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PREDICTION OF THE PROPERTIES OF HIGH-ENERGY POLYMER MATERIALS BASED ON OLEOCHEMICAL PRODUCTS

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A series of oleochemical products, namely amide derivatives of fatty acids from vegetable oils based on diethanolamine, diethylenetriamine, piperazine, and morpholine, was synthesized. The synthesized products are considered as potential components of mixed solid missile fuels: plasticizers, surfactants, and combustion regulators. To evaluate their applicability, the predicted energy characteristics of mixed compositions containing the synthesized oleochemical products were calculated, including the composition of transformation products, heat of combustion, combustion temperature, and specific volume of combustion products. The method of calculation is presented. The obtained characteristics of the compositions based on oleochemical products are comparable to the calculated values for a known composition based on liquid rubber and dioctyl adipate plasticizer: heat of combustion of 5860 kJ/kg, combustion temperature of 3450 K, and specific volume of combustion products of 0.818 m^3/kg.

Keywords: fatty acid amides, energy calculations, oleochemical products, mixed solid missile fuel, combustion.

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Introduction

Among the wide variety of polymer composite materials, a special place is occupied by high-energy materials on a polymer binder, in particular propellants – mixed missile solid fuels (MMSF). The vast majority of such compositions are a mixture of ammonium perchlorate and other functional additives in a polymer fuel-binder, which can harden after preparation of the composition, forming a solid mass [1,2].

The integral components of MMSF formulations are plasticizers and surfactants (SAS), which determine the required level of technological and operational characteristics. They are introduced into fuel mixtures to intensify the dispersion of powdery components and reduce viscosity. The most common MMSF plasticizers are the well-known dibutyl phthalate, dioctyl phthalate, dioctyl sebacinate, and, in some cases, energy-rich low molecular weight compounds such as nitroalkanes, azides, etc. In particular, amine-containing derivatives of fatty acids, sulfosuccinates, polyoxyethylene, etc. are used as SAS [3]. The raw material base for the production of such compounds is fossil hydrocarbons [4]. In addition, as evidenced by the experience of dealing with MMSF and the results of research, the plasticizers used above do not have sufficient thermodynamic affinity with the fuel-binder. Therefore, they are prone to diffusion from the fuel to the binding and heat-shielding layers of combustion chambers of solid-fuel missile engines (SFME), which affects the energy, thermophysical, and physical-mechanical properties of charges and structural elements of SFME [5].

In order to successfully counter external aggression, Ukraine needs to increase the volume of domestic production and use of SFME. However, a significant restraining factor is the actual lack of own component base even for existing productions. In addition, most of the components of modern MMSF (fuel-binder components, plasticizers, SAS) are

synthetic products of processing non-renewable fossil raw materials, and their production causes a negative impact on the environment. Therefore, research in the direction of creating a domestic component base for MMSF based on renewable ecological raw materials is definitely relevant.

Vegetable oils can be considered one of the most popular types of renewable raw materials today. Accordingly, an independent direction, oleochemistry, was formed within the limits of organic and polymer synthesis. Based on vegetable oils, various products are already produced in significant volumes. Many thorough publications, in particular refs. [6–8], are devoted to this topic, and their number increases every year.

Ukraine has great potential for the production of renewable raw materials suitable for processing into chemical products for various purposes, in particular vegetable oils. In view of the above, the aim of this study is the synthesis of products based on vegetable oils as promising components of the domestic component base for MMSF, as well as forecasting the energy characteristics of solid fuel compositions based on these products. Calculation methods are widely used to predict the energy characteristics of missile fuels, especially in the early stages of their design [9,10].

Experimental and calculations

Compounds, which are predictable components of MMSF oleochemical products (OP), are characterized in Table 1.

