Thermal Uniformity Analysis of Polar and Non-polar Solvents During Heating Based on Numerical Calculation

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It is a key issue to obtain uniform heating in certain regions of an applicator. In this paper, the non-polar (CCl_4) and polar (water) solvents are heated together in same container. The silicon-carbide is chose to be a vessel. The uniformities of temperature were analyzed using finite-element method under different configurations during heating. The results show that the temperature uniformity is influenced by solvent volume size and volume ratio and the thermal energy transfers from the non-polar to polar solvent for temperature difference. When the improvement in temperature uniformity is not obvious, it can improve significantly the uniformity of temperature by changing the volume or volume ratio.

Key Words: Thermal uniformity, Polar and Non-polar Solvents, Numerical calculation, Silicon carbide.

INTRODUCTION

It is known that solvents are classified on the basis of their polarity. Molecules with large dipole moments and high dielectric constants are considered polar and those with low dipole moments and low dielectric constants are considered non-polar.

(1) Highly polar molecules have a network of hydrogen bonding between their molecule *e.g.* water; (2) Polar solvents have a replaceable hydrogen atom and an element like nitrogen or oxygen, *e.g.* methanol; (3) Intermediately polar solvents have an element like nitrogen or oxygen, but no replaceable hydrogen atom, *e.g.* acetonitrile; (4) Non-polar compounds neither have replaceable hydrogen nor electronegative element in their molecule *e.g.* benzene or other hydrocarbons.

Interestingly carbon tetra chloride, despite of having chlorine in it is a non-polar compound, since the structure of the compound is such that the there is nullification of dipole moments due to identical and opposite bonds between carbon and chlorine.

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. However, the non-polar solvents are also commonly used in a number of chemical reactions.

In this paper, the method of heating is not traditional heating, but microwave heating. Compared with traditional heating, microwave energy is delivered directly to materials through molecular interactions with the electromagnetic field[3]. Thus microwave heating has the advantages such as lesser time and energy savings, easy to control as well as clean heating *etc.*, which present an impressive application prospects[4].

In this paper, a numerical model is presented to study the temperature distribution of heterogeneous mixture reaction solution under microwave radiation. The uniformity is well analyzed when the solvent of polar and non-polar is mixed.

EXPERIMENTAL

In the simulation of microwave heating on chemical reactions, we have to know the function of the effective permittivity with respect to temperature. Generally, the effective permittivity of reactants changes with temperature. The coupled Maxwell's equations, fluid field equations and heat transport equations were solved by using finite-element method. The flow chart of the numerical calculation of multiphysics is shown in Fig. 1 and the calculation model is shown in Fig 2.

In this paper, CCl_4 is a typical non-polar solvent widely used in synthetic chemistry research. The permittivity of water was taken from reference[5], which is $\varepsilon_r = 2.24-j*0.002$. The silicon-carbide (SiC) is chose to be a vessel. 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[6]. The permittivity of SiC changes with temperatures, so it is necessary to establish a function between the permittivity and temperature. From the work of Damm and Kappe[7,8], the relation between ε_r and temperature is gained as formula (1) by the method of curve-fitting.

$$\varepsilon_r = 6.52 - j*(-6.40786 + 0.02347*T) \qquad (1)$$

where T is the temperature.

Water is a typical polar solvent widely used in synthetic chemistry research. This paper therefore focused on the heating of water and CCl_4 in SiC container with different configurations and size.
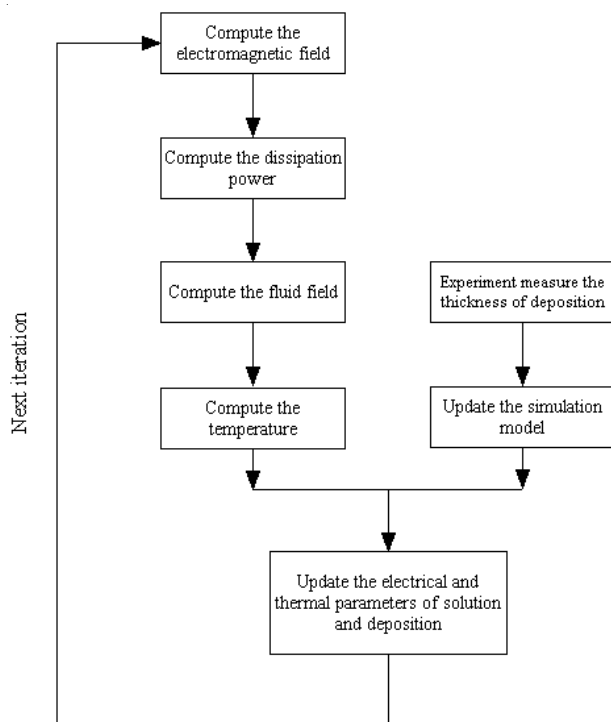

Fig. 1. Flow chart of the numerical calculation of multiphysics

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 = 5s. Relative parameters which are used to solve the case are listed in Table-1.

