NUMERICAL SIMULATION OF UNSTEADY DETONATION PROCESSES IN A SHOCK-WAVE TUBE WITH A REACTING SUBSTANCE – HMX

D. V. Begashev, A. V. Ershov, V. V. Tashlanov

FSUE «RFNC – VNIITF named after Academ. E. I. Zababakhin», Snezhinsk, Russia

E-mail: vniitf@vniitf.ru

A shock-wave tube (SWT) is one of the main elements of non-electric blasting systems widely used in blasting operations on the ground surface, in underground mines, and shafts. SWT can be used also in systems for triggering various pyrotechnic devices. The SWT under consideration is a plastic tube (waveguide) of small diameter with HMX layer applied to its inner surface, containing of 1 to 7% of aluminium powder.

To ensure reliable operation of the SWT, it is necessary to thoroughly understand how detonation processes are formed and evolved in it. One of the methods that make it possible to study in detail unsteady detonation processes in the SWT is a numerical simulation based on mathematical models (MM) of multidimensional flows of chemically reacting multicomponent gas mixtures (GM) with detonation waves. In this work, the mathematical description of the processes under study is based on the RANS (Reynolds Averaged Navier-Stokes) [1], the modified Menter's *k*-ω turbulence model SST (Shear Stress Transport) [2], and the proposed two-stage kinetic model of the thermal decomposition of HMX, including forward chemical reactions of the first order in both condensed and gas phases. The Reynolds stresses in Menter's SST turbulence model are related to average flow parameters according to Boussinesq hypothesis through the apparent scalar eddy viscosity μ_T, which is determined by the Bradshaw formula [2]. Proposed MM allows us to simulate slow combustion modes – deflagrations, as well as the transition to detonation.

The RANS equations are closed by the equation of state for a mixture of ideal gases:

$$\overline{p} = R\sum_{i=1}^{S} M_i^{-1}\left(\overline{\rho}\tilde{\omega}_i\tilde{T} + \overline{\rho\omega_i T''}\right) \tag{1}$$

and the two-parameter turbulence model SST, including the transport equations for the kinetic turbulence energy *k* and the specific dissipation rate of the kinetic turbulence energy ω [2].

In equation (1), the following notations are adopted: *p* – pressure, Pa; *R* – universal gas constant, J/(mol·K); M_i – molecular mass of the *i* – component GM, kg/mol; ρ – GM density, kg/m³; ω_i – mass fraction of the *i* – component GM; *T* – thermodynamic temperature, K; *S* – number of components GM symbols «–» and «~» respectively mean Reynolds and Favre averaging, while the symbol «″» indicates the Favre fluctuation.

Below is presented the two-stage kinetic model of decomposition of HMX in condensed and gas phases, based on the analysis of the works of G. A. Avakyan, F. I. Dubovitsky, B. L. Korsunsky, N. E. Ermolin, V. E. Zarko, A. A. Paletsky, and others:

$$\begin{aligned}&\mathrm{HMX_S} \xrightarrow{k_1} 1{,}817\mathrm{NO} + 1{,}103\mathrm{H_2O} + 0{,}919\mathrm{CO} + 0{,}905\mathrm{HCN} + 0{,}757\mathrm{H_2} + 0{,}508\mathrm{N_2O} + 0{,}421\mathrm{N_2} + \\ &+ 0{,}345\mathrm{HMX_V} + 0{,}309\mathrm{NO_2} + 0{,}240\mathrm{CO_2} + 0{,}298\mathrm{CH_2O} + Q_\mathrm{c};\end{aligned} \tag{2}$$

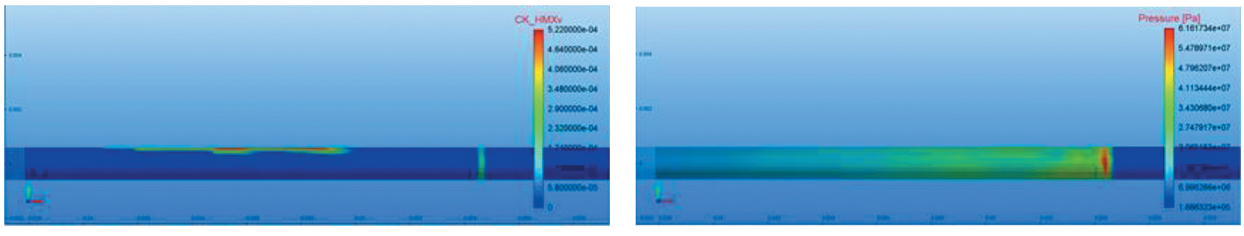
$$\mathrm{HMX_V} \xrightarrow{k_2} 0{,}945\mathrm{CO_2} + 2{,}603\mathrm{CO} + 0{,}452\mathrm{C(т)} + 3{,}507\mathrm{H_2O} + 0{,}493\mathrm{H_2} + 4\mathrm{N_2} + Q_\mathrm{g}, \tag{3}$$

