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Optimization of the Characteristics of High-Energy Materials

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Abstract. In work explored effect of mixed metallic fuel on the thermodynamic and ballistic characteristics of High-Energy Materials (HEMs). Efficiency of mixed metallic fuel estimated in relation to the characteristics of HEMs, containing conventional metallic fuel - aluminum. The main criteria of comparison are the specific impulse and the composition of the combustion products HEMs.

Keywords: perchlorate high-energy materials, mixed metallic fuel, specific impulse, condensed combustion products, hydrogen chloride.

1. INTRODUCTION

Modern HEMs compositions are based on three components: the inert fuel-binder –butadiene rubber SKDM-80; the oxidizer – ammonium perchlorate (AP); metallic fuel – individual metals and mechanical mixtures on their basis [1].

The main energy component of HEMs is the metallic fuel. Metallic fuel determines the energy characteristics of fuels (specific impulse, the temperature in the combustion chamber and at the nozzle outlet) and influences the composition of the gaseous combustion products and the content of condensed substances. Along with energy characteristics the metals and metal-containing substances increases the density of the fuel, which also increases the efficiency of its application in rocket engines based on solid fuel [2].

The main requirements to modern HEMs:

1) specific impulse of not less than 250 c;

2) reduction of the hydrogen chloride (HCl) content in the gaseous combustion products of HEMs in comparison with the systems containing the initial aluminum;

3) minimization of the content of condensed substances in the combustion products of HEMs;

4) optimization of the ratio of fuel mass to the mass of the engine, i.e. the use of heavy metallic fuel.

The efficiency of fuel is dependent on the heat of formation of products of complete oxidation of metallic fuel. Table 1 shows the characteristics of metallic fuels and their oxides, taken from [3].

Table 1. Characteristics of metallic fuels and metallic oxides

	metallic fuel	ρ_{Me}, кг/м^3	Me_nO_m	ρ_{MenOm}, kg/m^3	Q, kJ\kg
1	Al	2.698	Al_2O_3	3.50-4.10	16.137
2	Mg	1.741	MgO	3.20-3.70	15.172
3	B	2.330	B_2O_3	1.84	20.985
4	Si	2.326	SiO_2	2.20-2.65	21.631
5	W	19.270	WO_3	7.00	4.568
6	Ti	4.505	TiO_2	3.84-4.26	11.418

On the basis of values of the densities of the metals and the heat of formation of metallic oxides for further study were selected the metallic fuels aluminum (Al), magnesium (Mg), boron (B), silicon (Si), titanium (Ti) and mixtures based thereon.

2. METHOD OF RESEARCH

The energy and thermodynamic characteristics of HEMs was determined by the results of thermodynamic calculation by software package "Astra-4" [4]. The initial data for thermodynamic calculations are: the content of components in HEMs (wt.%), the equivalent formulas of HEMs and the enthalpies of formation ΔH. The calculations are carried out at a predetermined pressure in the combustion chamber $p_к$ and at the nozzle outlet p_a. The calculations were carried out at a pressure in the combustion chamber 4.0 MPa and at the nozzle outlet 0.1 MPa.

We considered HEMs, containing 15 wt. % metallic fuel with oxidizer excess coefficient (α) equal to 0.5. Table 2 shows the compositions, the equivalent formulas and the enthalpies of formation of investigated HEMs.

Table 2. Composition, the equivalent formula and the enthalpy of formation of HEMs.

