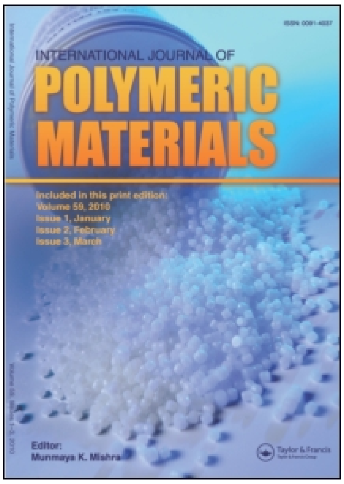

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Effect of Electronic Charge on Oxygen Atom of Oxygen-Containing Oxidizers on Characteristics of Reactive Rocket Fuels

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The calculations of typical oxygen-containing oxidizers of rocket fuels OF_2, O_2, ClO_3F, H_2O_2, N_2O_4, HNO_3, were carried out by quantum chemical semi-empirical MNDO method in Dewar and Teel parameterization with minimization of total energy of molecular system by Davidon-Fletcher-Powell method. The optimized electronic and geometric structure of these oxidizers was obtained. We established correlative dependencies between some parameters of the following reactive fuels ($H_2, N_2H_4, N_2\ H_2(CH_3)_2$ $\sim CH_2 \sim$, $Al\ H_3, B_5H_9, Be\ H_2$): and minimum electronic charge on oxygen atom $q_O^{\min}$ of oxygen-containing oxidizers. The latter being calculated by the MNDO method.

Keywords: Reactive fuels; rockets; oxidizers; electronic charge; quantum chemical calculations; MNDO method

1. BACKGROUND

Typical Oxygen-containing oxidizers of reactive fuels are combinations of the type: OF_2, O_2, H_2O, ClO_3F, N_2O_4, HNO_3 [1]. Despite the existing quantum-chemical calculations of some oxidizers, in

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*Corresponding author.

particular by CNDO/2 method [1, 2], there is not systematic research in this field.

Quantum chemical calculation of oxygen-containing rocket fuels were carried out by classical semi-empiric MNDO method, to determine their optimized electronic and geometrical structure and compare the quantum-chemical parameters, for example; the electronic charge on oxygen atom $q_O^{\min}$ (Tab. I) with parameters of combustion of rocket fuels. These combustion parameters include; specific traction in atmosphere P_1, specific traction in vacuum P_i^{∞}, specific impulse of pressure I_p, combuster temperature T_c, *etc.* (Tabs. II – VII). We expected that

TABLE I The some quantum-chemical parameters of oxygen-containing oxidizers

N	*Oxidizers*	E_0, *kJ/mole*	$q_O^{\min}$
1	OF_2	– 123004	0.146
2	O_2	– 61795	0.0
3	H_2O_2	– 64740	– 0.194
4	N_2O_4	– 163601	– 0.215
5	HNO_3	– 114232	– 0.348

E_0 – the total energy of system.
$q_O^{\min}$ – the minimum electronic charge on oxygen atom.

TABLE II The specific traction in atmosphere – P_1 of some reactive fuels in various oxidizers [5]

			Oxidizers, P_1 *s*			
Fuels	ClO_3F	OF_2	O_2	H_2O_2	N_2O_4	HNO_3
H_2	344.0	412.2	391.1	322.4	340.7	319.7
N_2H_4	295.3	345.9	312.9	286.9	291.1	279.1
$H_2N_2(CH_3)_2$	289.6	352.2	309.7	283.7	285.2	272.4
$—CH_2—$	280.6	351.9	300.1	278.2	275.7	263.4
AlH_3	293.7	326.5	310.8	318.4	300.5	301.3
B_5H_9	299.3	361.6	319.7	309.1	299.3	293.7
BeH_2	309.5	342.9	331.4	353.1	316.1	322.1

TABLE III The specific traction in vacuum – P_i^{∞} of some reactive fuels in various oxidizers [5]

			Oxidizers, P_i^{∞}*s*			
Fuels	ClO_3F	OF_2	O_2	H_2O_2	N_2O_4	HNO_3
H_2	398.7	478.3	456.0	374.8	494.9	370.8
N_2H_4	347.4	408.4	369.7	337.6	342.0	327.4
$H_2N_2(CH_3)_2$	341.8	416.6	368.2	335.9	337.0	321.6
$—CH_2—$	331.9	413.4	358.5	329.8	326.2	312.0
AlH_3	353.6	393.4	375.7	383.1	362.8	363.6
B_5H_9	395.5	433.2	385.2	373.2	359.6	352.3
BeH_2	377.5	417.1	406.5	430.0	384.9	394.8

TABLE IV The specific impulse of pressure – I_p of some reactive fuels in various oxidizers [5]

			Oxidizers, $I_p s$			
Fuels	ClO_3F	OF_2	O_2	H_2O_2	N_2O_4	HNO_3
H_2	219.6	261.3	247.9	205.1	217.7	204.1
N_2H_4	183.0	213.3	192.8	178.8	181.5	174.8
$H_2N_2(CH_3)_2$	178.9	217.8	189.3	174.8	175.9	168.7
$—CH_2—$	173.0	218.5	182.7	171.2	169.7	162.0
AlH_3	177.6	197.4	186.4	192.2	180.7	181.3
B_5H_9	182.0	220.8	193.2	186.9	181.7	178.8
BeH_2	181.5	202.5	195.6	206.9	188.9	190.0

