# THERMODYNAMIC MODELING OF DETONATION OF HYDRAZINE-NITROMETHANE LIQUID MIXTURES

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Liquid explosive mixtures containing hydrazine are used as components of rocket propellents and also in other technical devices. Detonation parameters of these mixtures are little investigated in comparison with detonation properties of the mixture individual components. Therefore, theoretical calculation of detonation of the liquid explosive mixtures in order to predict their detonation behavior is of great interest.

In this work we carried out thermodynamic modeling of the detonation parameters of binary hydrazine-nitromethane mixtures.

It has been shown that binary mixtures of hydrazine and nitromethane contain molecules of not only the source components, but also molecules of an associate. The formation of the associate considerably affects the thermodynamic properties and detonation parameters of these explosive mixtures. Furthermore, the presence of the associate molecules is a major factor that determines the shock sensitivity of the studied solutions.

We have developed an equation of state (EOS) of hydrazine-nitromethane system. This EOS takes into account a possibility of formation of associate molecules due to interactions between hydrazine and nitromethane molecules. We have determined possible chemical formula of the associate as well as its standard state heat of formation and entropy. Thermodynamic calculations of detonation parameters of hydrazine-nitromethane binary systems have been done for a wide range of hydrazine content in explosive mixture (from 0 to 75 weight-percent). It is shown that using of the obtained EOS considerably improves an accuracy of predicted detonation properties of hydrazine-nitromethane mixtures and gives excellent agreement between computed and experimental detonation velocities [1]. This EOS also allows to predict the shock sensitivity of the hydrazine-nitromethane solutions in close agreement with the measured data. The presence of the associate molecules in the hydrazine-nitromethane mixtures allows to explain why the experimental shock sensitivity of this binary system has maximum value at hydrazine concentration of about 25 weight-percent.

The detonation products of the studied binary mixtures were found to contain nanoparticles of solid carbon. The phase state of nano-size carbon crystals (i.e. graphite or diamond) depends on the composition of the explosive mixture. Our calculations predict that at some compositions of the mixtures their detonation occurs in the anomalous mode [2], that causes a sharp change of slope in the dependence of detonation velocity on mixture composition and corresponding breaks in values of pressure behind the detonation front.

For the gaseous detonation products we used BKW EOS with our own set of coefficients BKW-RR [3]. Although the BKW EOS has a weak basis in statistical mechanics, the BKW-RR model is useful in practical applications because its coefficients were calibrated to accurately reproduce experimental data on detonation parameters for a collection of condensed explosives.

To describe thermodynamic properties of solid carbon phases more accurately we have obtained new EOS for graphite and diamond with the Grüneisen gamma depending on specific volume only [4]. All available experimental data on thermal expansion, heat capacity, shock-wave and static compression have been used to determine the best EOS parameters. These EOS have been applied to calculate the graphite-diamond equilibrium line in a wide range of pressures and temperatures. The computed phase equilibrium line fits available experimental data and theoretical calculations. This confirms that the EOS obtained for graphite and diamond are physically reasonable.

The EOS of gaseous and condensed detonation products used in the present work allowed to obtain sufficiently precise results for the solutions of hydrazine and nitromethane. We suppose that these EOS can be used to calculate reasonable detonation properties also for other CHNO liquid explosive systems. To predict detonation parameters of explosive mixture more reliably, it is desirable to have experimental data on its density and enthalpy of mixing.