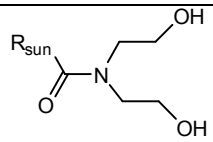
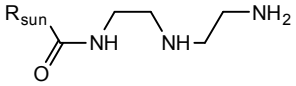
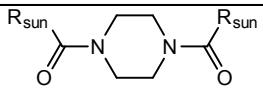
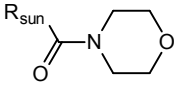
Amide derivatives of fatty acids listed in the Table 1 were synthesized according to ref. [8].

To determine the prospects of using the specified oleochemical products in the formulations of high-energy mixed compositions, the following calculation method for predicting the energy characteristics of MRSF is proposed:

– fuel combustion heat, Q_V, quantitative heat generated during the combustion of 1 kg of MRSF without the access of an oxidant from the outside and under the condition of cooling the combustion products

Table 1

Studied OP and their characteristics

Designation	Compound [a]	$\overline{M}$ [b]	δ_2 [c]	$\frac{\delta_a}{\delta_2}$ [d]	$-\Delta_f H^0$ [e]	Predicted functional purpose in MRSF
DEAFA		367.4	22.35	0.684	870.5	surfactant which is a crystal surface modifier PCA
DTAFA		365.5	25.03	0.727	564.5	hardener; burning rate regulator component
PAFA		610.6	17.95	0.402	1053.0	plasticizer
MAFA		349.4	18.84	0.464	692.5	plasticizer
RO	Ricinic oil $C_{57}H_{104}O_{87}$	928.6	19.63	0.578	2878.0	structure-forming agent
OA	$H_3C(CH_2)_7CH{=}CH(CH_2)_7COOH$	282.5	19.10	0.554	764.8	modifier

Notes: [a] – R_{san} stands for hydrocarbon residues of sunflower oil acids; [b] – $\overline{M}$ is the average molar mass of the product (g/mol); the values are given taking into account the average acid composition of sunflower-seed oil; [c] – solubility parameter of compounds, $MJ^{0.5}\cdot m^{-1.5}$; calculated as shown in ref. [11]; [d] – the contribution of the associative solubility parameter to the total solubility parameter; calculated according to ref. [12]; [e] – standard enthalpy of formation, $kJ\cdot mol^{-1}$; the value is calculated by Benson's additive scheme, taking into account the values given in ref. [13].

to standard temperature;

– temperature of fuel combustion products, T_1, the temperature of the final combustion products directly at the time of their formation;

– the specific volume of fuel combustion products, W_1, the volume of gaseous and vaporous products formed as a result of the combustion of 1 kg of MRSF in an inert environment close to normal thermodynamic conditions (water in the combustion products is conventionally considered to be steam).

The averaged MMSF formulation according to refs. [1,3,14] is taken as the base for comparison. Its component composition and some characteristics are given in Table 2.

As formulations of experimental MMSF obtained from the base by replacing, certain functional components with OP were considered. The conclusion regarding the possibility of using specific OP instead of DOA in fuel masses was drawn on the closeness of the values of δ_2 and δ_a/δ_2 (Tables 1 and 2), which is an empirical criterion of the closeness of the thermodynamic affinity of the specified plasticizers with the rest of the MMSF components.

The energy calculation algorithm assumes the following assumptions:

– the combustion process takes place under isentropic and isochoric conditions. Although it is known that combustion occurs under isobaric conditions, the representation of combustion as an adiabatic isochoric thermodynamic process makes it possible to perform calculations using the laws of conservation of energy and mass, as well as equations for the equilibrium constants of chemical reactions;

– the end products of MMSF combustion, in addition to metal oxides, are gaseous and vaporous products;

– metals in the composition of MMSF are completely transformed into oxides, chlorine into hydrogen chloride, nitrogen into molecular nitrogen.