Where $\mathrm{HMX_S}$ – is HMX in the solid phase; $\mathrm{HMX_V}$ – is HMX vapor; $k_1 = 1{,}58\cdot10^{11}\exp\left(-158687{,}3/RT\right)$ – the rate constant for the gasification reaction of HMX, s⁻¹; $k_2 = 1{,}58\cdot10^{14}\exp\left(-165386{,}5/RT\right)$ – the rate constant for the thermal decomposition reaction of HMX in the gas phase, s⁻¹; Q_c, Q_g – the thermal effects of the reactions J/mol.

The thermal effects of reactions (2) and (3) were calculated based on the standard enthalpies of formation of the substances involved in the reactions, taking into account the reactions occurring at constant volume.

The numerical analysis of proposed MM for the studied processes was conducted using the software package "LOGOS" [3]. Figures 1 and 2 present some results of numerical simulation of HMX combustion in the SWT with inner diameter of 1.2 mm. The initiation of the SWT was modeled by introducing a mass flow of propellant gases at the entrance of the waveguide with a temperature of 2936 K. It was established

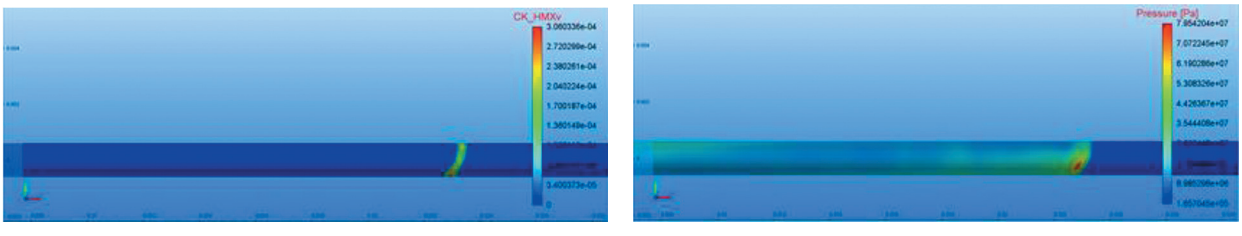
that the transition to detonation occurs according to the scheme: *deflagration* → *flow cumulation* → *ignition (thermal explosion)* → *overdriven detonation* (Fig. 1) → *steady-state spin detonation* (Fig. 2). A characteristic feature of the structure of the spin detonation wave is the existence of pressure maxima at the wall – of the spin's "head", which rotates around the axis of the waveguide simultaneously with the translational motion of the detonation wave front. The detonation velocity determined from the calculations satisfactorily agrees with the experimental data on measuring the detonation velocity in the SWT.



a *b*

Fig. 1. Distribution of parameters of the thermal decomposition process of HMX in SWT during the transition from deflagration to detonation:

a – mass fraction of HMX vapors; *b* – pressure in the GM



a *b*

Fig. 2. Distribution of parameters of the thermal decomposition process of HMX in SWT in the steady-state spin detonation mode:

a – mass fraction of HMX vapors; *b* – pressure in the GM

References

1. **Warnatz, U.** Combustion. Physical and Chemical Aspects, Modelling, Experiments, Formation of Pollutants [Text] / U. Warnatz, U. Maas, R. Dibble ; translated from English by G. L. Agafonov ; ed. by P. A. Vlasov. – M. : FISMATLIT, 2003. – 352 pp.

2. **Menter, F. R.** Ten years of experience with the SST turbulent model [Text] / F. R. Menter, M. Kuntz, R. Lantry ; ed. by K. Hanjalic, Y. Nagano, M. Tummers // Turbulence, Heat and Mass Transfer 4. – Begell House Inc, 2003.

3. **Kozelkov, A. S.** Multifunctional Software Package LOGOS: Physical and Mathematical Models for Solving Problems in Aerohydrodynamics and Heat Transfer [Text] : Preprint. RFNC – VNIIEF No. 111 / A. S. Kozelkov, Yu. N. Deryugin, D. K. Zelensky, et al. – Sarov : RFNC – VNIIEF, 2013. – 67 pp.