Numerical Optimization of Microwave Reactor Parameters for Direct Methane Aromatization

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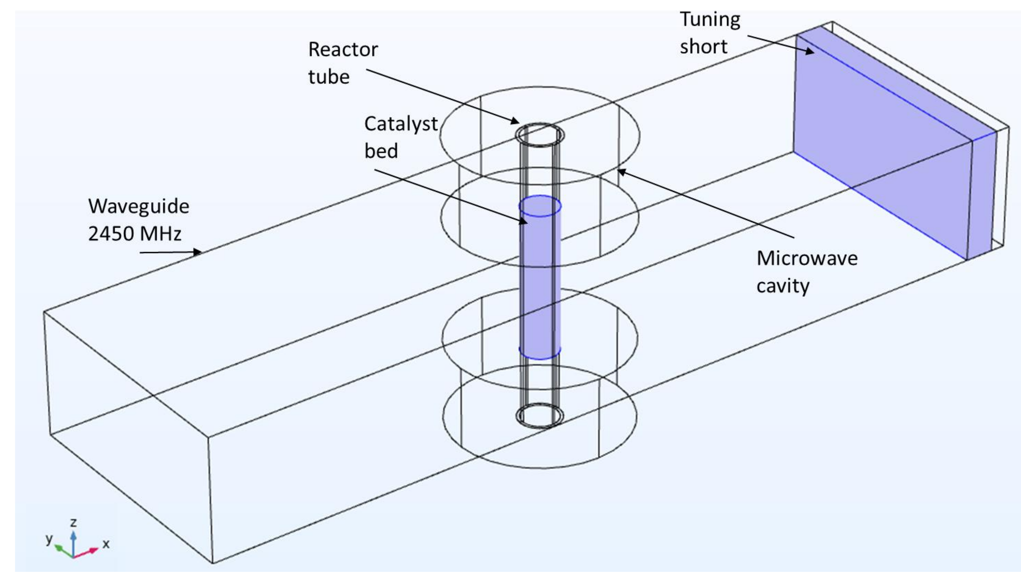
Introduction

Direct methane aromatization (DMA) using Mo-ZSM-5 catalyst is an effective method for methane conversion. Microwave-assisted DMA offers quick reaction times, higher methane conversion and product selectivity and efficient catalyst activation due to direct microwave-active sites interactions. In order to achieve best catalytic performance, the microwave reactor should be optimized for various parameters that govern the microwave heating process[1].

