2D Fluid Dynamics Modeling Of A Pyrolysis Microreactor

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Abstract

Accumulation of plastic solid waste is a large share of municipal solid waste (MSW). Thermochemical treatment processes are a vital component of a sustainable integrated MSW management since they reduce the volume of the waste 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), the temperature by thermal camera input to a PID loop and measure the upstream and the downstream pressures. The outlet flow is supersonic (high Mach number) due to expansion into vacuum.
We use the thermodynamics interface in COMSOL Multiphysics® Chemical Reaction Engineering Module 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 interface 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 allows us to predict the pressure and the temperature profiles as a function of flow rate and reactor heating using a parametric sweep. In addition, we can compare different fluids (such as He, Ar and N2) and mixtures. The model results are in agreement with preliminary experimental results.
In the future we plan to add the model Reaction Engineering interface to describe chemical reactions that will take place in the reactor.
In conclusion, 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.

Figures used in the abstract

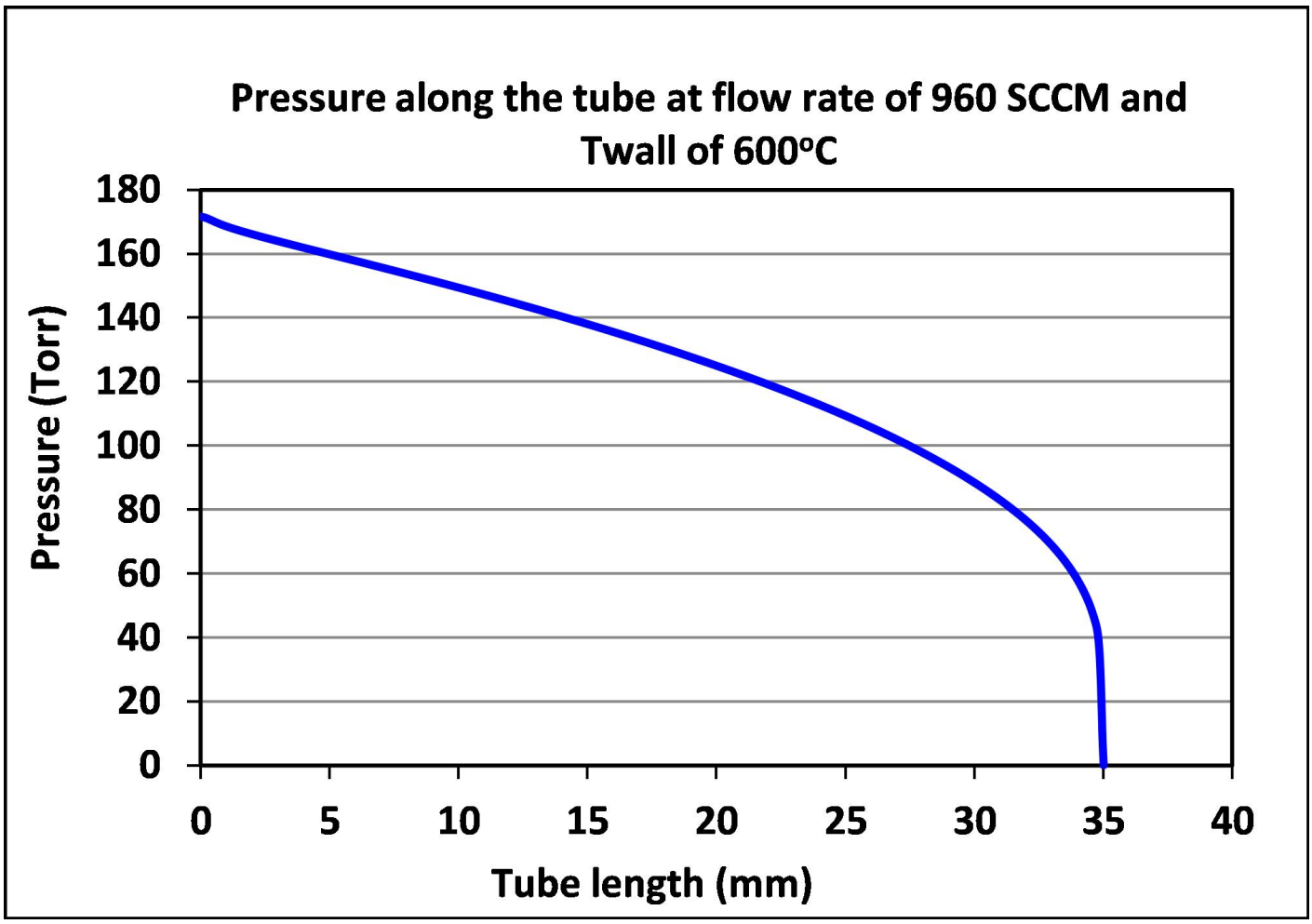

Figure 1 : Modeling results obtained for 35 mm long, 1mm inner diameter micro-reactor in the center (R=0), Helium gas under a flow rate of 960 SCCM: simulated pressure along the tube length

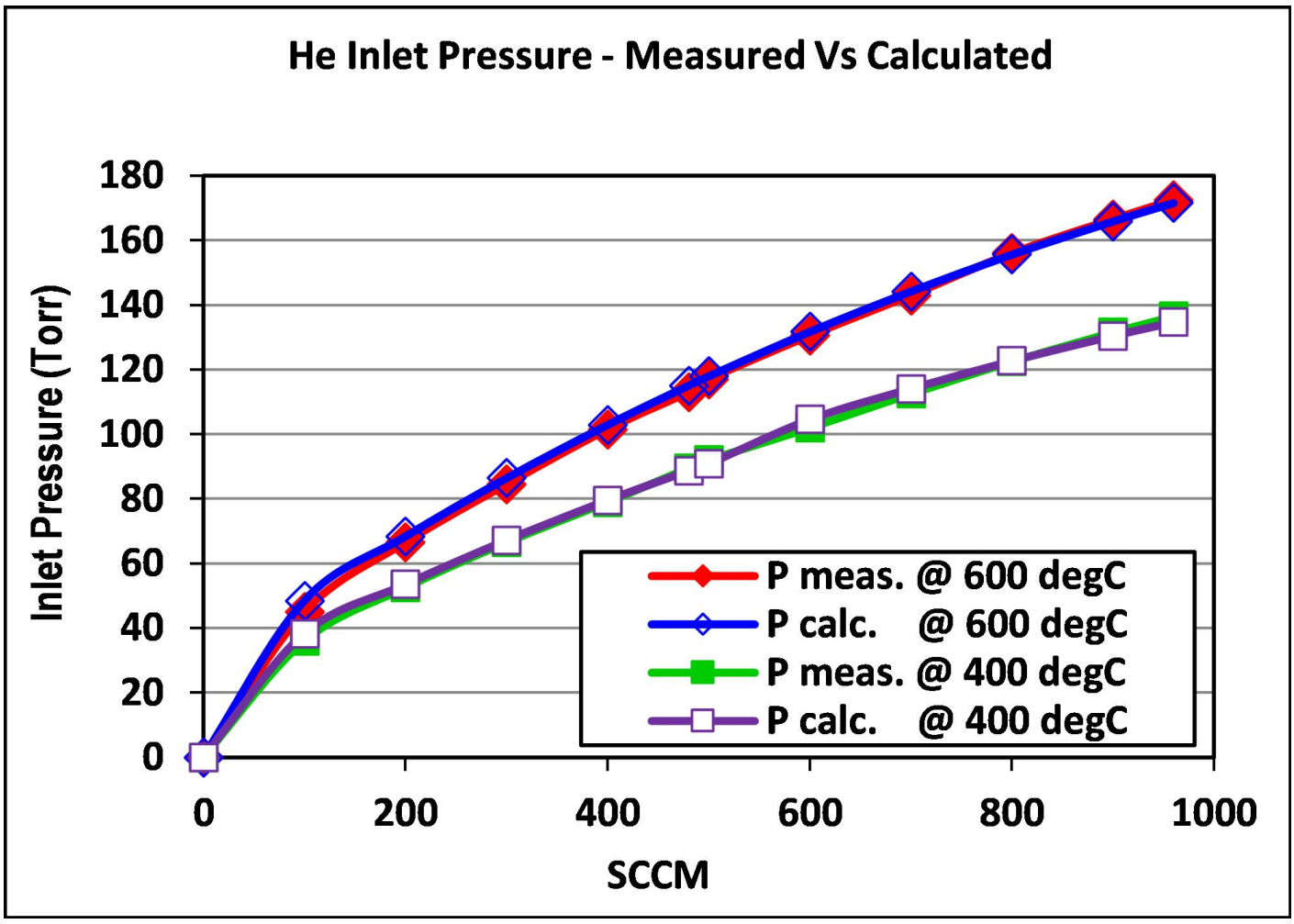

Figure 2 : Modeling results obtained for 35 mm long, 1mm inner diameter micro-reactor in the center (R=0: comparison of measured vs. simulated inlet pressure of Helium gas