TABLE V The combustor temperature – T_c of some reactive fuels in various oxidizers [5]

			Oxidizers, $T_c^\circ K$			
Fuels	ClO_3F	OF_2	O_2	H_2O_2	N_2O_4	HNO_3
H_2	3003	3547	2977	2419	2640	2474
N_2H_4	3467	4047	3406	2927	3247	3021
$H_2N_2(CH_3)_2$	3657	4493	3608	3008	3415	3147
$—CH_2—$	3720	4716	3686	3006	3438	3147
AlH_3	4061	4340	4301	3834	4179	3993
B_5H_9	4242	5009	4160	2969	3913	3588
BeH_2	3205	3300	3352	3205	2831	3358

TABLE VI The combustor-exit temperature – T_e of some reactive fuels in various oxidizers [5]

			Oxidizers, $T_e^\circ K$			
Fuels	ClO_3F	OF_2	O_2	H_2O_2	N_2O_4	HNO_3
H_2	1288	1622	1355	1050	1106	1043
N_2H_4	1921	2435	1974	1533	1703	1530
$H_2N_2(CH_3)_2$	2114	2705	2280	1731	1966	1746
$—CH_2—$	2221	2670	2457	1745	2016	1838
AlH_3	2904	3200	3232	2707	3090	2914
B_5H_9	2930	3408	2969	2094	2653	2311
BeH_2	2669	2682	2857	2656	2402	2816

TABLE VII The increment of ideal velocity of rocket flight – ΔV of some reactive fuels in various oxidizers [5]

			Oxidizers, $\Delta V m/s$			
Fuels	ClO_3F	OF_2	O_2	H_2O_2	N_2O_4	HNO_3
H_2	2350	2669	2057	2324	2111	2144
N_2H_4	4233	4830	3980	4003	3985	3883
$H_2N_2(CH_3)_2$	4087	4816	3749	3930	3823	3739
$—CH_2—$	4217	5067	3823	4010	3901	3815
AlH_3	4617	5004	4428	4806	4537	4595
B_5H_9	4136	4866	3686	3839	3846	3820
BeH_2	4037	4338	3744	4285	3721	4060

these correlations there parameters will provide guidelines for development of new more efficient fuels, oxidizers for rocket fuels.

2. METHODOLOGY

To calculate the mentioned oxidizers we used MNDO method in Dewar and Teel parameterization [3]. This method gives quite precise values of valent angles and realistic sequence of levels of molecular orbitals. The MNDO calculation also gives adequate results for hydrazine type molecules combinations of fluorine, especially those containing F-O and F-N bonds. The minimization of the total energy of molecular system has been performed by Davidon-Fletcher-Powell method with optimization at all geometric parameters.

The calculations were performed in classical approximation of isolated molecule in a gas phase.

3. RESULTS AND DISCUSSION

The calculated quantum-chemical parameters of oxygen-containing oxidizers (Tab. I) and the electronic charge on oxygen atom, in particular, were compared with the published parameters of burning of reactive fuels (Tabs. II – VI) and correlative dependences between them were established.

Quantum-chemical characteristics of models of oxygen-containing oxidizers of rocket fuels are represented in Table I, and optimal electronic and geometric structure is shown in Figure 1.

The Table I shows that the lowest negative charge on oxygen atom of all investigated models of oxygen-containing oxidizers of reactive fuels is with the nitric acid $q_{\mathrm{O}}^{\mathrm{min}} = -0.348$. The highest (and even a positive) charge on oxygen atom is found with oxygen difluorid $q_{\mathrm{O}}^{\mathrm{min}} = +0.146$. For O_2 oxidizer, the $q_{\mathrm{O}}^{\mathrm{min}} = 0$.

3.1. Specific Traction in Atmosphere (P_1) and in Vacuum (P_i^{∞})

With all considered fuels: H_2, N_2H_4, $H_2N_2(CH_3)_2$, $-CH_2-$, AlH_3, B_5H_9 the OF_2 and O_2 oxidizers are exhibit highest values of specific

