3D Material Response Analysis of PICA Pyrolysis Experiments

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Abstract

The PICA decomposition experiments of Bessire and Minton [1] are investigated using 3D material response analysis. The steady thermoelectric equations have been added to the CHAR code to enable analysis of the Joule-heated experiments and the DAKOTA optimization code is used to define the voltage boundary condition that yields the experimentally observed temperature response. This analysis has identified a potential spatial non-uniformity in the PICA sample temperature driven by the cooled copper electrodes and thermal radiation from the surface of the test article (Figure 1). The non-uniformity leads to a variable heating rate throughout the sample volume that has an effect on the quantitative results of the experiment. Averaging the results of integrating a kinetic reaction mechanism with the heating rates seen across the sample volume yield a shift of peak species production to lower temperatures that is more significant for higher heating rates (Figure 2) when compared to integrating the same mechanism at the reported heating rate. The analysis supporting these conclusions will be presented along with a proposed analysis procedure that permits quantitative use of the existing data. Time permitting, a status on the in-development kinetic decomposition mechanism based on this data will be presented as well.

Keywords: Pyrolysis, PICA, Heat Transfer, Non-Equilibrium, CHAR, Thermoelectric

References


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Figure 1: Computational domain and temperature field at end of 25 K/s run.

Figure 2: $H_2O$ gas production rate for Arrhenius model integrated at reported heating rate (dashed lines) and the volume-averaged integration of the same Arrhenius model (solid lines) compared to measured data. Colors denote different reported heating rates.