Erroneous use of balance equations in combustion theory of energetic materials

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The problem is discussed of erroneous using the balance equations in studies dealing with determination of energetic materials (EMs) high temperature kinetic parameters and calculation of dependency of burning rate on radiant flux. High temperature kinetic parameters are widely used in caculations of ignition and combustion characteristics. Unfortunately, classical thermal analysis methods (heating rate ca. 1 K/s) could not provide adequate data for evaluating the EM burn rate because typically the EMs heating rate during combustion is much higher than 1000 K/s. The solution to the problem was proposed by A.G. Merzhanov [1] who suggested determining kinetic parameters from calculation of ignition criterion when using the data on EM ignition delays. This criterion states that at the ignition instant the heat flux generated by condensed phase (global) reaction equals in magnitude to the external heat flux. Unfortunately, mathematical justification for that approach has not been performed. In present work numerical calculations were performed using mathematical model of EM's ignition and the results of virtual experiments were processed using Merzhanov's ignition criterion. It was found [2] that the use of simple heat balance gives wrong magnitude of kinetic parameters and ignition criterion should be complemented with the fitting coefficient, which depends on the values of heat flux and kinetic parameters.

Dependencies of burn rate on initial temperature and radiant flux are widely used in technical applications and for verification of combustion models. In some earlier works [3,4] the assumption has been made on the basis of simplified heat balance equation that the combustion of transparent EM under radiant flux q_r is equaling to combustion at enhanced initial temperature $T_o^* = T_o + q_r / \rho c r(q_r)$, where ρ = density, c = heat capacity and $r(q_r)$ = burn rate. Processing the dependencies $r(T_0)$ and $r(q_r)$ obtained in physical experiments [3] has shown that using a simplified heat balance equality gives not correct results and explanation has been found very recently based on detailed combustion modeling, which showed necessity of implementing proper fitting coefficients in balance equation.

[1] A.G. Merzhanov, *Combustion and Flame* **1967**, *11(3)*, pp. 201-211.

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[3] E.V. Konev, Combustion, Explosion, and Shock Waves, **1965**, *1 (2)*, pp. 53 – 56.

[4] I.G. Assovsky, Physics of combustion and internal ballistics. M, Science, **2005**.