Pyrolis of $C_{10}H_7Br$ in high temperature microreactor: experiment and modelling

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One of the key stages in combustion of compound hydrocarbon fuels is pyrolysis, or thermal decomposition, which initiate and drive the complex chemistry in the combustion. But this phase is quite poorly investigated. One of the promising tools of research that phenomena are high-temperature micro-reactors.

In present work, we investigate experimentally and theoretically the efficiency of bromonaphthalene pyrolysis in high-temperature 'chemical reactor' incorporated into a molecular beam machine equipped with Wiley-McLaren reflectron time-of-flight mass spectrometer. The principal part of the apparatus is a gas-flow tube made of SiC with an internal diameter of 1 mm, with a total length of 38 mm. The length of the section of the micro-reactor with the zone of ohmic heating up to 1300-1500 K is 13.2-33.2 mm from the entrance. The analysis of pyrolysis products was carried out with the help of PIMS. Theoretical calculation of the distribution of temperature, pressure, flow rate in the micro-reactor were carried out using the Comsol Multiphysics package [1]. The following processes were simultaneously modelled: the electric current and ohmic heating, the Navier-Stokes and heat transfer problems, the kinetics of the pyrolysis process. Reaction rates constants for the $C_{10}H_7Br$ dissociation were calculated using variable reaction coordinate transition state theory VRC-TST with help of ROTD [2] and MESS [3] software.

Calculations demonstrated high values of the temperature, pressure and velocity gradients in axial direction. Intensive pyrolysis took place in the 20-27 mm zone from the gas inlet of the SiC micro-reactor, in which the gas temperature was more than 1400 K, the gas velocity varied from 200 m/s to 400 m/s, the pressure dropped from 55 Torr to 30 Torr. The residence time of the gas in this zone was about 50 μs. Closer to the reactor outlet there was a sharp drop in pressure, temperature and acceleration of the gas flow, which practically led to the cessation of pyrolysis of bromonaphthalene. According to calculations, the efficiency of pyrolysis of bromonaphthalene was 16% at temperature of 1500K. The increase in temperature to 1600K led to an increase in pyrolysis efficiency to 56%. The result obtained is in satisfactory agreement with the experimental value of 40% pyrolysis efficiency at a micro reactor temperature of about 1500K.

1. COMSOL, Inc., Comsol multiphysics. https://www.comsol.com.
2. Y. Georgievskii, S.J. Klippenstein, Transition state theory for multichannel addition reactions: multifaceted dividing surfaces, J. Phys. Chem. A 107 (2003) 9776-9781.
3. Y. Georgievskii, S.J. Klippenstein, Master Equation System Solver (MESS), 2015, http://tcg.cse.anl.gov/papr.