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PHYSICOCHEMICAL PRINCIPLES OF THE TECHNOLOGY OF MODIFIED PYROTECHNIC COMPOSITIONS TO REDUCE THE CHEMICAL POLLUTION OF THE ATMOSPHERE

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This paper presents the results of determination of conditions for the production of modified pyrotechnic compositions that allow initiating atmospheric precipitation, neutralizing their acidity and scavenging toxic substances from the atmosphere. Taking into account the requirements of environmental protection, the use of Mg as a fuel and KNO_3 as an oxidizing agent in the pyrotechnic composition was suggested. The combustion of the proposed two-layer pyrocomposition impedes the release of chemically hazardous combustion products (NH_3 and HCl). Using TERMO-CALC software package, the content of ammonia and hydrogen chloride in the combustion products of the proposed mixtures was determined at the best fuel-oxidizing agent ratio. The thermodynamic calculations were performed to determine the best reducing/oxidizing agent mass fraction ratio which was stated to be 1:8. The experimental study of the main parameters of high-temperature oxidation (temperature and burning rate) of pyrotechnic compositions was carried out. A two-layer structure of the explosive charge with a highly flammable primary layer is proposed, which substantially increases the probability of ignition of the pyrotechnic mixture triggered by an electric spark. In order to intensify a decrease of the acidity of atmospheric precipitation, a technology for modifying pyrotechnic compositions by adding KOH and cellulose was proposed. The modification of the developed composition with the use of NaOH allows effectively neutralizing such dangerous gases as chlorine and phosgene. The established physicochemical basics of the technology for modifying pyrotechnic compositions for complex purposes allow developing multi-functional explosive compositions aimed at artificial initiation of precipitation and chemical neutralization of hazardous substances in the atmosphere.

Keywords: pyrotechnic composition, calculation, combustion temperature, initiation of precipitation, neutralization of phosgene, chemical neutralization of acid rains.

Introduction

In case of large-scale emergencies, a huge amount of hazardous chemical substances enters the atmosphere [1−3], the composition and physical and chemical properties of which depend on the nature of the emergency [4,5]. It is essential to increase the rate of the atmosphere cleaning by discharging special chemical reagents into the atmosphere that increase the rate of sorption of dangerous (poisoning, radioactive) particles of rain drops or neutralize their negative impact. Therefore, the development of the technology of special modified pyrotechnic compounds (PCs) initiating artificial precipitation and reducing the degree of negative effects of air

pollutants, is an urgent task.

When technogenic accidents on the objects of the chemical industry take place, the release of such hazardous substances as Cl_2 and $COCl_2$ occurs. Their neutralization is carried out by spraying aqueous solutions of NaOH and $C_6H_{10}O_5$ [4].

Another characteristic of accidents are fires. The qualitative and quantitative compositions of the combustion products depend substantially on the type of fuel and the combustion conditions. The main components of the combustion products in fires are CO_2, CO, NO, NO_2, SO_2, soot and ashes [6,7]. The atmospheric precipitation is known to efficiently sorb not only dangerous chemical but also radioactive

substances and precipitate them from the atmosphere [8]. The effectiveness of cleaning the atmosphere due to precipitation depends on the precipitation rate and the physical and chemical properties of the precipitated substances [9,10]. Various reagents are used to artificially initiate the precipitation. The most effective way of delivering and spraying reagents in the atmosphere is the use of pyrotechnic compositions designed as aerosol generators or explosive cartridges [11,12]. An analysis of the latest achievements and publications has shown that the substantiation of physical and chemical approaches in the theory of modification and features of kinetics of PC modification reactions has already been given [13,14]. However, the existing compounds of explosive cartridges are not very effective or cannot be used to neutralize or reduce the negative impact of pollutants.
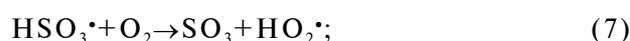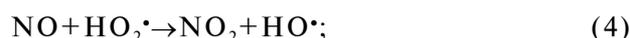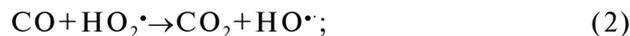
In view of the above, the aim of this paper is to establish the process conditions for the modification of pyrotechnic compositions that have both enhanced properties of initiating atmospheric precipitation and neutralization of their acidity and toxic components in the atmosphere.

