UNIFIED KINETIC MODEL OF SOOT FORMATION DURING PYROLYSIS AND OXIDATION OF ALIPHATIC AND AROMATIC HYDROCARBONS IN SHOCK WAVES

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Abstract: Experimental and kinetic simulation studies on soot formation and product distribution for the pyrolysis and oxidation of a number of aliphatic (C_2H_2, C_2H_4, C_2H_6, CH_4, C_3H_8, and C_3H_6) and aromatic (benzene, toluene, and ethylbenzene) hydrocarbons over a temperature range of 1500–2800 K behind reflected shock waves are performed. Along with the experimental measurements of the soot yield and the temperature of soot particles, a direct comparison of the experimentally measured and calculated product distributions for the pyrolysis and oxidation of various hydrocarbons was carried out. The proposed unique detailed kinetic model of soot formation, according to which soot precursors are formed from both aromatic and unsaturated aliphatic hydrocarbons, quantitatively describes the authors' experimental results on soot formation. All kinetic parameters of kinetic model are kept constant. The kinetic parameters are adjusted only once, for a 4.8% C_2H_2/95.2% Ar mixture.

Keywords: soot formation; shock tube; pyrolysis and oxidation of hydrocarbons; kinetic simulation

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