# Using reliable empirical methods in predicting performance of pure and mixed explosive formulations on the basis of heat of formation

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## ABSTRACT

Some reliable empirical methods have been introduced so that they can combined in form of a new computer code for predicting performance of pure and mixed explosive formulations. If condensed phase heat of formation of explosive was not available, computer code can calculate gas phase heat of formation of explosive and use appropriate method to evaluate its performance. Detonation pressures at various loading densities, heats of detonation and detonation temperatures as important detonation parameters can be calculated by new computer code. Predicted results show good agreement with experimental values. The results of new computer code for detonation pressures and detonation temperatures also give comparable results with respect to the computed outputs obtained by complex computer code using BKWR and BKWS equations of state.

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## INTRODUCTION

Detonation pressure, heat and temperature are three important detonation performance parameters which can be determined by complicated computer codes or empirical methods. In an effort to make the best use of limited resources and to minimize the waste ensuing from experimental measurements, various methods have been developed to aid in formulations of advanced propellants and explosives. Elimination of poor candidate energetic compounds before investing in synthesis and testing will go far toward achieving this goal. The development of new simple and reliable computer codes to predict properties related to performance allow screening upon the conception of a new energetic compound.

Detonation products can be obtained at high pressures and temperatures simultaneously which covers a wide range of pressures, ~1-100 GPa, and temperatures, ~1000-5000K[1]. Complicated thermochemical/hydrodynamic computer codes such as BKW[2] and RUBY[3] and latter's offspring TIGER[4], CHEQ[5], and CHEETAH[6] (a C version of TIGER) with an appro-
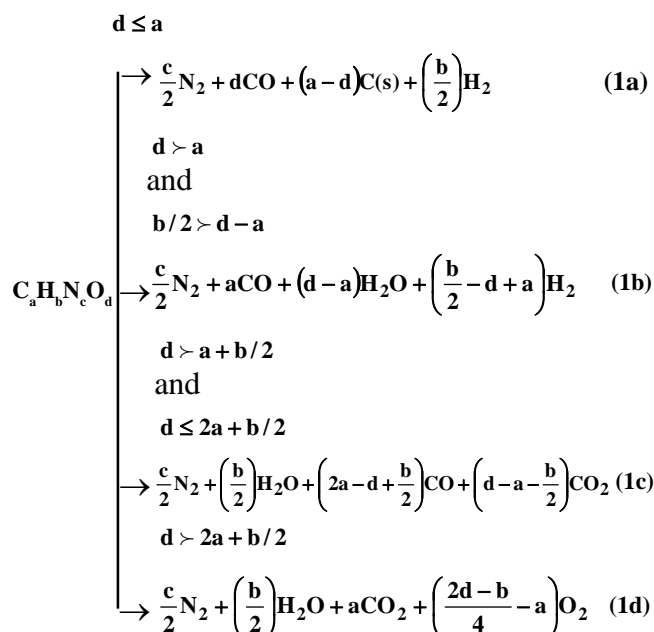
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priate empirical equation of state such as Becker-Kistiakosky-Wilson (BKW-EOS)[7], the Jacobs-Cowperthwaite-Zwisler (JCZ-EOS)[8] and Kihara-Hikita-Tanaka (KHT-EOS)[9,10] can be used to determine detonation properties. Of mentioned equations of states, the BKW-EOS in spite of its weak theoretical basis is used extensively to calculate detonation properties of high explosives. Three different parameteriza tions of the BKW-EOS are the BKWC-EOS[6], BKWR-EOS[11] and BKWS-EOS[12]. Of theses, the BKWS-EOS is one of the best equations of states for predicting detonation temperatures. The computation of detonation parameters by thermochemical/hydrodynamic computer codes in spite of its complexity usually requires measured condensed heat of formation of the explosive.