The tasks of PC modification are defined based on a preliminary analysis of the expected effects of interparticle interaction under the conditions of forced condensation of water vapor and the absorption of acid molecules and toxic components by condensate drops.

The research objectives were as follows: (i) to model the best composition (Ox/Red ratio) at the maximum combustion temperature and the PC combustion rate; (ii) to increase the effectiveness of pyrocomposition to neutralize acidic atmospheric precipitation, and (iii) to study the features of a PC with new additives, such as NaOH and $C_6H_{10}O_5$, for the neutralization of $COCl_2$ and Cl_2.

Theory

Among the gaseous products of high-temperature oxidation released into the atmosphere, CO, NO, NO_2 and SO_2 have the highest reactivity. When discharged to the atmosphere, these combustion products react with atmospheric gases. The lower troposphere, except for H_2O, O_2 and almost non-reactive CO_2 and N_2, contains highly active radicals, such as hydroxyl $HO^\bullet$, hydroperoxide $HO_2^\bullet$, and nitrate ions NO_3^- [5]. Such radicals appear in the atmosphere due to ultraviolet radiation. Chemically active components of combustion products react with radicals according to the following reaction schemes:

$$CO + HO^\bullet \rightarrow CO_2 + H^\bullet; \tag{1}$$

$$CO + HO_2^\bullet \rightarrow CO_2 + HO^\bullet; \tag{2}$$

$$NO + HO^\bullet \rightarrow NO_2 + H^\bullet; \tag{3}$$

$$NO + HO_2^\bullet \rightarrow NO_2 + HO^\bullet; \tag{4}$$

$$NO_2 + HO^\bullet \leftrightarrow HNO_3; \tag{5}$$

$$SO_2 + HO^\bullet \rightarrow HSO_3^\bullet; \tag{6}$$

$$HSO_3^\bullet + O_2 \rightarrow SO_3 + HO_2^\bullet; \tag{7}$$

$$SO_3 + H_2O \leftrightarrow H_2SO_4. \tag{8}$$

Due to chemical transformation of NO, NO_2, SO_2 according to (1)−(8), nitric and sulfuric acids are formed in the atmosphere and sorbed by small water drops. Under certain weather conditions, drops of aqueous solutions of acids fall out causing significant damage to crops and other vegetation. Therefore, we propose a method of neutralizing the acid before it is on the earth surface by spraying fine-dispersed alkali contained in the pyrotechnic composition of the explosive cartridge [14].

In studying the combustion processes of multicomponent pyrotechnic compositions for artificial influence on atmospheric processes, the development of a theoretical model that takes into account all the main factors affecting the combustion process is an extremely difficult task. Therefore, we analyze below the main factors affecting the combustion process and existing models for describing this process based on experimental data and the use of specialized models.

Ammonium perchlorate (NH_4ClO_4) and ammonium nitrate (NH_4NO_3) are mainly used as an oxidizer in solid pyrotechnic compositions. Ammonium perchlorate has the highest oxidizing activity. However, when it burns, a harmful halide HCl is released. The replacement of NH_4ClO_4 with NH_4NO_3 leads to a sharp decrease in the burning rate and reactive thrust. Therefore, oxide-coated dispersible alkali and alkaline-earth metals are used as fuels for explosive charges. The most used are beryllium (Be), sodium (Na), magnesium (Mg) and aluminum (Al). Among the listed substances, sodium is unstable in the air and flammable, and beryllium releases extremely toxic products during combustion. Among the stable metals, magnesium has the largest heat and highest burning rate; that is why it is so often used as a fuel for explosive charges [13,14]. When artificially influencing the atmospheric precipitation, aluminum compositions are often used. Nevertheless, all previous studies on the development

