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SHORT COMMUNICATION

Theoretical evaluation of TKX-50 as an ingredient in rocket propellants

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Dedicated to Professor Christoph Janiak on the occasion of his 60th birthday

Dihydroxylammonium-5,5′-bistetrazolyl-1,1′-diolate (TKX-50), is one of the most promising energetic materials that has been reported in recent time. TKX-50 shows great potential for future application as a secondary explosive, due to its sensitivity and explosive performance data. In this work, we report initial computational results which have been undertaken to investigate the viability of the application of TKX-50 as an energetic ingredient in rocket propellants.

Out of the many reports of new explosive compounds which have been published in the literature in recent time, TKX-50 must be considered to be one of the most exciting new energetic materials which has been developed in the past decade, since it shows great promise for future application as a secondary explosive. Not only does TKX-50 show the desired combination of low impact sensitivity and friction sensitivity with high thermal stability, density and detonation velocity, it can also be prepared using a facile, inexpensive synthesis. Additionally, TKX-50 shows low toxicity. All of these properties combined makes TKX-50 particularly attractive as an explosive of the future which combines increased safety with high-performance.[1,2] Although the first report about TKX-50 was published as recently as 2012,[3–5] the interest in TKX-50 has been considerable since this initial report, and many important aspects of the chemical and physical properties of TKX-50 have since been extensively investigated and reported by groups from all over the world.[6]

Generally speaking, composite rocket propellants usually consist of a powdered oxidizer (e.g. ammonium perchlorate, AP), powdered metal fuel (e.g. aluminum, Al) and a plasticized binder (e.g. HTPB).[7,8] The category of propellants known as high-energy composite (HEC) propellants in addition add a high-energy explosive (e.g. RDX, HMX or CL-20) to the formulation and partly replace AP with these high-energy materials.[9–13] Although this results in an increase in the specific impulse (I_{sp}), implementation of HECs is limited due to the increased hazard that the high-energy explosive additives bring with them, since they are impact and friction sensitive additives.[9–13]

It has been reported in the literature, that computational results for TKX-50-based solid rocket propellant formulations (22% energetic binder, 20% oxidizer, 18% Al, 40% TKX-50) indicated that TKX-50 shows a higher density impulse than HMX, but is lower than that of CL-20.[14] The NASA SP-273 computer code was used to predict the parameters of rocket propellant formulations, and was able to show that TKX-50 containing formulations showed a superior specific impulse value compared to corresponding formulations in which TKX-50 was replaced by other common explosives.[14] Based on this work, the authors concluded that the theoretically predicted data indicated that TKX-50 has potential for application in rocket and gun propellants.[14]

The properties of composite propellants containing TKX-50 have been investigated experimentally with different mass fractions of TKX-50 particles – specifically on TKX-50/HTPB binder slurries and AP/HTPB/Al propellant slurries.[15] It is possible with the inclusion of specially selected energetic materials to increase the gravimetric specific impulse or the density specific impulse of propellants, however, the energetic materials chosen for this purpose must show low sensitivity to external stimuli such as impact and friction. Since TKX-50 shows a high detonation velocity, but at the same time a low sensitivity to friction (comparable to or lower than those of RDX, HMX and CL-20) and impact (lower than those of HMX, RDX and CL-20), it is an interesting candidate not only as an explosive, but also as an ingredient in propulsion compositions.[15] In addition, the effects of TKX-50 on the properties of HTPB-based composite solid propellants have been studied computationally.[16] It has been concluded that TKX-50 particles could be used as the energetic components which would improve the combustion properties of the composite propellant.[16]

In order to assess the potential of TKX-50 as a possible future component of solid rocket motors, we calculated (EXPLO5)[17] the performance of TKX-50 in various solid rocket propellant formulations.

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A typical composite propellant formulation (70% AP, 16% Al, 12% HTPB and 2% epoxy) with real-life applications has a calculated specific impulse of 264 s. The calculated specific impulses of the pure (100%), individual energetic ingredients are the following: NG 259 s, HMX 266 s, CL-20 272 s and TKX-50 268 s.

In this work, we have now evaluated high-energy composite (HEC) propellants with the following composition:

Glycidyl azide polymer	(GAP)	10%
Nitroglycerin	(NG)	15%
Aluminum	(Al)	18%
Energetic filler	(HMX, CL-20, TKX-50)	X%
Ammonium perchlorate	(AP)	Y%

The percentage ratios X+Y=57% were optimized in order to obtain an oxygen balance with respect to CO_2 of −33%, which corresponds to that of the above mentioned typical composite propellant formulation (70% AP, 16% Al, 12% HTPB and 2% epoxy) with real-life applications. The results are summarized in Table 1.

It is shown in Table 1, that the high-energy composite (HEC) propellant formulation based on TKX-50 is calculated to have the highest specific impulse, exceeding those of the corresponding HMX and CL-20-based formulations. In addition, the typical composite propellant formulation of 70% AP, 16% Al, 12% HTPB and 2% epoxy only has a calculated specific impulse of 264 s. This means that, all of the three HECs shown in Table 1 were calculated to possess higher specific impulses than that of the secondary explosive-free standard composite propellant formulation. However, it must be pointed out that importantly, TKX-50 is less impact and friction sensitive than CL-20, and this is important, since it should result in a significant reduction in the hazard of the propellant formulation in comparison with the same propellant composition containing CL-20 instead of TKX-50. A further safety aspect which is of importance is that TKX-50 shows a relatively low acute toxicity and no mutagenicity.[19–12] These initial findings should instigate and encourage experimental studies into the above-mentioned HECs, in order to verify the obtained computational results.

Table 1. EXPLO5 calculation results for various high-energy composite (HEC) propellant formulations, as well as sensitivity data for the individual secondary explosives (HMX, CL-20 and TKX-50) taken form the literature.

High-energy explosive component	HMX	CL-20	TKX-50
Impact sensitivity [J][18]	7.4	3–4	20
Friction sensitivity [N][18]	120	ca. 96	120
ESD [J][18]	0.2	ca. 0.1	0.1
Formulation	10% GAP, 15% NG, 18% Al, 45% HMX, 12% AP	10% GAP, 15% NG, 18% Al, 54% CL-20, 3% AP	10% GAP, 15% NG, 18% Al, 41% TKX-50, 16% AP
Oxygen balance [%]	−33	−33	−33
Specific impulse [s]	274	275	278
Isochoric combustion temperature [K]	3806	3964	3701
Heat of combustion [kJ/kg]	6094	5971	5996
Exhaust velocity [m/s]	2690	2694	2723

Experimental Section

All calculations were carried out with the thermochemical equilibrium code EXPLO5 (version 6.05.02).[17] Theoretical rocket performances were calculated for an infinite-area combustion chamber model, taking the assigned pressure ratio (p_c/p_e) to be 70 (assigned chamber pressure 7 MPa and exit pressure 0.1 MPa). The calculation is performed assuming equilibrium flow conditions.

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