The Application of the Huang Method in the Analysis of Microwave Heating

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In this paper, acetone iodation was carried out and the Huang method based on experimental results was employed to calculate the effective permittivity of acetone iodation system as a function of temperature and reaction time. The coupled electromagnetic field equations, reaction kinetics equations, and heat transport equation were solved to simulate the microwave heating on chemical reaction. Here, the finite difference time domain (FDTD) method was used. Finally, the calculated results were compared with the measured results to verify this calculation. This method offers high potential applications in the explanation of some specific phenomena in the microwave heating on chemical reactions and instructs the design of microwave chemistry reactor.

Most chemical reactions are sensitive to temperature; therefore, using microwaves to heat reactants presents an impressive application prospect.[1] Unfortunately, some difficulties arise in the application of high-power microwaves in chemistry.[2,3] Obviously, it is necessary to develop some methods in this challenging field to simulate microwave heating on chemical reactions. Nowadays, a number of numerical approaches have been used to study microwave heating,[4–7] but most of the traditional numerical simulations of microwave heating are limited to use of coupled electromagnetic and thermal equations. Only a few methods have been used to simulate microwave heating in chemical reactions to instruct the design of microwave chemistry reactors and give reasonable explanations for the specific effects of microwaves in chemical reactions.[8,9] For the microwave heating on chemical reactions, the main difficulty is that the effective permittivity of the reactantion system changes with not only temperature but also reaction time. The most important previous work in simulation is to obtain the effective permittivity of chemical reaction system as a function of temperature and reaction time. In this paper, the Huang method[10] based on experimental results was employed to calculate the effective permittivity of acetone iodation reaction system as a function of temperature and reaction time. Meanwhile, coupled electromagnetic field equations, reaction kinetics equations, and heat transport equation have been used to study the microwave heating of chemical reactions for the first time. Here, FDTD method was employed. To verify this method, the temperature rising inside the acetone iodation reaction system under microwave irradiation was measured with an optical fiber thermometer. The calculated results were compared with the measured results. Good agreement can be seen between the measured and calculated results. This method offers high potential applications in the explanation of some specific phenomena in the microwave heating of chemical reaction systems and instructs the design of microwave chemistry reactors.

Generally, the effective permittivity of reactants changes with not only temperature but also reaction time. In the simulation of microwave heating on chemical reactions, we have to know the effective permittivity as a function of temperature and reaction time. Huang proposed a method based on experimental results to calculate the effective permittivity of chemical reaction systems as a function of temperature and reaction time.[10]

In this paper, acetone iodation was carried out because it is a carefully studied chemical reaction and because significant change of effective permittivity can be observed. The reaction was carried out at four constant temperatures of 30, 37, 44, and 52 °C, respectively. By using the Huang method, the permittivity of a mixture during the acetone iodation reaction at 915 MHz can be obtained.

We used a Banpo-1 solid-state source to generate power, the frequency stability is up to 10^{-8}. The maximum output power of the generator is 100 W. In order to avoid very fast temperature rise and convection of the solution, less than 5-W power was used. The measurement was performed at 915 MHz. A coaxial probe was inserted in the solution and used to heat the reaction system. A power meter with two channels was used to measure the input and reflected power. A UMI-8 optical fiber thermometer with diameter of 1 mm was employed to measure the temperature near the top of the coaxial probe. A PC was used to record the rising temperature. It should be noted that the height and diameter of the beaker must be larger than two wavelengths of microwave in the solution to avoid the influence of microwave reflection from the wall of the beaker and air–solution interface. Generally, the reflection decays rapidly owing to the lossy solution. The experimental system is shown in Figure 1.

According to the experiment conditions, a numerical model used to calculate the rising temperature in the acetone iodation system is shown in Figure 2.

In the model, the optical fiber is considered. In the calculation presented in the following section, the diameters of the inner and outer conductor of the coaxial line are taken to be $D4 = 3.04$, $D2 = 9.8$, and $D3 = 16$ mm. The diameter of the extended inner conductor is assumed to be $D1 = 1$ mm. The height and diameter of the calculation domain are $H = 210$ and $D = 140$ mm.

Figure 1. The experimental system.