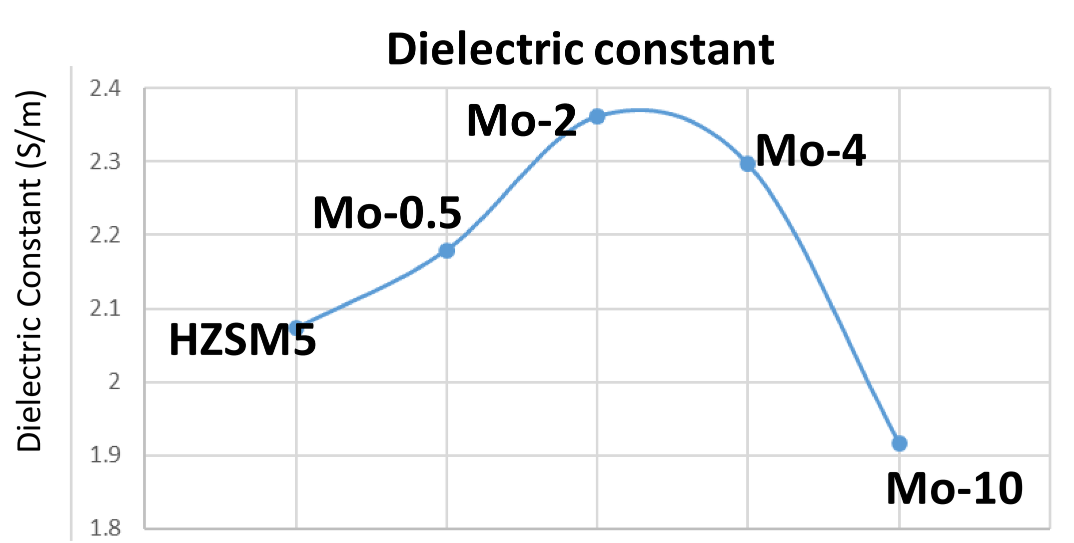
Modeling Methods

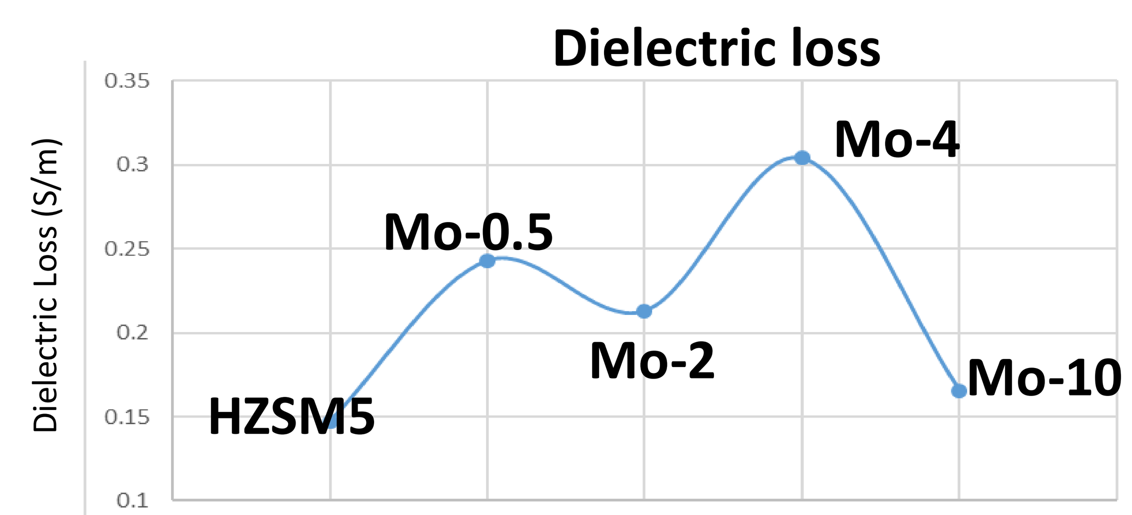
- COMSOL Multiphysics was used to model microwave heating of Mo-ZSM-5 catalyst at 2450 MHz[2,3]
- Effect of tuning short position, reactor tube diameter, catalyst bed design, addition of SiC as absorber and, cavity design were studied
- Dielectric properties of catalyst were measured using Vector Network Analyzer using a two-probe method[4]



Dielectric Properties

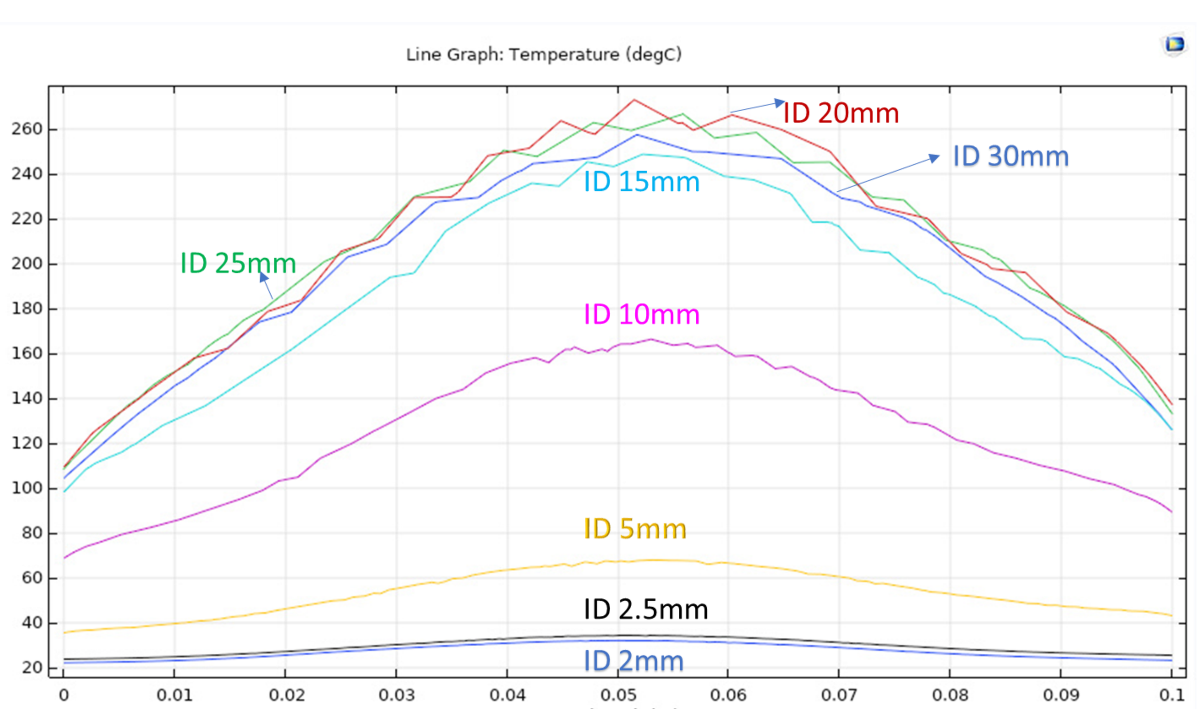
- Properties of fresh ZSM-5, and ZSM-5 loaded with Mo (0.5, 2, 4, 10 wt%) at 2450 MHz at room T
- Mo-ZSM-5 with 4 wt% loading has highest dielectric loss