of pyrotechnic compositions for the artificial initiation of precipitation paid very little attention to the physicochemical principles of the combustion of the main components that determine the effective ratio of the fuel and oxidizing agent, the burning rate, the chemical composition of combustion products, their surface properties, etc.
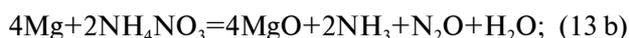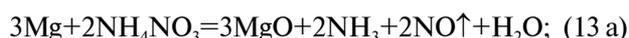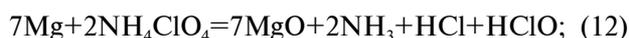
Since metal oxides have significantly higher melting and boiling points than the metals themselves, oxide film will reduce the rate and temperature of combustion.

Based on the fact that metals particles are small, the effect of the oxide film on the combustion will be significant. The dynamics of the destruction of the oxide film will depend on its thickness and porosity determined by the storage conditions and the combustion temperature.

One of the main parameters of an effective pyrotechnic composition is an optimal ratio of the mass of the fuel and the oxidizing agents. However, it is often underestimated since the air components take part in combustion. To obtain a formal stoichiometric ratio, we use the set of thermodynamic calculation programs for multicomponent systems TERMO-CALC. We take the maximum PC combustion temperature as a criterion for estimating reaching the stoichiometry of the combustion process (Fig. 1).

As shown in Fig. 1, the high-temperature oxidation (combustion temperature) of magnesium (Fig. 1,a) with all of the oxidants is much higher than the combustion temperature of aluminum (Fig. 1,b). At the same time, ammonium perchlorate is the most reactive among the oxidizing agents, and the reactivity scheme of the oxidizers is as follows: $NH_4ClO_4>NH_4NO_3>KNO_3$. The temperature of effective combustion shifts towards a decrease in the oxidizer content when magnesium is burned with

ammonium perchlorate, whereas an inverse relation is observed when using ammonium nitrate. When the oxidant content is less than 3 weight parts, practically all the mixtures do not burn. The use of ammonium oxidizers, especially ammonium perchlorate and nitrate, can lead to the release of highly toxic NH_3 and HCl:

$$14Al+6NH_4ClO_4= \\ =7Al_2O_3+6NH_3+3HCl+3HClO; \qquad (9)$$

$$2Al+2NH_4NO_3=Al_2O_3+2NH_3+2NO\uparrow+H_2O; \quad (10\,a)$$

$$8Al+6NH_4NO_3=4Al_2O_3+6NH_3+3N_2O+3H_2O; \quad (10\,b)$$

$$2Al+2KNO_3=Al_2O_3+2NO\uparrow+K_2O, \\ K_2O+H_2O(atm.)=2KOH; \qquad (11)$$

$$7Mg+2NH_4ClO_4=7MgO+2NH_3+HCl+HClO; \quad (12)$$

$$3Mg+2NH_4NO_3=3MgO+2NH_3+2NO\uparrow+H_2O; \quad (13\,a)$$

$$4Mg+2NH_4NO_3=4MgO+2NH_3+N_2O+H_2O; \quad (13\,b)$$

$$3Mg+2KNO_3=3MgO+2NO\uparrow+K_2O, \\ K_2O+H_2O(atm.)=2KOH. \qquad (14)$$

The most realistic reaction paths (9)−(14) are presented on the basis of experimental data in a climate chamber using a Drager Xam−5000 gas analyzer with gas detectors on NO, NH_3, HCl, Cl_2.