The composition of the remaining combustion products (PC) depends on the equilibrium reactions that take place with the participation of the primary products of the oxidation process after their formation. Among the possible equilibrium reactions, the formation of the final composition is mainly influenced by the reaction of water gas, which determines the equilibrium between the products CO, CO_2, H_2 and H_2O. In this case, the combustion process of 1 kg of MRSF can be represented by the following generalized chemical reaction:

$$C_aH_bN_cO_dAl_eCl_fFe_g \rightarrow xCO + yCO_2 + zH_2 + uH_2O + \frac{c}{2}N_2 + \frac{e}{2}Al_2O_3 + fHCl + \frac{g}{2}Fe_2O_3, \quad (1)$$

where a, b, c, d, e, f, and g are the numbers of gram-atoms of the corresponding chemical element in 1 kg of MMSF.

The ratio of the first four compounds in the combustion products formed by the above reaction is related to the equilibrium constant of the water gas reaction in the following way:

$$K_{w.g.} = \frac{\vartheta_{CO} \cdot \vartheta_{H_2O}}{\vartheta_{CO_2} \cdot \vartheta_{H_2}}, \quad (2)$$

where $K_{w.g.}$ is the equilibrium constant of the water gas reaction; and ϑ is the number of moles of the corresponding subscripted compound in the combustion products of 1 kg of MMSF.

The method of calculating the energy characteristics of the compositions provides the following features:

(a) drawing up the conversion equation of 1 kg of MMSF (Eq. (1)) with determination of the coefficients (number of moles) of PC through the value of $K_{w.g}$ (Eq. (2)) for T_1, which is close to the real combustion temperature of MRSF:

Table 2

Composition of the basic formulation of MMSF and characteristics of its components

Component	Part by weight	Empirical formula	$\overline{M}$	δ_2	$\frac{\delta_a}{\delta_2}$	$-\Delta_fH^0$
Ammonium perchlorate	0.650	H_4ClNO_4	117.49	–	–	298.3
Aluminum powder	0.185	Al	26.98	–	–	0
Butadiene rubber with terminal hydroxyl groups (HTPB)	0.090	$C_{225.967}H_{340.951}O_2$	3089.7	17.0	0.27	1070.0 [a]
Dioctyl adipate (DOA)	0.064	$C_{22}H_{42}O_4$	370.57	17.4	0.43	396.5
Isophorondiisocyanate	0.005	$C_{12}H_8N_2O_2$	212.21	23.0	0.47	288.17
Catalyst DAF-2	0.006	$C_{14}H_{18}Fe$	242.15	21.1	0.46	921.0

Note: [a] – in kJ/kg.

$$u = \frac{B \pm \sqrt{B^2 - 4 \cdot A \cdot \Gamma}}{2 \cdot A},$$

where $A=K_{w.g}-1$; $B=K_{w.g.}(0.5b'+d'-a)+2a-d$; $\Gamma=K_{w.g.}\cdot 0.5b'(d'-a)$; $b'=b-f$; $d'=d-3(g+e)/2$; $y=d'-(a+u)$; $x=a-y$; $z=0.5b'-u$; and $K_{w.g.} = \frac{x \cdot u}{y \cdot z}$;

(b) calculation of Q_V according to the complex equation of transformation by the following equation:

$$Q_V = -\Delta_f H^0_{(PC)} - \left(-\Delta_f H^0_{(MMSF)}\right) - j_n RT, \quad (3)$$

where $\Delta_f H^0_{(PC)}$ is the sum of the standard enthalpies of formation of PC per 1 kg of MMSF (kJ/kg); $\Delta_f H^0_{(MMSF)}$ is the sum of the standard enthalpies of formation of the components MMSF (kJ/kg); j_n is the number of moles of gaseous simple substances which form 1 kg MMSF and PC; R is the universal gas constant ($kJ\cdot mol^{-1}\cdot K^{-1}$); and T is the thermodynamic temperature (K);

(c) checking the correctness of the choice of the assumed T_1 according to the equation:

$$T_1 = \frac{Q_V}{\sum \vartheta_m \bar{c}v_{\mu_m}} + T_0,$$

where ϑ_m is the number of moles of the m-th compound in the PC of 1 kg of the composition (that is x, y, z, u, c/2, e/2, f, g/2); $\bar{c}v_{\mu_m}$ is the average isochoric molar heat capacity of the m-th compound in PC in the temperature range T_1-T_0, where T_0 is the standard temperature (298 K).