It should be noted that the accuracy of predictive methods are not necessarily enhanced by greater complexity. Some new empirical methods have been recently introduced for calculation of detonation pressure, heat and temperature[13-27]. Gas phase or condensed phase heats of formation can be used in new procedures to predict mentioned detonation parameters. The purpose of this work was to introduce a simple computer code for estimating detonation pressure at specified loading density, detonation heat and temperature of various $C_aH_bN_cO_d$ explosives. The predicted results of detonation pressures and heats for some well-known explosives will be compared with experimental data as well as computer outputs of two equations of state, namely the BKWS-EOS and BKWR-EOS. The present computer code uses Joback's method[28] to calculate gas phase heat of formation of energetic compounds. It can also be used for pure and mixed explosive formulations without any difficulties.

**Prediction of detonation pressure**

**1. Using condensed phase heat of formation**

The equilibrium composition of gaseous products can be determined through experimental measurement, thermochemical equilibrium or by suggesting an appropriate detonation reaction. Since thermochemical calculations indicate that 94% of gaseous products consist of CO, $H_2O$, $H_2$, $N_2$ and $CO_2$[29], it was shown that the following decomposition reactions is suitable for $C_aH_bN_cO_d$ energetic compounds[16]:

$$d \leq a$$

$$\rightarrow \frac{c}{2}N_2 + dCO + (a-d)C(s) + \left(\frac{b}{2}\right)H_2 \qquad (1a)$$

$$d \succ a$$
$$\text{and}$$
$$b/2 \succ d-a$$

$$C_aH_bN_cO_d \rightarrow \frac{c}{2}N_2 + aCO + (d-a)H_2O + \left(\frac{b}{2}-d+a\right)H_2 \qquad (1b)$$

$$d \succ a+b/2$$
$$\text{and}$$
$$d \leq 2a+b/2$$

$$\rightarrow \frac{c}{2}N_2 + \left(\frac{b}{2}\right)H_2O + \left(2a-d+\frac{b}{2}\right)CO + \left(d-a-\frac{b}{2}\right)CO_2 \qquad (1c)$$

$$d \succ 2a+b/2$$

$$\rightarrow \frac{c}{2}N_2 + \left(\frac{b}{2}\right)H_2O + aCO_2 + \left(\frac{2d-b}{4}-a\right)O_2 \qquad (1d)$$

Experiments show that the C-J detonation pressure is roughly proportional to the loading density squared[2]. One of the most important properties of an explosive is the solid state density, which determines the performance of the explosive. The C-J detonation pressure can be correlated linearly with the heat of detonation as well as the number moles of gaseous products and loading density as follows[16]:

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$$P_{det} = 15.88\alpha(MQ_{det})^{1/2}\rho_0^2 - 11 \qquad (2)$$

where $P_{det}$ is the C-J detonation pressure in kbar, $\alpha$ is the number of moles of gaseous products of detonation per gram of explosive, M is the average molecular weight of gaseous products, $Q_{det}$ and $\rho_0$ are heat of detonation and loading density, respectively. The $Q_{det}$ can be defined as the negative of the enthalpy change of the detonation reaction which is determined from the heat of formation of reactant and decomposition products of the explosive through the relation:

$$Q_{det} \cong -\frac{[\Delta H_f(\text{detonation products}) - \Delta H_f(\text{explosive})]}{\text{formula weight of explosive}} \qquad (3)$$

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To predict detonation pressure, appropriate decomposition pathway according to Eqs. (1a) to (1b) for a pure or composite explosive can be selected and heat of detonation can be calculated by using condensed phase heat of formation of explosive and the standard heats of formation of assumed detonation products. It should be mentioned that a positive heat of formation (per unit weight) is favorable for an explosive because it leads to a greater release of energy upon detonation.

## 2. Using gas phase heat of formation

No precise prediction of gas phase heat of formation was required here in order to reproduce the experimental data within the error limits ascribed to that of data. The following equation was used to find detonation pressure[18]:

$$P_{det} = -2.6 + \left(-1026a' + 226b' + 1031c' + 3150d' + 30.7\Delta H_f^{\circ'}(g)\right)\rho_0^2 \quad (4)$$

are a, b, c, d and gas phase heat of formation of explosive divided by molecular weight of explosive, respectively. As seen in Eq. (4), detonation pressure is relatively insensitive to large variation in the gas phase heat of formation of the unreacted explosive that is significant in view of the uncertainty often associated with different methods of calculation of the heats of formation by additivity rules.

