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Influence of Vessel Configuration and Size of Vessel Wall Based on the Numerical Analysis of Polar Solvent Heated by Microwave

J. SHU[1], X.Q. YANG[1,*], K.M. HUANG[1], G.Z. JIA[2], K. LI[1] and J.L. ZHANG[1]

[1]College of Electronics and Information Engineering, Sichuan University, Chengdu 610065, P.R. China
[2]Sichuan Normal University, Chengdu 610068, P.R. China

*Corresponding author: Fax: +86 28 85408779; Tel: +86 28 85408779; E-mail: yyxxqq_mail@163.com; sdill2005@126.com

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The choice of vessel is vital for heating polar solvent. In this paper, water at silicon carbide or glass vessel with three different configurations and size of vessel wall were heated by microwave. The uniformities of temperature were analyzed using COMSOL Multiphysics under different configurations and size of vessel wall during microwave heating. It was concluded that the temperature uniformities were influenced by the parameters of different configurations and size of vessel wall, when the improvement in temperature uniformity is not obvious for one configuration, it can be significantly improved by changing to another specific configuration and size of vessel wall.

Key Words: Microwave heating, Polar solvent, Temperature uniformity, Multiphysics.

INTRODUCTION

In the early 1980's, microwaves were proposed to be used for accelerating chemical reactions by their efficient heating of some reactants. Many recent reports indicated that microwave could evidently accelerate reactions, and the rate enhancement factor could reach over one thousand. Most chemical reactions are sensitive to temperature, therefore using microwaves to heat reactants presents an impressive application prospect[1,2]. At present, in the reactions assisted and catalyzed, the majority of reaction solvents are polar in order that they are heated preferably.

During heating reactions, it might cause heterogeneous temperature distribution in chemical syntheses. Thus, it is necessary to analyze some parameters influencing temperature uniformities using numerical calculation.

Due to the high microwave absorptivity, with regard to SiC, materials (*i.e.* a solvent or a reaction mixture) contained inside the container will be effectively shielded from the electromagnetic field[3]. The heat flow through the walls of the reaction vessel and subsequent heat exchange with the reaction mixture contained inside is exceptionally fast based on high thermal conductivity and diffusibility of silicon carbide[4].

Water is a typical polar solvent and glass is a main vessel widely used in synthetic chemistry research. This paper therefore focused on the heating of water in silicon carbide or glass container with different constructions and size. The uniformity of temperature is investigated during heating. The study will provide further assists and references for the system of microwave promoting polar solvent reaction.

Besides, there is a vital problem for microwave heating that the dielectric heating process represents a coupled electrothermal problem. According to the classification made by Kumbhar and Kulkarni[5] the coupling of electromagnetic and thermal fields is week, due to the large difference in the time constants of the two problems. Thus it is necessary to consider the two problems which are the results of the electric field analysis allowing the determination of the source term for the heat diffusion equation and the analysis of the temperature distribution in the load enabling a re-evaluation of the physical constants (permittivity, loss angle, *etc.*), which in turn will modify the electric field distribution[6]. COMSOL can solve effectively the coupled electrothermal problem and it is chosen finally for this study.

METHODS AND SIMULATIONS

In this paper, the COMSOL software based on FEM is used to analyze the uniformity of temperature.

The permittivity of water was taken from reference[7]. The permittivity of silicon carbide changes with temperatures, so it is necessary to establish a function between the permittivity and temperature. From the reported work[4], the relation between tan δ and temperature is gained as Fig. 1. The values of seven special points from the curve of silicon carbide are analyzed in Table-1.

According to the definition of loss tangent, tan δ is imaginary part dividing real part of the permittivity. It is assumed ε_r = a-j*b, so tan δ = b/a. The real part of silicon carbide permittivity, which is obtained from literature is a = 6.52, and its imaginary part which is obtained by linear fit (Table-1) is b= -6.40786+0.02347*T. Finally, the permittivity of SiC is ε_r = 6.52-j*(-6.40786 + 0.02347* T). During all the computational process, the input power at the waveguide feeding has been set to P = 700 W. The microwave heating time is t = 8s.

