PARTIAL OXIDATION OF A MODEL BIOGAS MIXTURE UNDER ADIABATIC COMPRESSION CONDITIONS

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Abstract: Partial oxidation of a model biogas mixture with a $CH_4/CO_2/N_2$ ratio of 60/30/10 (vol./vol.) was investigated under adiabatic compression conditions. Oxygen was used as the oxidizer at an oxidizer-to-fuel equivalence ratio of $\alpha = 0.4$. Both major (H_2, CO, and H_2O) and minor reaction products, including C_2–C_7 hydrocarbons and C_1–C_2 oxygen-containing organic compounds, were determined. The conversion of the mixtures, calculated based on the total yield of all products, ranged from 1% to 52%. Based on the results of the chemical analysis, a good convergence of the balance for elements C, H, and O was obtained. Kinetic modeling was performed using the NUIG Mech1.3_C2 kinetic mechanism. It was shown that in experiments without ignition, the calculated pressure dependence satisfactorily agreed with the experimental one. In ignition experiments, the pressure rise occurred earlier in time and the pressure reached higher values than in the experiment.

Keywords: biogas; methane; CO_2; ignition; oxidation; adiabatic compression; synthesis gas; hydrogen

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Figure Captions

Figure 1 Pressure dependences during adiabatic compression of the mixture: *1* — driver pressure of 8 atm; *2* — 8.5; *3* — 9; *4* — 9.4; *5* — 9.5, *6* — 9.6; and *7* — driver pressure of 10 atm. The curve numbers *1–7* correspond to the numbers of experiments 1–7

Figure 2 Dependence of residual content of O_2 (*1*), CH_4 (*2*), CO_2 (*3*), and C_2H_6 (*4*) and yields of methane partial oxidation products as a function of maximum compression ratio $\varepsilon_{\max}$ for mixture No. 2: *5* — CO; *6* — H_2O; *7* — C_2H_4; *8* — C_2H_2; *9* — H_2; *10* — benzene; *11* — C_3H_8; *12* — C_3H_6; *13* — methylacetylene; *14* — allene; *15* — CH_3CHO; *16* — CH_3OH; *17* — C_2H_5OH; *18* — methyl formate $HCOOCH_3$; *19* — vinylacetylene; *20* — diacetylene; *21* — n-butane; *22* — isobutane; *23* — 1,3-butadiene; *24* — but-1-ene; *25* — isobutene; *26* — cyclopentadiene; *27* — toluene; *28* — the sum of unidentified C_5–C_7 hydrocarbons; *29* — isopentane; *30* — n-pentane; *31* — $trans$-but-2-ene; *32* — cis-but-2-ene; *33* — pentene sum except 2-methylbut-1-ene; *34* — keten CH_2CO; *35* — ethylene oxide; *36* — 2-methylbut-1-ene; *37* — but-1-yne;, *38* — isoprene; *39* — but-2-yne; *40* — hexane sum except n-hexane; *41* — n-hexane; *42* — neopentane; and *43* — hexene sum

Figure 3 The balance of elements C, H, and O

Figure 4 Conversion degrees of O_2 (*1*), CH_4 (*2*), and CO_2 (*3*) and the conversion degree by total product (*4*) as functions of the maximum compression ratio $\varepsilon_{\max}$

Figure 5 Pressure profiles $P(t)$ of the investigated mixtures at $P_{\text{driver}} = 8.5$ (*a*), 9.5 (*b*), and 10 atm (*c*): experimental pressure (*1*) and calculation results in KinYac (*2*), in Comsol (*3*), in Comsol taking into account the thermal conductivity of the mixture (*4*) (all — at $T_0 = 393$ K), and in Comsol taking into account the thermal conductivity of the mixture at $T_0 = 373$ K (*5*)

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