## Predicting detonation temperature

### 1. Using condensed phase heat of formation

Typical detonation products of high explosives with the elements carbon, hydrogen, nitrogen and oxygen at high pressures and temperatures simultaneously are CO, $N_2$, $CO_2$, $H_2O$, solid carbon, etc. Complex chemical reactions are initiated to sustain the detonation process. Detonation temperature is maximum temperature that can be obtained by assuming that heat of decomposition of explosive is used entirely to heat the products. To predict detonation temperature, based on decomposition reactions given in Eqs. (1a) to (1d), four correlations can be used to estimated detonation temperature according to the following conditions[21]:

**(i)** If, then d$\leq$a

$$T_{det} = 298 + \frac{\Delta H_f - 529.4d}{10.95 \times 10^{-3}a - 0.1132b + 13.35 \times 10^{-3}c - 99.1 \times 10^{-3}d} \quad (5a)$$

**(ii)** If $d \succ a$ and $b/2 \succ d - a$, then

$$T_{det} = 298 + \frac{\Delta H_f - 943.4a + 1229.5d}{-0.1914a + 59.67 \times 10^{-3}b + 16.87 \times 10^{-3}c + 0.2224d} \quad (5b)$$

**(iii)** If $d \succ a + b/2$ and $\leq 2a+b/2$, then

$$T_{det} = 298 + \frac{\Delta H_f - 1158.3a - 252.3 + 847.9d}{-0.2964a + 55.09 \times 10^{-3}b + 18.66 \times 10^{-3}c + 0.1911d} \quad (5c)$$

**(iv)** If $d \succ 2a + b/2$ then,

$$T_{det} = 298 + \frac{\Delta H_f + 625.2a - 142.8b}{59.05 \times 10^{-3}a - 43.81 \times 10^{-3}b + 18.66 \times 10^{-3}c + 20.36 \times 10^{-3}d} \quad (5d)$$

where $T_{det}$ is detonation temperature in K and $\Delta H_f$ is condensed heat of formation. It is worthwhile to note that the present method is exceedingly simple and at the same time gives the results that are comparable with respect to the other methods involving the equations of state of the products.

## 2. Using gas phase heat of formation

Since condensed phase heat of formation can correlate with gas phase heat of formation for some classes of explosives[30], crystal effects can also be excluded for determining the detonation temperature in this manner. Two following correlations (6) and (7) can be obtained for aromatic and non-aromatic explosives, respectively:

$$T_{det} = \begin{pmatrix} -75.8 + 950.8a' + 12.3b' + 1114.9c' \\ +1324.5d' + 1.2\Delta H_f^{\circ'}(g) \end{pmatrix} \times 10^3 \quad (6)$$

$$T_{det} = \begin{pmatrix} 149.0 - 1513.9a' - 196.5b' - 206.6c' \\ -2346.2d' + 1.2\Delta H_f^{\circ'}(g) \end{pmatrix} \times 10^3 \quad (7)$$

## Prediction of heat of detonation on the basis of gas phase heat of formation

It was also shown that the heat of detonation of a high explosive as one of detonation parameters can most appropriately be expressed as its elemental composition and heat of formation of explosive in gas phase rather than the condensed phase. It was found that the same as detonation temperature, two optimized correlations can be derived for non-aromatic and aromatic explosives, respectively[22], in which $H_2O$ is in liquid state as follows:

$$Q_{det} = 58.722a' - 55.011b' - 21.234c' + 250.92d' + 4.485\Delta H_f^{\circ'}(g) \quad (8)$$

$$Q_{det} = 61.781a' - 51.317b' + 30.656c' + 91.446d' - 0.2791\Delta H_f^{\circ'}(g) \quad (9)$$

As seen, Eqs. (8) and (9) require no prior knowledge of any measured, estimated or calculated physical, chemical or thermochemical properties of explosive and assumed detonation products other than simply calculated gas phase heat of formation by additivity rule.

