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

Wen-Hsuan Lee[1], Klavs F. Jensen[1]

1. Massachusetts Institute of Technology, Department of Chemical Engineering, 77 Mass Ave, Cambridge, MA

Goal is to design a microreactor for a microwave unit in order to acheive:

- High-throughput organic synthesis, reaction screening
- Kinetic modeling of microwave reactions

Original Design:

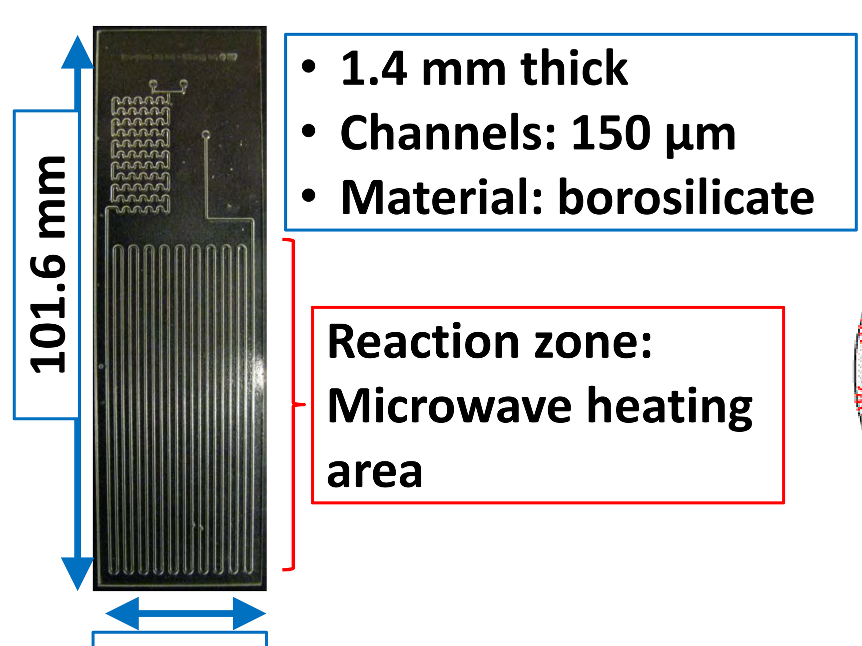

Figure 1. Microreactor

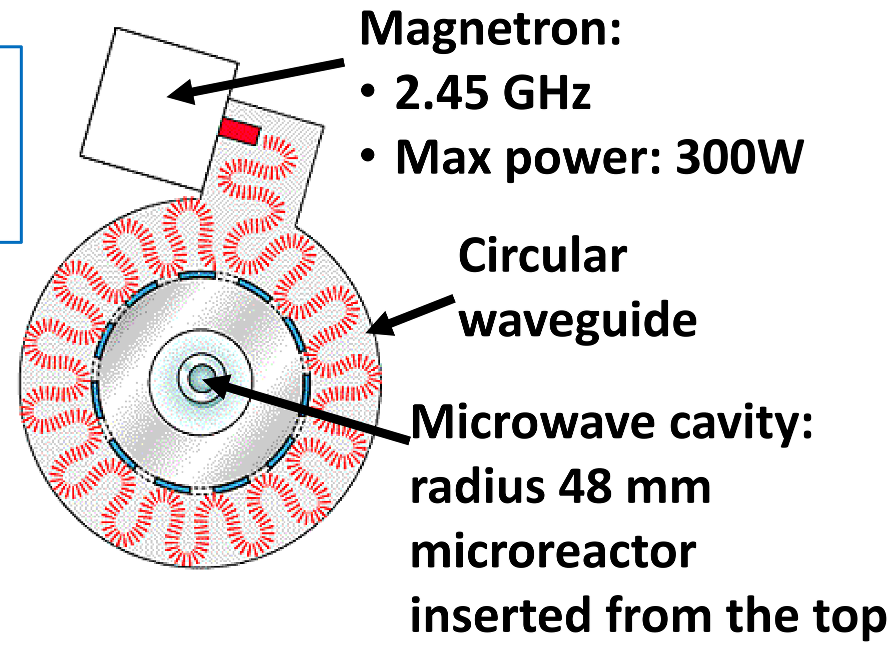

Figure 2. Top view of microwave unit[1]

Heating Issues:

- Uneven temperature distribution across reactor; center of the reactor is hottest.
- Maximum steady-state temperatures too low for desired chemical reactions

