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The Empirical Nitrogen Equivalent Equations for Predicting the Detonation Velocity and Detonation Pressure of CHNO Explosives with Approaching the Results of Kamlet-Jacobs Equations

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Abstract: We have suggested two empirical nitrogen equivalent equations for predicting the detonation velocity (D) and detonation pressure (p) of CHNO explosives with more approaching the results of Kamlet-Jacobs equations than common used nitrogen equivalent equations

Key words: CHNO explosives; detonation velocity; detonation pressure; nitrogen equivalent equations

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In 1964, Guo Yuxian proposed a nitrogen equivalent (NE) equation for predicting the detonation velocity (D) of CHNO explosives. In the early 1980's, Guo Yuxian and Zhang Housheng[1-2] proposed two NE equations for predicting the D and detonation pressure (p) of CHNO explosives. Here we plan to propose two empirical NE equations for predicting the values of D and p with more approaching the values of D and p in Kamlet-Jacobs equations than Guo Yuxian-Zhang Housheng's NE equations.

By substituting the 1631 sets of original data (Table S2), D_i, M_i, ρ_i and x_i, $i=1, 2, \cdots, 1631$, for 324 CHNO single-compound explosives (Table S1) into eqns. (1), (3), (5) and (7), eqns. (2), (4), (6) and (8) are obtained via solution of eqns. (1), (3), (5) and (7) using the trust region approach.

$$\min_{a,b,N_{N_2},N_{H_2O},N_{CO_2},N_{CO},N_{H_2},N_{O_2},N_C} \sum_{i=2}^{n} \left[D_i - \frac{100}{M}(a+b\rho)\left(x_{N_2}N_{N_2}+x_{H_2O}N_{H_2O}+x_{CO_2}N_{CO_2}+x_{CO}N_{CO}+x_{H_2}N_{H_2}+x_{O_2}N_{O_2}+x_C N_C\right)\right]^2$$

s.t. $690.00\leqslant a\leqslant 690.01$, $1160\leqslant b\leqslant 1160.01$, $1.000\leqslant N_{N_2}\leqslant 1.001$, $0.5400\leqslant N_{H_2O}\leqslant 0.5401$, $1.3500\leqslant N_{CO_2}\leqslant 1.3501$, $0.7800\leqslant N_{CO}\leqslant 0.7801$, $0.2900\leqslant N_{H_2}\leqslant 0.2901$, $0.5000\leqslant N_{O_2}\leqslant 0.5001$, $0.1500\leqslant N_C\leqslant 0.1501$ (1)

$$D=\frac{100}{M}(690+1160\rho)\left(1.00x_{N_2}+0.54x_{H_2O}+1.35x_{CO_2}+0.78x_{CO}+0.29x_{H_2}+0.50x_{O_2}+0.15x_C\right) \quad (2)$$

where D is the detonation velocity, $m\cdot s^{-1}$; M is the mole weight of explosive, $g\cdot mol^{-1}$; 690 and 1160 are constants; ρ is the initial densities of explosives, $g\cdot cm^{-3}$; 1.00, 0.54, 1.35, 0.78, 0.29, 0.50, 0.15 are the nitrogen equivalent coefficient of gaseous detonation products N_2, H_2O, CO_2, CO, H_2, O_2, C of explosive; x_i(i = N_2, H_2O, CO_2, CO, H_2, O_2, C) is the numbers of moles of gaseous detonation products.

Equation (2) is known as Guo Yuxian-Zhang Housheng's NE equation for predicting the value of D of CHNO explosives.

The relative error ($\Delta\delta$) of eqn. (2) is:

$$\Delta\delta=\sqrt{\sum_{i=1}^{n}\left[D_{cald,i}-D_{K\text{-}J,i}\right]^2 / \sum_{i=1}^{n} D_{K\text{-}J,i}^2}=0.0499$$

$$\min_{c,N_{N_2},N_{H_2O},N_{CO_2},N_{CO},N_{H_2},N_{O_2},N_C,d} \sum_{i=2}^{n} \left\{p_i - c\left[\rho\frac{100}{M}\left(x_{N_2}N_{N_2}+x_{H_2O}N_{H_2O}+x_{CO_2}N_{CO_2}+x_{CO}N_{CO}+x_{H_2}N_{H_2}+x_{O_2}N_{O_2}+x_C N_C\right)\right]^2+d\right\}^2$$

s.t. $1.09200\leqslant c\leqslant 1.09201$, $1.000\leqslant N_{N_2}\leqslant 1.001$, $0.5400\leqslant N_{H_2O}\leqslant 0.5401$, $1.3500\leqslant N_{CO_2}\leqslant 1.3501$, $0.7800\leqslant N_{CO}\leqslant 0.7801$, $0.2900\leqslant N_{H_2}\leqslant 0.2901$, $0.5000\leqslant N_{O_2}\leqslant 0.5001$, $0.1500\leqslant N_C\leqslant 0.1501$, $0.57400\leqslant d\leqslant 0.57401$ (3)

$$p=1.092\left[\rho\frac{100}{M}\left(1.00x_{N_2}+0.54x_{H_2O}+1.35x_{CO_2}+0.78x_{CO}+0.29x_{H_2}+0.50x_{O_2}+0.15x_C\right)\right]^2-0.574 \quad (4)$$

where p is the detonation pressure, GPa; 1.092 and 0.574 are constants.