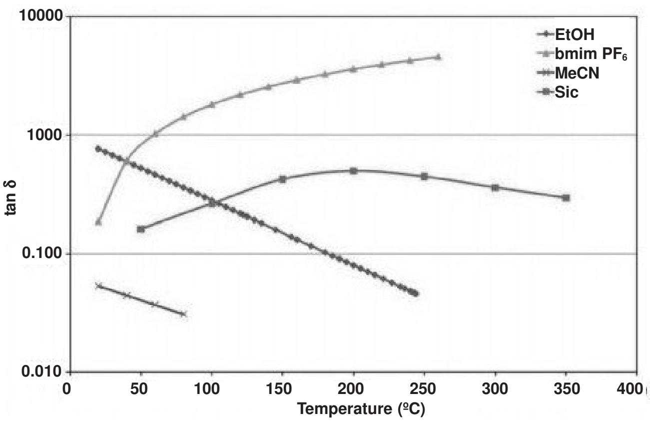

Fig. 1. Tan δ as a function of temperature for the silicon carbide

TABLE-1
LOSS TANGENT δ FROM THE SiC CURVE

T (ºC)	50	100	150	200	250	300	350
Tan δ	0.18	0.33	0.6	0.69	0.63	0.51	0.46

After calculation, the results such as maximum and minimum value of temperature were recorded during heating. Then the uniformities of electric field and temperature were obtained respectively by formula (1). The average temperature was achieved by formula (2).

Finally, comparing synthetically the all configurations and different thickness of vessel wall, the best uniformity of temperature is gained.

$$\text{Temperature uniformity} = \sqrt{\frac{T_{max}^2 - T_{min}^2}{T_{max}^2}} \quad (1)$$

T_{max} is the maximum temperature and T_{min} is minimum temperature.

$$\text{Average temperature} = \frac{\sum_{i=1}^{\infty} T_1}{V} \quad (2)$$

T_i is the temperature for every grid of heated solvent and V is the total volume.

RESULTS AND DISCUSSION

The three different configurations were calculated and the following reports during heating. Three configurations are separately presented to measure in detail the uniformity of the temperature in the solvent. Their physical models are shown in Fig. 2-4.

Configuration 1: The problem to be solved consists of a 267 × 270 × 188 mm^3 metallic rectangular applicator. In this model, the inside solvent is water and the outer vessel is silicon carbide. The cubage of water is $V_{water} = \pi * r^2 * h$ and the cubage of silicon carbide is $V_{SIC} = \pi * R^2 * h_1 - \pi * r^2 * h$. R is the radius of big cylinder, r is the radius of small cylinder and h_1 is the height of silicon carbide and h is the height of water.

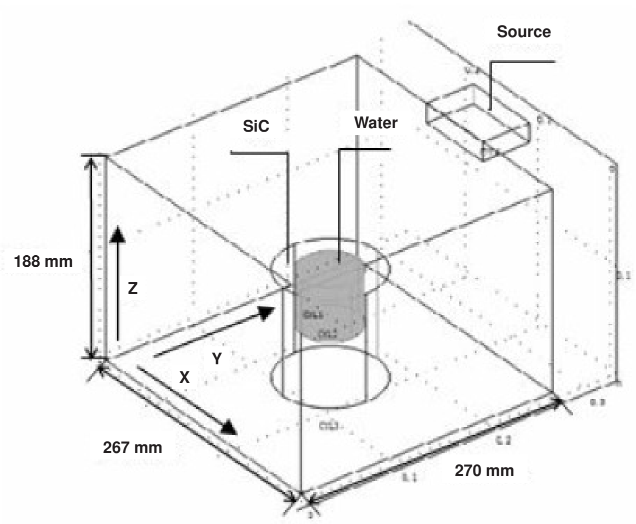

Fig. 2. Inside solvent is water and the outer is silicon carbide

Configuration 2: The problem to be solved consists of a 267 × 270 × 188 mm^3 metallic rectangular applicator. In this model, the inside solvent is water and the outer vessel is glass. The cubage of water is $V_{water} = \pi * r^2 * h$ and the cubage of glass is $V_{glass} = \pi * R^2 * h_1 - \pi * r^2 * h$. R is the radius of big cylinder, r is the radius of small cylinder, and h_1 is the height of glass and h is the height of water.

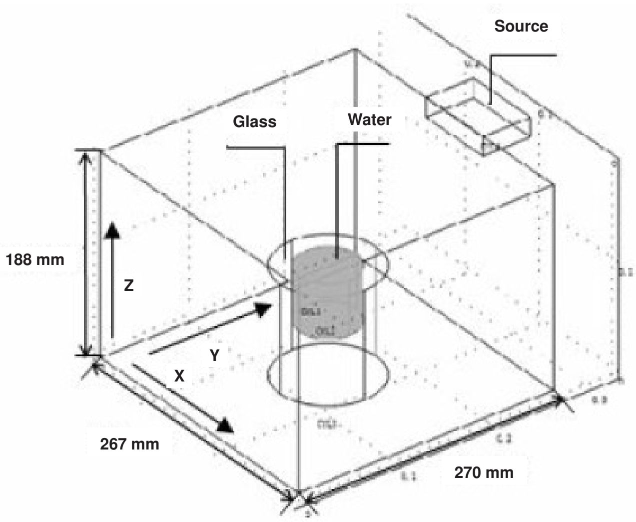

Fig. 3. Inside solvent is water and the outer vessel is glass

Configuration 3: The problem to be solved consists of a 267 × 270 × 188 mm^3 metallic rectangular applicator. In this model, the outer vessel is glass and inside material is silicon carbide and the middle solvent is water. The cubage of SiC is $V_{SiC} = \pi * r^2 * h$ and the cubage of water is $V_{water} = \pi * R^2 * h_1$-

