EFFECT OF H_2 AND CO ADDITIVES ON THE PROCESS OF SOOT FORMATION DURING PYROLYSIS OF ETHYLENE AND METHANE

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Abstract: The effect of H_2 and CO additives on the formation of soot nuclei and soot particles during the pyrolysis of ethylene and methane in experiments behind reflected shock waves is considered. A direct comparison of the experimental results obtained in the shock tube with the results of kinetic simulations of the soot formation process according to the kinetic model of soot formation developed by the present authors has been carried out. Comparison of experiments and simulations has shown a significant decrease in the volume fraction and soot yield during pyrolysis of ethylene and methane when hydrogen is added to the reaction mixture. A detailed kinetic mechanism of the influence of hydrogen on the soot formation process has been established. The presence of hydrogen leads to a noticeable decrease in the concentration of soot nuclei and soot particles, without changing the mechanism of their surface growth and the induction period of the soot formation process. When CO is added, it is not involved in the chemical mechanism of soot formation but acts only as a diluent gas, without affecting the soot yield.

Keywords: pyrolysis; methane; ethylene; soot; shock waves; soot formation mechanism

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Figure Captions

Figure 1 Experimentally measured in [3] (*1*) and calculated by the authors using a unified kinetic model of soot formation [4] (*2*) time dependences of the soot volume fraction for mixtures of $2\%C_2H_4 + Ar$ ($T_5 = 1993$ K and $p_5 = 4.65$ bar) (*a*), $2\%C_2H_4 + 0.5\%H_2 + Ar$ ($T_5 = 1994$ K and $p_5 = 4.48$ bar) (*b*), and $2\%C_2H_4 + 1\%H_2 + Ar$ ($T_5 = 1995$ K and $p_5 = 4.58$ bar) (*c*)

Figure 2 Experimentally measured in [3] (filled signs) and calculated using a unified kinetic model of soot formation [4] (empty signs), temperature dependences of the soot yield for a reaction time of 2 ms for mixtures of $2\%C_2H_4 + Ar$ (*1*), $2\%C_2H_4 + 0.5\%H_2 + Ar$ (*2*), and $2\%C_2H_4 + 1\%H_2 + Ar$ (*3*): curves — approximations of experimental points

Figure 3 Calculated temporal dependences of the concentration of soot particle nuclei (*1*) and total concentration of particles (nuclei + soot particles) (*2*) for mixtures of $5\%C_2H_4 + Ar$ (*a*) and $5\%C_2H_4 + 10\%H_2 + Ar$ (*b*), $T_5 = 2300$ K, $p_5 = 5$ bar, and reaction time of 2 ms

Figure 4 Contribution of the main reactions of formation and consumption of soot particle nuclei CH[ ] for mixtures of $5\%C_2H_4$ (*a*) and $5\%C_2H_4 + 10\%H_2$ (*b*) in argon at temperature and pressure behind the reflected shock wave $T_5 = 2300$ K and $p_5 = 5$ bar

Figure 5 Calculated temporal dependences of the concentration of soot particle nuclei (*1*) and total concentration of particles (nuclei + soot particles) (*2*) for mixtures of $10\%CH_4 + Ar$ (*a*) and $10\%CH_4 + 10\%H_2 + Ar$ (*b*), $T_5 = 2600$ K, $p_5 = 5$ bar, and reaction time of 2 ms

Figure 6 Contribution of the main reactions of formation and consumption of soot particle nuclei CH[ ] for mixtures of $10\%CH_4 + Ar$ (*a*) and $10\%CH_4 + 10\%H_2 + Ar$ (*b*) at $T_5 = 2600$ K, $p_5 = 5$ bar, and reaction time of 2 ms

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