2D Fluid Dynamics Modeling of a Pyrolysis Micro-Reactor

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INTRODUCTION: Plastic solid waste is a large share of accumulating municipal solid waste (MSW). Thermochemical treatment processes are a vital component of a sustainable integrated MSW management since they reduce waste volume significantly. In conjunction with our efforts to develop improved treatment processes, we investigate chemical reaction mechanisms. Our system includes a pyrolysis microreactor that is primarily defined by its ability to isolate initial steps in a high temperature process, which dramatically simplifies analysis of reaction networks. This key feature stems from the brief residence time within the reactor, which can be made short compared to the reaction timescale. We control the upstream flow rate by a mass flow controller (MFC) and the temperature by thermal camera input to a PID loop, while we measure the upstream and the downstream pressures. The outlet flow is supersonic (high Mach number) due to choked flow expansion into vacuum.

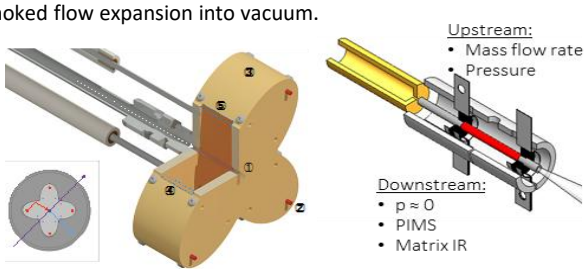

Figure 1. Microreactor design : ① Transparent tube; ② Heating element; ③ Elliptical mirror; ④ Slit for Optical access; ⑤ Second optical axis

COMPUTATIONAL METHODS: We use the thermodynamics interface in the *Chemistry* module of COMSOL to calculate the physical properties of the inlet mixture. These properties are calculated as a function of temperature, pressure, and molar fractions of species. We also use the *High Mach Number Flow, Laminar* module to solve the pressure, velocity, and temperature along the reactor length. The geometry is 2D with a symmetry axis in the center of the reactor. The model solves the mass, momentum and the total energy described by the continuity equation (Navier-Stokes equations):

$$\rho(\mathrm{u}\cdot\nabla)\mathrm{u} = \nabla\cdot[P\mathrm{I}+\mathrm{K}]+\mathrm{F}$$

$$\nabla\cdot(\rho\mathbf{u}) = 0$$

$$\mathrm{d}_z\rho C_p\mathbf{u}\cdot\nabla\boldsymbol{T}+\nabla\cdot\mathrm{q} = \mathrm{d}_z\mathrm{Q}+q_0$$

$$\mathrm{q} = -\mathrm{d}_z k\nabla\mathrm{T}$$

Where:

ρ is the density (SI unit: kg/m³)

u is the velocity vector (SI unit: m/s)

p is the pressure (SI unit: Pa)

F is the volume force vector (SI unit: N/m³)

C_p is the specific heat capacity at constant pressure (SI unit: J/(kg·K))

T is the temperature (SI unit: K)

K is the thermal conductivity (SI unit: W/m/K)

q is the heat flux vector (SI unit: W/m²)

Q contains the heat sources (SI unit: W/m³)

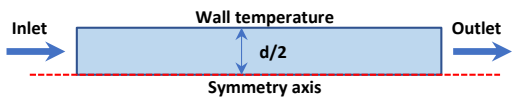

Figure 2. 2D Microreactor geometry

Table 1. Model parameters

Fluid	Inlet flow, [SCCM]	Wall Temp., [°C]
He, Ar, N_2 He-NO mixture @ various compositions	100 - 960	15 - 600

RESULTS: Modeling results obtained for 35 mm long, 1 mm inner diameter microreactor.

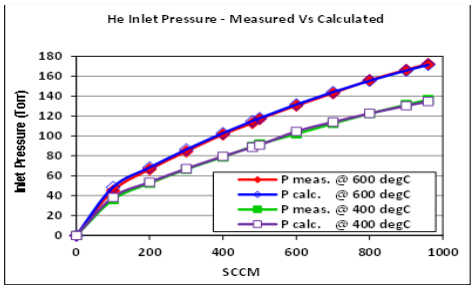

Figure 2. Simulated inlet pressure vs. measured results at two different wall temperature, Helium gas under a flow rate of 960 SCCM

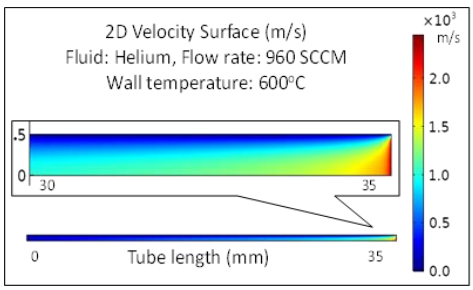

Figure 3. Simulated 2D surface velocity along the tube length

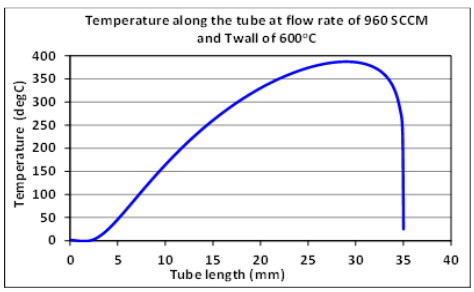

Figure 4. Simulated temperature in the center (R=0) of the reactor, Helium gas under a flow rate of 960 SCCM

Calculation of mixture physical properties: a parametric auxiliary sweep for temperature and NO mass fraction calculates the density, thermal conductivity, heat capacity and the viscosity of the mixture.

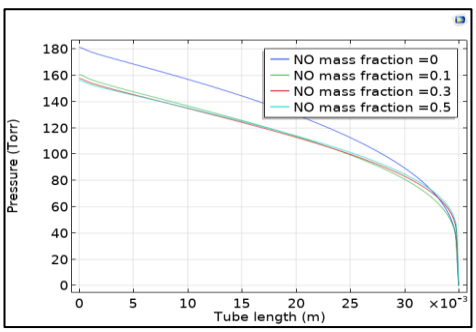

Figure 5. Simulated pressure vs. NO mass fraction

CONCLUSIONS: The model allows us to predict the pressure and the temperature profiles as a function of flow rate and reactor heating. In addition, we can compare different fluids (such as He, Ar and N_2) and mixtures. The model results are in agreement with preliminary experimental results. Incorporating a computational model provides substantial complementary information in support of the experimental data and leads to better understanding of the scientific problem. In addition, it is of great practical assistance for the design of future system setups and tests. In the future we plan to add the model *Reaction Engineering* interface to describe chemical reactions that will take place in the reactor.

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