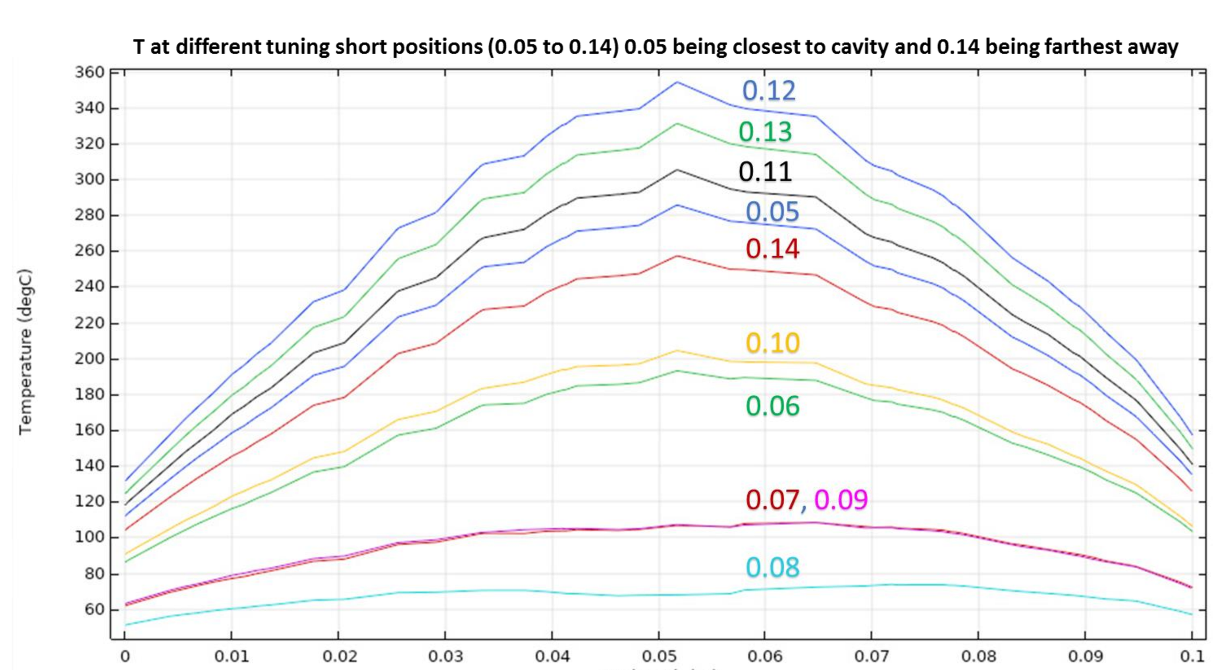
Effect of Reactor Tube Geometry

- T increases with increase in tube diameter up to 20 mm, then decreases
- Penetration depth of Mo-ZSM-5 is 19.1 mm
- Not enough material to absorb MW effectively at lower tube diameter
- >20mm ID, too much material and maximum T-drops