Using the TERMO-CALC software package, we will estimate the content of ammonia and hydrogen chloride in the combustion products of the mixtures under study at the best fuel-oxidizing agent ratio (Table 1). The calculations showed that a rather large amount of toxic ammonia and hydrogen chloride releases when pyrocompositions burn with
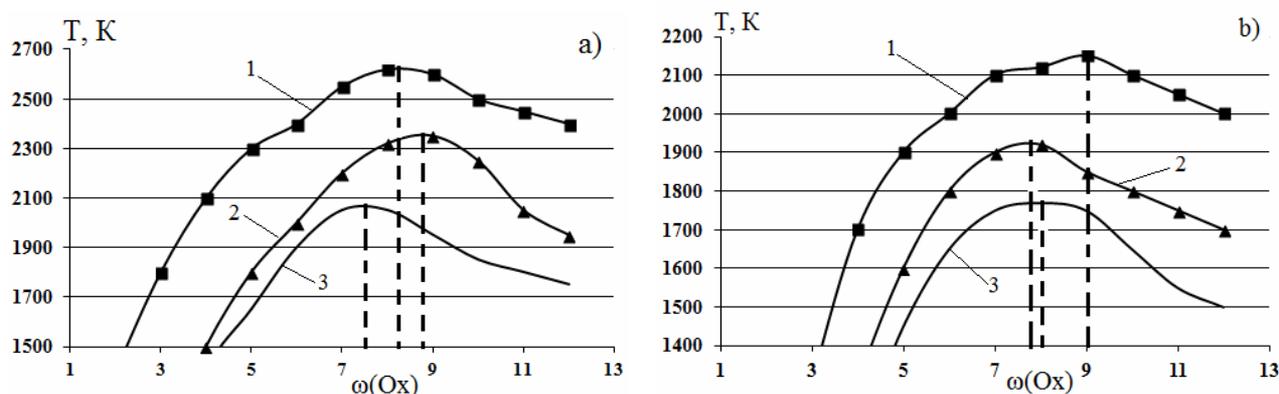

Fig. 1. Temperature of combustion of pyrotechnic compositions as a function of fuel-oxidizing agent ratio (Red/Ox ratio) where Red: (a) Mg, (b) Al; Ox: (1) NH_4ClO_4, (2) NH_4NO_3, (3) KNO_3. w(Ox) is the mass ratio of Ox (w(Ox)/w(Red) at w(Red)=1)

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ammonium oxidizing agents.

Content of NH_3 and HCl in the pyrocomposition combustion products

| Compositions	mol/kg	
	NH_3	HCl
PC-0-1 [Al+NH_4ClO_4 (1:9)]	18.22	6.34
PC-0-2 [Al+NH_4NO_3 (1:7.8)]	22.73	–
PC-0-3 [Al+KNO_3 (1:8.1)]	–	–
PC-0-4 [Mg+NH_4ClO_4 (1:8.4)]	13.51	8.31
PC-0-5 [Mg+NH_4NO_3 (1:8.9)]	15.42	–
PC-0-6 [Mg+KNO_3 (1:7.3)]	–	–

Table 1 shows that it is preferable to use compositions based on potassium nitrate as an oxidizing agent (11) and (14) to improve environmental safety when using pyrotechnic compositions for the purpose of artificial precipitation.

Such modifying additives as fine powders of alkali (NaOH, KOH) do not participate in the combustion process. As a result of combustion of the explosive charge, alkali particles are sprayed, contact with the acidic atmospheric aquatic formations and neutralize their excessive acidity.

Since the boiling temperature of these alkalis is high (T_{boil}(NaOH)=1676 K, T_{boil}(KOH)=1600 K), the explosive charge burning makes them subliming, which leads to an additional dispersion of alkali particles.

The overall process of high-temperature oxidation of pyrocompositions can be considered as a two-stage process: pyrocompositions reactants interact under conditions of a closed thermodynamic system (I), but the combustion reaction products and modifiers (NaOH, KOH) interact with atmospheric components under the conditions of an open thermodynamic system (II).
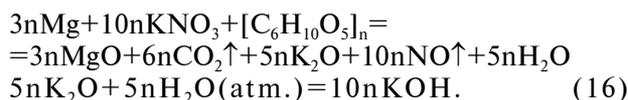
An additional amount of alkali in the thermodynamic system (II) can be released as a result of the combustion reaction of metals burning with alkali metal nitrates in the thermodynamic system (I):

$$3Mg+2KNO_3+H_2O=3MgO\downarrow+2KOH+2NO$$
or
$$3Mg+2KNO_3+4H_2O=$$
$$=3Mg(OH)_2\downarrow+2KOH+2NO. \qquad (15)$$
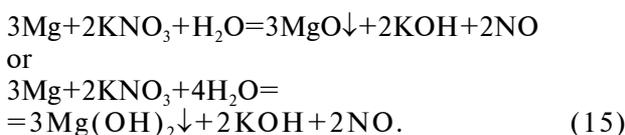
However, as equations (15) show, the additional release of potassium hydroxide requires water. Despite the fact that moisture is always in the atmosphere, entry of water molecules into the fire reaction zone

of the explosive charge is extremely difficult due to the escape of a powerful stream of superheated reaction products from the charge nozzle.

