Effects of coupling radiation on detonation parameters of inert explosive: a MC+thermodynamics study

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Abstract. Influences of neutron & γ mixing radiation field on decomposition speed and detonation parameters of long-term storage explosive molecular have been performed by a combined MC+thermodynamics method. The results show that energy deposition of neutron & γ transport in explosive components has a negligible effect on the decomposition speed, detonation speed and detonation pressure, but it significantly improves the detonation temperature of the explosive. The findings can be helpful for deeply understanding aging mechanisms for long-term storage explosive component, and improving its safety and reliability.

1. Introduction
Inert explosive may be exposed to cumulative damage effects induced by various radiations during long-term storage, and its self-heating readily results in increasing temperature of the storage environment. Therefore, nuclear radiations can cause many consequences for explosive, such as changing molecular structure parameters and physicochemical properties of explosive molecular, accelerating decomposition speed, reducing explosive strength, increasing creep speed, decreasing density and stability, varying parameters of constitutive equations, thus affecting detonation performance. However, as far as we know, few people pay attention to the influence of nuclear radiation on detonation performance. We adopt a model of Chen et al in[1] to analyze influences of nuclear radiation, especially neutron & γ mixing radiation field, on decomposition speed and detonation parameters of inert explosive (PETN type in this paper) during long-term storage based on a combined Monte Carlo plus thermodynamics method.

2. Computational details
For n & γ radiations (α & β particles can be ignorable because they are subjected to strong absorption, shielding and scattering effects), we perform particle transport calculations for energy deposition implemented in GEANT4 code[2] which is mainly based on Monte Carlo methods and written in the C++ language[3]. Then, we utilize the Arrhenius formula to analyze influence of energy deposition on decomposition speed of a representative inert explosive (PETN explosive). For effects of energy deposition on the detonation parameters, we consider energy deposition as a perturbation term of chemical equilibrium equations set for solving detonation parameters, use the minimization principle of Gibbs free energy to solve the compositions of detonation products. Detonation parameters at C-J point are computed according to the thermodynamics method.
2.1 Calculations for influences of n & γ radiation on decomposition speed of explosive

It is well known that decomposition speed of explosive follows the famous Arrhenius formula[4,5]

\[ k = A e^{-E/RT} f(x) \]  \hspace{1cm} (1)

where \( k \) is decomposition speed (year\(^{-1}\)), \( A \) pre-exponential factor (dimensionless), \( E \) activation energy of a reaction (in eV), \( R \) gas constant (\( R = 8.314 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1} \)), \( T \) absolute temperature (K), \( f(x) \) reaction excitation function (dimensionless), can be viewed as a constant when conversion rate is relatively low, \( f(x) \) is also called the frequency factor.

Relationship for temperature change and change of internal energy is given by

\[ \Delta T = \left( m C_p \right)^{-1} \Delta H \]  \hspace{1cm} (2)

where \( \Delta T \) is temperature change (in K), \( m \) mass of explosive component (Kg), \( C_p \) specific heat capacity (in \( \text{J} \cdot \text{Kg}^{-1} \cdot \text{K}^{-1} \)), \( \Delta H \) is change of internal energy (in eV).

Differentiating of Eq.(1) can yields

\[ dk = \frac{AE}{RT^2} e^{-E/RT} f(x) dT \]  \hspace{1cm} (3)

When the temperature is very small, Eq.(3) can be simplified into

\[ \Delta k = \frac{AE}{RT} e^{-E/RT} f(x) \Delta T \]  \hspace{1cm} (4)

Assuming rate of energy deposition \( \mu \) in explosive component keeps constant during n & γ particle transport, and relationship for \( \mu \), change of internal energy \( \Delta H \) and reaction time \( \Delta t \) is

\[ \Delta H = \mu \Delta t \]  \hspace{1cm} (5)

According to transport theory for n & γ particles, \( \mu \) is equivalent to mathematical expectation of n & γ emergent rate

\[ \mu = \int_0^\infty (O_n(E)f_n(E) + O_\gamma(E)f_\gamma(E))dE \]  \hspace{1cm} (6)

where \( O_n(E) \) and \( O_\gamma(E) \) are n, \( \gamma \) emergent rate on radiation source surface, respectively. \( f_n(E) \) and \( f_\gamma(E) \) denote n, \( \gamma \) probability distributions for rate of energy deposition \( \mu \) in explosive component, respectively. For practical purposes, n particle transport obeys Maxwell distribution, while \( f_\gamma(E) \) can be determined by \( \gamma \) particle energy and its branching ratio emitted from radiation source