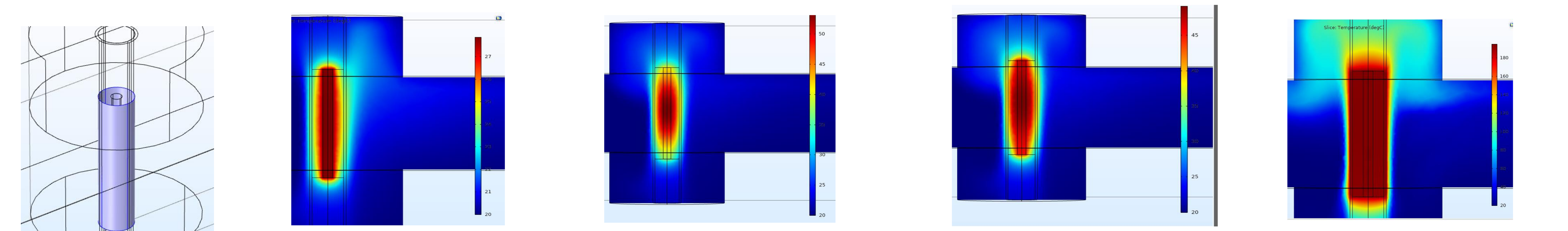
Effect of Tuning Short Position

- Tuning short maximize the e-field in the catalyst bed
- T changes with change in tuning short position
- Changing short position affects standing wave pattern
- 0.12 is the optimum position for Mo-ZSM-5 catalyst in 2m waveguide at 2450 MHz
- No effect on T-profile



Annular Catalyst Design to Improve Uniformity

- To increase uniformity of outer catalyst zone, annular design was tested with different materials
- SiC, glass, and Alumina on the inner region and Mo-ZSM-5 on the outer region
- SiC on the outer and Mo-ZSM-5 on the inside resulted in most uniform T profile



Outer region: Mo-ZSM-5
Inner region : SiC
Power in : 25 W for 30 min
Tmax : 27 C

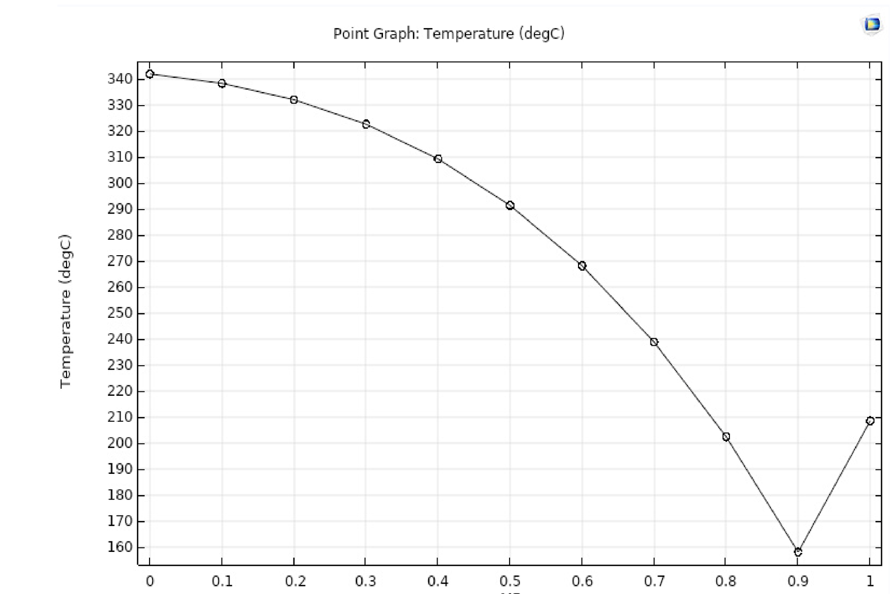
Outer region: Mo-ZSM-5
Inner region : quartz
Power in : 200 W for 30 min
Tmax : 55 C

Outer region: Mo-ZSM-5
Inner region : Alumina
Power in : 200 W for 30 min
Tmax : 50 C

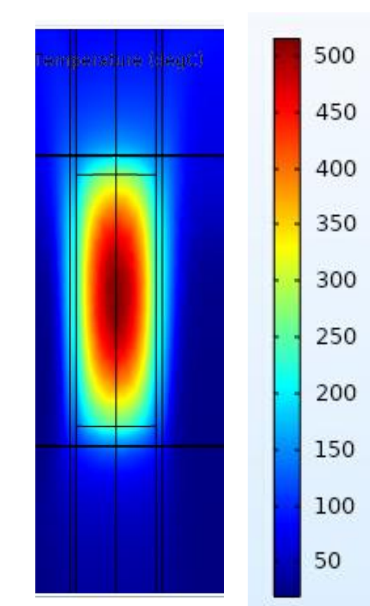
Outer region: SiC
Inner region : Mo-ZSM-5
Power in : 25 W for 30 min
Tmax : 200 C

