

# REGULARITIES OF CATALYSTS'S EFFECT ON THE COMBUSTION OF ENERGY-SATURATED MATERIALS OF DIFFERENT STRUCTURES CONTAINING NITRO GROUPS

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## Relevance of the research topic

The widespread use of ballistic propellants (BP) as solid propellants became possible due to the introduction of catalysts into their composition, which not only increase their burning rate ( $U$ ), but, most importantly, significantly reduce its dependence on pressure ( $p$ ) and on the initial temperature charge ( $T_0$ ). The use of such propellants has significantly improved the performance of rocket systems. Therefore, it is understandable why numerous studies have been devoted to the study of the regularities and mechanism of the influence of catalysts on the combustion of fuels, in which various points of view on the mechanism of combustion catalysis were proposed, especially on the key issue - in which combustion zone do catalysts operate, as a result of which the combustion rate and its dependence on pressure change.

In Mendeleev's University of Chemical Technology of Russia (MUCTR) at the department of chemistry and technology of high molecular compounds (CTHMC) it was found that catalysis of BP's combustion occurs only when two conditions are met: the first is the formation of a developed carbon skeleton on the combustion surface, on which there is a significant accumulation of catalyst particles without their agglomeration; and secondly, the coefficient of thermal conductivity of this frame ( $\lambda_{\text{frame}}$ ) should be significantly (by  $\sim 2$  or more times) higher than for the gas zone ( $\lambda_{\text{gas}}$ ) above the combustion surface of powders without catalysts. Only in this case does an increase in the heat flux from the framework zone into the condensed phase (c-phase) occur, leading to an increase in the combustion rate. With increasing pressure, the possibility of forming a framework decreases and, accordingly, the effectiveness of the catalyst decreases, which leads to a decrease in the value of the coefficient " $\nu$ " in the combustion rate law ( $U = Bp^\nu$ ).

It can be assumed that BP combustion catalysts should similarly affect the combustion of most energy-saturated materials (EMs) containing nitro groups (NO<sub>2</sub>), despite the fact that in many properties they can significantly differ from the main components of BP, which are nitroesters, in terms of burning rate and thermal decomposition. The results of these studies can show that the combustion catalysis of most EMs, including mixed systems, during the combustion of which heat is released as a result of redox reactions, occurs according to the same mechanism as for BP, i.e. is one. This will make it possible to more purposefully address the issue of regulating the burning rate of various EMs.

### **Purpose and tasks of the work**

The purpose of this work was to clarify the fundamental question of the applicability of the combustion catalysis mechanism proposed for BP to the combustion of various EMs containing nitro groups.

To achieve this purpose, the following tasks were solved in the work:

1. Study of the regularities of the effect of BP combustion catalysts individually and in combination with soot and carbon nanotubes on the combustion rate of various explosives;
2. Study of the effect of catalysts on the temperature profile in the combustion wave of aromatic nitro compounds to clarify the mechanism of combustion catalysis;
3. Study of the structure and elemental composition of the framework on the surface of quenched samples of aromatic nitro compounds;
4. Study of the effect of catalysts on the flash point, flash delay time and thermal decomposition of aromatic nitro compounds.

### **Scientific novelty of the work**

For the first time, the effect of high-performance BP catalysts on the combustion of ten individual compounds containing –NO<sub>2</sub> groups, which differ significantly in thermal stability, combustion rate, and temperature, has been systematically studied. It

is shown that the regularities of the effect of catalysts on the combustion of these explosives do not qualitatively differ from those for BP:

- catalysts without soot and CNTs affect the combustion of only some explosives, while their efficiency is low ( $Z_2 = 1.2 - 1.4$ ), which significantly (1.5 - 3 times) increases with the introduction of soot and, especially, CNTs.
- for high-energy explosives with increased burning rate and temperature, the effect of catalysts, as for BP, manifests itself only when they are introduced together with soot and, especially, with CNTs. In this case, the efficiency of the combined catalyst is determined by their ratio: the dependence  $Z$  (% of carbon materials) passes through a maximum, as in the case of BP.
- as for BP, the value of  $Z$  in the pressure range of 2 – 18 MPa decreases, as a result of which the value of „ $v$ ” decreases by 1.5 – 4 times. In the area of lower pressure (less than  $P \leq 2$  MPa), for some explosives, the value of  $Z$  can increase with increasing pressure, i.e. the dependence  $Z(p)$  passes through a maximum, therefore, in this region, the value of “ $v$ ” is much higher than for samples without catalysts.

It has been shown for the first time that the effect of catalysts on the parameters of the combustion wave of trinitrotoluene (TNT), trinitrophenol (TNP) and trinitroresorcin (TNR) is the same as for BP: the catalyst increases the temperature gradient and the rate of heat release in the framework zone, but only this cannot increase the heat supply from the framework zone ( $q_\lambda = (\lambda/\rho U) \cdot dT/dx$ ) into the c-phase, since the burning rate increases to a greater extent than  $dT/dx$ .

It was shown for the first time that, as for BP, there is a sooty framework on the surface of quenched TNP and TNR samples, on which catalyst particles are significantly accumulated, as a result of which its thermal conductivity coefficient is ~ 2.4 times higher for TNP and ~ 7 times higher for TNR than the zones above the combustion surface of samples without catalysts.

It was shown for the first time that for the studied samples with a relatively small amount of catalysts (up to 4%), as well as for BP, there is no relationship between their

effect on the combustion rate and thermal decomposition. This confirms that catalysis during their combustion occurs on the framework, and not in the c-phase.

On the example of TNR, it is shown that the ability to burn EMs has a significant effect not only on the diameter of the charge, but also on the magnitude of the ignition pulse.

### **Theoretical and practical significance of the work**

Based on previously obtained data for BP of various compositions, the results of this work, as well as the results obtained at the MUCTR for mixed samples based on perchlorate ammonium (PCA), it can be assumed that combustion catalysis for all EMs, during the combustion of which heat is released as a result of redox reactions, proceeds according to a single mechanism: a soot skeleton should form on the combustion surface, on which catalyst particles accumulate, increasing the rate of heat release, and the thermal conductivity of the frame. As a result, the burning rate increases.

The proposed mechanism of combustion catalysis allows more purposefully and in a shorter time to combine various fuels with a controlled burning rate and its dependence on pressure and initial temperature of the charge. For example, this paper shows the real possibility of developing nitroglycerine-free fuels containing ~ 30% TNT (including batches of explosives intended for disposal) for gas generators and rocket systems intended for economic purposes. These compositions have a low dependence of the combustion rate on pressure ( $\nu = 0.36 - 0.33$ ) and low cost. Charges from these propellants can be obtained using rolling and through-pressing.