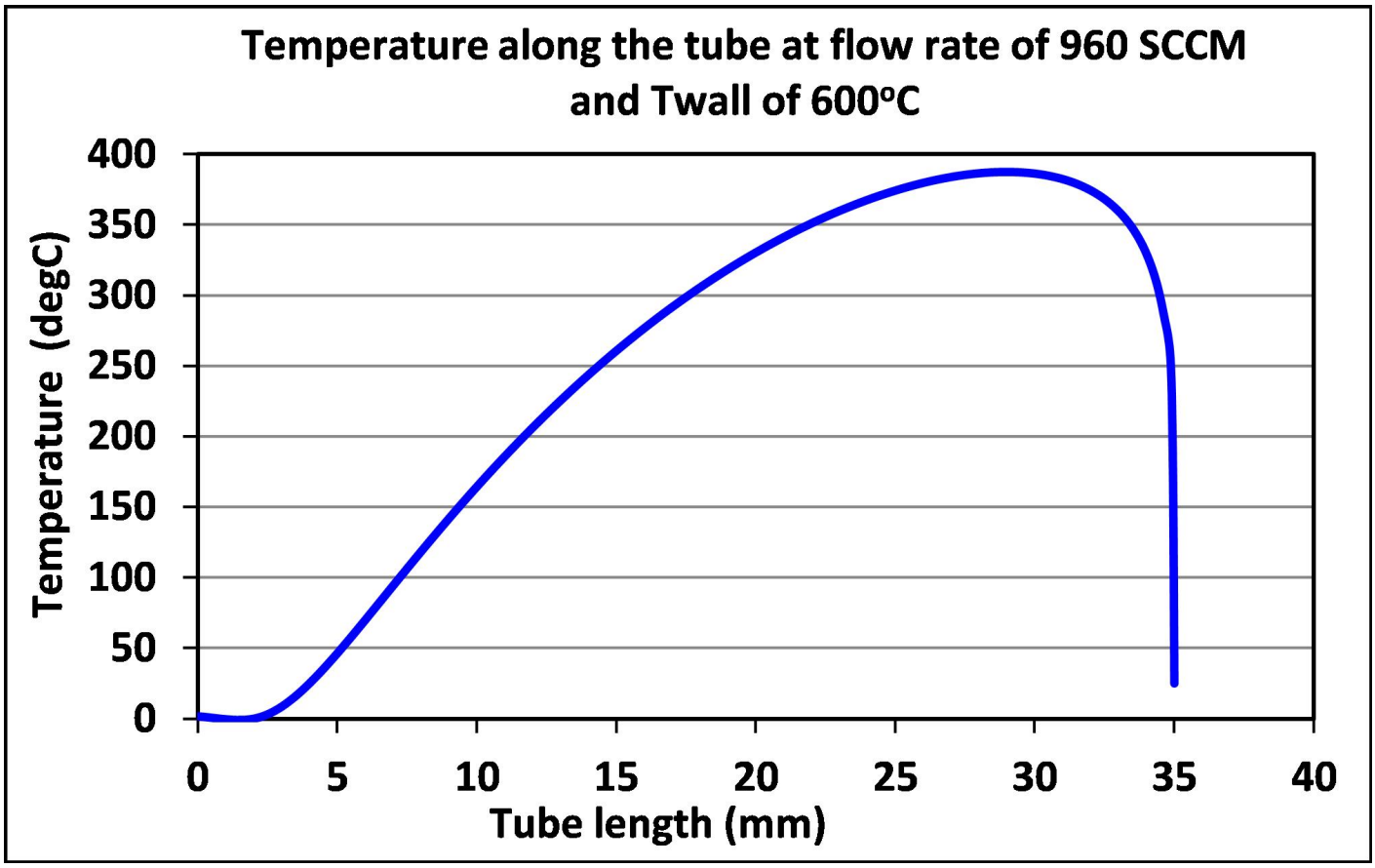

Figure 3 : Modeling results obtained for 35 mm long, 1mm inner diameter micro-reactor in the center (R=0), Helium gas under a flow rate of 960 SCCM: simulated temperature along the tube length