№	metallic fuel	Content of components, %			Equivalent formula	ΔH, kJ\kg
		metallic fuel	SKDM-80	AP		
1	Al	15	16	69	$C_{11.527}H_{44.256}S_{0.023}O_{23.589}Cl_{5.897}Al_{5.556}N_{5.897}$	-1908.926
2	Mg	15	17	68	$C_{12.247}H_{45.207}S_{0.024}O_{23.248}Cl_{5.812}Mg_{6.168}N_{5.812}$	-1829.384
3	B	15	11	74	$C_{7.925}H_{39.508}S_{0.016}O_{25.299}Cl_{6.325}B_{13.863}N_{6.325}$	-1980.239
4	Si	15	17	68	$C_{12.247}H_{45.207}S_{0.024}O_{23.248}Cl_{5.812}Si_{5.340}N_{5.812}$	-1829.384
5	Ti	15	17	68	$C_{12.247}H_{45.207}S_{0.024}O_{23.248}Cl_{5.812}Ti_{3.132}N_{5.812}$	-1829.384
6	Al/Mg	7.5/7.5	16	69	$C_{11.527}H_{44.256}S_{0.023}O_{23.589}Cl_{5.897}Al_{2.778}Mg_{3.084}N_{5.897}$	-1908.926
7	Al/B	7.5/7.5	13	72	$C_{9.366}H_{41.407}S_{0.019}O_{24.615}Cl_{6.154}Al_{2.778}B_{6.932}N_{6.154}$	-1951.714
8	Al/Si	7.5/7.5	16	69	$C_{11.527}H_{44.256}S_{0.023}O_{23.589}Cl_{5.897}Al_{2.778}Si_{2.670}N_{5.897}$	-1908.926
9	Al/Ti	7.5/7.5	16	69	$C_{11.527}H_{44.256}S_{0.023}O_{23.589}Cl_{5.897}Al_{2.778}Ti_{1.566}N_{5.897}$	-1908.926
10	Al/Mg/B	5/5/5	14	71	$C_{10.000}H_{44.273}O_{24.273}Cl_{6.068}Al_{1.852}Mg_{2.056}B_{4.621}N_{6.068}$	-1937.452
11	Al/Mg/Si	5/5/5	16	69	$C_{11.429}H_{46.446}O_{23.589}Cl_{5.897}Al_{1.852}Mg_{2.056}Si_{1.780}N_{5.897}$	-1908.926
12	Al/B/Si	5/5/5	14	71	$C_{10.000}H_{44.273}O_{24.273}Cl_{6.068}Al_{1.852}B_{4.621}Si_{1.780}N_{6.068}$	-1937.452
13	Al/Ti/Mg	5/5/5	16	69	$C_{11.429}H_{46.446}O_{23.589}Cl_{5.897}Al_{1.852}Ti_{1.044}Mg_{2.056}N_{5.897}$	-1908.926
14	Al/Mg/B	7/5/3	15	70	$C_{10.714}H_{45.361}O_{23.932}Cl_{5.983}Al_{2.593}Mg_{2.056}B_{2.773}N_{5.983}$	-1923.189
15	Al/Mg/B	3/5/7	14	71	$C_{10.000}H_{44.273}O_{24.273}Cl_{6.068}Al_{1.111}Mg_{2.056}B_{6.469}N_{6.068}$	-1937.452

In the analysis of calculated data focuses on the following characteristics: specific impulse I_{sp}, the combustion temperature in the chamber T_{eq} and at the nozzle outlet T_{ad}, the content of condensed combustion products and hydrogen chloride, the average molar mass of the combustion products.

3. RESULTS AND DISCUSSION

The efficiency of investigated HEMs was determined by the formula

$$K = \frac{B_{Me}}{B_{Al}},$$

where B_{Me} – characteristic of HEMs, containing the investigated metallic fuel; B_{Al} – characteristic of HEMs, containing 15 wt. % aluminum [5].

Table 3 shows the results of thermodynamic calculations of HEMs, containing individual metallic fuel.

Table 3. Thermodynamic characteristics of HEMs, containing individual metallic fuel

	metallic fuel	T_{eq}, K	T_{ad}, K	I_{sp}, sec	K_{Isp}	The average molar mass, g/mol	Content, %		$K_{cond.\ phase}$	K_{HCl}
							condensed phase (Z)	HCl		
1	Al	3051	1733	268	1.00	18.215	28.3	21.5	1.00	1.00
2	Mg	2725	1569	257	0.96	18.954	23.3	18.5	0.82	0.86
3	B	2590	1965	259	0.97	21.359	22.4	20.4	0.79	0.95
4	Si	2944	1636	265	0.99	16.956	32.0	21.1	1.13	0.98
5	Ti	2627	1357	244	0.91	18.954	23.7	21.2	0.84	0.99

Introduction into the fuel 15 wt. % aluminum provides specific impulse at the level 268 seconds and the temperature in the combustion chamber of the order of 3050 K. However, in the combustion products of such fuels contains up to 28 wt. % condensed substances as alumina and up to 21 wt. % hydrogen chloride vapor, which in real conditions leads to a reduction of the specific impulse and contradicts the requirements of ecological purity of combustion products of HEMs.