TABLE-1
RELATIVE PARAMETERS

Parameter	SiC	CCl_4	Water
Heat conduction: k (w/m*K)	20	0.106	0.6096
Density: ρ (kg/m³)	3200	1595	997
Atmospheric heat capacity: C_p (J/(kg*K))	170	854	4181

By 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 (2). The average temperature was achieved by formula (3).

$$\text{Temperature uniformity} = \sqrt{\frac{T^2_{max} - T^2_{min}}{T^2_{max}}} \qquad (2)$$

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

$$\text{Average temperature} = \frac{\sum_{i=1}^{\infty} T_i}{V} \qquad (3)$$

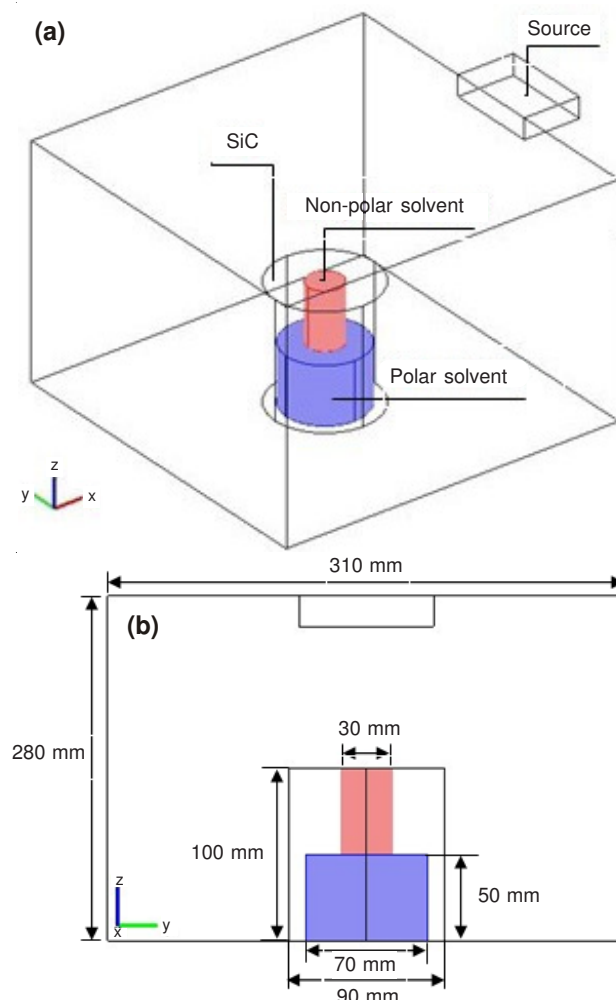T_i is the temperature for every grid of heated solvent and V is the total volume.

Fig. 2. Physical model of experiment system: (a) 3D model; (b) 2D model

RESULTS AND DISCUSSION

By calculation, the resulted temperature distributions under the different proportion with non-polar and polar solvent were shown in Fig. 3.

It is observed that the heated effect of CCl_4 is more obvious than water and the temperature is high relatively. As we can see, the energy is flowing from CCl_4 to water. It is proved that the thermal energy transfers from non-polar solvent to polar solvent.

According to calculation results, the maximum and minimum values of the temperature were recorded during the heating process. Finally, the uniformity of the temperature was calculated by the formula (2). The results from different radius and volume ratio for the CCl_4 and water are listed in Tables 2 and 3.