The problem of providing water to the explosive charge is solved by introducing combustible hydrogen-containing components directly into the explosive charge. Organic compounds can be used for such purpose. From a technological point of view, explosive charge organic substances must be solid and highly dispersed under normal conditions. Cellulose can be used as such an additive. The explosive charge burning with cellulose added at the molecular level releases MgO, CO_2, K_2O, NO and H_2O. Since cellulose is a typical polymer, it is more correct to make the equation for high-temperature oxidation of Mg and $[C_6H_{10}O_5]_n$ taking into account the degree of polymerization (n), i.e. of monomers in a polymer molecule:

$$3nMg+10nKNO_3+[C_6H_{10}O_5]_n=$$
$$=3nMgO+6nCO_2\uparrow+5nK_2O+10nNO\uparrow+5nH_2O$$
$$5nK_2O+5nH_2O(atm.)=10nKOH. \qquad (16)$$

Almost all potassium atoms in the process of combustion of EC release potassium oxide, which, when entering the atmosphere, further increases the concentration of alkali and also increases the degree of neutralization of acidic atmospheric formations.

After selecting the components for the explosive charge, it is necessary to determine the mass composition. Determination of the effective mass composition was carried out experimentally by measuring the parameters of the high-temperature oxidation process (burning rate and combustion temperature).

Experimental

To make a solid explosive charge, ASD-4 aluminum powder and MPF-4 magnesium powder with a size of 20−80 microns were used as fuels, KNO_3 salt ground and screened with a size of 50−100 microns was used as an oxidizing agent, and granulated butadiene-nitrile rubber SKN-26 was used as a binder. The content of components in the composition was as follows (wt.%):

PC-1-3: ASD-4 − 10; KNO_3 − 80; and SKN-26 − 10;

PC-1-6: MPF-4 − 11; KNO_3 − 79; and SKN-26 − 10.

The components of explosive charges were qualified as "pure". The composition was formed as a cylindrical elongated test piece with a diameter of d=20 mm and a length of l=150 mm.

The explosive charge was ignited with an electric

spark. The burning rate was determined by measuring the burning time of the PC mass between the control marks. The combustion temperature was determined using a high-temperature pyrometer Flus, IR866 [15]. The experiments were performed in an isolated chamber. The measurements were carried out three times for each composition.

Experimental results and discussion

The results of experiments on the study of the parameters of PC combustion in the stoichiometric ratio are shown in Table 2.

Table 2

Parameters of PCs combustion

PC	Combustion parameters	
	Burning rate, 10^3 m·s^{-1}	Combustion temperature, K
PC-1-3	3.1±0.1	1690±20
PC-1-6	3.5±0.1	2060±20
PC-1-31	3.1±0.1	1695±20
PC-1-61	3.4±0.1	2050±20

The experiment results confirmed the assumption that adding a binder reduces the burning rate (the measured combustion temperature is lower than the predicted one). This fact should be taken into account for future development of the composition of multicomponent solid pyrotechnic charges, in which some components do not participate in the combustion process.

The decrease in the combustion rate is affected by an oxide film which was not taken into account in the calculations. For this reason, the experiments showed a low probability of ignition of pyrocharges PS-1-3 and PS-1-6 by an electric spark. The probability of ignition of PC-1-3 composition was ~50%, and ~30% for PS-1-6 composition. This is also related to the presence of an oxide film, which prevents initiation of combustion. The melting point of the MgO film is much higher than that of the aluminum oxide film; that apparently affects the low probability of ignition of PC-1-6.