Magnesium and boron decreases the content of condensed substances on (18-21) % relative to the initial aluminum, and the introduction of silicon increases the content of condensed phase by 13%. Magnesium decreases the hydrogen chloride content in the combustion products by 14%.

Table 4 shows the calculated thermodynamic characteristics of HEMs, containing mixed metallic fuel in the form of a mechanical mixture of different metals.

6-9 – fuel compositions, containing mixtures of double metals in the ratio 1/1, and 10-13 – fuel compositions, containing mixtures of triple metals in the ratio 1/1/1.

Table 4. Thermodynamic characteristics of HEMs, containing mixed metallic fuel

	metallic fuel	T_{eq}, K	T_{ad}, K	I_{sp}, sec	The average molar mass, g/mol	Content, %		$K_{cond.\ phase}$	K_{HCl}
						condensed phase (Z)	HCl		
6	Al/Mg	2896	1664	262	19.164	24.6	17.8	0.87	0.83
7	Al/B	2865	1933	266	19.961	24.6	21.5	0.87	1.00
8	Al/Si	3013	1710	267	17.756	30.2	21.5	1.07	1.00
9	Al/Ti	2878	1573	258	18.806	26.0	21.5	0.92	1.00
10	Al/Mg/B	2855	1765	265	20.245	20.0	14.6	0.71	0.68
11	Al/Mg/Si	2954	1665	267	17.792	28.5	21.2	1.01	0.99
12	Al/B/Si	2877	1852	268	18.517	27.7	21.7	0.98	1.01
13	Al/Ti/Mg	2850	1575	260	18.411	24.5	21.0	0.87	0.98

The results show that the most interesting and effective is the triple mixture Al/Mg/B, taken in the ratio 1/1/1. Application of the triple mixture Al/Mg/B results in a marked decrease of condensed substances (29%) and chlorine compounds in the combustion products (32%) compared with the initial aluminum, which increases ecological purity of combustion products of HEMs. It should be noted that the change of the specific impulse of fuel is insignificantly.

In work performed the optimization of a mixture Al/Mg/B due to the change of the ratios of its components (table. 5).

Table 5. Thermodynamic characteristics of HEMs, containing the triple mixture Al/Mg/B

	Metallic fuel content in HEMs, %			T_{eq}, K	T_{ad}, K	I_{sp}, sec	The average molar mass, g/mol	Content, %		$K_{cond.\ phase}$	K_{HCl}
	Al	Mg	B					condensed phase (Z)	HCl		
10	5	5	5	2855	1765	265	20.245	20.0	14.6	0.71	0.68
14	7	5	3	2881	1687	264	19.469	21.2	16.3	0.75	0.76
15	3	5	7	2728	1808	264	20.074	20.9	11.7	0.74	0.54

One of possible reason of influence of the triple mixture Al/Mg/B in the ratio 3/5/7, i.e. with an excess of boron in relation to magnesium, may be the formation in the combustion wave of magnesium boride, which according to [6] is a combustion catalyst of HEMs.

4. CONCLUSIONS

1. The use of mixed metallic fuel allows to optimize the characteristics of perchlorate HEMs in the predetermined direction.
2. The selection of the initial components of the mixed metallic fuel is advisable to carry out based on the analysis of their effect on the thermodynamic characteristics of HEMs on the predetermined direction.
3. It was established that the use of mixed metallic fuel Al/Mg/B in the ratio 3/5/7 allows to reduce the hydrogen chloride content in 1.9 times and the content of condensed substances by 1.4 times.

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