If the calculated T_1 differs from the expected one by no more than 50^0, its value is taken as final; otherwise, the above calculations are repeated for $K_{w.g}$, which corresponds to the calculated temperature;

(d) determination of the specific volume of fuel combustion products W_1 ($m^3\cdot kg^{-1}$), according to the following formula:

$$W_1 = 0.02241 \cdot \sum l_j,$$

where l_j is the number of moles of the j-th gaseous and vaporous (including water) compound in PC 1 kg of the composition.

Results and discussion

The results of the calculations of the energy characteristics of the basic composition and those obtained by replacing the plasticizer DOA in the basic composition with the corresponding OP are summarized in Table 3.

The data listed in Table 3 show that the replacement of the DOA plasticizer in the basic composition with OP does not significantly reduce Q_V (by 2.3–4.4%) and T_1 (by 2.1–4.0%), but increases the W_1 value (by 0.4–1.7%).

Further calculations revealed that it is possible to prepare MMSF with better energy indicators than MMSF of the basic formulation by selecting combinations of synthesized OP with other available fuel-binders. The predicted characteristics of imaginary compositions were calculated, in which the content of PCA and aluminum corresponds to the content in the basic composition, and the basis of the liquid-viscous part is OP in combination with polyisocyanate (PIC), for example, based on hexamethylene

Table 3

Calculated PS composition and energy characteristics of the base MMSF and obtained by replacing DOA with OP

Empirical formula of 1 kg MMSF	Number of moles of combustion products and energy characteristics of 1 kg MRSF							
	CO	CO_2	H_2	H_2O	N_2	A_2O_3	HCl	Fe_2O_3
basic composition								
$C_{11.004}H_{39.944}N_{5.580}O_{22.932}$ $Al_{6.856}Cl_{5.532}Fe_{0.025}$	10.881	0.122	15.722	1.484	2.790	3.428	5.532	0.012
	Q_V=5860 kJ/kg; T_1=3450 K; W_1=0.818 m^3							
composition with DEAFA instead of DOA								
$C_{11.021}H_{39.983}N_{5.754}$ $O_{22.764}Al_{6.856}Cl_{5.532}Fe_{0.025}$	10.912	0.109	15.914	1.311	2.877	3.428	5.532	0.012
	Q_V=5725 kJ/kg; T_1=3376 K; W_1=0.821 m^3							
composition with PAFA instead of DOA								
$C_{11.378}H_{40.208}$ $N_{5.789}O_{22.451}Al_{6.856}Cl_{5.532}$ $Fe_{0.025}$	11.320	0.058	16.645	0.693	2.895	3.428	5.532	0.012
	Q_V=5615 kJ/kg; T_1=3314 K; W_1=0.832 m^3							
composition with MAFA instead of DOA								
$C_{11.201}H_{39.993}N_{5.763}O_{22.608}$ $Al_{6.856}Cl_{5.532}Fe_{0.025}$	11.135	0.084	16.246	0.984	2.881	3.428	5.532	0.012
	Q_V=5605 kJ/kg; T_1=3313 K; W_1=0.826 m^3							

diisocyanate trimer or epoxy resin of the ED-22 type (ER) with a content of epoxy groups of 22.1-23.6% with a hardener of the ethylene polyamine brand HEPA-S120.

The qualitative composition and the results of calculations of energy characteristics of experimental compositions are given in Table 4. As follows from the data given in Table 4, MMSF based on PIC and OP have energy characteristics, the values of which are practically equal to those of the basic MRSF. In the case of a fuel-binder based on ER, the calculation results yielded insignificantly lower Q_V values (0.4–0.8%), but higher T_1 values (0.5–0.7%).

