Implication of COMSOL® to Laser Powered Non-Isothermal Reactors for Pyrolysis in the Gas Phase

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INTRODUCTION: The Infrared Laser Powered Homogeneous Pyrolysis (IR LPHP) is a widely implemented approach in Chemistry [1] to investigate pyrolysis reactions of diverse type of organics. The main advantage of the LPHP reactor is the establishment of a strong homogeneous environment in the gas phase allowing to avoid any unwanted, secondary processes accompanying the pyrolysis of, for instance biomass and its components like cellulose, lignin. These pyrolysis processes occur at non-isothermal conditions and the prediction of the temperature distribution in LPHP reactors are crucial. The objective of this work is to numerically calculate temperature distribution of photochemically sensitized by SF6 pyrolysis of pulverized Lignin in horizontal (or vertical) located LPHP reactors using COMSOL Multiphysics [2].

COMPUTATIONAL METHODS:

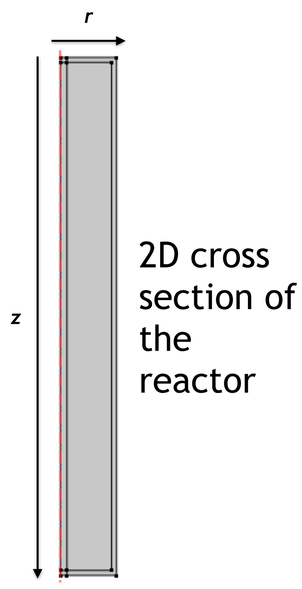
- Heat transfer in fluids module coupled to Laminar flow module is implemented to model the temperature distribution of SF6 in the LPHP reactor
- The temperature is determined by solving the heat equation

$$\partial T/\partial t + D(T)\,\nabla^2 T = Q \quad \Longleftrightarrow \quad \frac{dI}{dz} = -\mu(T) I(z)$$

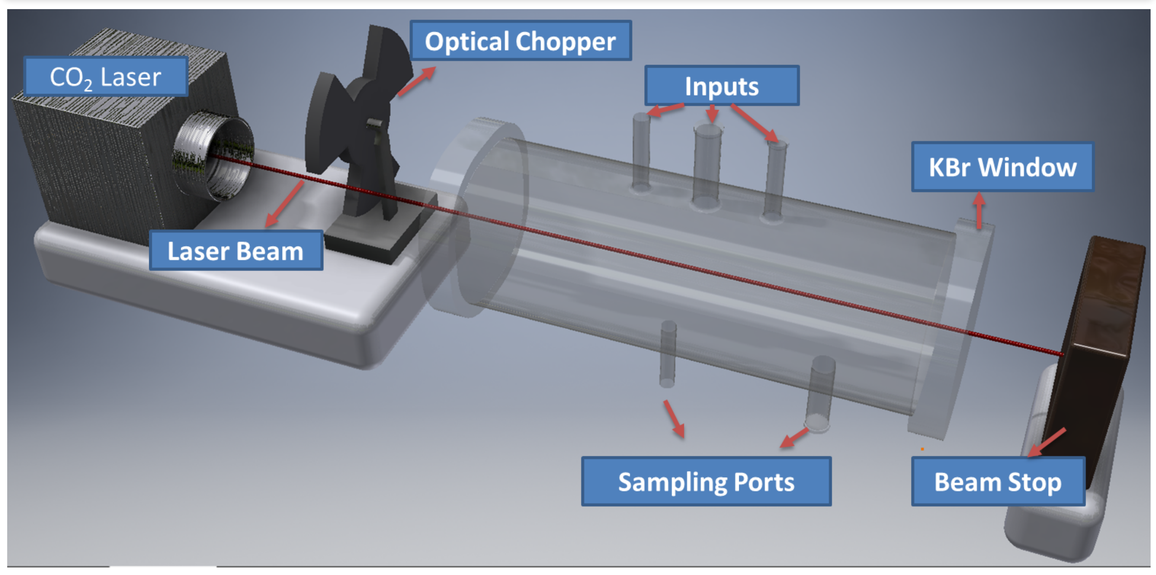
- The heat source is determined through the laser intensity by implementing the General PDE and solving for the intensity of the laser beam
- The heat loss on the surface of the reactor is accounted for through grey body-radiation and external natural air convection
- The laminar flow is used to model the internal convection by including the effect of the gravity
- Because gravity acts along the height of the cylinder, the heat equation is azimuthally symmetric
- This symmetry allows us to model the reactor as a rectangular 2D surface

Variable	Value	Units
SF6 Pressure	8.7	torr
Laser Beam Radius	1.25	mm
Ambient Temperature	300	K
Ambient Pressure	1	atm