$\pi*r^2*h$ and the cubage of glass is $V_{glass} = \pi*R'^2*h_2-\pi*R^2*h_1$. R' is the radius of big cylinder and R is the radius of middle cylinder, r is the radius of small cylinder and h_2 is the height of big cylinder and h_1 is the height of middle cylinder and h is the height of small cylinder.

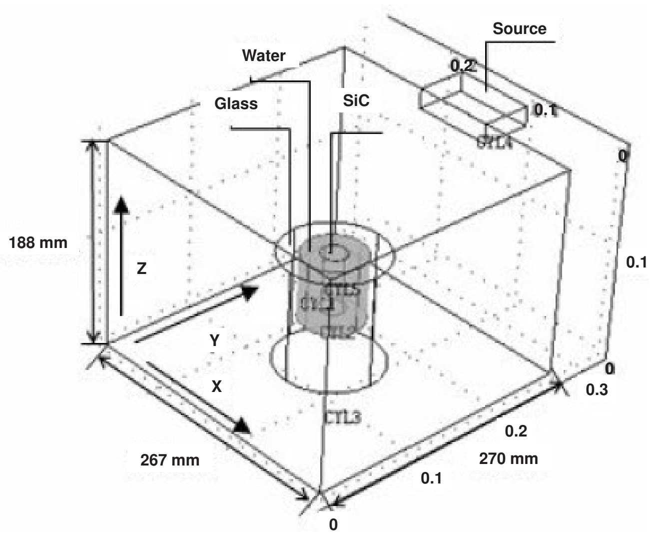

Fig. 4. Outer vessel is glass and inside material is silicon carbide and the middle solvent is water.

Analysis and comparison: According to simulation results, the maximum and minimum value of the temperature were recorded during the microwave heating process. Finally, the uniformity of the temperature were calculated by the formula (1). The results from three configurations for the temperature are listed in Tables 2-4.

By comparing the datum in Tables 2-4, it is observed that the effect of heating solvent is desired using SiC as the vessel material, and especially when the thickness of vessel wall is 0.01m, the temperature uniformity is lowest and the effect of heating solvent is best. However, when glass is used for vessel, the variety of temperature uniformity is not obvious, even though the thickness of vessel is changed.

TABLE-2
GLASS VESSEL

Thickness of vessel (m)	T_{max} (ºC)	T_{min} (ºC)	Average temp.: T_{avg} (ºC/m^3)	Temperature uniformity
0.005	428.761	321.576	330.880	0.661
0.010	390.920	319.257	330.469	0.577
0.020	404.256	319.980	330.817	0.611
0.030	426.428	318.858	329.794	0.664

TABLE-3
SILICON CARBIDE VESSEL

Thickness of vessel (m)	T_{max} (ºC)	T_{min} (ºC)	Average temp.: T_{avg} (ºC/m^3)	Temperature uniformity
0.005	482.000	239.892	324.070	0.867
0.010	329.209	322.107	323.200	0.206
0.020	368.945	321.420	324.019	0.483
0.030	330.651	322.861	323.360	0.215

TABLE-4
GLASS AND SILICON CARBIDE VESSEL

Thickness of vessel (m)	T_{max} (ºC)	T_{min} (ºC)	Average temp.: T_{avg} (ºC/m^3)	Temperature uniformity
0.005	386.184	321.040	330.662	0.560
0.010	441.092	321.500	331.128	0.684
0.020	382.110	322.223	331.370	0.537
0.030	371.905	322.180	329.469	0.499

From above, it is obvious that the temperature uniformities were influenced by different configurations and size of vessel wall, the uniformity of temperature can be highly improved by changing the configuration and the thickness of vessel wall.

Conclusion

This paper used silicon carbide with the high microwave absorption properties as the heated container and water as the polar solvent. Three configurations were designed to heat water assisted by silicon carbide or glass. Best vessel configuration and thickness of wall with uniformity of temperature was achieved. It is the configuration that water is surrounded by silicon carbide and the thickness of vessel wall is 0.01 m.

By calculation, the three configurations with different thickness of wall are integrally compared in the uniformity of temperature field. When the improvement in temperature uniformity is not obvious, it can improve significantly the uniformity of temperature by changing the configuration and thickness of vessel wall.

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