To eliminate this issue, it is proposed to use a two-layer charge with a thin layer of initiating composition based on potassium perchlorate and graphite ($KClO_4$+C) in the ignition zone and the main working composition based on potassium nitrate and dispersed metals (Fig. 2).

The results of testing two-layer compositions PC-1-31 and PC-1-61 (Table 2) show that the introduced changes (i.e. two-layer PC) do not influence the burning rate within the measurement accuracy, and the probability of ignition in all tests was 100%.
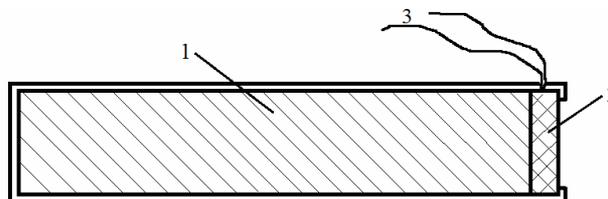

Fig. 2. Two-layer explosive charge: 1 − main composition; 2 −ignition composition; 3 − electric ignition

The results of experimental studies of explosive charges with modifying additives KOH and $C_6H_{10}O_5$ are given in Tables 3 and 4. Initially, a composition was studied with the addition of potassium alkali only as the main acid neutralizer.

Table 3

Basic parameters of PC burning to neutralize acidity without adding cellulose

Composition	KOH content, wt.%	Combustion rate, ×10^3 m·s^{-1}	Burning rate, K
PC-2-0	0	3.3±0.1	1870±20
PC-2-1	10	3.1±0.1	1850±20
PC-2-2	20	3.1±0.1	1820±20
PC-2-3	30	2.9±0.1	1820±20
PC-2-4	40	2.7±0.1	1810±20
PC-2-5	50	2.6±0.1	1800±20
PC-2-6	60	2.3±0.1	1780±20
PC-2-7	70	~2.1 (blow-off)	1750±20
PC-2-8	80	~2.0 (blow-off)	1720±20

Table 4

Basic parameters of PC burning to neutralize acidity with cellulose added

Composition	KOH content, wt.%	Cellulose content, wt.%	Combustion rate, ×10^3 m·s^{-1}	Burning rate, K
PC-2-51	50	5	2.4±0.1	1790±20
PC-2-52	50	10	2.4±0.1	1780±20
PC-2-53	50	15	2.4±0.1	1760±20
PC-2-61	60	5	2.1±0.1	1750±20
PC-2-62	60	10	(blow-off)	1720±20
PC-2-63	60	15	(blow-off)	1710±20
PC-2-71	70	5	(blow-off)	1700±20

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The experimental results showed that the addition of potassium alkali to 60−65 wt.% allows maintaining stable burning of the pyrotechnic composition.

Due to the addition of cellulose, the parameters of EC combustion decrease because of the replacement of a certain amount of reactive combustible components with cellulose. However, the combustion of the composition of PS-2-61 with 60% of KOH and 5% of cellulose is stable and this composition can be used to neutralize acid precipitates. In addition, magnesia and alumina released during combustion are the centers of drop formation which leads to an additional initiation of precipitation. The precipitation process can also be accelerated by adding AgI or NaCl to the pyrotechnic composition assuming that the total number of modifying additives should not exceed 65 wt.%.

The use of the proposed composition for artificial precipitation allows initiating the precipitation over the zones of large natural and man-made fires which leads to the precipitation of harmful combustion products from the atmosphere and prevents the formation of acidic atmospheric precipitation by neutralizing them.

Chlorine and phosgene form a separate group of toxic substances. Unlike the solubility in water of ammonia, those of chlorine (Cl_2) and phosgene ($COCl_2$) are extremely low. A low solubility of chlorine and phosgene in water leads to a low rate of precipitation of these gases by atmospheric precipitation. Therefore, neutralizing agents must be added in order to increase the rate of the atmosphere transformation into the aqua-condensate.

Sodium thiosulfate is the most active chlorine neutralizer according to the following reaction:

$$Na_2S_2O_3 + 4Cl_2 + 5H_2O = 2H_2SO_4 + 2NaCl + 6HCl, \quad (17)$$

but it makes precipitation more acid.