We substitute Eqs.(2) and (5) into Eq.(4) to obtain

\[ \Delta k = \frac{AE}{mC_p RT^2} e^{-E/RT} f(x) \mu \Delta t \]  \hspace{1cm} (7)

Substituting of Eq.(1) into Eq.(7) yields

\[ \Delta k = k \frac{E \mu \Delta t}{mRT^2 C_p} \]  \hspace{1cm} (8)

2.2 Calculations for detonation parameters of explosive

2.2.1 Chemical equilibrium equations set

For a chemical equilibrium system composed of \( t \) constituents, including \( s \) gases, \( p \) solids, and \( c \) chemical elements, various constituents can be expressed in term of linear representation for individual elements. For generality, molecular formula for \( i \)th constituent can be given by[6]

\[ y_i = x_{i1}^\alpha x_{i2}^\beta \ldots x_{in}^\nu \]  \hspace{1cm} (9)

where \( x_k \) denotes \( k \)th element, \( a_k \) atom numbers for \( k \)th element in molecular formula of \( i \)th constituent.

Vector representation for molecular formula of \( i \)th constituent is[6]

\[ y_i = (\alpha_{i1} \alpha_{i2} \ldots \alpha_{ic}) \]  \hspace{1cm} (10)

For a certain chemical reaction, atom numbers of various elements in reactants is equal to corresponding elements in products, and can be expressed in term of molecular formula vector as[6]

\[ \sum_{i=1}^s \alpha_{ij} n_i + \sum_{i=s+1}^t \alpha_{ij} n_i = q_j \]  \hspace{1cm} (11)
where $j=1,\ldots,c$, $n_i$ is mole number of $i$th constituent, and $q_j$ total mole number of $j$th element in the system.

Chemical equilibrium conditions require that chemical potential of reactants should be equal to that of products. Similar to molecular formula of individual constituent, chemical potential of each constituent can be determined by chemical potential of corresponding element in the system. Supposing chemical potentials of various element are $\lambda_i$, chemical potentials of each constituent can be represented by

$$\mu_i = \sum_{j=1}^{c} \alpha_{ij} \lambda_i \quad j = 1, \ldots, t$$

Gibbs free energy is minimal value when the system is in chemical equilibrium state, and we can obtain the following chemical equilibrium equations set[7,8]

$$\frac{n_i}{n_i^0} - \frac{n}{n^0} + \sum_{k=1}^{c} \alpha_{ik} \lambda_k = -f_i(n^0) \quad i = 1, \ldots, s$$

$$\sum_{k=1}^{c} \lambda_k \alpha_{ik} = -G_i(n^0) \quad i = s + 1, \ldots, t$$

$$\sum_{i=1}^{t} \alpha_{ij} n_i = b_j \quad j = 1, \ldots, c$$

$$\sum_{i=1}^{s} n_i - n = 0$$

$$n^0 = \sum_{i=1}^{s} n_i$$

$$n^0 = \sum_{i=1}^{t} n_i^0$$

$$\varepsilon = \sum_{i=1}^{s} |n_i^0 - n_i| < 10^{-8}$$

where $n_i$ is mole number of $i$th constituent after an iteration, $n_i^0$ mole number of $i$th constituent before an iteration, $n$ total mole number of gas products after an iteration, $n^0$ total mole number of gas products after an iteration, $f_i(n^0)$ free energy of $i$th gas product, $G_i(n^0)$ free energy of $i$th solid product.

2.2.2 Gibbs free energy of detonation product

We choose PETN explosive (chemical formula is $C_5H_8N_4O_12$) as a representative inert explosive. For this type of explosive, we consider detonation products to be composed of $H_2O$, $CO_2$, $CO$ and $N_2$ gas phases. As we all know, Gibbs free energies of detonation products are correlated with equation of state, one can determine equilibrium products based on the chemical equilibrium method. Therefore, one can calculate Gibbs free energies of detonation products for PETN explosive to obtain the detonation parameters.

Formula for free energy of $H_2O$, $CO_2$, $CO$ and $N_2$ gas phases is given by[9]

$$G = G_0 + RT \ln S$$

where $R$ is gas constant, $S$ reaction entropy, $G_0$ reference free energy ($G_0=0$ here).