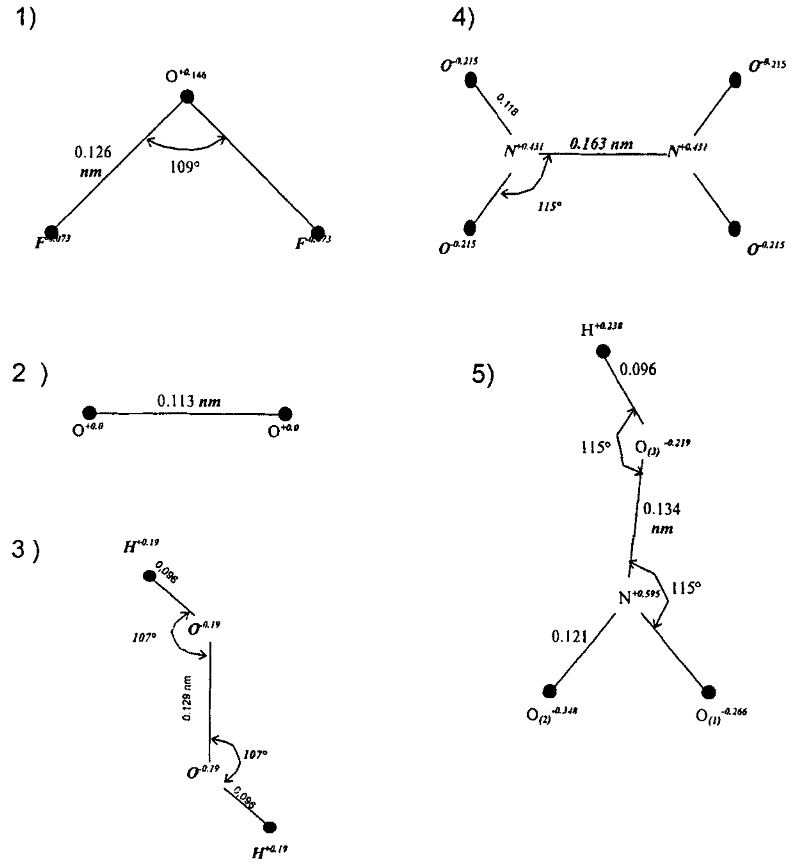

FIGURE 1 The optimal electronic and geometric structure of molecules of oxygen-containing oxidizers of reactive fuels.

traction in atmosphere – P_1 and specific traction in vacuum – P_i^{∞} (Tabs. II, III). The lowest values of P_1 and P_i^{∞} are characteristic for the nitric acid. In addition, the increases of negative charge on oxygen atom $q_{\mathrm{O}}^{\min}$ of oxygen-containing oxidizers leads to decreases of the values P_1 and P_i^{∞}. These findings confirm the merits of correlative relations between parameters of combustion of rocket fuels (Tabs. II, III) and electronic charge $q_{\mathrm{O}}^{\min}$ on oxygen atom calculated by MNDO method (Tab. I).

The analysis of quantum-chemical parameters of oxidizers allowed us to establish that O_2 and OF_2 have the minimum electronic charge on oxygen atom, and moreover for OF_2 $q_O^{min} > 0$. These oxidizers are characterized by the maximum values of specific traction in atmosphere – P_l and specific traction in vacuum – P_i^{∞}.

The comparison of calculated data of oxygen-containing oxidizers (Tab. I) and literature data of parameters of combustion of rocket fuels (Tabs. II, III) showed that there is complex relationship between these parameters and q_O^{min}.

For specific traction in atmosphere – P_l and specific traction in vacuum – P_i^{∞} we obtained the following correlative dependences on q_O^{min} for H_2, N_2H_4, $H_2N_2(CH_3)_2$, —CH_2— and B_5H_9:

$$\mathrm{H_2}\left|\begin{array}{l} P_l = P_l^{\max}[0.919 + 0.575(q_O^{\min}) + 0.383(q_O^{\min})^2], \\ P_l^{\max}(\mathrm{OF_2}) = 412.2\,\mathrm{s.}, R = 0.964 \\ P_i^{\infty} = P_i^{\infty\,\max}[0.922 + 0.571(q_O^{\min}) + 0.341(q_O^{\min})^2], \\ P_i^{\infty\,\max}(\mathrm{OF_2}) = 478.3\,\mathrm{s.}, R = 0.963 \end{array}\right.$$

$$\mathrm{N_2H_4}\left|\begin{array}{l} P_l = P_l^{\max}[0.922 + 0.387(q_O^{\min})], \\ P_l^{\max}(\mathrm{OF_2}) = 345.3\,\mathrm{s.}, R = 0.965 \\ P_i^{\infty} = P_i^{\infty\,\max}[0.923 + 0.341(q_O^{\min})], \\ P_i^{\infty\,\max}(\mathrm{OF_2}) = 408.4\,\mathrm{s.}, R = 0.973 \end{array}\right.$$

$$\begin{array}{c}\mathrm{H_2N_2}\\ \mathrm{(CH_3)_2}\end{array}\left|\begin{array}{l} P_l = P_l^{\max}[0.872 + 0.449(q_O^{\min})], \\ P_l^{\max}(\mathrm{OF_2}) = 352.2\,\mathrm{s.}, R = 0.965 \\ P_i^{\infty} = P_i^{\infty\,\max}[0.909 + 0.454(q_O^{\min})], \\ P_i^{\infty\,\max}(\mathrm{OF_2}) = 416.6\,\mathrm{s.}, R = 0.971 \end{array}\right.$$

$$—\mathrm{CH_2}—\left|\begin{array}{l} P_l = P_l^{\max}[0.872 + 0.671(q_O^{\min}) + 0.966(q_O^{\min})^2], \\ P_l^{\max}(\mathrm{OF_2}) = 351.9\,\mathrm{s.}, R = 0.990 \\ P_i^{\infty} = P_i^{\infty\,\max}[0.900 + 0.484(q_O^{\min})], \\ P_i^{\infty\,\max}(\mathrm{OF_2}) = 413.4\,\mathrm{s.}, R = 0.965 \end{array}\right.$$

$$\mathrm{B_5H_9}\left|\begin{array}{l} P_l = P_l^{\max}[0.902 + 0.501(q_O^{\min}) + 0.744(q_O^{\min})^2], \\ P_l^{\max}(\mathrm{OF_2}) = 361.6\,\mathrm{s.}, R = 0.970 \\ P_i^{\infty} = P_i^{\infty\,\max}[0.907 + 0.482(q_O^{\min}) + 0.658(q_O^{\min})^2], \\ P_i^{\infty\,\max}(\mathrm{OF_2}) = 433.2\,\mathrm{s.}, R = 0.977 \end{array}\right.$$

3.2. Specific Impulse of Pressure (I_p) and Combustor Temperature (T_c)

With all considered fuels: H_2, N_2H_4, $H_2N_2(CH_3)_2$, $—CH_2—$, AlH_3, B_5H_9 the oxidizers OF_2 and O_2 exhibit the highest values of specific impulse of pressure – I_p and combustor temperature – T_c (Tabs. IV, V). The minimum values of I_p and T_c are found with the nitric acid. Note also that the increase of negative charge on oxygen atom $q_O^{\min}$ of oxygen-containing oxidizers leads to a decrease of the values I_p and T_c.