## REFERENCES

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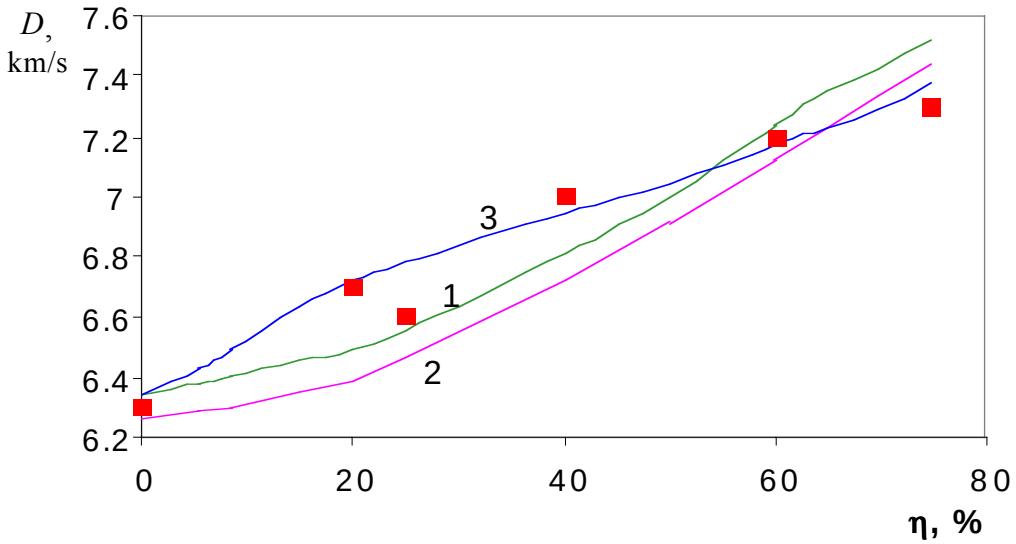


FIG. 1. Detonation velocity $D$ of hydrazine-nitromethane (H-NM) solutions vs weight fraction of hydrazine in source (before mixing) system η. Line 1 - calculation for ideal H-NM solutions and EOS of graphite and diamond nanoparticles. Line 2 - calculation for ideal H-NM solutions and EOS of non-disperse graphite and diamond. Line 3 - calculation for EOS of H-NM solutions and EOS of graphite and diamond nanoparticles. Points - experiment [1].

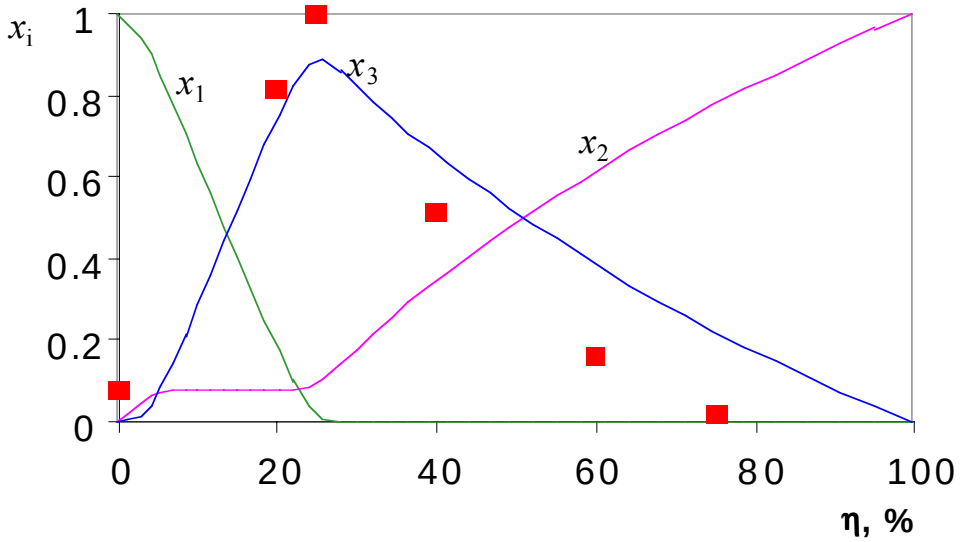


FIG. 2. Calculated mole fractions of components of hydrazine-nitromethane solutions ($x_1$ - nitromethane, $x_2$ - hydrazine, $x_3$ - associate) at $T$ = 298.15 K, $p$ = 1 atm vs weight fraction of hydrazine in source (before mixing) system η.
Points - experiment [1] on shock sensitivity of the solutions in relative units (gap values divided by 105 mm).