OXIDATION AND COMBUSTION OF FUEL-RICH *N*-BUTANE–OXYGEN MIXTURE IN A STANDARD 20-LITER EXPLOSION VESSEL

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ABSTRACT

Experiments on forced ignition of extremely fuel-rich n-butane–oxygen mixture with the equivalence ratio of 23 in the standard 20-liter spherical vessel at elevated initial pressure (4.1 bar) and temperature (500 K) reveal the nonmonotonic influence of the forced ignition delay time (IDT) on the maximum explosion pressure and the maximum rate of pressure rise [1].

The objective of the study reported herein is better understanding of oxidation and combustion of such a mixture by means of mathematical modeling of the phenomena in the 20-liter vessel, namely, mixing caused by injection of oxygen to n-butane, forced ignition, flame propagation, preflame oxidation, heat transfer, and natural convection. Based on CFD simulations of the mixing process and natural convection of the ignition kernel, as well as on the analyses of the detailed reaction mechanism of n-butane oxidation, laminar flame propagation, and self-ignition, possible explanations for the observed phenomena have been suggested.

The test mixture was found to be flammable. At the initial conditions, the mixture had the laminar burning velocity of about 3.4 cm/s with the temperature of combustion products of 911 K. Its self-ignition was found to exhibit a two-stage behavior with a cool flame and hot explosion arising at about 1000 and 1300 s after oxygen injection termination. Since the burning velocity was very low, mixture combustion in the vessel after forced ignition was affected by buoyancy. The buoyant flame kernel dissipated completely during 1–2 s after ignition. As a result, combustion of the test mixture was always incomplete: a maximal explosion pressure ratio was only 1.6 instead of the thermodynamic value of 6.21. Thus, the nonmonotonic dependence of the maximum explosion pressure on the IDT could be explained primarily by the variation of the mixture laminar burning velocity with increasing the IDT.

The mixture preparation procedure used in [1] implied a possibility of obtaining excessive (as compared to the mean value) oxygen concentration at an IDT between 3 and 100 s. This could be a reason for the first maximum at the explosion pressure curve, obtained at an IDT of about 40 s. Further temporal relaxation of the oxygen mass fraction in the vessel center to the mean value resulted in decreasing the burning velocity and the maximal explosion pressure to the minimal value at an IDT of about 360 s. The subsequent increase in the maximal explosion pressure with the IDT exceeding 360 s could be explained by the growing influence of preflame reactions. The second maximum of the explosion pressure arising at an IDT of 1000 s was seemingly caused by faster flame propagation in the mixture at its forced ignition during the cool-flame conversion. The decrease of the maximal explosion pressure at the IDT exceeding 1000 s was caused by lower reactivity and exothermicity of the mixture passed through cool-flame oxidation.

The results of the study indicate that apparently inflammable mixtures can nevertheless become hazardous depending on the mixture preparation procedure and forced ignition timing.

REFERENCES

[1] A. A. Pekalski, E. Terli, J. F. Zevenbergen, S. M. Lemkowitz, and H. J. Pasman, Combustion Institute Proceedings, **30**, 1133–1139 (2005).