The analysis of quantum-chemical parameters of oxidizers allowed us to establish that O_2 and OF_2 have the minimum electronic charge on oxygen atom, and moreover for OF_2 $q_O^{\min} > 0$. These oxidizers are characterized by the maximum values of specific impulse of pressure – I_p and combustor temperature – T_c.

The comparison of calculated data of oxygen-containing oxidizers (Tab. I) and literature data of parameters of combustion of rocket fuels (Tabs. IV, V) showed that there is complex relationship between these parameters and $q_O^{\min}$.

For specific impulse of pressure – I_p and combustor temperature – T_c we obtained the following correlative dependences on $q_O^{\min}$ for H_2, N_2H_4, $H_2N_2(CH_3)_2$, $— CH_2 —$ and B_5H_9:

$$\mathrm{H_2}\left|\begin{array}{l} I_p = I_p^{\max}[0.919 + 0.559(q_O^{\min}) + 0.390(q_O^{\min})^2],\\ I_p^{\max}(\mathrm{OF_2}) = 261.3\,\mathrm{s.}, R = 0.962\\ T_c = T_c^{\max}[0.837 + 0.907(q_O^{\min}) + 1.478(q_O^{\min})^2],\\ T_c^{\max}(\mathrm{OF_2}) = 3547^\circ\mathrm{K}, R = 0.982 \end{array}\right.$$

$$\mathrm{N_2H_4}\left|\begin{array}{l} I_p = I_p^{\max}[0.924 + 0.356(q_O^{\min})],\\ I_p^{\max}(\mathrm{OF_2}) = 213.3\,\mathrm{s.}, R = 0.961\\ T_c = T_c^{\max}[0.853 + 0.765(q_O^{\min}) + 1.393(q_O^{\min})^2],\\ T_c^{\max}(\mathrm{OF_2}) = 4047^\circ\mathrm{K}, R = 0.959 \end{array}\right.$$

$$\begin{array}{c}\mathrm{H_2N_2}\\ \mathrm{(CH_3)_2}\end{array}\left|\begin{array}{l} I_p = I_p^{\max}[0.882 + 0.615(q_O^{\min}) + 0.914(q_O^{\min})^2],\\ I_p^{\max}(\mathrm{OF_2}) = 217.8\,\mathrm{s.}, R = 0.992\\ T_c = T_c^{\max}[0.819 + 0.926(q_O^{\min}) + 1.777(q_O^{\min})^2],\\ T_c^{\max}(\mathrm{OF_2}) = 4493^\circ\mathrm{K}, R = 0.961 \end{array}\right.$$

$$\text{—CH}_2\text{—}\left|\begin{array}{l} I_p = I_p^{\max}[0.856 + 0.737(q_{\mathrm{O}}^{\min}) + 1.222(q_{\mathrm{O}}^{\min})^2], \\ I_p^{\max}(\mathrm{OF}_2) = 218.5\,\mathrm{s.}, R = 0.987 \\ T_c = T_c^{\max}[0.799 + 1.028(q_{\mathrm{O}}^{\min}) + 1.965(q_{\mathrm{O}}^{\min})^2 \\ \qquad +13.924(q_{\mathrm{O}}^{\min})^3], \\ T_c^{\max}(\mathrm{OF}_2) = 4716^{\circ}\mathrm{K}, R = 0.966 \end{array}\right.$$

$$\mathrm{B_5H_9}\left|\begin{array}{l} I_p = I_p^{\max}[0.897 + 0.525(q_{\mathrm{O}}^{\min}) + 0.870(q_{\mathrm{O}}^{\min})^2], \\ I_p^{\max}(\mathrm{OF}_2) = 220.8\,\mathrm{s.}, R = 0.978 \end{array}\right.$$

3.3. Specific Traction in Atmosphere (P_1) and Combustor Temperature (T_c)

With all considered fuels: $H_2, N_2H_4, H_2N_2(CH_3)_2$, —$CH_2$—, AlH_3, B_5H_9 the oxidizers OF_2 and O_2 exhibit characterized highest values of specific traction in atmosphere – P_1 and combustor temperature – T_c (Tabs. II–VI). The lowest values of P_1 and T_c are found with nitric acid. In addition, the increases of negative charge on oxygen atom $q_{\mathrm{O}}^{\min}$ of oxygen-containing oxidizers leads to decreases of the values P_1 and T_c. The oxidizers O_2 and OF_2 are characterized by the maximum values of specific traction in atmosphere – P_1 and combustor temperature – T_c.

The comparison of calculated data of oxygen-containing oxidizers (Tab. I) and literature data of parameters of combustion of rocket fuels (Tabs. II, VI) showed that there is complex relationship between these two parameters and $q_{\mathrm{O}}^{\min}$.

