EFFECT OF SYNGAS COMPOSITION ON ITS IGNITION IN THE TEMPERATURE RANGE $T \leq 1000$ K

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Abstract: Analysis of the dependence of the self-ignition delay of syngas on its composition in the temperature range $T \leq 1000$ K on the basis of available experimental results and kinetic modeling has shown that the ignition of syngas up to a concentration of $[\mathrm{CO}] \approx 80\%$ in it is mainly determined by the process of hydrogen ignition. In the range from 800 to 1000 K, there is a transition from a low-temperature to a high-temperature ignition mechanism determined by the corresponding transition in the hydrogen oxidation mechanism. In the low-temperature part of this range, an increase in the concentration of CO has a promotional effect and in the high-temperature part — an inhibitory effect. In the low-temperature part of the studied range, an increase in pressure to 10 atm significantly increases the ignition delay but with a further increase in pressure, its gradual decrease is observed. In the high-temperature part of this range, an increase in pressure monotonically reduces the ignition delay. The unavoidable presence in the syngas of almost any composition of hydrogen and unreacted hydrocarbons makes the ignition delay time not very sensitive to the presence of water vapor, carbon dioxide, nitrogen, and other chemically inactive diluents. Their role at these relatively low temperatures is manifested in an increase in the heat capacity of the mixture and their effectiveness in recombination and dissociation reactions.

Keywords: syngas; hydrogen; carbon monoxide; ignition delay; shock waves; kinetic modeling

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Figure Captions

Figure 1 Comparison of experimental results (signs) on the temperature dependence of the self-ignition delay of syngas and its calculation (curves) by various mechanisms: (*a*) syngas $80\%\,\mathrm{CO} + 20\%\,\mathrm{H_2}$, $P = 2.6$ atm (according to [7]); and (*b*) syngas of various compositions, $P = 20$ atm (according to [9])

Figure 2 Temperature dependence of the self-ignition delay time for compositions with different CO concentration ((*a*) 0%; (*b*) 25%; (*c*) 50%; and (*d*) 75%): curves — calculation for the conditions of a constant volume bomb; *1* — experiment; and *2* — calculation for the conditions of reflected shock waves from [19]

Figure 3 The calculated dependence of the ignition delay time of syngas stoichiometric mixture with air on its composition for the conditions of a constant volume bomb, $P = 1$ atm, and $\varphi = 1.0$: (*a*) $T_0 = 800$ K; and (*b*) $T_0 = 1000$ K

Figure 4 The calculated dependence of the ignition delay time of the syngas of composition $60\,\%(\mathrm{mol.})\,\mathrm{H_2} + 40\,\%(\mathrm{mol.})\,\mathrm{CO}$ on pressure, $\varphi = 1.0$: (*a*) $T_0 = 800$ K, and (*b*) $T_0 = 1000$ K

Figure 5 Kinetics of concentrations of $\mathrm{HO_2}$, H, and OH during ignition of syngas of composition $90\%\,\mathrm{CO} + 10\%\,\mathrm{H_2}$, $\varphi = 0.5$, $T = 1050$ K, and P = 14.9 atm (according to [7])

Figure 6 The effect of water vapor admixture on the ignition of CO (100%) and syngas of composition $95\%\,\mathrm{CO} + 5\%\,\mathrm{H_2}$; $P = 1$ atm; and $\varphi = 0.5$ (according to [7])

Figure 7 Calculation of the temperature dependence of the ignition delay time at $P = 1$ atm of stoichiometric mixture of syngas $60\%\,\mathrm{H_2} + 40\%\,\mathrm{CO}$ with air (*1*), the same mixture with the addition of $\sim 13\%\,\mathrm{CO_2}$ (*2*), and the same mixture with the addition of $\sim 13\%\,\mathrm{H_2O}$ (*3*)

Table Captions

Table 1 Composition of the mixtures under study (%(mol.))

Table 2 Autoignition delay time (s)

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