> **Input parameters for pure explosives:**
> – **The number of moles of carbon, hydrogen, nitrogen and oxygen in general form $C_aH_bN_cO_d$**
> – **Initial density of explosive**

> **Input parameters for mixed explosive formulations:**
> – **Mass fraction of components**
> – **The number of moles of carbon, hydrogen, nitrogen and oxygen in general form $C_aH_bN_cO_d$ for components**
> – **Initial density of mixed explosive**

> **If condensed phase of pure explosive or components of mixed explosive were available, they can be entered in computer code to calculate detonation parameters.**

> **If condensed phase of pure explosives or components of mixed explosives were not available, computer code calculate their gas phase heat of formation.**

> **Determination of detonation pressure, temperature and heat on the basis of condensed and gas phase heat of formation of explosive.**
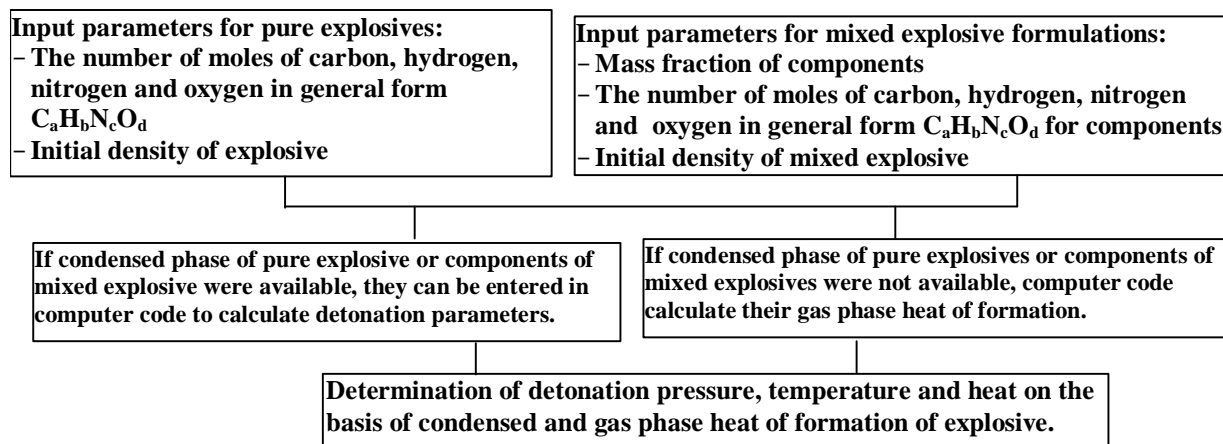
**Figure 1: Schematic depiction in the prediction of detonation pressure, temperature and heat through condensed phase and gas phase heat of formation of pure or mixed explosives**

## RESULTS AND DISCUSSION

Complicated thermochemical/hydrodynamic computer codes require knowledge of the equation of state of the system that can accurately reflect the thermodynamic properties of multicomponent mixtures at several thousand Kelvin and hundreds of kbar, as well as at much lower temperatures and pressures obtained during expansion of the reaction products. They are convincing evidence of the utility of them for engineering calculations of detonation properties of explosives. They have some shortcomings such as their complexity for chemists, selecting appropriate equations of state to obtain reliable results for desired detonation parameters, using condensed phase heat of formation of explosive, etc. The present computer code has several advantages which can be considered as: (a) much simple to use; (b) calculation of gas phase heat of formation of explosives; (c) predicting detonation parameters on the basis of condensed and calculated gas phase heat of formation; and (d) using reliable new empirical methods.