For specific traction in atmosphere – P_1 and combustor temperature – T_c, we obtained the following correlative dependences on $q_{\mathrm{O}}^{\min}$ for investigated fuels.

$$\mathrm{H_2}\left|\begin{array}{l} P_1 = P_1^{\max}[0.919 + 0.575(q_{\mathrm{O}}^{\min}) + 0.383(q_{\mathrm{O}}^{\min})^2], \\ P_1^{\max}(\mathrm{OF}_2) = 412.2\,\mathrm{s.}, R = 0.964 \\ T_c = T_c^{\max}[0.837 + 0.907(q_{\mathrm{O}}^{\min}) + 1.478(q_{\mathrm{O}}^{\min})^2], \\ T_c^{\max}(\mathrm{OF}_2) = 3547^{\circ}\mathrm{K}, R = 0.982 \end{array}\right.$$

$$\mathrm{N_2H_4}\left|\begin{array}{l} P_1 = P_1^{\max}[0.922 + 0.387(q_{\mathrm{O}}^{\min})], \\ P_1^{\max}(\mathrm{OF}_2) = 345.3\,\mathrm{s.}, R = 0.965 \\ T_c = T_c^{\max}[0.853 + 0.765(q_{\mathrm{O}}^{\min}) + 1.393(q_{\mathrm{O}}^{\min})^2], \\ T_c^{\max}(\mathrm{OF}_2) = 4047^{\circ}\mathrm{K}, R = 0.959 \end{array}\right.$$

$$\begin{array}{r|l}
 & P_1 = P_1^{\mathrm{max}}[0.872 + 0.449(q_{\mathrm{O}}^{\mathrm{min}})], \\
 & P_1^{\mathrm{max}}(\mathrm{OF_2}) = 352.2\,\mathrm{s.}, R = 0.965 \\
\mathrm{H_2N_2} & T_c = T_c^{\mathrm{max}}[0.819 + 0.926(q_{\mathrm{O}}^{\mathrm{min}}) + 1.777(q_{\mathrm{O}}^{\mathrm{min}})^2], \\
\mathrm{(CH_3)_2} & T_c^{\mathrm{max}}(\mathrm{OF_2}) = 4493^{\circ}\mathrm{K}, R = 0.961
\end{array}$$

$$\begin{array}{r|l}
 & P_1 = P_1^{\mathrm{max}}[0.872 + 0.671(q_{\mathrm{O}}^{\mathrm{min}}) + 0.966(q_{\mathrm{O}}^{\mathrm{min}})^2], \\
 & P_1^{\mathrm{max}}(\mathrm{OF_2}) = 351.9\,\mathrm{s.}, R = 0.990 \\
-\mathrm{CH_2}- & T_c = T_c^{\mathrm{max}}[0.799 + 1.028(q_{\mathrm{O}}^{\mathrm{min}}) + 1.965(q_{\mathrm{O}}^{\mathrm{min}})^2 \\
 & \qquad +13.924(q_{\mathrm{O}}^{\mathrm{min}})^3], \\
 & T_c^{\mathrm{max}}(\mathrm{OF_2}) = 4716^{\circ}\mathrm{K}, R = 0.966
\end{array}$$

$$\begin{array}{r|l}
 & P_1 = P_1^{\mathrm{max}}[0.902 + 0.501(q_{\mathrm{O}}^{\mathrm{min}}) + 0.744(q_{\mathrm{O}}^{\mathrm{min}})^2], \\
\mathrm{B_5H_9} & P_1^{\mathrm{max}}(\mathrm{OF_2}) = 361.6\,\mathrm{s.}, R = 0.970
\end{array}$$

3.4. Specific Impulse Pressure (I_p) and Specific Traction in Vacuum (P_i^{∞})

With all considered fuels the oxidizers OF_2 and O_2 exhibit highest values of specific impulse of pressure – I_p and specific traction in vacuum – P_i^{∞} (Tabs. III, IV). The lowest values of I_p and P_i^{∞} are found with nitric acid. It should be noted that increases of negative charge on oxygen atom $q_{\mathrm{O}}^{\mathrm{min}}$ of oxygen-containing oxidizers lead to decreases of the values I_p and P_i^{∞}. These O_2 and OF_2 oxidizers are characterized by the maximum values of specific impulse of pressure – I_p and specific traction in vacuum – P_i^{∞}.

The comparison of calculated data of oxygen-containing oxidizers (Tab. I) and literature data of parameters of combustion of rocket fuels (Tabs. III, IV) indicates a complex dependence between these parameters and $q_{\mathrm{O}}^{\mathrm{min}}$.

For specific impulse of pressure – I_p and specific traction in vacuum – P_i^{∞} we obtained the following correlative dependences on $q_{\mathrm{O}}^{\mathrm{min}}$ for H_2, N_2H_4, $H_2N_2(CH_3)_2$, $—CH_2—$, and B_5H_9.