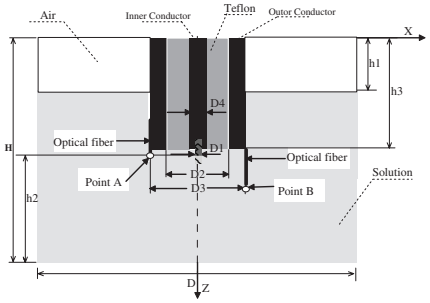


Figure 2. The numerical model to simulate the microwave heating in acetone iodation system.

The heights of $h1$, $h2$, and $h3$ are 50, 109, and 100 mm, respectively. Two optical fibers were employed to measure the rising temperature. One was placed at point A (−8 mm, 101 mm); another was placed at point B (8 mm, 111 mm). The coupled electromagnetic field equations, reaction kinetics equations, and heat transport equation were solved to simulate the microwave heating on the chemical reaction by FDTD.[9] The electromagnetic fields in reactant satisfy Maxwell's equations as follows:

$$-\frac{\mathrm{d}C_{\mathrm{CH_3COCH_3}}}{\mathrm{d}t} = K_{\mathrm{rate}} \times C_{\mathrm{CH_3COCH_3}} \times C_{\mathrm{H^+}} \quad (1)$$

The heat transport equation is given by

$$\begin{aligned} \nabla \times \vec{H} &= \frac{\partial \vec{D}}{\partial t} + \sigma(t)\vec{E} \\ \nabla \times \vec{E} &= -\frac{\partial \vec{B}}{\partial t} \\ \nabla \cdot \vec{D} &= \rho \\ \nabla \cdot \vec{B} &= 0 \end{aligned} \quad (2)$$

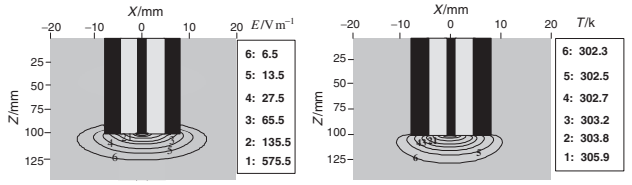
where $P_{\mathrm{e}}(\vec{r},t)$ is the releasing power per unit volume produced by the reaction, $P_{\mathrm{d}}(\vec{r},t)$ is the electromagnetic power dissipated per unit volume, ρ_{m} is the medium density, C_{m} is the specific heat of the medium, k_{t} is thermal conductivity of the medium. The thermal properties of the medium in the model can be found in published reference.[11] The reaction kinetics equation can be given by

$$\rho_{\mathrm{m}} C_{\mathrm{m}} \frac{\partial T(\vec{r},t)}{\partial t} = k_{\mathrm{t}} \nabla^2 T(\vec{r},t) + P_{\mathrm{d}}(\vec{r},t) + P_{\mathrm{e}}(\vec{r},t) \quad (3)$$

where the concentration of acetone is $C_{\mathrm{CH_3COCH_3}}$, the concentration of pH indicator is $C_{\mathrm{H^+}}$, K_{rate} is the rate constant of acetone iodation reaction.

By simulation, we have obtained the distribution of electric field and temperature after 10 s with 0.3-W absorbing power. The results are shown in Figure 3.

By experiment, we measured the rising temperature at point A and B in Figure 2. The measured results are compared with the calculated results with 0.3-W absorbing power. The comparisons are shown in Figure 4.



(a) Distribution of electric field (b) Distribution of temperature

Figure 3. The electric field and temperature distribution after 10 s with 0.3-W absorbing power.

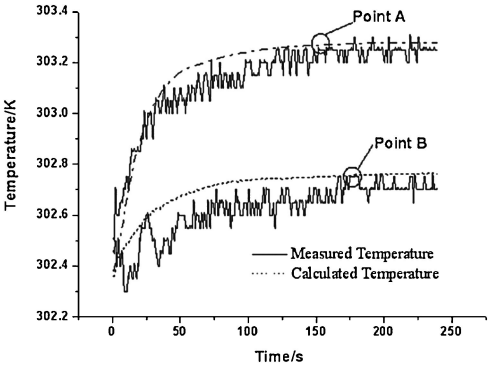


Figure 4. Temperature rising at point A and B.

From Figure 4, good agreement can be seen between the measured and calculated results. It verifies the feasibility of the method. This method offers high potential applications in the explanation of some specific phenomena in the microwave heating of chemical reaction systems and instructs the design of microwave chemistry reactors.

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