On the basis of the above-mentioned procedures in previous sections, the algorithm of the computer programming for prediction of detonation pressure, temperature and heat is shown in figure 1 as a flowchart. New computer code has been written as a C programming language. The computer program, named DPPME (Determination of Performance of Pure and Mixed Explosives), is designed to calculate three mentioned $\Delta H_f^{o'}(g)$ detonation parameters of $C_aH_bN_cO_d$ explo-
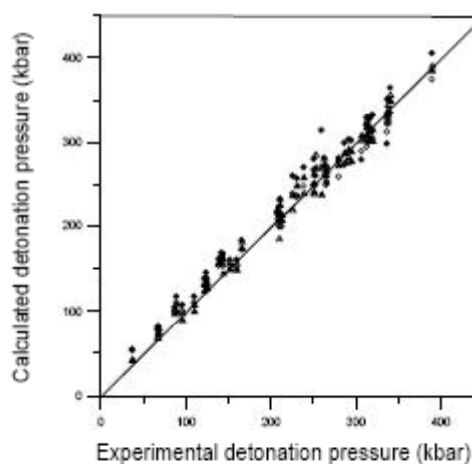


**Figure 2: Predicted detonation pressure of $C_aH_bN_cO_d$ explosives at various loading densities vs. experimental values[12]. The solid lines represent exact agreement between predictions and experiment. Solid and hollow circles denote calculated detonation pressure by BKWR-EOS and BKWS-EOS computations[12], respectively. Filled and hollow triangles denote calculated detonation pressure using condensed and gas phase heat of formation of explosives, respectively**

sives. Since the contributions of small in all of correlations which uses gas phase heats of formation in determination detonation parameters, there is no need to use precise value of gas phase heat of formation of explosives. However, computer code uses Joback's method [28] to calculate gas phase heats of formation.

Comparison of calculated detonation pressures, temperatures and heat for underoxidized and overoxidized pure as well as mixed explosives with ex-
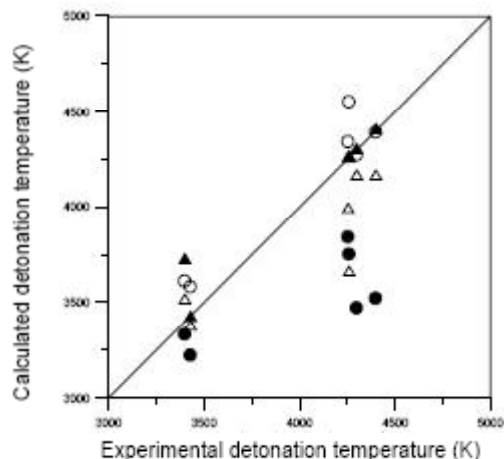
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**Figure 3: Predicted detonation temperature of $C_aH_bN_cO_d$ explosives vs. experimental values, where measured data were available[12]. The solid lines represent exact agreement between predictions and experiment. Solid and hollow circles denote calculated detonation temperature by BKWR-EOS and BKWS-EOS computations[12], respectively. Filled and hollow triangles denote calculated results using condensed and gas phase heat of formation, respectively**
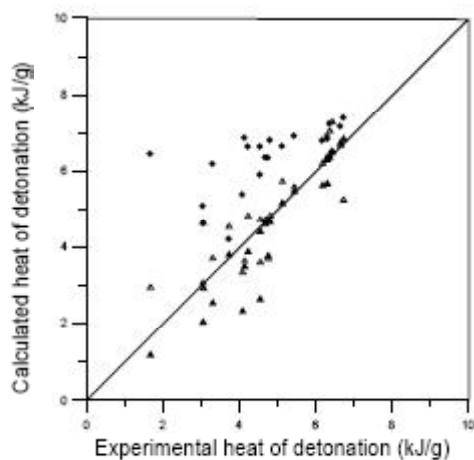


**Figure 4: Predicted heat of detonation of $C_aH_bN_cO_d$ explosives vs. experimental values[34]. The solid lines represent exact agreement between predictions and experiment. Solid circles denote calculated detonation temperature by Kamlet's method[31]. Filled and hollow triangles denote calculated results using condensed and gas phase heat of formation, respectively**

