STUDY OF THE KINETICS OF HIGH-TEMPERATURE OXIDATION OF TETRAHYDROFURAN BEHIND SHOCK WAVES BY ATOMIC RESONANCE ABSORPTION SPECTROSCOPY

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Abstract: This work provides new information on the kinetics of tetrahydrofuran (C_4H_8O) oxidation. Concentration profiles of the formation and consumption of atomic oxygen (O) during tetrahydrofuran oxidation by molecular oxygen (O_2) in a mixture of 10 ppm C_4H_8O + 10 ppm O_2 + Ar in the temperature range 1650–4150 K at pressures 1.6–2.8 bar have been measured and analyzed using Atomic Resonance Absorption Spectroscopy (ARAS). Predictive capabilities of kinetic combustion schemes of Somers *et al.* (2013) and Wu *et al.* (2020) were evaluated on the basis of the obtained experimental data and were also used to find out and study the key reaction pathways determining the oxidation dynamics of fuel mixture under the studied conditions.

Keywords: biofuel; tetrahydrofuran; combustion; oxidation; kinetics; atomic resonance absorption spectroscopy (ARAS); shock tube; shock waves

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Figure Captions

Figure 1 Calibration curves (*1* — 2000 K; *2* — 2200; *3* — 2700; *4* — 3100; *5* — 3600 (verification); and *6* — 4200 K (verification)) of the absolute oxygen concentration $[\mathrm{O}] = f[A]$ in the investigated temperature range (signs): *1* — 2000 ± 50 K; *2* — 2200 ± 50 K; *3* — 2700 ± 50 K; *4* — 3100 ± 50 K; *5* — 3621K (verification); and *6* — 4204 K (verification)

Figure 2 A typical experimental signal in the studied mixture 10 ppm O_2 + 10 ppm C_4H_8O + Ar: *1* — O-atom absorption profile; and *2* — pressure profile behind shock wave ($T_5 = 2924$ K; $p_5 = 1.935$ bar)

Figure 3 Experimental concentration profiles of the formation and consumption of atomic oxygen in a mixture of 10 ppm O_2 + 10 ppm C_4H_8O + Ar at different temperatures and pressures: *1* — $T_5/p_5 = 1642/2.799$; *2* — 1854/2.686; *3* — 2069/2.606; *4* — 2227/2.423; *5* — 2468/2.412; *6* — 2731/2.099; *7* — 3180/1.909; *8* — 3514/1.789; *9* — 3763/1.644; and *10* — $T_5/p_5 = 4157/1{,}609$

Figure 4 Experiments (*1*; *2* — dispersion) and simulated profiles of [O] (*3* — [28]; and *4* — [17]) in a mixture of 10 ppm O_2 + 10 ppm C_4H_8O + Ar at temperatures T_5 = 1642–4157 K and pressures 1.6–2.8 bar: (*a*) $T_5 = 1642$ K, $p_5 = 2.799$ bar; (*b*) $T_5 = 1854$ K, $p_5 = 2.686$ bar; (*c*) $T_5 = 2069$ K, $p_5 = 2.606$ bar; (*d*) $T_5 = 2227$ K, $p_5 = 2.423$ bar; (*e*) $T_5 = 2468$ K, $p_5 = 2.412$ bar; (*f*) $T_5 = 2731$ K, $p_5 = 2.099$ bar; (*g*) $T_5 = 2924$ K, $p_5 = 1.935$ bar; (*h*) $T_5 = 3180$ K, $p_5 = 1.909$ bar; (*i*) $T_5 = 3377$ K, $p_5 = 1.824$ bar; (*j*) $T_5 = 3514$ K, $p_5 = 1.789$ bar; (*k*) $T_5 = 3763$ K, $p_5 = 1.644$ bar; and (*l*) $T_5 = 4157$ K, $p_5 = 1.609$ bar

Figure 5 Analysis of the rate of [O] production by the phases of its active formation (0–400 μs) (*a*) and consumption (400–1000 μs) (*b*) and normalized coefficients of [O] sensitivity for the phases of its active formation (0–400 μs) (*c*) and consumption (400–1000 μs) (*d*), $T_5 = 2069$ K, $p_5 = 2.606$ bar: *1* — [28]; and *2* — [17]

Figure 6 Analysis of the rate of [O] production by the phases of its active formation (0–300 μs) (*a*) and consumption (300–1000 μs) (*b*) and normalized coefficients of sensitivity [O] for the phases of its active formation (0–300 μs) (*c*) and consumption (300–1000 μs) (*d*), $T_5 = 2731$ K, $p_5 = 2{,}099$ bar: *1* — [28]; and *2* — [17]

Figure 7 Analysis of the rate of [O] production by the phases of its active formation (0–300 μs) (*a*) and consumption (300–1000 μs) (*b*) and normalized coefficients of sensitivity [O] for the phases of its active formation (0–300 μs) (*c*) and consumption (300–1000 μs) (*d*), $T_5 = 3514$ K; $p_5 = 1{,}789$ bar: *1* — [28]; and *2* — [17]

Figure 8 Analysis of the rate of [O] production by the phases of its active formation (0–300 μs) (*a*) and consumption (300–1000 μs) (*b*) and normalized coefficients of sensitivity [O] for the phases of its active formation (0–300 μs) (*c*) and consumption (300–1000 μs) (*d*), $T_5 = 4157$ K, $p_5 = 1{,}609$ бар: *1* — [28]; and *2* — [17]

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