From Fig. 3 and Table-2, one can observe that the uniformity radius 40 mm is superior to others when the volume ratio of CCl_4 and water is 1:1. The effect of heating solvent is desired
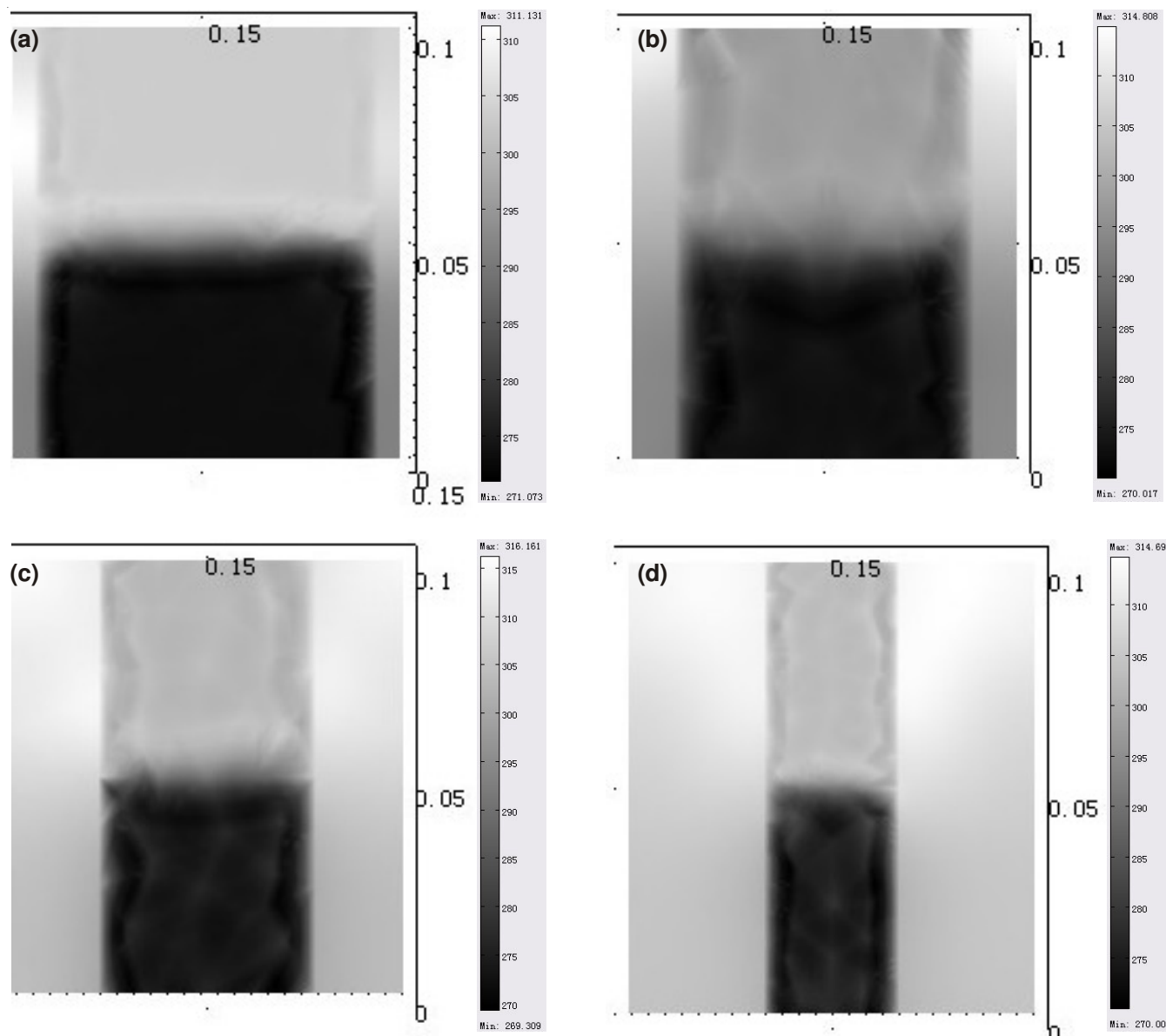
Fig. 3.　Temperature distribution with different radius when the volume ratio is 1:1(unit: K); (a) The radius of CCl_4 and water is 40 mm; (b) The radius of CCl_4 and water is 35 mm; (c) The radius of CCl_4 and water is 25 mm (d) The radius of CCl_4 and water is 15 mm

using SiC as the vessel material. It is proved that the container will be effectively shielded from the electromagnetic field. The thermal energy in SiC container is found to transfer from CCl_4 to water. Besides, by comparing with different volume ratio of CCl_4 and water from Fig. 4 and Table-3, the uniformity is best when the volume ratio of CCl_4 and water is 49: 9. So it is obvious that the temperature uniformities were influenced by different solvent volumes, the uniformity of temperature can be highly improved by changing the volume.

TABLE-3
RESULTS WITH DIFFERENT VOLUME
RATIO OF CCl_4 AND WATER

The volume ratio of CCl_4 and water	T_{max}(K)	T_{min}(K)	Average temperature: T_{avg}(K/m³)	Temperature uniformity
9:49	320.477	270.148	295.375	0.538
49:9	307.396	269.871	288.656	0.479
25:64	324.132	270.773	297.485	0.550
64:25	311.251	269.098	290.192	0.503

