Prediction of the Temperature Distribution in a Laser Powered Homogeneous Pyrolysis Reactor Using COMSOL Multiphysics

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INTRODUCTION: Laser Powered Homogenous Pyrolysis (LPHP), a non-isothermal wall-less plug flow reactor using cw-IR CO 2 laser heating by fast vibrational–translational (V–T) energy transfer, is a new technique for high temperature pyrolysis in the gas phase with minimal heterogeneous catalytic effect of hot surfaces. In LPHP reactor, the vibrational energy of IR laser is absorbed by the introduction of a photosensitizer gas such as SF_6 to the reacting mixture (N_2 as carrier gas) where it rapidly converts into heat (translational energy) via efficient relaxation processes. The generated heat is then transferred via conduction or collisions between photosensitizer and reagent gases and further convected or distributed in the reactor environment. Due to the small diameter of laser ray in comparison to the LPHP reactor, the hot zone is confined in almost the center of the reactor whereas the walls stay at approximate room temperature. Analysis of temperature distribution in the LPHP reactor then becomes a complex problem as a result of extremely high temperature gradient along the radius of the reactor. Therefore, the application of COMSOL Multiphysics v5.3a to simulate the reactor environment under various experimental conditions such as reactor configuration and dimension, laser power, photosensitizer gas concentration, and carrier gas flow direction can be implemented in order to avoid the unnecessary technical difficulties and experimental errors in direct temperature measurements using thermocouples or other physical tools. A detailed thermal analysis of the gas media with consideration of all heat transfer modules (conduction, convection and radiation) on the temperature distribution was performed under specific flow conditions, in continuation of our previous effort for non-flow condition [1].

COMPUTATIONAL METHODS:

Laminar flow module was coupled with heat transfer in fluids and General PDE modules to determine the temperature distribution of SF_6 gas in LPHP reactor by introducing the heating source through solving the heat equation based on the intensity of the laser beam and Beer-Lambert law.

$$\rho C_p \frac{\partial T}{\partial t} - \nabla \cdot (k \nabla T) = Q = \alpha(T) I \Longleftrightarrow \frac{\partial I}{\partial z} = \alpha(T) I$$

The surface heat loss of the reactor is defined through grey body-radiation and external natural air convection. The effect of the gravity on the internal convection was considered in the laminar flow module.

The laser beam was assumed to have a Gaussian profile (see equations), where *r* is the radial coordinate, *σ* is the radius of the laser beam, 0.9 is transmission coefficient of the KBr window, P is the laser power, and I_0 is the initial laser beam intensity.

$$I = 0.9 I_0 Exp\left(-\frac{r^2}{\sigma^2}\right)$$

$$I_0 = \frac{P}{\pi \sigma^2}$$

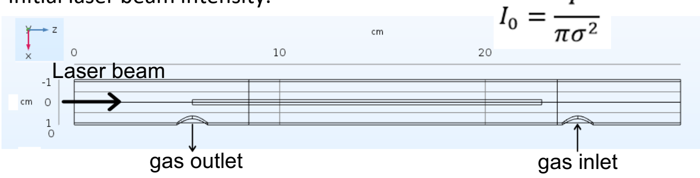

Figure 1. Geometry of the reactor

Variable	Value	Unit
SF_6 content	2%	--
Ambient pressure	1	atm
Ambient Temperature	300	K
Laser Beam radius	1.25	mm
Wall temperature	573.15	K

RESULTS: The computation was performed for various laser beam powers and the results are shown below.

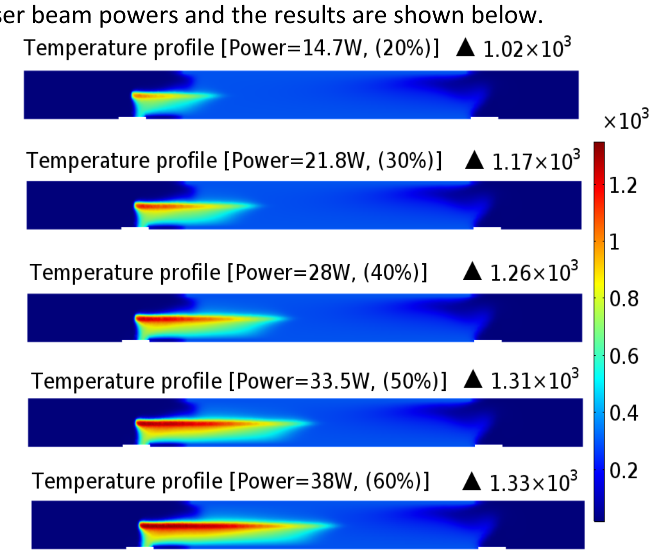

Figure 2. Temperature distribution in the LPHP reactor (in ℃). Maximum values at each power level are indicated next to ▲ symbol).

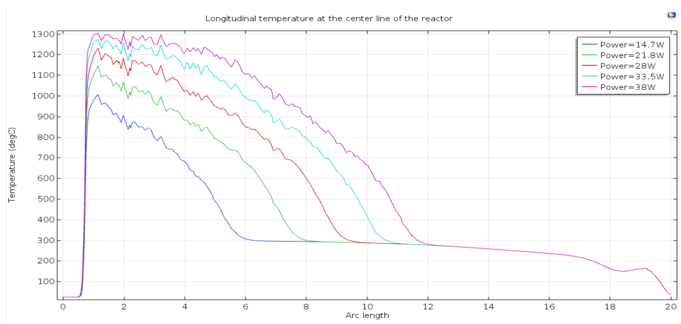

Figure 3. Longitudinal temperature distribution in the LPHP reactor. (Arclenght represents the length of the reactor. Beam entrance is at Arclenght=0). Higher power results in higher temperatures distributed over longer distances in the reactor)

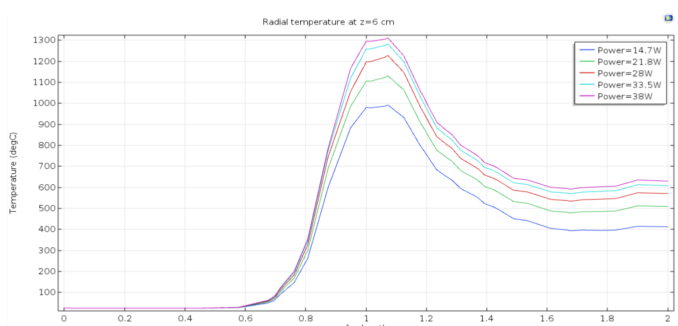

Figure 4. Radial temperature distribution in the LPHP reactor at z=6 cm (Arclength = diameter of the reactor, reactor top: Arclength=0 cm). The effect of the vacuum pulling the gas at the outlet is reflected in the skewed distribution of the temperatures toward the reactor bottom

CONCLUSIONS:

COMSOL predicted the temperature distribution in the LPHP reactor with reasonable accuracy in continuation of the previous study in stagnant condition.

REFERENCES:

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2. L. Khachatryan, M. Barekati-Goudarzi, D. Kekejian, G. Aguilar, R. Asatryan, G. Stanley, D. Boldor, Pyrolysis of Lignin in Gas-Phase Isothermal and cw-CO2 Laser Powered Non-Isothermal Reactors, Energy & Fuels 2018 32 (12), 12597-12606

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