$$\begin{array}{r|l}
 & I_p = I_p^{\mathrm{max}}[0.919 + 0.559(q_{\mathrm{O}}^{\mathrm{min}}) + 0.390(q_{\mathrm{O}}^{\mathrm{min}})^2], \\
 & I_p^{\mathrm{max}}(\mathrm{OF_2}) = 261.3\,\mathrm{s.}, R = 0.962 \\
\mathrm{H_2} & P_i^{\infty} = P_i^{\infty\,\mathrm{max}}[0.922 + 0.571(q_{\mathrm{O}}^{\mathrm{min}}) + 0.341(q_{\mathrm{O}}^{\mathrm{min}})^2], \\
 & P_i^{\infty\,\mathrm{max}}(\mathrm{OF_2}) = 478.3\,\mathrm{s.}, R = 0.963
\end{array}$$

$$\mathrm{N_2H_4}\left|\begin{array}{l} I_p = I_p^{\max}[0.924 + 0.356(q_{\mathrm{O}}^{\min})], \\ I_p^{\max}(\mathrm{OF_2}) = 213.3\,\mathrm{s.}, R = 0.961 \\ P_i^{\infty} = P_i^{\infty\max}[0.923 + 0.341(q_{\mathrm{O}}^{\min})], \\ P_i^{\infty\max}(\mathrm{OF_2}) = 408.4\,\mathrm{s.}, R = 0.973 \end{array}\right.$$

$$\begin{array}{c}\mathrm{H_2N_2} \\ \mathrm{(CH_3)_2}\end{array}\left|\begin{array}{l} I_p = I_p^{\max}[0.882 + 0.615(q_{\mathrm{O}}^{\min}) + 0.914(q_{\mathrm{O}}^{\min})^2], \\ I_p^{\max}(\mathrm{OF_2}) = 217.8\,\mathrm{s.}, R = 0.992 \\ P_i^{\infty} = P_i^{\infty\max}[0.909 + 0.454(q_{\mathrm{O}}^{\min})], \\ P_i^{\infty\max}(\mathrm{OF_2}) = 416.6\,\mathrm{s.}, R = 0.971 \end{array}\right.$$

$$-\mathrm{CH_2}-\left|\begin{array}{l} I_p = I_p^{\max}[0.856 + 0.737(q_{\mathrm{O}}^{\min}) + 1.222(q_{\mathrm{O}}^{\min})^2], \\ I_p^{\max}(\mathrm{OF_2}) = 218.5\,\mathrm{s.}, R = 0.987 \\ P_i^{\infty} = P_i^{\infty\max}[0.900 + 0.484(q_{\mathrm{O}}^{\min})], \\ P_i^{\infty\max}(\mathrm{OF_2}) = 413.4\,\mathrm{s.}, R = 0.965 \end{array}\right.$$

$$\mathrm{B_5H_9}\left|\begin{array}{l} I_p = I_p^{\max}[0.897 + 0.525(q_{\mathrm{O}}^{\min}) + 0.870(q_{\mathrm{O}}^{\min})^2], \\ I_p^{\max}(\mathrm{OF_2}) = 220.8\,\mathrm{s.}, R = 0.978 \\ P_i^{\infty} = P_i^{\infty\max}[0.907 + 0.482(q_{\mathrm{O}}^{\min}) + 0.658(q_{\mathrm{O}}^{\min})^2], \\ P_i^{\infty\max}(\mathrm{OF_2}) = 433.2\,\mathrm{s.}, R = 0.977 \end{array}\right.$$

3.5. Specific Traction in Vacuum (P_i^{∞}) and Combustor Exit Temperature (T_e)

With all considered fuels: the oxidizers $\mathrm{OF_2}$ and $\mathrm{O_2}$ exhibit the highest values of specific traction in vacuum – P_i^{∞} and combustor-exit temperature – T_e (Tabs. III, VI). The minimum values of P_i^{∞} and T_e are noted with nitric acid. Moreover, the increases of negative charge on oxygen atom $q_{\mathrm{O}}^{\min}$ of oxygen-containing oxidizers lead to decreases of the values P_i^{∞} and T_e. The $\mathrm{O_2}$ and $\mathrm{OF_2}$ oxidizers are characterized by the maximum values of specific traction in vacuum – P_i^{∞} and combustor-exit temperature – T_e.

The comparison of calculated data of oxygen-containing oxidizers (Tab. I) and literature data of parameters of combustion of rocket fuels (Tabs. III, VI) showed that there is complex dependence between these parameters and $q_{\mathrm{O}}^{\min}$.

For specific traction in vacuum – P_i^{∞} and combustor-exit temperature – T_e we obtained the following correlative dependences on $q_{\mathrm{O}}^{\min}$ for investigated fuels.

H_2

$$\begin{aligned}&P_i^{\infty} = P_i^{\infty\,\max}[0.922 + 0.571(q_{\mathrm{O}}^{\min}) + 0.341(q_{\mathrm{O}}^{\min})^2],\\ &P_i^{\infty\,\max}(\mathrm{OF_2}) = 478.3\,\mathrm{s.}, R = 0.963\\ &T_e = T_e^{\max}[0.821 + 1.043(q_{\mathrm{O}}^{\min}) + 1.493(q_{\mathrm{O}}^{\min})^2],\\ &T_e^{\max}(\mathrm{OF_2}) = 1622^{\circ}\mathrm{K}, R = 0.993\end{aligned}$$

N_2H_4

$$\begin{aligned}&P_i^{\infty} = P_i^{\infty\,\max}[0.923 + 0.341(q_{\mathrm{O}}^{\min})],\\ &P_i^{\infty\,\max}(\mathrm{OF_2}) = 408.4\,\mathrm{s.}, R = 0.973\\ &T_e = T_e^{\max}[0.819 + 1.011(q_{\mathrm{O}}^{\min}) + 1.407(q_{\mathrm{O}}^{\min})^2],\\ &T_e^{\max}(\mathrm{OF_2}) = 2435^{\circ}\mathrm{K}, R = 0.97\end{aligned}$$