**TABLE 1: List of explosives used in new computer code to calculate detonation pressure, temperature and heat**

| Name | Formula | Calculated detonation parameter |
|---|---|---|
| Bi-trinitroethylurea (BTNEU) | $C_5H_6N_8O_{13}$ | $Q_{det}$ |
| Cyclomethylene trinitramine (RDX) | $C_3H_6N_6O_6$ | $P_{det}$, $T_{det}$, $Q_{det}$ |
| Cyclotetramethylene tetranitramine (HMX) | $C_4H_8N_8O_8$ | $P_{det}$, $Q_{det}$ |
| 1,3-Diamino-2,4,6-trinitrobenzene (DATB) | $C_6H_5N_5O_6$ | $P_{det}$, $Q_{det}$ |
| Di-ethyeleglycol dinitrate (DEGN) | $C_4H_8N_2O_7$ | $Q_{det}$ |
| Dioxyethylnitramine dinitrate (DINA) | $C_4H_8N_4O_8$ | $Q_{det}$ |
| Dipentaerythritol hexanitrate (DIPEHN) | $C_{10}H_{16}N_6O_{19}$ | $Q_{det}$ |
| Ethriol trinitrate | $C_4H_6N_4O_{12}$ | $Q_{det}$ |
| Ethylenedinitramine (EDNA) | $C_2H_6N_4O_4$ | $Q_{det}$ |
| Mannitol hexanitrate(MHN) | $C_6H_8N_6O_{18}$ | $Q_{det}$ |
| Metyl nitrate | $CH_3NO_3$ | $Q_{det}$ |
| Nitroethane | $C_2H_5NO_2$ | $Q_{det}$ |
| Nitroglycerine (NG) | $C_3H_5N_3O_9$ | $P_{det}$, $T_{det}$, $Q_{det}$ |
| Nitromethane (NM) | $CH_3NO_2$ | $P_{det}$, $Q_{det}$ |
| Nitrourea | $CH_3N_3O_3$ | $Q_{det}$ |
| N-Methyl-N-nitro-2,4,6-trinitroaniline (TETRYL) | $C_7H_5N_5O_8$ | $P_{det}$, $T_{det}$, $Q_{det}$ |
| Pentaerythritol tetranitrate (PETN) | $C_5H_8N_4O_{12}$ | $P_{det}$, $T_{det}$, $Q_{det}$ |
| 1,3,5-Triamino-2,4,6-trinitrobenzene (TATB) | $C_6H_6N_6O_6$ | $P_{det}$, $Q_{det}$ |
| Triethyleneglycol dinitrate (TEGN) | $C_6H_{12}N_2O_8$ | $Q_{det}$ |
| 2,4,6-Trinitrotoluene (TNT) | $C_7H_5N_3O_6$ | $P_{det}$, $T_{det}$, $Q_{det}$ |
| 63/36/1 RDX/TNT/wax (COMP B) | $C_{2.03}H_{2.64}N_{2.18}O_{2.67}$ | $P_{det}$ |
| 60/40 RDX/TNT (COMP B-3) | $C_{2.04}H_{2.50}N_{2.15}O_{2.68}$ | $P_{det}$ |
| 78/22 RDX/TNT (CYCLOTOL-78/22) | $C_{1.73}H_{2.59}N_{2.40}O_{2.69}$ | $P_{det}$ |
| 77/23 RDX/TNT (CYCLOTOL-77/23) | $C_{1.75}H_{2.59}N_{2.38}O_{2.69}$ | $P_{det}$ |
| 75/25 RDX/TNT (CYCLOTOL-75/25) | $C_{1.78}H_{2.58}N_{2.36}O_{2.69}$ | $P_{det}$ |
| 65/35 RDX/TNT (CYCLOTOL-65/35) | $C_{1.96}H_{2.53}N_{2.22}O_{2.68}$ | $P_{det}$ |
| 50/50 RDX/TNT (CYCLOTOL-50/50) | $C_{2.22}H_{2.45}N_{2.01}O_{2.67}$ | $P_{det}$ |

perimental data are given in figures 2 to 4. Detonation pressures at various loading densities are also compared with computed results of BKWR-EOS and BKWS-EOS. As seen, the introduced new computer code using both gas and condensed heat of formation of explosives give good results as compared to outputs of complicated computer codes BKWR-EOS and BKWS-EOS.