Mo-ZSM-5 + SiC

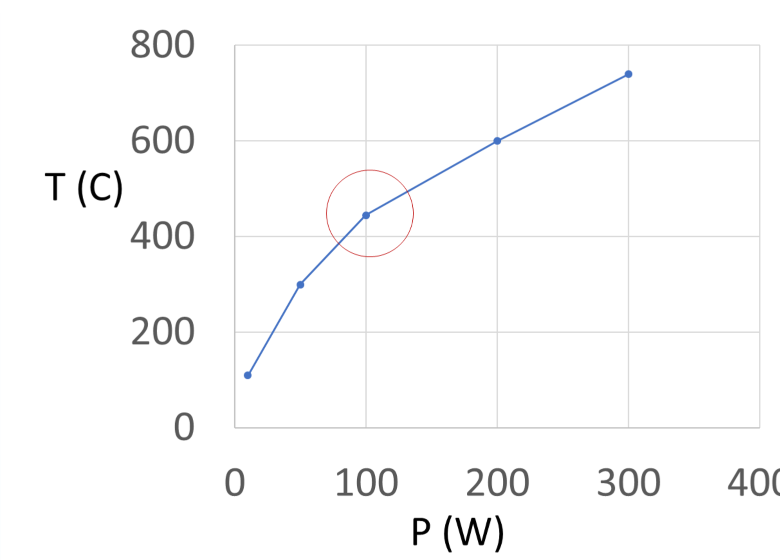
- Catalyst bed 1.5 in long and ID 0.5 in at 100 W
- Highest T at the center of the catalyst bed, non-uniform T
- Adding SiC in small quantities to Mo-ZSM-5 can help
- Dielectric properties calculated by COMSOL from Maxwell – Wagner mixture rule
- Uniform T but lower T achieved compared to SiC at 100 W



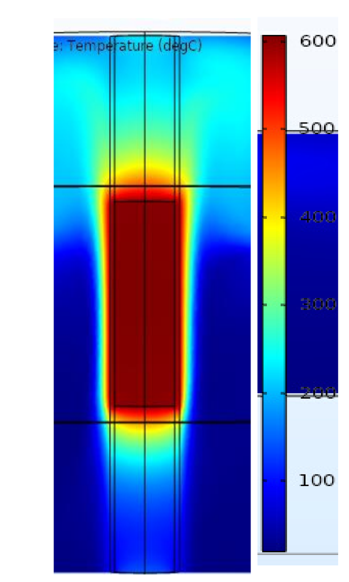
Mo-ZSM-5 Mass Fraction



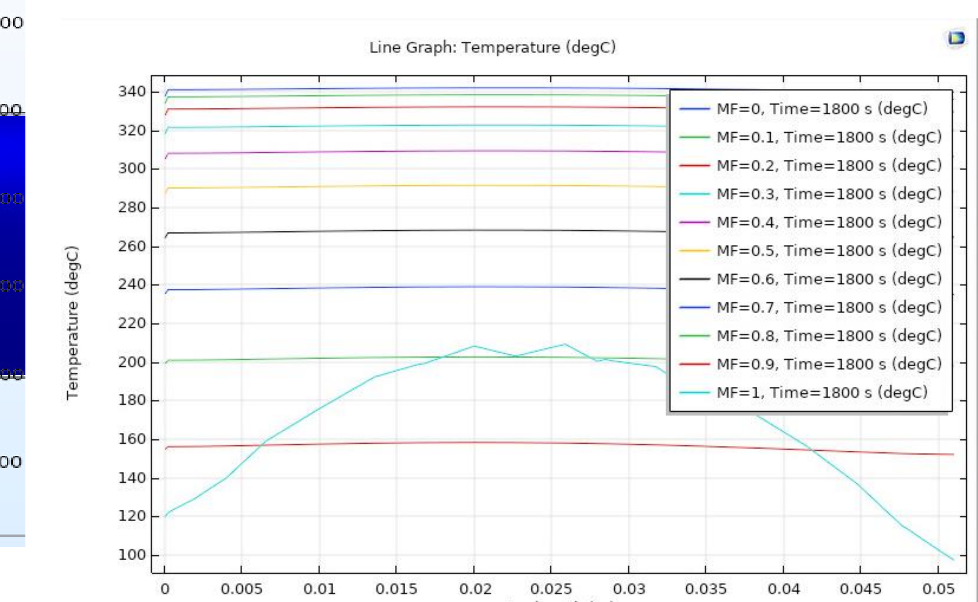
Mo-ZSM-5 T-profile



SiC heating; T vs Power



SiC T-profile



Conclusions

- Microwave reactor geometry has significant impact on T profile in a Mo-ZSM-5 catalyst bed
- Reactor tube diameter should be selected based on material penetration depth
- Tuning short position should be optimized
- Adding SiC and h-field can result in uniform T profile

Disclaimer

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