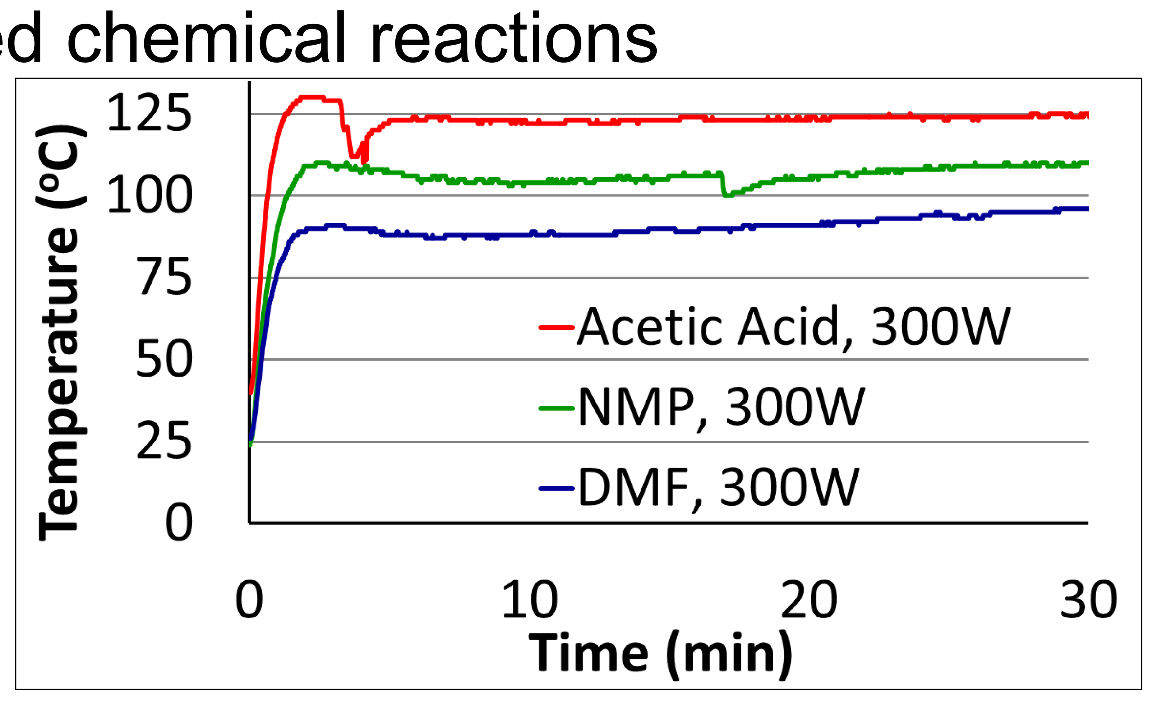

Figure 3. Heating profile of the reactor surface center with different solvents (measured by fiber optic probe)

Computational Model:

- The RF module: microwave heating and electromagnetic waves physics

$$\nabla \times \mu_r^{-1}(\nabla \times \mathbf{E}) - k_o^2\left(\varepsilon_r - \frac{j\sigma}{\omega\varepsilon_o}\right)\mathbf{E} = \mathbf{0}$$

→solve electric field

→heat source: $Q = \frac{1}{2}\omega\varepsilon_o\varepsilon''\mathbf{E}\cdot\mathbf{E}^*$

- Single-Phase Flow Module:

$$\nabla \cdot \mathbf{v} = 0$$

$$\rho\frac{D\mathbf{v}}{Dt} = \rho\mathbf{g} - \nabla P + \nabla\cdot\boldsymbol{\tau}$$

→velocity of air convection in waveguide

- Heat Transfer Module:

$$\rho C_p\left(\frac{\partial T}{\partial t} + \mathbf{v}\cdot\nabla T\right) = \nabla\cdot(k\nabla T) + Q$$