Since experimental data for detonation temperatures are scarce, few comparisons with measured detonation temperatures are given in figure 3. As indicated,

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the same as detonation pressure, relatively good agreements with respect to measured data are observed as compared to computed results of BKWR-EOS and BKWS-EOS.

A visual comparison of the predicted heats of detonation with experiment is also given in figure 4. Figure 4 shows the comparison between experiment and predictions in which the $H_2O$ product in liquid state. As evident in Figure 4, the new computer code shows good agreement with experimental data using gas and condensed heat of formation of explosives. Using reliable detonation products, which counted the other detonation products such as CO and $H_2$ for oxygen lean explosives, give better predicted heats of detonation than those obtained by Kamlet and Jacobs procedure[31]. However, the results are also compared with Kamlet and Jacobs[31] decomposition reaction. The results confirm that four decomposition paths of Eqs. (1a) to (1d) give better predictions. Predicting fairly accurate heats of detonation, by new computer code, are highly desired for calculating the various detonation parameters of energetic compounds. Moreover, their calculated values are useful in comparing the relative heat releasing of one explosive with respect to the other.

It is worthwhile to note that by considering large percent deviations generally attributed to experimental measurements of detonation temperature and pressure, the good agreement between calculated and measured values given in figures 2 and 3 are also satisfactory. It is felt that the introduced computer code represents a significant advance in a priori estimation of explosive performance because its simplicity for explosive's users.

## CONCLUSIONS

There is a continuing need to have simple procedures for predicting behavior of energetic materials and an improved diagnostic capability to measure the complex chemical and hydrodynamic process during detonation. A new simple computer code has been introduced to calculate detonation pressure, temperature and heat as three important detonation parameters. It uses recent methods to estimate detonation pressure, temperature and heat of pure and mixed explosives, which require as input information only the elemental compositions and loading density. If condensed phase heat of formation of explosive was not available, computer code uses Joback's method to calculate detonation performance. Since the contribution of $\left|\Delta H°'_f(g)\right|$ of the explosive is small relative to the elemental composition of the $C_aH_bN_cO_d$ explosive in using methods, Joback's method can used without any difficulties. However, the new computer code is very simple in form and easy to use in a practical sense. Since the values of condensed heat of formation are hardly known experimentally for new energetic materials of interest which are usually needed for available methods, the present computer code can be used easily to estimate detonation performance.

## REFERENCES

[1] M.S.Abdualazeem; High Temp. High Press., **30**, 387 **(1998)**.

[2] C.L.Mader; 'Numerical Modeling of Explosives and Propellants', CRC Press, 2nd edition, **(1998)**.

[3] H.B.Levine, R.E.Sharples; Operator's Manual for RUBY, Lawrence Livermore Laboratory report UCRL-6815, Livermore, CA, **(1962)**.

[4] M.Cowperthwaite, W.H.Zwisler; TIGER computer program documentation, Stanford Research Institute, SRI publication number 2106, **(1973)**.

[5] A.L.Nichols, F.H.Ree; CHEQ 2.0 User's Manual, UCRL-MA-106754, Lawrence Livermore National Laboratory, Livermore, CA, **(1990)**.

[6] L.E.Fried, W.M.Howard, P.C.Souers; CHEETAH 2.0 User's Manual, Lawrence Livermore National Laboratory, Livermore, CA, **(1998)**.

[7] C.L.Mader; Detonation properties of condensed explosives computed using the Becker-Kistiakosky-Wilson equation of state, Los Alamos Scientific Laboratory Report LA-2900, New Mexico, **(1963)**.