H_2N_2
$(CH_3)_2$

$$\begin{aligned}&P_i^{\infty} = P_i^{\infty\,\max}[0.909 + 0.454(q_{\mathrm{O}}^{\min})],\\ &P_i^{\infty\,\max}(\mathrm{OF_2}) = 416.6\,\mathrm{s.}, R = 0.971\\ &T_e = T_e^{\max}[0.833 + 0.979(q_{\mathrm{O}}^{\min}) + 1.271(q_{\mathrm{O}}^{\min})^2],\\ &T_e^{\max}(\mathrm{OF_2}) = 2705^{\circ}\mathrm{K}, R = 0.973\end{aligned}$$

$—CH_2—$

$$\begin{aligned}&P_i^{\infty} = P_i^{\infty\,\max}[0.900 + 0.484(q_{\mathrm{O}}^{\min})],\\ &P_i^{\infty\,\max}(\mathrm{OF_2}) = 413.4\,\mathrm{s.}, R = 0.965\\ &T_e = T_e^{\max}[0.914 + 1.013(q_{\mathrm{O}}^{\min}) - 0.591(q_{\mathrm{O}}^{\min})^2\\ &\qquad -7.947(q_{\mathrm{O}}^{\min})^3],\\ &T_e^{\max}(\mathrm{OF_2}) = 2670^{\circ}\mathrm{K}, R = 0.961\end{aligned}$$

B_5H_9

$$\begin{aligned}&P_i^{\infty} = P_i^{\infty\,\max}[0.907 + 0.482(q_{\mathrm{O}}^{\min}) + 0.658(q_{\mathrm{O}}^{\min})^2],\\ &P_i^{\infty\,\max}(\mathrm{OF_2}) = 433.2\,\mathrm{s.}, R = 0.977\end{aligned}$$

3.6. Combustor (T_e) and Combustor Exit Temperature (T_e)

With all considered fuels: H_2, N_2H_4, $H_2N_2(CH_3)_2$, —CH_2—, AlH_3, B_5H_9 the oxidizers OF_2 and O_2 exhibit the highest values of combustor and combustor-exit temperature – T_c, T_e (Tabs. II, III). The lowest values of T_c and T_e are found with nitric acid. Note also that the increase of negative charge on oxygen atom $q_{\mathrm{O}}^{\min}$ of oxygen-containing oxidizers leads to a decrease of the values T_c and T_e. The O_2 and OF_2 oxidizers are characterized by the maximum values of combustor and combustor-exit temperature – T_c, T_e.

The comparison of MNDO calculated data of oxygen-containing oxidizers (Tab. I) and literature data of parameters of combustion of rocket fuels (Tabs. V, VI) showed that there is complex relationship between these two parameters and $q_{\mathrm{O}}^{\min}$.

For H_2, N_2H_4, $H_2N_2(CH_3)_2$, $—CH_2—$ and B_5H_9 we extracted for combustor and combustor-exit temperature ($T_c - T_e$) the following correlative dependences on $q_{\mathrm{O}}^{\min}$.

$$\mathrm{H_2}\left|\begin{array}{l} T_c = T_c^{\max}[0.837 + 0.907(q_{\mathrm{O}}^{\min}) + 1.478(q_{\mathrm{O}}^{\min})^2], \\ T_c^{\max}(\mathrm{OF_2}) = 3547°\mathrm{K}, R = 0.982 \\ T_e = T_e^{\max}[0.821 + 1.043(q_{\mathrm{O}}^{\min}) + 1.493(q_{\mathrm{O}}^{\min})^2], \\ T_e^{\max}(\mathrm{OF_2}) = 1622°\mathrm{K}, R = 0.993 \end{array}\right.$$

$$\mathrm{N_2H_4}\left|\begin{array}{l} T_c = T_c^{\max}[0.853 + 0.765(q_{\mathrm{O}}^{\min}) + 1.393(q_{\mathrm{O}}^{\min})^2], \\ T_c^{\max}(\mathrm{OF_2}) = 4047°\mathrm{K}, R = 0.959 \\ T_e = T_e^{\max}[0.819 + 1.011(q_{\mathrm{O}}^{\min}) + 1.407(q_{\mathrm{O}}^{\min})^2], \\ T_e^{\max}(\mathrm{OF_2}) = 2435°\mathrm{K}, R = 0.97 \end{array}\right.$$

$$\begin{array}{c}\mathrm{H_2N_2} \\ \mathrm{(CH_3)_2}\end{array}\left|\begin{array}{l} T_c = T_c^{\max}[0.819 + 0.926(q_{\mathrm{O}}^{\min}) + 1.777(q_{\mathrm{O}}^{\min})^2], \\ T_c^{\max}(\mathrm{OF_2}) = 4493°\mathrm{K}, R = 0.961 \\ T_e = T_e^{\max}[0.833 + 0.979(q_{\mathrm{O}}^{\min}) + 1.271(q_{\mathrm{O}}^{\min})^2], \\ T_e^{\max}(\mathrm{OF_2}) = 2705°\mathrm{K}, R = 0.973 \end{array}\right.$$

$$—\mathrm{CH_2}—\left|\begin{array}{l} T_c = T_c^{\max}[0.799 + 1.028(q_{\mathrm{O}}^{\min}) + 1.965(q_{\mathrm{O}}^{\min})^2 \\ \qquad +13.924(q_{\mathrm{O}}^{\min})^3], \\ T_c^{\max}(\mathrm{OF_2}) = 4716°\mathrm{K}, R = 0.966 \\ T_e = T_e^{\max}[0.914 + 1.013(q_{\mathrm{O}}^{\min}) - 0.591(q_{\mathrm{O}}^{\min})^2 \\ \qquad -7.947(q_{\mathrm{O}}^{\min})^3], \\ T_e^{\max}(\mathrm{OF_2}) = 2670°\mathrm{K}, R = 0.961 \end{array}\right.$$