Conclusion

In this paper, due to microwave absorption of the non-polar and polar solvent is different, silicon carbide with the high microwave absorption properties is used to be the heated vessel and CCl_4 as the non-polar solvent and water as polar solvent. By calculation, it is proved that the temperature uniformity is influenced by solvent volume size and volume ratio when the non-polar and polar solvents are heated together
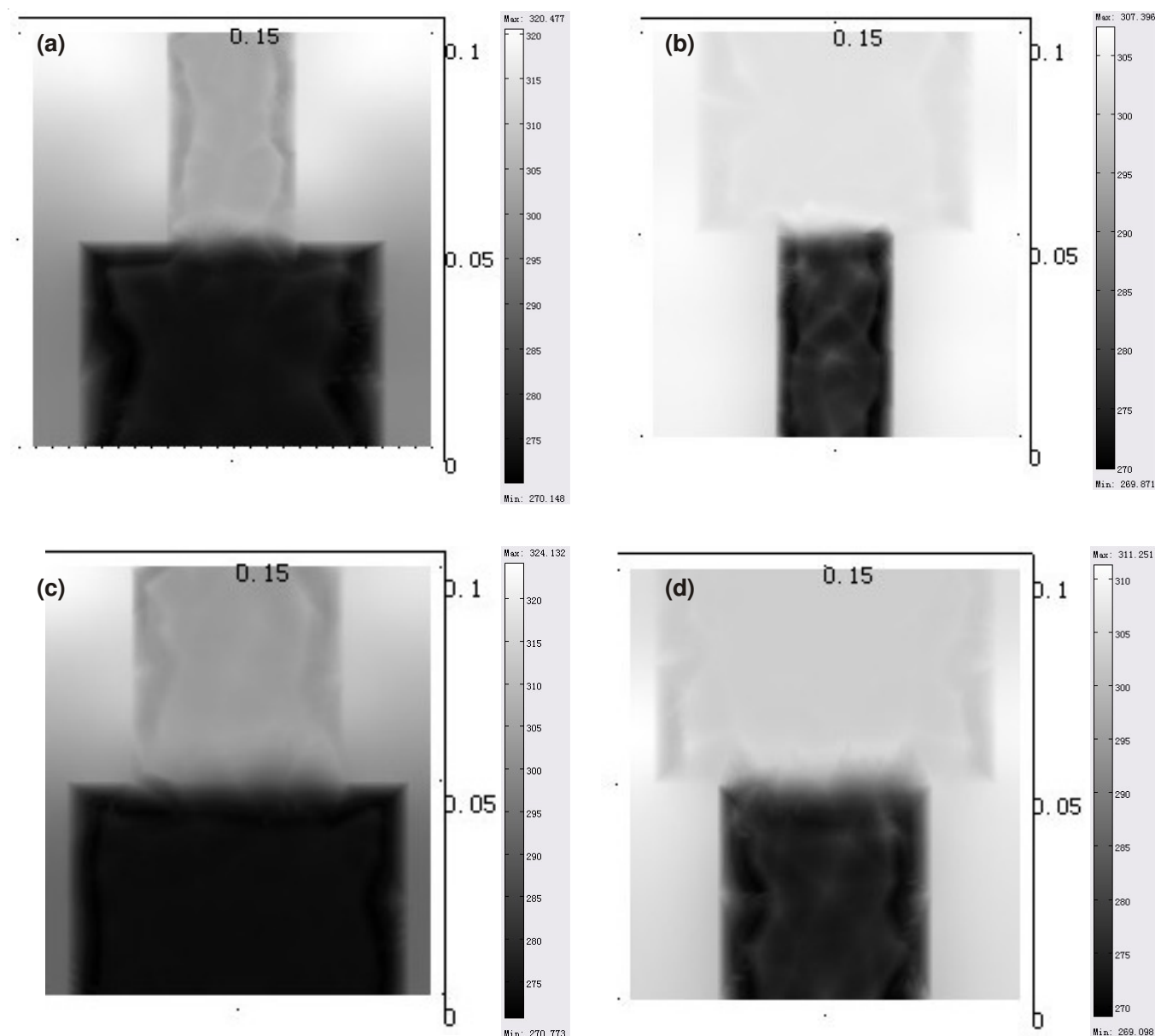
TABLE-2
RESULTS WITH DIFFERENT RADIUS OF CCl_4
AND WATER (THE VOLUME RATIO 1:1)

Radius (mm)	T_{max}(K)	T_{min}(K)	Average temperature: T_{avg}(K/m³)	Temperature uniformity
40	311.131	271.073	291.142	0.491
35	314.808	270.017	292.431	0.858
25	316.161	269.309	292.752	0.852
15	314.698	270.003	292.324	0.856

Fig. 4. Temperature distribution with different volume ratio (unit: K); (a) The volume ratio of CCl$_4$ and water is 9:49. (b) The volume ratio of CCl$_4$ and water is 49:9. (c) The volume ratio of CCl$_4$ and water is 25:64. (d) The volume ratio of CCl$_4$ and water is 64:25

in same container. Besides, it is occurred that the thermal energy transfers from the non-polar to polar solvent for temperature difference. When the improvement in temperature uniformity is not obvious, it can improve significantly the uniformity of temperature by changing the volume or volume ratio.

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