EFFECT OF HYDROGEN ADDITION ON OXIDATIVE PYROLYSIS OF ETHANE UNDER ADIABATIC COMPRESSION CONDITIONS

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Abstract: The effect of hydrogen addition on the oxidative pyrolysis of ethane under adiabatic compression conditions in the temperature range of 1180–1420 K has been studied. The composition of the investigated mixture (%(vol.)): $C_2H_6/O_2/H_2/N_2 = 2.0/0.7/0.7/96.6$ and oxidizer excess ratio $\alpha = 0.095$. The range of total degrees of conversion is 32.6%–85.2%. The major (ethylene, hydrogen, methane, and CO) and minor reaction products, including soot formation precursors (acetylene and its homologs, C_3–C_5 dienes, and benzene) were determined. No soot was detected in the products. Dependences of reaction product yield on the maximum compression ratio $\varepsilon_{\max}$ and selectivity of products formation on the degree of formation were obtained. It was found that in the gas-phase process, equimolar hydrogen addition relative to oxygen ($H_2/O_2 = 1$) has no significant effect on ethane oxidation, ethane conversion degree, and product yield, while the selectivity of ethylene formation decreases in the whole range of conversion degrees studied.

Keywords: ethane; oxidative pyrolysis; rapid compression machine (RCM); ethylene; hydrogen

DOI: 10.30826/CE24170104 **EDN:** KXRVAP

Figure Captions

Figure 1 Dependence of conversion degree of O_2 (*1*), C_2H_6 (*2*) and by total product (*3*); residual content of O_2 (*4*) and C_2H_6 (*5*); and yields of ethane oxypyrolysis products as a function of maximum compression ratio $\varepsilon_{\max}$: *6* — C_2H_4, *7* — H_2O (on balance), *8* — CO, *9* — CH_4, *10* — H_2, *11* — C_2H_2, *12* — C_3H_6, *13* — 1,3-butadiene, *14* — C_3H_8, *15* — n-butane, *16* — benzene, *17* — but-1-ene, *18* — vinylacetylene, *19* — methylacetylene, *20* — allene, *21* — pent-1-ene, *22* — cyclopentadiene, *23* — the sum of unidentified C_5–C_7 hydrocarbons, *24* — the sum of unidentified C_{8+} hydrocarbons, *25* — trans-but-2-ene, *26* — cis-but-2-ene, *27* — trans-pent-2-ene, *28* — cis-pent-2-ene, *29* — 3-methylbut-1-ene, *30* — cyclopentene, *31* — 2-methylbut-2-ene, *32* — 2-methylbut-1-ene, *33* — isoprene, *34* — but-1-yne, *35* — but-2-yne, *36* — diacetylene, *37* — isobutene, *38* — isopentane, *39* — isobutane, *40* — n-pentane, and *41* — n-hexane

Figure 2 Selectivity of carbon-containing products of ethane oxypyrolysis with H_2 addition: *6–41* are the same as for Fig. 1

Figure 3 Effect of hydrogen addition on the degree of ethane conversion (*1*) and yield of major products in ethane oxypyrolysis: *2* — C_2H_4; *3* — CO; *4* — CH_4; *5* — C_2H_2; *I* — mixture $C_2H_6/O_2/N_2 = 2.0/0.7/97.3$; and *II* — mixture $C_2H_6/O_2/H_2/N_2 = 2.0/0.7/0.7/96.6$

Figure 4 Effect of hydrogen addition on the ethylene selectivity in ethane oxypyrolysis. Homogeneous simulation [9]: *1* — mixture $C_2H_6/O_2 = 2/1$; *2* — mixture $C_2H_6/O_2/H_2 = 2/1/1$; experiment (adiabatic compression): *3* — mixture $C_2H_6/O_2/N_2 = 2.0/0.7/97.3$ [16]; and *4* — mixture $C_2H_6/O_2/H_2/N_2 = 2.0/0.7/0.7/96.6$ (this work)

Acknowledgments

The work was carried out under the State Order for TIPS RAS.

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Received December 13, 2023

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