3.7. Specific Impulse Pressure (I_p) and Increment of Ideal Rocket Velocity (ΔV)

With all considered fuels: H_2, N_2H_4, $H_2N_2(CH_3)_2$, $—CH_2—$, AlH_3, B_5H_9 the oxidizers OF_2 and O_2 exhibit the values of specific impulse of pressure – I_p (Tabs. IV, VII). The minimum values of I_p are characterized the nitric acid. Here, the increase of negative charge on oxygen atom $q_{\mathrm{O}}^{\min}$ of oxygen-containing oxidizers leads to a decrease of the values I_p and ΔV. These O_2 and OF_2 oxidizers are characterized by the maximum values of specific impulse of pressure – I_p.

The comparison of calculated data of oxygen-containing oxidizers (Tab. I) and literature data of parameters of combustion of rocket fuels (Tabs. IV, VII) showed that there is complex relationship between these two parameters and $q_O^{\min}$.

For H_2, N_2H_4, $H_2N_2(CH_3)_2$, $—CH_2—$ and B_5H_9 fuels we extracted for specific impulse of pressure – I_p and increment of ideal velocity of flight of a rocket – ΔV the following correlative dependences on $q_O^{\min}$.

$$\mathrm{H_2}\ \left|\begin{array}{l} I_p = I_p^{\max}[0.919 + 0.559(q_O^{\min}) + 0.390(q_O^{\min})^2], \\ I_p^{\max}(OF_2) = 261.3\,\text{c.}, R = 0.962 \end{array}\right.$$

$$\mathrm{N_2H_4}\ \left|\begin{array}{l} I_p = I_p^{\max}[0.924 + 0.356(q_O^{\min})], \\ I_p^{\max}(OF_2) = 213.3\,\text{c.}, R = 0.961 \\ \Delta V = \Delta V^{\max}[0.783 + 0.418(q_O^{\min}) \\ \qquad +5.55(q_O^{\min})^2 + 12.013(q_O^{\min})^3], \\ \Delta V^{\max}(OF_2) = 4830\,\text{м/с}, R = 0.999 \end{array}\right.$$

$$\begin{array}{c}\mathrm{H_2N_2}\\ \mathrm{(CH_3)_2}\end{array}\ \left|\begin{array}{l} I_p = I_p^{\max}[0.882 + 0.615(q_O^{\min}) + 0.914(q_O^{\min})^2], \\ I_p^{\max}(OF_2) = 217.8\,\text{c.}, R = 0.992 \\ \Delta V = \Delta V^{\max}[0.779 + 0.489(q_O^{\min}) + 5.308(q_O^{\min})^2 \\ \qquad +11.315(q_O^{\min})^3], \\ \Delta V^{\max}(OF_2) = 4816\,\text{м/с}, R = 0.994. \end{array}\right.$$

$$—\mathrm{CH_2}—\ \left|\begin{array}{l} I_p = I_p^{\max}[0.856 + 0.737(q_O^{\min}) + 1.222(q_O^{\min})^2], \\ I_p^{\max}(OF_2) = 218.5\,\text{c.}, R = 0.987 \\ \Delta V = \Delta V^{\max}[0.756 + 0.559(q_O^{\min}) + 5.824(q_O^{\min})^2 \\ \qquad +12.211(q_O^{\min})^3], \\ \Delta V^{\max}(OF_2) = 5067\,\text{м/с}, R = 0.995. \end{array}\right.$$

$$\mathrm{B_5H_9}\ \left|\begin{array}{l} I_p = I_p^{\max}[0.897 + 0.525(q_O^{\min}) + 0.870(q_O^{\min})^2], \\ I_p^{\max}(OF_2) = 220.8\,\text{c.}, R = 0.978 \\ \Delta V = \Delta V^{\max}[0.758 + 0.556(q_O^{\min}) + 5.854(q_O^{\min})^2 \\ \qquad +11.587(q_O^{\min})^3], \\ \Delta V^{\max}(OF_2) = 4866\,\text{м/с}, R = 0.999. \end{array}\right.$$

4. CONCLUSIONS

Examples of rocket fuel performance presented above show that

1. MNDO method for calculating molecular characteristic such as geometric and electronic structure of rocket fuel oxidizer yields meaningful data relative to reactive fuel characteristics.
2. The calculated charge on oxygen atom is an important characteristic of oxygen-containing oxidizers, relative to fuel performance.
3. Useful correlative relations exist between parameters of rocket fuels combustion and negative charge on oxygen atom.
4. The established correlations between fuel combustion parameters such as: specific traction in atmosphere, specific traction in vacuum, specific impulse pressure, combustor temperature, combustor exit temperature, and increment of ideal rocket velocity prove the technological merits of these calculations and provide guidelines for future rocket fuel research.

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