Implication of COMSOL® to Laser Powered Non-Isothermal Reactors for Pyrolysis in the Gas Phase

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Abstract

The IR CO2 laser powered chemical conversions in the gas phase are intriguing and the researchers' attention was focused on this transformation a while ago. The method, known as Infrared Laser Powered Homogeneous Pyrolysis, or IR LPHP opened reaction pathways not reached by conventional techniques. In a LPHP reactor the energy is absorbed within a vibrational mode of the photosensitizer (mostly SF6), and rapidly converted into heat (translational energy) via efficient relaxation processes. Energy is then transferred to the reagent molecules via collisions mostly in the same manner as in conventional pyrolysis. The small dimensions aid the rapid establishment of a steady state temperature and redistribution of reactants and products in the cell due to elimination of wall effects on the reactions. However, the calculation of temperature distribution in LPHP reactors is a complex problem, involving many factors. The application of COMSOL Multiphysics to model the temperature distribution in the gas phase in LPHP reactor opens new perspectives to accurately predict the temperature profile in horizontally or vertically aligned LPHP reactors at static and dynamic conditions. A detailed analysis of thermal conductivity of the gas media with and without thermal gaseous convection on temperature distribution was performed. Different experimental approaches such as direct thermocouple measurements, implication of "chemical thermometer" were applied to validate the COMSOL predictions.