Single-pulse shock tube investigation on the pyrolysis of n-heptane and benzene

A. Hamadi, W. Sun, S. Abid, N. Chaumeix, A. Comandini

Institut de Combustion Aérothermique Réactivité Environnement (ICARE) - CNRS
1C Avenue de la Recherche Scientifique, 45071 Orléans, France

Among the different detection techniques used to perform kinetic studies with conventional shock tubes (ST), gas chromatography (GC) and mass spectrometry (MS) have been widely implemented for the measurement of stable intermediates from the pyrolysis and the oxidation of fuel components and mixtures[1-2]. In the present work, the single-pulse operation of a new ST-GC/MS facility is tested. First, the effects of the dump tank and the buffer gas on the pressure profiles will be presented. The facility was also used to study the thermal decomposition of n-heptane behind reflected shock waves under highly-diluted, pyrolytic conditions (100 ppm of n-heptane in argon bath gas), for temperatures between 900 K and 1900 K, nominal pressures of 10 bar, and reaction times of around 4 ms. The experimental profiles for both the decomposition of n-heptane and the formation of the main intermediate compounds are in good agreement with the simulation results obtained with recent chemical kinetic models. n-Heptane chemistry has been widely studied for decades now and the kinetic models have reached high level of accuracy, thus this first part of the study constitutes a validation of our experimental set-up. Additional experiments were performed on the pyrolysis of benzene at similar conditions to the ones considered for n-heptane. In particular, the work will focus on the formation of polycyclic aromatic hydrocarbons (PAHs), including biphenyl, acenaphthylene, indene, and naphthalene. The data will be analyzed using kinetic modeling and mechanisms for the PAH formation will be tested and proposed.

References

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2. Shock Waves in Chemistry; Lifshitz, A., Ed.; Marcel Dekker, New York, 1981.