Conclusions

According to the results of the performed calculations, it is possible to consider the synthesized OP as promising components of the domestic component base for mixed missile solid fuels.

Based on the results of the performed calculations, the synthesized amide derivatives of fatty acids of plant origin can be considered promising starting compounds for creating mixed missile solid fuels based on the domestic component base. With the use of considered OP as plasticizers, surfactants, and structure formers, it is possible to create new types of MMSF on isocyanate or epoxy fuel-binders, which have energy characteristics no worse than the characteristics of known MMSF. In particular, MMSF with imaginary formulations have values of heat of combustion in the range of 5800–5900 kJ/kg, combustion temperature of 3410–3475 K, and specific volume of combustion products of up to 0.79 m^3/kg.

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Table 4

Calculated RS composition and energy characteristics of imaginary MMSF based on OP

Empirical formula of 1 kg MRSF	The qualitative composition of the liquid-viscous part, the number of moles of combustion products and energy characteristics of 1 kg of MRSF							
	CO	CO_2	H_2	H_2O	N_2	A_2O_3	HCl	Fe_2O_3
PIC; RO; PAFA; adduct FeC_2O_4–DTAFA								
$C_{10.579}H_{41.097}N_{6.263}O_{23.786}Al_{6.856}Cl_{5.532}Fe_{0.031}$	10.358	0.221	15.128	2.654	3.132	3.428	5.532	0.016
	Q_V=5895 kJ/kg; T_1=3411 K; W_1=0.829 m^3							
ER; hardener HEPA-S120; OA; FeC_2O_4								
$C_{10.044}H_{37.798}N_{6.736}O_{22.744}Al_{6.856}Cl_{5.532}Fe_{0.028}$	9.860	0.184	13.944	2.189	3.380	3.428	5.532	0.014
	Q_V=5811 kJ/kg; T_1=3469 K; W_1=0.786 m^3							
ER; hardener HEPA-S120; DEAFA; OA; adduct FeC_2O_4–DTAFA								
$C_{10.009}H_{38.141}N_{6.760}O_{22.770}Al_{6.856}Cl_{5.532}Fe_{0.028}$	9.821	0.187	14.056	2.287	3.368	3.428	5.532	0.014
	Q_V=5835 kJ/kg; T_1=3475 K; W_1=0.789 m^3							

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ПРОГНОЗУВАННЯ ВЛАСТИВОСТЕЙ ВИСОКОЕНЕРГЕТИЧНИХ ПОЛІМЕРНИХ МАТЕРІАЛІВ НА ОСНОВІ ОЛЕОХІМІЧНИХ ПРОДУКТІВ

К.Є. Варлан, О.В. Черваков, К.М. Сухий, О.А. Бєляновська

Синтезовано низку олеохімічних продуктів – амідних похідних жирних кислот рослинних олій на основі діетаноламіну, діетилентріаміну, піперазину, морфоліну. Синтезовані продукти розглянуто як можливі компоненти сумішевих ракетних твердих палив: пластифікатори, поверхнево-активні речовини, регулятори горіння. Для цього виконано розрахунки прогнозованих енергетичних характеристик сумішевих композицій, що містять синтезовані олеохімічні продукти: склад продуктів перетворення, теплоту, температуру та питомий об'єм продуктів горіння. Наведено відповідну методику розрахунків. Отримані значення характеристик композицій на основі олеохімічних продуктів практично дорівнюють розрахованим значенням відомої композиції на основі рідкого каучуку і пластифікатору – діоктиладипінату: теплота згоряння 5860 кДж/кг; температура горіння 3450 К; питомий об'єм продуктів згоряння 0,818 м^3/кг.

Ключові слова: аміди жирних кислот, енергетичні розрахунки, олеохімічні продукти, сумішеве ракетне тверде паливо, горіння.

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Keywords: fatty acid amides; energy calculations; oleochemical products; mixed solid missile fuel; combustion.

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