THE LOWEST LIMITS OF NO CONCENTRATIONS AND THE CONDITIONS FOR THEIR ACHIEVEMENT DURING COMBUSTION OF LEAN AND RICH $H_2O/O_2/N_2$ MIXTURES OF METHANE INDUCED BY O_3 AND H_2O_2

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Abstract: The work is devoted to the calculation of the concentration of NO formed during combustion of lean and rich H_2O–air mixtures of CH_4 under controlled chemical ignition by H_2O_2 or O_3. The plug flow reactor and adiabatic conditions are used for the calculations. The concentration of NO is determined at the moment of time corresponding to the exhaustion of fuel and/or O_2. The same moment of time is used as the residence time of the mixture in the combustion chamber. The calculations demonstrate that the lowest yields of NO in lean and rich mixtures are observed in the case of using O_3 for the ignition. According to these calculations, the concentration of NO under the most favorable conditions, from the point of view of decreasing NO emission (the leanest or richest mixtures, the temperature of initial mixtures $T_0 \cong 700$ K), is near 2–3 ppm at the exit of the combustion chamber. These values of NO concentrations correspond to its lower limit which can be achieved during the combustion of CH_4 mixtures with $T_0 \geq 700$ K.

Keywords: NOx; $\tau_{\rm ign}$; H_2O_2; O_3; controlled chemical induction; rich and lean CH_4 air mixtures

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Figure Captions

Figure 1 Example of temperature profile calculated for the initial H_2O–air–CH_4 mixture ($CH_4/O_2 = 0.423$) containing 0.005 m.f. of H_2O_2 and used for the determination of $\tau_{\rm ign}$ as well as the dynamics of T changes (inset) at the moment of CH_4 exhaustion ($T_{\max}$)

Figure 2 Dependence of $T_{\max}$ (*a*) and $\tau_{\rm ign}$ (*b*) upon T_0 and ratio ($[CH_4]/[O_2]$) of initial mixture with 0.005 m.f. of $[H_2O_2]_o$ or $[O_3]_o$; red circles — $T_0 = 700$ K

Figure 3 The dynamics of formation of NO calculated for the stoichiometric (*1*), rich ($CH_4/O_2 = 0.521$ (*2*)), and lean ($CH_4/O_2 = 0.4794$ (*3*) and $CH_4/O_2 = 0.423$ (*4*)) mixtures containing 0.005 m.f. of O_3 at $T_0 = 700$ K

Figure 4 The dynamics of formation of CO and the values of $\tau_{\rm st}$ determined for the stoichiometric (*1*) and lean ($CH_4/O_2 = 0.4794$ (*2*)) mixtures at $T_0 = 700$ K

Figure 5 Dependence of concentrations of $NO_{\rm st}$ (*a*) and $CO_{\rm st}$ (*b*) upon T_0 and ratio CH_4/O_2 of initial mixture calculated at $[H_2O_2]_o = 0.005$ m.f. or $[O_3]_o = 0.005$ m.f. (red circles)

Figure 6 Dependencies of $[NO]_{\tau \rm st}$, $[CH_4]/(T_{\max} - T_0)$, and $\tau_{\rm ign}$ upon composition $[CH_4/O_2]$ and T_0 of initial mixture calculated at $[H_2O_2]_o = 0.005$ m.f. (from bottom to top: 1st sign (○) — 423; 2nd (○) — 0.437; 3rd (▽) — 0.451; 4th (▽) — 0.465; 5th (□) — 0.479; 6th (□) — 0.493; 7th (◊) — 0.5; 8th (◊) — 0.507; 9th (△) — 0.521; 10th (△) — 0.535; 11th (○) — 0.549; and 12th sign (○) — 0.556): *1* — $T_0 = 700$ K; *2* — 750; *3* — 800; *4* — 847; and *5* — $T_0 = 900$ K

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