Equation (4) is known as Guo Yuxian-Zhang Housheng's NE equation for predicting the value of p of CHNO explosives.

The relative error ($\Delta\delta$) of eqn. (4) is:

$$\Delta\delta=\sqrt{\sum_{i=1}^{n}\left[p_{cald,i}-p_{K\text{-}J,i}\right]^2 / \sum_{i=1}^{n} p_{K\text{-}J,i}^2}=0.0885$$

$$\min_{a,b,N_{N_2},N_{H_2O},N_{CO_2},N_{CO},N_{H_2},N_{O_2},N_C} \sum_{i=2}^{n} \left[D_i - \frac{100}{M}(a+b\rho)\left(x_{N_2}N_{N_2}+x_{H_2O}N_{H_2O}+x_{CO_2}N_{CO_2}+x_{CO}N_{CO}+x_{H_2}N_{H_2}+x_{O_2}N_{O_2}+x_C N_C\right)\right]^2$$

s.t. $650\leqslant a\leqslant 695$, $1150\leqslant b\leqslant 1165$, $0.800\leqslant N_{N_2}\leqslant 1.001$, $0.340\leqslant N_{H_2O}\leqslant 0.640$, $1.150\leqslant N_{CO_2}\leqslant 1.350$, $0.250\leqslant N_{CO}\leqslant 0.780$, $0.110\leqslant N_{H_2}\leqslant 0.290$, $0.010\leqslant N_{O_2}\leqslant 0.500$, $0.110\leqslant N_C\leqslant 0.150$ (5)

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$$D=\frac{100}{M}(695+1150\rho)(1.00x_{N_2}+0.64x_{H_2O}+1.34x_{CO_2}+0.72x_{CO}+0.18x_{H_2}+0.50x_{O_2}+0.12x_C) \quad (6)$$

where 695 and 1150 are constants; 1.00, 0.64, 1.34, 0.72, 0.18, 0.50, 0.12 are the nitrogen equivalent coefficient of gaseous detonation products N_2, H_2O, CO_2, CO, H_2, O_2, C of explosive.

Equation (6) is known as the empirical NE equation for predicting the value of D of CHNO explosives

The relative error ($\Delta\delta$) of eqn. (6) is:

$$\Delta\delta=\sqrt{\sum_{i=1}^{n}[D_{cald,i}-D_{K\text{-}J,i}]^2/\sum_{i=1}^{n}D_{K\text{-}J,i}^2}=0.0373$$

$$\min_{c,N_{N_2},N_{H_2O},N_{CO_2},N_{CO},N_{H_2},N_{O_2},N_C,d}\sum_{i=2}^{n}\left\{p_i-c\left[\rho\frac{100}{M}(x_{N_2}N_{N_2}+x_{H_2O}N_{H_2O}+x_{CO_2}N_{CO_2}+x_{CO}N_{CO}+x_{H_2}N_{H_2}+x_{O_2}N_{O_2}+x_CN_C)\right]^2+d\right\}^2$$

s.t. $1.060\leqslant a\leqslant1.500$, $1.000\leqslant N_{N_2}\leqslant1.001$, $0.6400\leqslant N_{H_2O}\leqslant0.6401$, $1.3400\leqslant N_{CO_2}\leqslant1.3401$, $0.7200\leqslant N_{CO}\leqslant0.7201$, $0.1800\leqslant N_{H_2}\leqslant0.1801$, $0.0.500\leqslant N_{O_2}\leqslant0.501$, $0.1200\leqslant N_C\leqslant0.1201$, $0.001\leqslant d\leqslant0.874$ (7)

$$p=1.060\left[\rho\frac{100}{M}(1.000x_{N_2}+0.64x_{H_2O}+1.34x_{CO_2}+0.72x_{CO}+0.18x_{H_2}+0.50x_{O_2}+0.12x_C)\right]^2-0.619 \quad (8)$$

where 1.060 and 0.619 are constants.

Equation (8) is known as the empirical NE equation for predicting the value of p of CHNO explosives

The relative error ($\Delta\delta$) of eqn. (8) is:

$$\Delta\delta=\sqrt{\sum_{i=1}^{n}[p_{cald,i}-p_{K\text{-}J,i}]^2/\sum_{i=1}^{n}p_{K\text{-}J,i}^2}=0.0682$$

Compared with the values of $\Delta\delta$ of eqns. (2) and (4), the ones of $\Delta\delta$ of eqns. (6) and (8) decrease by 25.2% and 23.0%, respectively, indicating that eqns. (6) and (8) can be used to predict the values of D and p of CHNO explosives with more approaching the values of D and p in Kamlet-Jacobs equations than common used nitrogen equivalent equations.

Associated Content: Supporting information

The supporting information of the structure formula (Table S1) and original data (Table S2) is available free of charge on the website of Chinese Journal of Energetic Materials.

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预测接近 Kamlet-Jacobs 方程结果的 CHNO 炸药的爆速和爆压的经验氮当量方程

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摘　要: 我们提出了两个比常用氮当量方程更接近 Kamlet-Jacobs 方程结果的预测 CHNO 炸药爆速(D)和爆压(p)的经验氮当量方程。

关键词: CHNO 炸药; 爆速; 爆压; 氮当量方程
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