→solve for temperature

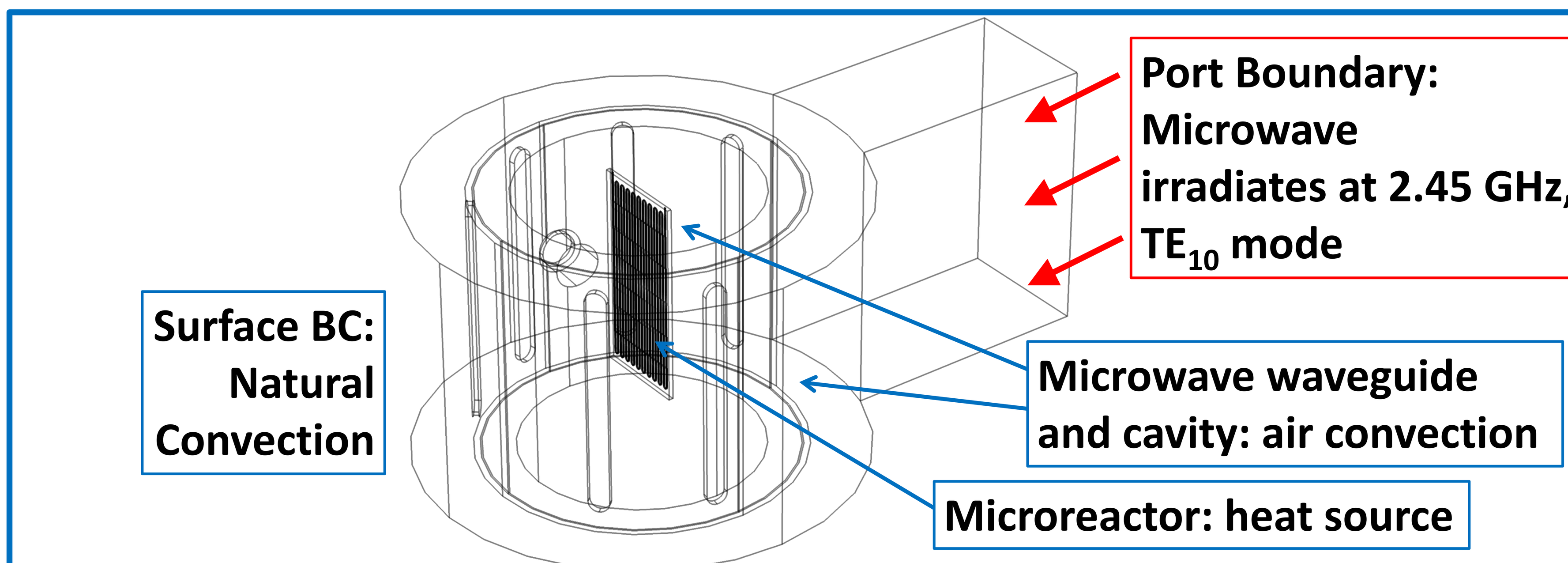

Figure 4. 3D geometry of computation model

Results:

