

A Pyroprobe Design For Millisecond Time-Scale Resolution Of Bio-Based Sustainable Reaction Products

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Abstract

Existing commercial pyrolysis systems do not have the capability to perform millisecond-scale temporal analysis of pyrolysis vapors that can provide time-resolved experimental data on the reactive and stable gas-phase intermediates predicted by models based on Density Functional Theory (DFT). To provide this capability, a novel experimental setup was designed by interfacing the probe rod from a CDS Analytical 5200 Series Pyroprobe system with a fast pulsing valve that can introduce micro-mole scale pulses of pyrolysis vapor into a synchrotron-based vacuum ultraviolet photoionization mass spectroscopy (SVUV-PIMS) instrument. Flow simulations for this modified pyroprobe system were performed using COMSOL Multiphysics® to investigate the effect of outlet pressure (50 - 760 Torr) and inlet volumetric flow rate on the flow regime inside the pyroprobe with helium as the carrier gas. The two-dimensional steady-state Navier-Stokes equations were solved using the Fluid Flow Module in COMSOL Multiphysics®. The Concentration of Diluted Species interface was used to solve the unsteady state equations of change from which the outlet gas pulse intensity (normal diffusive flux) was evaluated. The length of the restrictor (0.25 mm ID tubing) required to maintain a constant outlet pressure was estimated by using self-diffusion theory. The results showed that the flow was predominantly in the laminar regime for most of the outlet pressures (200 - 760 Torr) considered in this work. The average residence time (τ) inside the probe was 180 ms for 280 ml/min inlet flow. This millisecond range residence time of the modified pyroprobe would be ideal to interrogate the primary fast pyrolysis reactions by mapping the time evolution profiles of both the nascent reactive and stable intermediates.