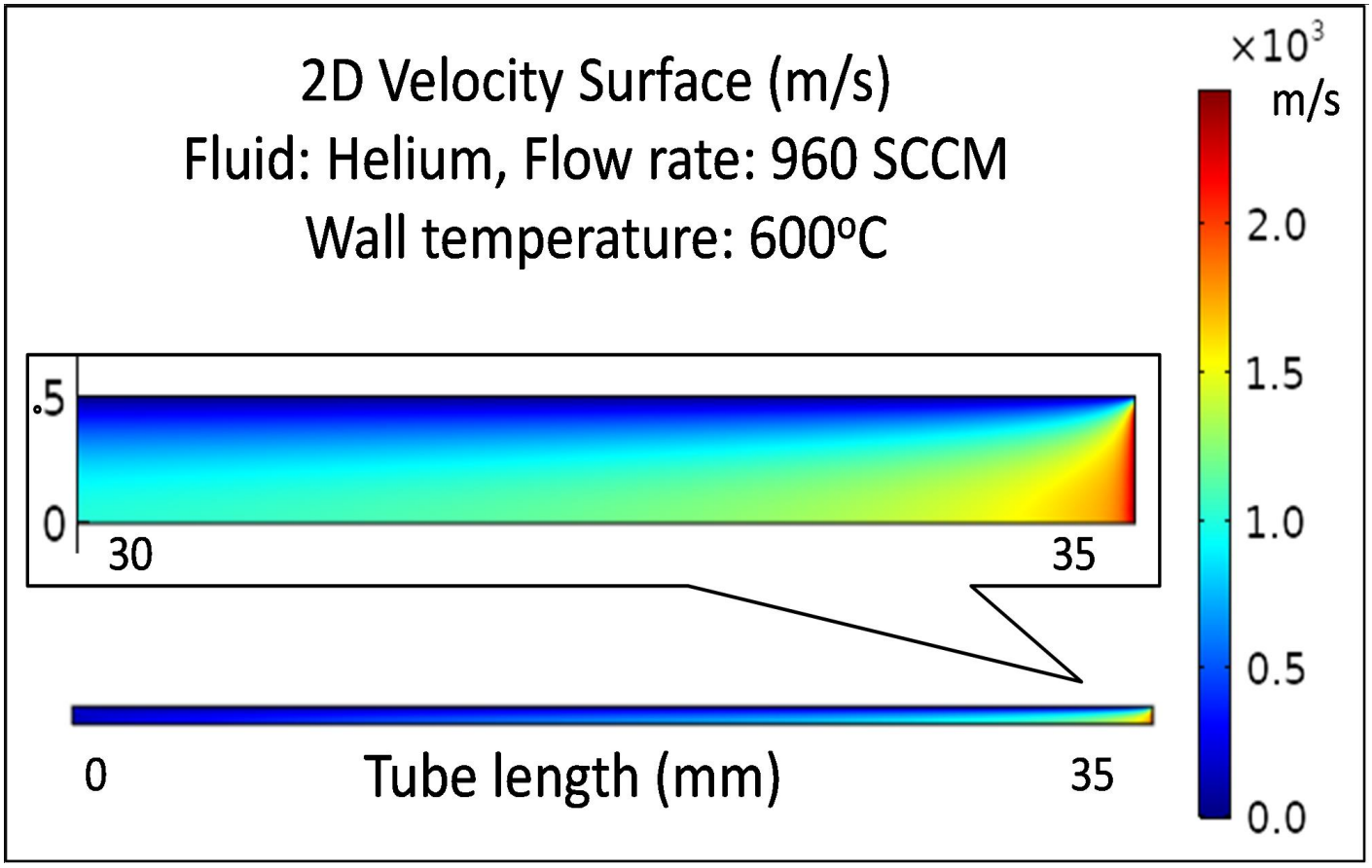

Figure 4 : Modeling results obtained for 35 mm long, 1mm inner diameter micro-reactor in the center (R=0), Helium gas under a flow rate of 960 SCCM: 2D velocity profile