide in the scatting field region, absorb boundary condition is use. Since absorb boundary is chosen to be far away from the test tube, only the principal mode can be transferred here. So the first order absorb boundary condition can be used well.

During the chemical reaction and the microwave

heating, temperature of the reaction system will increase enormously. To make temperature dependent medium into consideration, first order Debye equation of dielectric constant and temperature relation is adopted in the $(FD)^2TD$ calculation.

$$\varepsilon^*(\omega) = \varepsilon_0(\varepsilon_r + \frac{\sigma}{j\omega\varepsilon_0} + \frac{\varepsilon_s - \varepsilon_r}{1 + j\omega\tau}) \qquad (9)$$

Here relaxation constant $\tau = \tau_0 exp(Wa/kT)$, Wa is the viscous resistance related energy.

For some given parameters, simulation was performed to get the temperature distribution and temperature time varying. A system shown as Fig. 1 has been simulated. BJ22 waveguide (a=109.2mm , b=54.6mm) is used. The frequency of input microwave is 2450 MHz with power 32.74W (amplitude 103 V/m). The radius of test tube is 5 mm. In the coarse grid, ΔS=3.64 mm, $\Delta t = 5.027\times10^{-12}$ s, while in the fine grid it is only one third of them. Time proportion $\alpha = 5\times10^{10}$

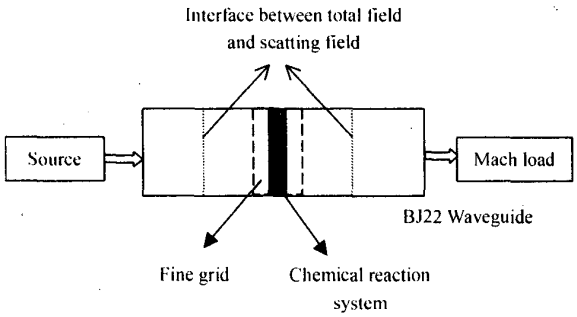

Fig. 1 Microwave chemical experimental system

Then for a given chemical reaction, the simulation can be performed. Fig. 2 shows the microwave reflection variation of a chemical reaction in the test tube. Fig. 3 shows the temperature distribution of a cross section of the tube. On the other hand, system reflection and electromagnetic distribution can be obtained simultaneously. We find that the temperature

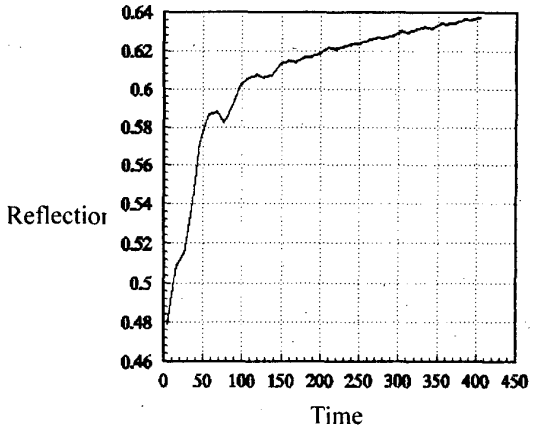

Fig. 2 Reflection variation due to dielectric constant change with chemical reaction

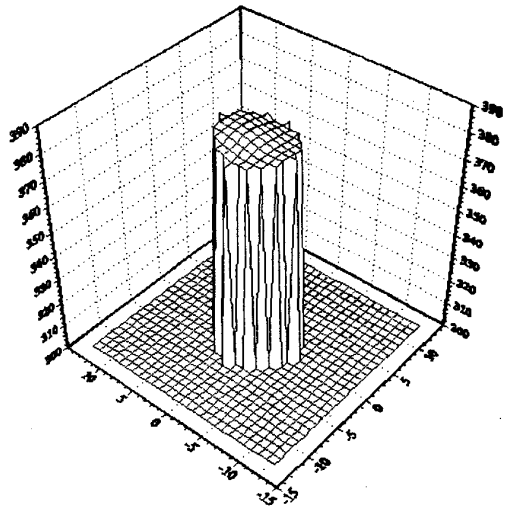

Fig. 3 Temperature distribution on a cross section of the test tube

rising is nonlinear with a nonlinear microwave reflection. Moreover, the temperature distribution in the tube is not uniform. Some rapid changes of the microwave reflection are found. Therefor, in the future application system, these effects should be considered.

In this method, it is the first step of using FDTD method to simulate the interaction between chemical reaction system and microwave. Some processes, such as the material transfer due to the concentration gradient, has not been taken into consideration, and the chemical reaction model is quite simple. So there is a long way to go to match simulation results with real experimental system data.

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