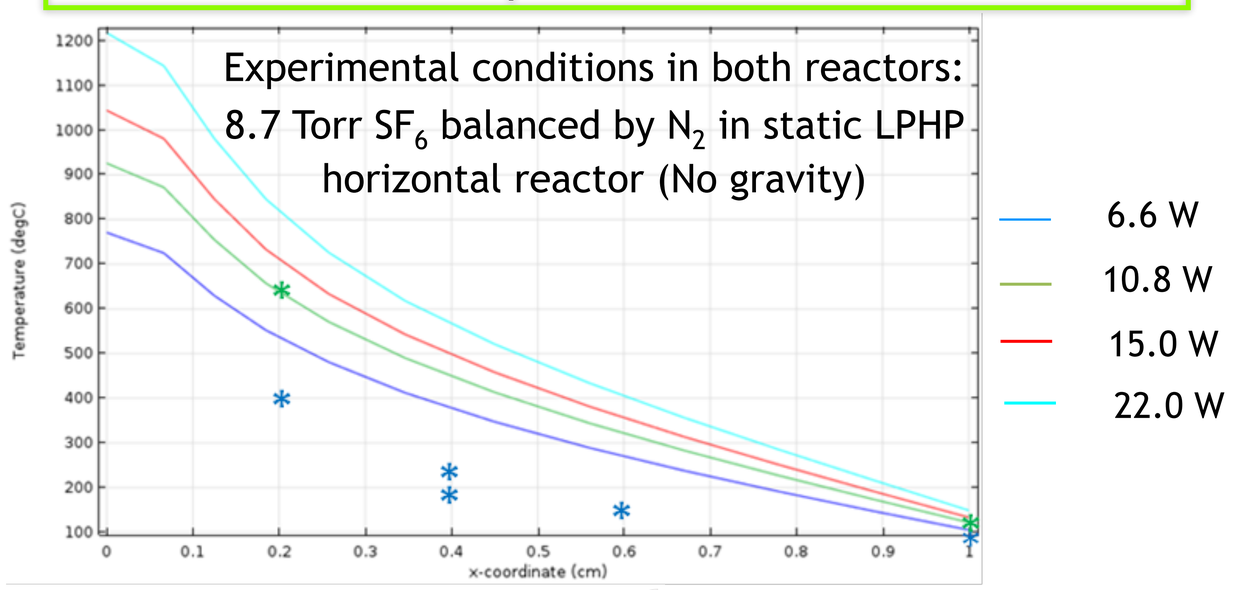
Figure 2. values of the parameters used

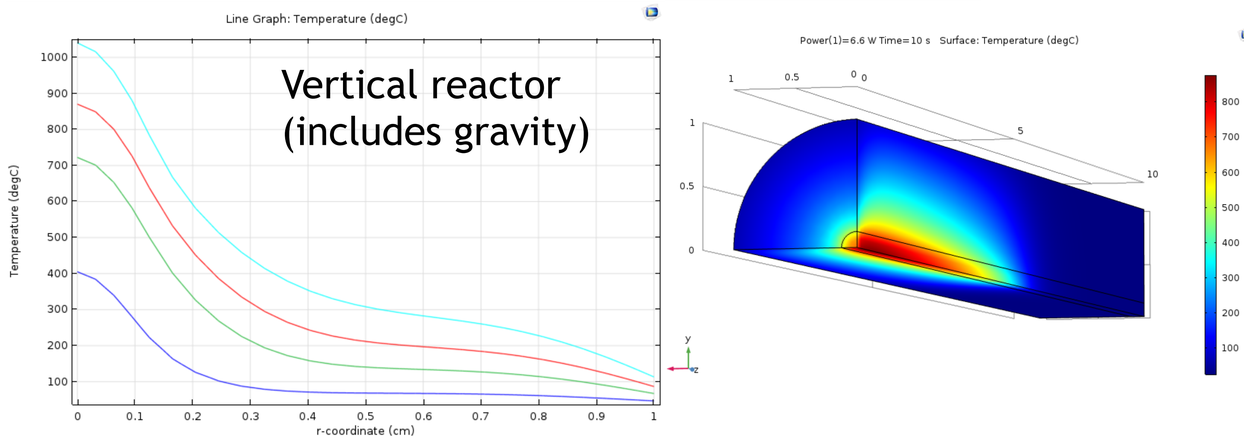


Experimental Setup: Below the LPHP reactor is represented which allows to operate in static (all ports are closed) as well as in flow conditions



RESULTS: The computation was carried out for different laser beam powers.





CONCLUSIONS:

- COMSOL with a reasonable accuracy, predicts the temperature distribution in the horizontal LPHP reactor in accordance with the thermocouple measurements.
- The consideration of convection phenomenon that may cause more accurate calculation in horizontal reactor (in progress) leads large changes in vertical reactor.

REFERENCES:

1. Shaub, W. H.; Bauer, S. H., Laser Powered Homogeneous Pyrolysis. *IEEE Journal of Quantum Electronics* **1975,** *11*, (8), 714-714.
2. Lavrent Khachatryan; Mohamad Barekati-Goudarzi; David Kekejian; Gustavo Aguilar; George G. Stanley; Boldor, D., Pyrolysis of Lignin in the Gas-Phase Isothermal and cw-CO2 Laser Powered Non-Isothermal Reactors. *Energy&Fuels* **2018,** *Submitted*.

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