According to Eq. (17), it takes almost 0.5 tons of $Na_2S_2O_3$ to neutralize 1 ton of chlorine. As seen from Eq. (17), the reaction proceeds in aqueous solutions. It must be taken into account that sodium thiosulfate is a combustible and explosive substance, it decomposes when heated to 220⁰C:

$$4Na_2S_2O_3 \overset{t}{=} 3Na_2SO_4 + Na_2S + 4S \downarrow \cdot \quad (18)$$
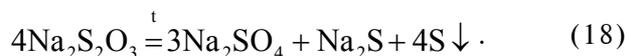
Due to the above, the use of $Na_2S_2O_3$ as an additive for explosive charges proves to be promising.

Sodium hydroxide is an effective neutralizer of chlorine:

$$Cl_2 + 2NaOH = NaCl + NaOCl + H_2O. \quad (19)$$

It takes 1.2 tons of NaOH to neutralize 1 ton of chlorine. Sodium hydroxide is highly soluble in water; therefore, aqueous solutions are usually used in aqueous degassing. As can be seen from Eq. (19), additional salts are formed when chlorine is neutralized with alkali; they are desublimated into hygroscopic crystals and water. It has been established that the formation of such reaction products (hygroscopic crystals) has a positive effect on the process of precipitation.

Despite the fact that phosgene is lowly soluble in water, like chlorine, it is actively neutralized by sodium hydroxide. Taking into account the hydrolysis of phosgene and the formation of HCl and CO_2, its neutralization proceeds according to the equation:

$$COCl_2 + 2NaOH = 2NaCl + H_2O + CO_2. \quad (20)$$

The reaction equation (20) shows that it takes 1.6 ton of sodium alkali or 16 tons of its 10% aqueous solution to neutralize 1 ton of phosgene.

Pyrotechnic compositions with alkali additives have been considered earlier. Similar properties of potassium and sodium alkalis allow replacing them in the composition of the explosive charge without significant changes in the combustion parameters. Thus, similarly with the composition of PC-2-6 with 60% of KOH as a non-combustible additive, the properties of the composition of PC-2-61 with 60% of NaOH were studied. As a result, it was established that this composition has a combustion rate of $(2.4\pm0.1)\cdot10^{-3}$ m·s^{-1} and a burning temperature of 1790 ± 20 K. Within the accuracy, these parameters correspond to the burning parameters of the composition of PC-1-6.

In case of unfavorable weather conditions for the artificial initiation of precipitation, it is expedient to use the method of spraying a finely dispersed reagent (NaOH) pneumatically from light-engineered manned and unmanned aerial vehicles.

Given that the molar masses of chlorine and phosgene are higher than the molar mass of air, the largest concentration of these dangerous gases is localized in the surface layer of the atmosphere. This makes it possible to efficiently use light-engine aircraft for seeding clouds of chlorine or phosgene, which permits significantly reducing material costs in eliminating the release.

Conclusions

This paper showed that the introduction of the pyrotechnic composition KNO_3 as an oxidizing agent of the combustion process in the technology of

production allows significantly reducing the degree of hazard of combustion products for living organisms.

The influence of the Ox/Red stoichiometric concentration on the stability of the high-temperature oxidation parameters was found and experimentally confirmed.

Based on physicochemical calculations and experimental results, the composition of the explosive charge with NaOH and KOH for artificial precipitation initiation was optimized to effectively neutralize the acidity of rains and fogs formed during large-scale natural and man-made fires. Pyrotechnic composition contains up to 65% of KOH, as well as cellulose, which contributes to the additional formation of alkali in the burning reaction of the explosive charge.

Thus, the novelty of this work consists in the expansion of the possibilities of pyrocompositions that have a complex of the following properties: precipitation initiation, neutralization of their acidity, removal from the atmosphere of toxic substances.

