DETONABILITY OF BORON- AND ALUMINUM-CONTAINING COMPOUNDS IN AIR, WATER, AND CARBON DIOXIDE

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Abstract: Contrary to the conventional chemical propulsion systems based on the controlled relatively slow (subsonic) combustion of fuel in a combustor, the operation process in pulsed detonation engines (PDEs) and rotating detonation engines (RDEs) is based on the controlled fast (supersonic) combustion of fuel in pulsed and continuous detonation waves, respectively. One of the most important issues for such propulsion systems is the choice of fuel with proper reactivity and exothermicity required for a sustained and energy-efficient operation process. Presented in the paper are the results of thermodynamic calculations of the detonation parameters of boron and aluminum containing compounds (B, B_2H_6, B_5H_9, $B_{10}H_{14}$, Al, AlH_3, $Al(C_2H_5)_3$, and $Al(CH_3)_3$) in air, water, and carbon dioxide. The results demonstrate the potential feasibility of using the considered compounds as fuels for air-, water-, and CO_2-breathing transportation vehicles powered with PDEs and RDEs. As a verification of the reliability of the calculated results, the detonation parameters of diborane, aluminum, and isopropyl nitrate in air were compared with experimental data available in the literature.

Keywords: ramjet; pulsed detonation engine; continuous detonation engine; thermodynamic calculation; detonation speed; detonability; oxidizing environment (air, water, CO_2); boron; diborane; pentaborane; decaborane; aluminum; aluminum hydrate; triethylaluminum; trimethylaluminum; isopropyl nitrate

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Figure Captions

Figure 1 Comparison of calculated (curves with (*1*) and without (*2*) NOx formation) and measured (signs [36, 37]) dependences of the detonation velocity D on the fuel-to-air equivalence ratio Φ for diborane–air mixtures at $P_0 = 0.1$ MPa and $T_0 = 300$ K; *3* — measurements [36] in a 19.1-millimeter tube; *4* — measurements [37] in a 31.8-millimeter tube; and *5* — measurements [37] in a 76.5-millimeter tube

Figure 2 Comparison of calculated (curves) and measured (signs [37]) dependences of the detonation velocity D on the fuel-to-air equivalence ratio Φ for diborane–air mixtures at $P_0 = 0.0025$ MPa (*1*), 0.015 MPa (*2*), and 0.05 MPa (*3*) and $T_0 = 300$ K: open signs — in tube sections of 31.75-millimeter diameter; and filled signs — in tube sections of 76.5-millimeter diameter

Figure 3 Comparison of the measured [37] (signs) hydrogen molar fraction in gaseous detonation products of diborane–air mixtures of different composition with the results of calculations based on the assumptions regarding the composition of detonation products: *1* — equilibrium at $T = T_{\mathrm{CJ}}$ (hot products); *2* — equilibrium at $T = T_0 = 300$ K (cooled products); and *3* — equilibrium at $T = T_0 = 300$ K with the “frozen” composition of boron compounds

Figure 4 Comparison of calculated (curves without (*1*, *3*) and with (*2*) NOx formation) and measured (signs) dependences of the detonation velocity on the initial concentration of aluminum particles in mixtures with air at $P_0 = 0.1$ MPa and $T_0 = 300$ K: *1*, *2*, *4*–*7* — 100% Al in powder (*4* — [46]; *5* — [47]; *6* — [48]; and *7* — [49]); *3* — 95%Al + 5%Al_2O_3 in powder; *8*–*10* — measurements [41] (*8* — Al powder 1650; *9* — 1650(BM); and *10* — 40XD); *11* and *12* — measurements [42] (*11* — Al powder PAP and *12* — UDA); *13* — measurements [44] (Al flakes 36 × 36 × 1 mm); *14* and *15* — measurements [45] (*14* — Al powder 0.1 mm and *15* — 2 mm); gray vertical band shows the stoichiometric concentration of aluminum powder in air, σ_{st}

Figure 5 Comparison of calculated (curves) and measured [74] (signs) dependences of the detonation velocity D on the fuel-to-air equivalence ratio Φ for the IPN–air mixtures at $P_0 = 0.1$ MPa and $T_0 = 373$ K: *1* — calculations of the present authors; *2* — calculations in [74]; and *3* and *4* — measurements in [74] (*3* — between sensors 1 and 2 and *4* — between sensors 2 and 3)

Figure 6 Dependences of TEA properties on temperature for data sets #1 to #6 in Table 7

Figure 7 Calculated dependences of the Chapman–Jouguet (CJ) detonation velocity D_{CJ} on the fuel-to-oxidizer equivalence ratio Φ for the TEA–air ($T_0 = 300$ K) (*a*) and TEA–water ($T_0 = 400$ K) (*b*) mixtures at $P_0 = 0.1$ MPa: *1* — calculations based on the experimental data of SRC for C_p(298 K), S(298 K), and ΔH_f°(298 K); and *2* to *6* — calculations based the experimental data for ΔH_f°(298 K) reported in [66] (*2*), [68] (*3*), [70] (*4*), [67] (*5*), and [69] (*6*). Functions $C_p(T)$, $S(T)$, and $[H(T) - \Delta H_f^*$(298 K)] are taken from [71]

Figure 8 Calculated dependences of the CJ detonation velocity D_{CJ} on the composition of the explosive mixtures TEA–air (*a*), TEA–water (*b*), and TEA–CO_2 (*c*) at $P_0 = 0.1$ MPa and $T_0 = 300$ (*1*); 400 (*2*); 500 (*3*); 600 (*4*); 700 (*5*); 800 (*6*), and 900 K (*7*); calculations are based on the experimental data of SRC for C_p(298 k), S(298 K), and ΔH_f^*(298 K) and functions $C_p(T)$, $S(T)$, and $[H(T) - \Delta H_f^*$(298 K)] taken from [71]

Figure 9 Calculated dependences of the CJ detonation velocity D_{CJ} on the composition of the explosive mixtures of B(s) (*1*), B_2H_6 (g) (*2*), B_5H_9 (l) (*3*), $B_{10}H_{14}$ (s) (*4*), AlH_3 (s) (*5*), Al (s) (*6*), TEA (l) (*7*), and TMA (l) (*8*) with air ($T_0 = 300$ K) (*a*), water ($T_0 = 400$ K) (*b*), and CO_2 ($T_0 = 300$ K) (*c*) at $P_0 = 0.1$ MPa. Calculations are based on the experimental data of SRC for C_p(298 K), S(298 K), and ΔH_f^*(298 K) and functions $C_p(T)$, $S(T)$, and $[H(T) - \Delta H_f^*$(298 K)] taken from [71]

Table Captions

Table 1 Overall reactions of B and Al containing compounds with air

Table 2 Overall reactions of B and Al containing compounds with water

Table 3 Overall reactions of B and Al containing compounds with carbon dioxide

Table 4 The list of species in the detonation products of B, Al, C, H, O, and N containing compounds and the references with their thermodynamic data

Table 5 Standard enthalpy of formation of TEA (liquid)

Table 6 Experimental data for the thermodynamic properties of TEA at normal conditions

Table 7 Data sets of the thermodynamic properties of TEA

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