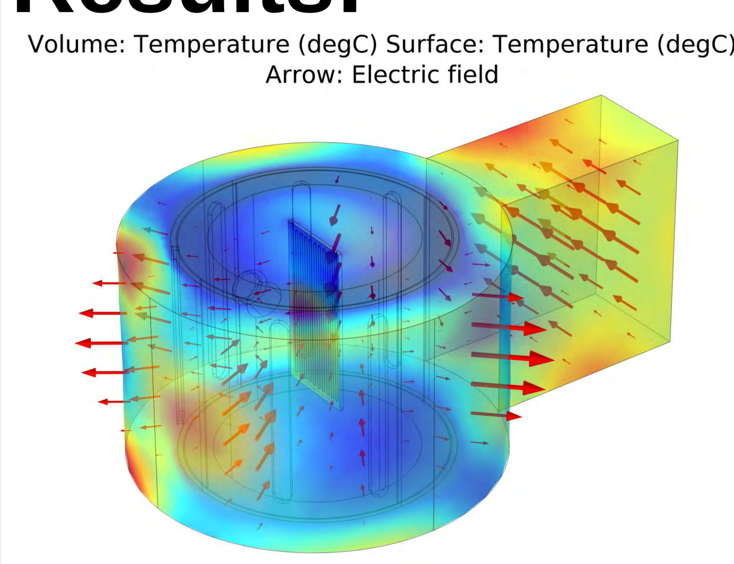

Figure 5. 3D view of result

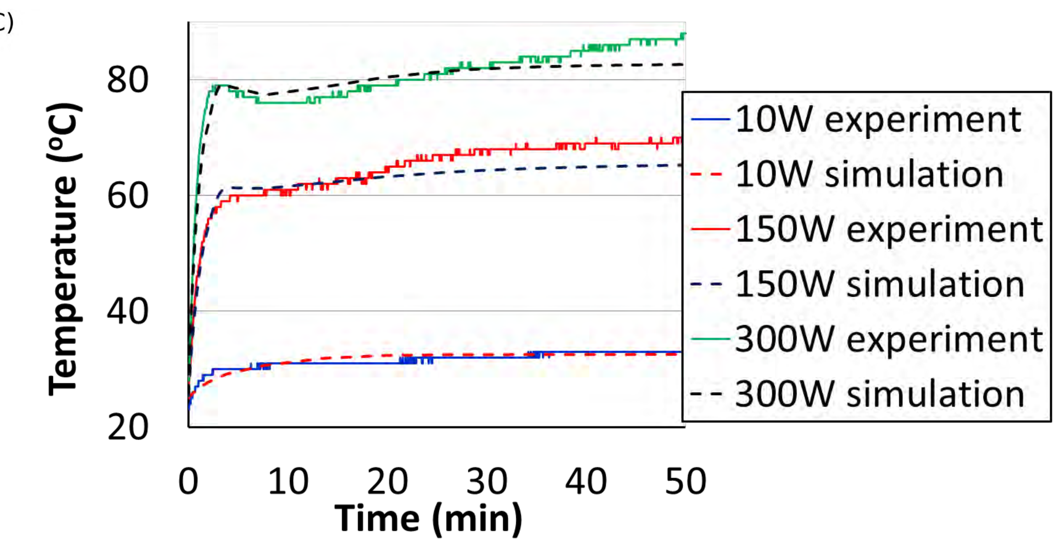

Figure 6. Temperature comparison of reactor surface center

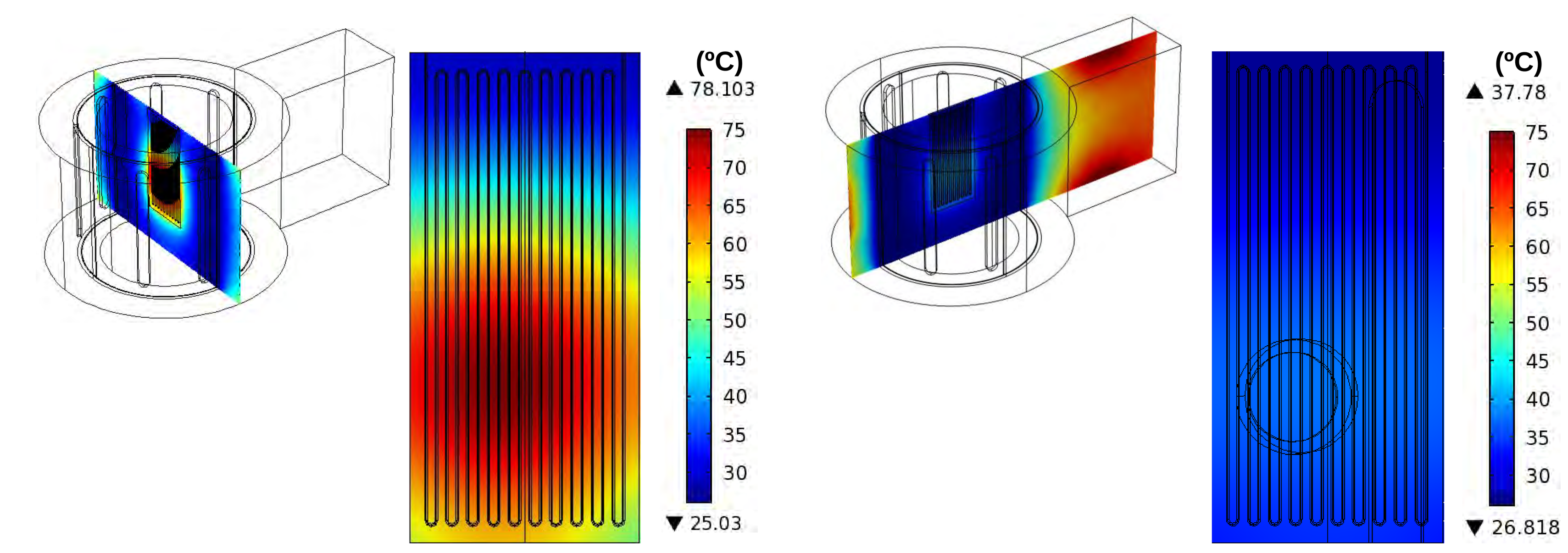

Figure 7. Reactor surface temperature varies with position

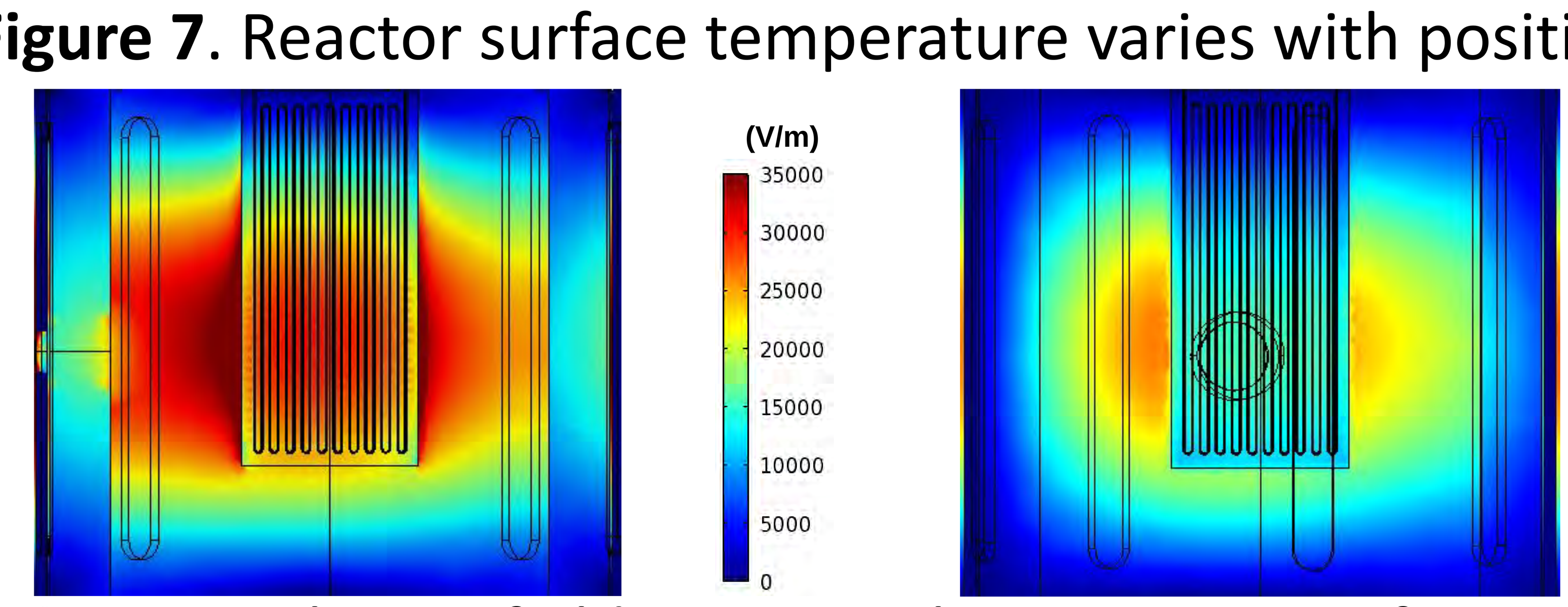

Figure 8. Electric field in cavity along reactor surfaces at the two positions shown in Figure 7

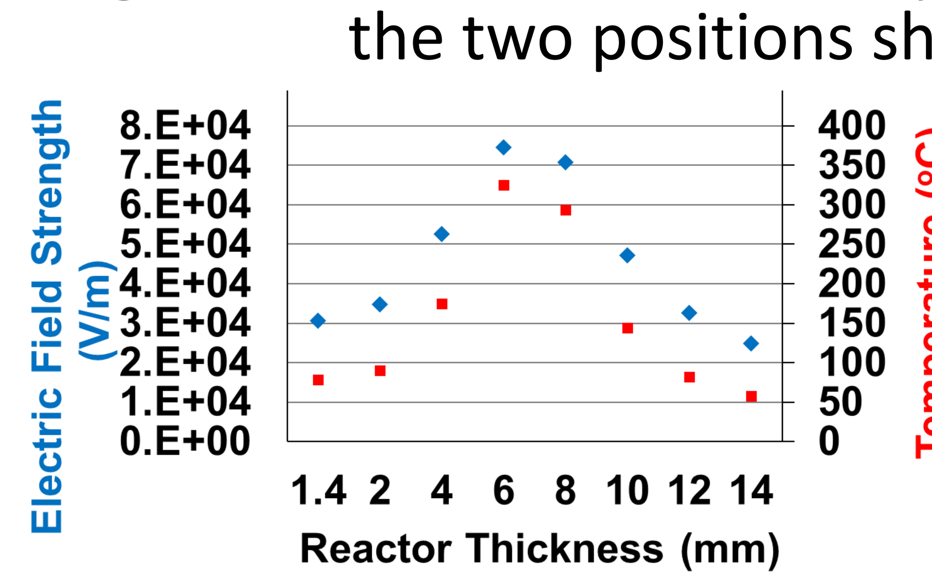

Figure 9. Electric field also varies with size of the reactor → used to improve design

Conclusion:

The simulation results match the measurements and uneven temperature distribution. The heating issues were caused by low electric field strength, which varies with the size and position of the reactor. A higher electric field strength could be induced by redesigning the reactor thickness.

Acknowledgement and Reference:

Thanks to NIH for funding and CEM for providing the microwave unit (1. Cavity top view picture from CEM company website: *www.cem.com*)