[8] M.Cowperthwaite, W.H.Zwisler; Sixth Symposium (International) on Detonation, Coronads, CA, Washington, DC, Office of the Chief of Naval Operations, **(1976)**.

[9] K.Tanaka; National Chemical Laboratory for Industry, Tsukuba Research Center, Yatabe, Tsukuba, Ibaraki, Japan, **(1983)**.

*Full Paper*

**[10]** K.Tanaka; Sixth Symposium (International) on Detonation, Albuquerque, New Mexico, Washington, DC, Office of the Chief of Naval Operations, **(1985)**.

**[11]** M.Fringer, E.Lee, F.H.Helm, B.Hayes, H.Hornig, R.McGuire, M.Kahara, M.Gudiry; Sixth Symposium (International) on Detonation, Coronads, CA, Washington, DC, Office of the Chief of Naval Operations, **(1976)**.

**[12]** M.L.Hobbs, M.R.Baer; Tenth Symposium (International) on Detonation, Boston, MA, **(1993)**.

**[13]** M.H.Keshavarz, M.Oftadeh; High Temp.High Press., **34**, 495 **(2002)**.

**[14]** M.H.Keshavarz, M.Oftadeh; Indian J.Eng.Mater. Sci., **10**, 236 **(2003)**.

**[15]** M.H.Keshavarz, M.Oftadeh; Bull.Korean Chem. Soc., **24**, 19 **(2003)**.

**[16]** M.H.Keshavarz, H.R.Pouretedal; Thermochim. Acta, **414**, 203 **(2004)**.

**[17]** M.H.Keshavarz; Asian J.Chem., **17**, 2085 **(2005)**.

**[18]** M.H.Keshavarz; J.Hazard.Mater A., **119**, 25 **(2005)**.

**[19]** M.H.Keshavarz; 'New Research on Hazardous Materials', Chapter 9, 'A Simple Theoretical Prediction of Detonation Velocities of Non-ideal Explosives only From Elemental Composition', Nova Science Publishers, Inc., **(2006)**.

**[20]** M.H.Keshavarz, H.R.Pouretedal; J.Chin.Inst.Eng., **29**, 145 **(2006)**.

**[21]** M.H.Keshavarz; Indian J.Eng.Mater.Sci., **12**, 158 **(2005)**.

**[22]** M.H.Keshavarz; Thermochim.Acta, **428**, 95 **(2005)**.

**[23]** M.H.Keshavarz, H.R.Nazari; J.Hazard.Mater.B, **133**, 129 **(2006)**.

**[24]** M.H.Keshavarz; J.Hazard.Mater.A, **137**, 1303 **(2006)**.

**[25]** M.H.Keshavarz; J.Hazard.Mater.A, **142**, 54 **(2007)**.

**[26]** M.H.Keshavarz; J.Hazard.MaterA., **143**, 549 **(2007)**.

**[27]** M.H.Keshavarz; Indian J.Eng.Mater.Sci., **14**, 77 **(2007)**.

**[28]** R.C.Reid, J.M.Prausnitz, B.E.Poling; 'The Properties of Gases and Liquids', 4th ed, McGraw-Hill, New York, **(1987)**.

**[29]** M.Rice, J.Hare; Thermochim.Acta, **384**, 377 **(2002)**.

**[30]** M.H.Keshavarz, M.Oftadeh; High Temp.High Press., **35/36**, 499 **(2003/2006)**.

**[31]** M.J.Kamlet, S.J.Jacobs; J.Chem.Phys., **48**, 23 **(1968)**.

**[32]** M.H.Keshavarz; J.Hazard.Mater.A, **136**, 145 **(2006)**.

**[33]** M.H.Keshavarz; J.Hazard.Mater., **A136**, 425 **(2006)**.

**[34]** R.Meyer, J.Köhler, A.Homburg; 'Explosives', Wiley-VCH, 5th edition, **(2002)**.