Computation of Microwave-Induced Temperature in Liquid Cylindrical Reactants

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The problem of efficient control over microwave-assisted chemical reactions is addressed in this paper through the development of a simple model capable of computing average temperature of a liquid reactant heated by microwaves and stirred by convection. The model is built for a three-medium concentric scenario typical for microwave equipment used for microwave-assisted chemistry. Computation is performed for water in a Pyrex vial held in a Teflon cup; modeling results are verified experimentally using the MiniFlow 200SS batch reactor from SAIREM and found to be in a very good agreement with the measurement.

Keywords: Concentric scenario, convection flow, liquid reactant, microwave heating, temperature, three-media model

INTRODUCTION

Microwave-assisted chemistry is a rapidly growing area utilizing microwaves (MW) as the means of enhancing and accelerating chemical reactions [1-2]. Currently, there exists a range of dedicated equipment for related lab studies [2]; however, the development of new reaction routes remains difficult because of lack of data on the interaction between the reactants and the MW structures. Modeling of the underlying electromagnetic and thermal characteristics has been suggested as a way to support development of such processes and of the design/scaling up of corresponding MW systems [3].

In our previous work [4], we developed an advanced model capable of solving the electromagnetic-thermal coupled problem and computing the 3D temperature fields in the reactant in the batch reactor *MiniFlow 200SS* designed and produced by SAIREM SAS. Experimental verification of the model, however, has revealed that, in liquid reactants, temperature fields are more uniform than in the model due to convection flows acting as an effective mechanism of averaging the reactant's temperature. Understanding the impact made by convection on temperature characteristics of the MW-induced reactions in liquid/low viscosity reactants therefore becomes a point of significant interest.

In this paper, we describe a simple model for computation of temperature in a cylindrical scenario typical for the systems in MW-assisted chemistry. The model allows

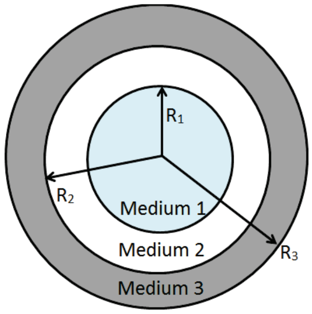


Figure 1. Three-medium geometry of the problem.

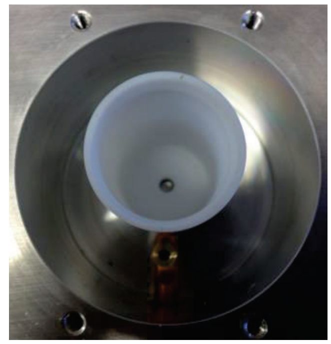


Figure 2. Internal view of the cylindrical cavity of the SAIREM's reactor *MiniFlow 200SS system.*

for determining the average temperature of a liquid reactant exposed to MW heating and stirred because of the convection effect.

THE MODEL

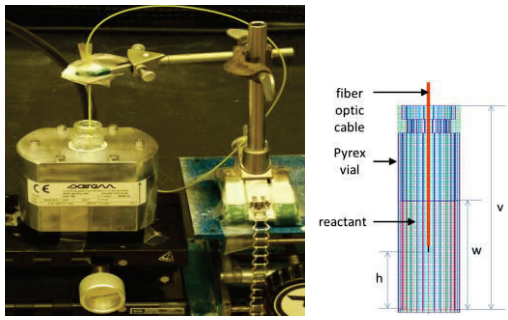
We consider a concentric 2D scenario (Figure 1) imitating a cross-section of a dielectric cup (Medium 3) holding a vial (Medium 2) with a liquid reactant (Medium 1). This setup is typical for the equipment currently used in the laboratory studies in MW-assisted chemistry and, at the same time, allows us to build a simple physics-based model for estimating the MW-induced temperature averaged by the convection flows. We also make a practically reasonable assumption that Medium 2 has a small mass and a low specific heat (so that the heat absorbed there is negligible).

In terms of boundary conditions, the system is considered insulated on the outer surface of Medium 3, and we assume perfect thermal contact (i.e., continuity of temperature and heat flux) at the interfaces of any two media. Under all these conditions, the electromagnetic-thermal coupled problem is separated into two independent ones, and the thermal problem is reduced to a linear system of ordinary differential equations whose solution is obtained by a computational procedure implemented in MATLAB.

COMPUTATION AND MEASUREMENT

Computations were performed for water (Medium 1) as a reactant in a Pyrex vial (Medium 2) held in a Teflon cup (Medium 3), and the values of R_1, R_2, and R_3 were taken as 10.0, 12.0, and 14.3 mm, respectively, from the *MiniFlow 200SS* reactor designed with a three-media structure as a core of the reactor (Figure 2) and employed for corresponding experiments. In computation, we used the values of not nominal, but actually absorbed MW power; this data was measured in the course of the experiments.

MW power was held constant (100 W), and the frequency was set to 2.45 GHz; these values of power and frequency were maintained by the control system of a solid-state generator of the *MiniFlow 200SS* system. In the experiment (Figure 3), a fiber optic cable was held inside a glass capillary in order to measure temperature at the points along the axis of the vial.



(a) (b)

Figure 3. Measuring temperature in *MiniFlow 200SS*: general outlook of the experimental setup (a) and a schematic view of the Pyrex vial with a fiber optic sensor.

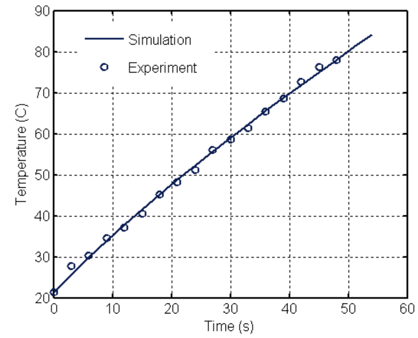


Figure 4. Measured and computed time characteristics of the average temperatures of water.

As it is shown in Figure 4, computational and experimental results are in an excellent agreement.

DISCUSSION

In contrast to the prediction by the coupled model [3] (which does not account for convection), the proposed approach suggests that temperature at different heights of the reactant are not very different from the experimental data. This confirms our hypothesis that the convection flows make a significant impact on the MW-induced temperature fields in liquid reactants. Our model is directly applicable to any low viscosity substances whose specific heat and thermal conductivity are known, as well as to other MW systems loaded with components of a similar concentric configuration.

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