Design of a Microreactor for Microwave Organic Synthesis Through Microwave Heating Simulations

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Abstract

Despite the popularity of microwave heating in chemistry, the mechanism of heating through electromagnetic interaction is not well understood and often not taken into account when designing the heating system. In this contribution, we will present the issues of a microreactor setup designed for microwave organic synthesis and demonstrate how simulation of microwave heating is used to improve the microreactor design.

Microwave-assisted organic synthesis has become increasingly popular due to the numerous advantages brought about by the unique mechanisms of microwave heating. Microwave heating dramatically increases the heating rate compared with conventional heating since molecules in the reaction mixtures can absorb the microwave energy directly within a microwave-transparent vessel. Novel reaction pathways and product distributions that differ from conventional heating can also be achieved through selective heating. The ability to collect data rapidly and potential to expand chemical space make microwave-assisted organic synthesis attractive to the fields of kinetic studies, high-throughput synthesis, and reaction optimization. Microreactors provides further benefits, such as reducing the amount of time and labor required, and providing simpler way of scaling up to avoid the penetration depth and energy efficiency limitations, by conducting microwave reactions in continuous flow formats. A microreactor was therefore designed to fit into the CEM Discover microwave unit. The original setup includes a micoreactor made of borosilicate glass, PEEK compressive packaging, and a Teflon holder for a fiber optic temperature detector. Validation reactions show unexpected low conversions that stem from an uneven temperature distribution across the microreactor and temperature limitations. In order to tackle the heating issues, a COMSOL Multiphysics® simulation of the whole setup is used to understand the mechanism of microwave heating (Figure 1).

The heating source in microwave heating is the power dissipation caused by the interaction between the electric field and the materials. The heating rate therefore depends on the magnitude of the electric field and the dielectric loss of the material. Using COMSOL, we solve the Maxwell equations that govern the electromagnetic field and then use the calculated heating rate to simulate the heat transfer scheme of the materials. The RF module was used for the electromagnetics and solid heat transfer simulations, while the Heat Transfer and CFD modules were used to estimate the heat convection of the air within the microwave cavity and fluids in the microreactor channels.

The results match the temperature measured experimentally (Figure 2) and reflect the experimental observation of the uneven temperature distribution (Figure 3). The heating limitation of the original microreactor is due to both the convection heat loss created by the air pocket and the low electrical field strength caused by the thinness of the reactor. By changing the thickness of the reactors in the simulation, we were able to find a design that will induce higher electric field strengths and lead to higher heating rates. The simulations allowed us to improve the design of the microreactor to overcome heating limits and obtain uniform temperature distribution in the reactor.

Figures used in the abstract

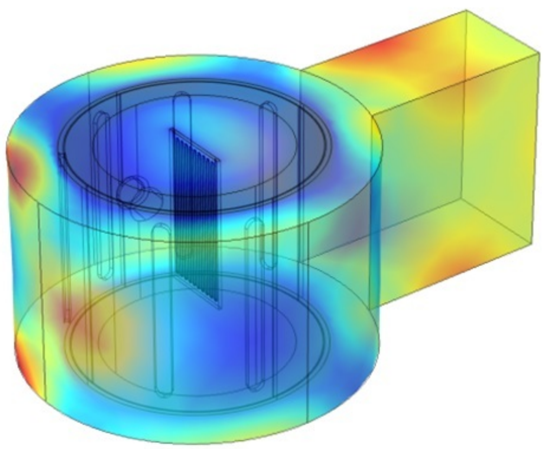

Figure 1: Geometry of the CEM Microwave Unit and Microreactor

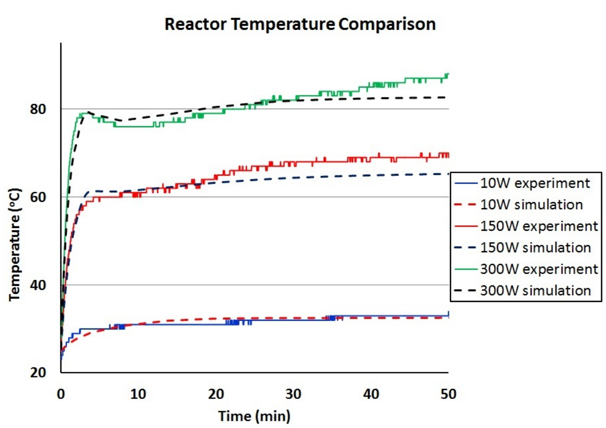

Figure 2: Temperature Measurements Comparison

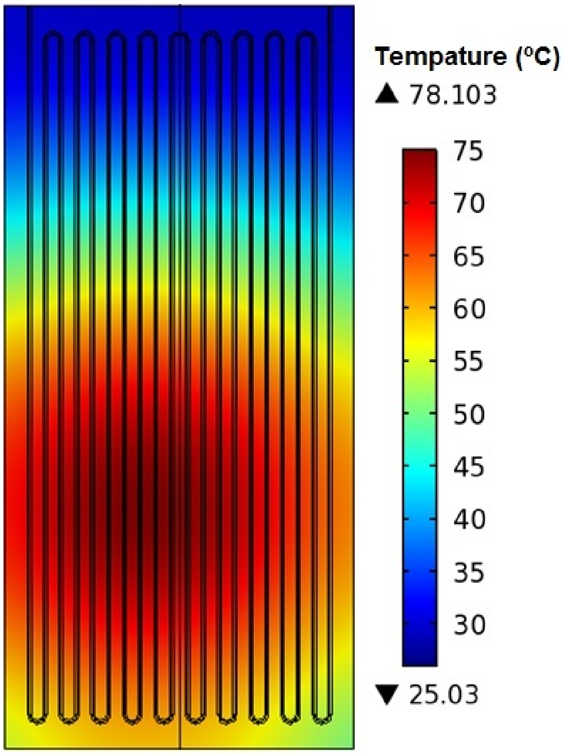

Figure 3: Temperature Distribution Across the Microreactor Surface at Steady State