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ФІЗИКО-ХІМІЧНІ ОСНОВИ ТЕХНОЛОГІЇ МОДІФІКОВАНИХ ПІРОТЕХНІЧНИХ СКЛАДІВ ДЛЯ ЗНИЖЕННЯ РІВНЯ ХІМІЧНОГО ЗАБРУДНЕННЯ АТМОСФЕРИ

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В роботі наведені результати встановлення технологічних умов виробництва модіфікованих піротехнічних складів, що володіють комплексом наступних властивостей: ініціювання атмосферних опадів, нейтралізація їх кислотності та вимивання токсичних компонентів, що містяться в атмосфері. З урахуванням вимог захисту навколишнього середовища, як пальне в піротехнічному складі запропоновано використовувати Mg, а як окислювач − KNO₃. При горінні запропонованого двошарового пірозкладу виключено утворення хімічно небезпечних продуктів горіння (NH₃ та HCl). За допомогою програмного комплексу «TERMO-CALC» здійснене оцінювання вмісту аміаку та гідроген хлориду в продуктах горіння запропонованих сумішей при оптимальних співвідношеннях пального та окисника. Виконані термодинамічні розрахунки для визначення оптимального співвідношення масових часток окисник/відновник, яке визначено рівним 1:8. Здійснено експериментальні дослідження основних параметрів високотемпературного окислення (температура та швидкість горіння) піротехнічних складів. Запропоновано двошарову структуру пірозаряду з легкозаймистим первинним шаром, що істотно підвищує ймовірність запалю-

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вання піросуміші електроіскровим методом. З метою посилен-
ня ефекту зниження кислотності атмосферних опадів запро-
понована технологія модифікування піротехнічного складу з
додаванням лугу КОН та целюлози. Модифікування розробле-
ного складу з використанням NaOH дозволяє ефективно ней-
тралізувати такі небезпечні гази, як хлор і фосген. Встанов-
лені фізико-хімічні основи технології модифікування піротех-
нічних складів комплексного призначення дозволяють розроб-
ляти склади пірозарядів багатофункціонального типу, спрямо-
вані на штучне ініціювання опадів та хімічну нейтралізацію
небезпечних речовин в атмосфері

Ключові слова: піротехнічний склад, розрахунок,
температура горіння, ініціювання опадів, нейтралізація
фосгену, хімічна нейтралізація кислотних дощів.

PHYSICOCHEMICAL PRINCIPLES OF THE TECHNOLOGY OF MODIFIED PYROTECHNIC COMPOSITIONS TO REDUCE THE CHEMICAL POLLUTION OF THE ATMOSPHERE

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This paper presents the results of determination of conditions for the production of modified pyrotechnic compositions that allow initiating atmospheric precipitation, neutralizing their acidity and scavenging toxic substances from the atmosphere. Taking into account the requirements of environmental protection, the use of Mg as a fuel and KNO₃ as an oxidizing agent in the pyrotechnic composition was suggested. The combustion of the proposed two-layer pyrocomposition impedes the release of chemically hazardous combustion products (NH₃ and HCl). Using TERMO-CALC software package, the content of ammonia and hydrogen chloride in the combustion products of the proposed mixtures was determined at the best fuel-oxidizing agent ratio. The thermodynamic calculations were performed to determine the best reducing/oxidizing agent mass fraction ratio which was stated to be 1:8. The experimental study of the main parameters of high-temperature oxidation (temperature and burning rate) of pyrotechnic compositions was carried out. A two-layer structure of the explosive charge with a highly flammable primary layer is proposed, which substantially increases the probability of ignition of the pyrotechnic mixture triggered by an electric spark. In order to intensify a decrease of the acidity of atmospheric precipitation, a technology for modifying pyrotechnic compositions by adding KOH and cellulose was proposed. The modification of the developed composition with the use of NaOH allows effectively neutralizing such dangerous gases as chlorine and phosgene. The established physicochemical basics of the technology for modifying pyrotechnic compositions for complex purposes allow developing multi-functional explosive compositions aimed at artificial initiation of precipitation and chemical neutralization of hazardous substances in the atmosphere.

Keywords: pyrotechnic composition; calculation; combustion temperature; initiation of precipitation; neutralization of phosgene; chemical neutralization of acid rains.

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