So Eq.(20) can be simplified into

$$G = RT \ln S$$

Parameters for equation of states for $H_2O$, $CO_2$, $CO$ and $N_2$ detonation gas products[10] are listed in Table 1.
2.2.3 Determination of detonation speed

Assuming a pair of \( P, T \) values, thermodynamics method is utilized to determine constituents of detonation product and mole number of \( i \)th constituent \( n_i \), detonation heat \( Q_v \), and internal energy \( e_0 \). \( e_0 \) is a function of specific volume \( V \) and temperature \( T \) \( (e=e(V, T)) \) because it is the sum of thermal internal energy and elastic internal energy\[8\]

\[
\frac{de}{dV} = C_v \frac{dT}{dV} + \left( \frac{\partial e}{\partial T} \right)_V \frac{dV}{dT} + \left( \frac{\partial e}{\partial T} \right)_T \frac{dT}{dV}
\]  

(22)

From the first rule of thermodynamics, one can obtain

\[
de = TdS - PdV
\]

(23)

Differentiating of definition for free energy function \( F=e-TS \) can yield

\[
dF = de - TdS - SdT = -PdV - SdT
\]

(25)

Therefore

\[
\left( \frac{\partial F}{\partial V} \right)_T = -P
\]

(26)

\[
\left( \frac{\partial F}{\partial T} \right)_V = -S
\]

(27)

\[
\left( \frac{\partial P}{\partial V} \right)_T = \frac{\partial^2 F}{\partial V \partial T} = \left( \frac{\partial S}{\partial T} \right)_V
\]

(28)

Substituting of Eq.(15) into Eq.(22) yields

\[
de = C_v dT + \left[ T \left( \frac{\partial P}{\partial T} \right)_V - P \right] dV
\]

(30)

Integrating of Eq.(30) yields

\[
e_i = \int_{T_i}^{T} C_v dT + \int_{V_i}^{V_c} \left[ T \left( \frac{\partial P}{\partial T} \right)_V - P \right] dV
\]

(31)

The first term in Eq.(31) is thermal internal energy, the second term, elastic internal energy, and the second term is a small amount relative to the first term, so Eq.(31) can be simplified into

\[
e_i \approx \int_{T_i}^{T} C_v dT
\]

(32)

Eq.(32) can be written into

\[
\int_{T_i}^{T} C_v dT = \int_{T_i}^{T} \left( \sum_{i=1}^{m} n_i C_{v_i} + n_c C_{v_c} \right)
\]

(33)

where \( C_{v_i} \) is average constant-volume heat capacity of \( i \)th constituent in detonation products, \( n_i \) mole number of \( i \)th constituent, \( n_c \) mole number of solid carbon, \( m \) species number of gas products.

Because we don't take solid carbon into account in detonation speed calculation for PETN explosive, so Eq.(33) can be simplified into

\[
\int_{T_i}^{T} C_v dT = \int_{T_i}^{T} \sum_{i=1}^{m} n_i C_{v_i}
\]

(34)

where \( C_{v_i} \) values are shown in Table 2.

According to the constituents of detonation products, total mole number of gas products is substituted into equation of state to calculate volume of gas products \( V_{gas} \), and product volume is the sum of volume of gas constants and that of solid constants\[10,11\]

\[
V_i = V_{gas} + V_e = V_{gas} + 5.4 n_e
\]

(35)

In fact, Eq.(35) can be simplified into \( V_i = V_{gas} \) because \( n_e = 0 \).

If one neglects \( e_0 \), and substitutes \( e_1, Q_v \) into Eq.(36), then can calculate \( V_0 \) according to
It is necessary to re-assume another \((P, T)\) values as long as \(V_0\) calculation value is consistent with initial density \(\rho_0\) (relative mass of explosive molecular). The above procedure is repeated until \(V_0\) value is in agreement with \(\rho_0\).

We choose an appropriate \((P, T)\) value \((P=20\text{ GPa}, T=3000\text{ K})\) in this paper. These values, together with parameter values in Table 2 and 5 are substituted into Eqs.(22)-(36) and the following detonation speed equation

\[
D = V_0 \sqrt{\frac{P_m - P_o}{V_0 - V_H}}
\]

We can obtain detonation speed without energy deposition \(D=8325\text{m} \cdot \text{s}^{-1}\).

2.2.4 Determination of other detonation parameters

After calculating detonation speed, we utilize equation of state (constant \(\gamma\)) to solve other detonation parameters[12,13]

\[
P = AV^{-\gamma} = A\rho^\gamma
\]

From Eq.(23) we can see that, \(TdS=0\) when only elastic energy (or elastic pressure) is taken into account, so

\[
d\varepsilon = -PdV
\]

\[
e - e_0 = \int_{V_0}^{V} PdV = -\int_{V_0}^{V} AV^{-\gamma}dV = \frac{PV}{\gamma - 1} - \frac{P_o V_0}{\gamma - 1}
\]

Hugoniot equation \((\alpha=1)\) is given by

\[
\frac{P_1 V_1}{\gamma - 1} - \frac{P_2 V_2}{\gamma - 1} = \frac{1}{2} (P_2 + P_o) (V_0 - V_2) + Q_0
\]

According to sound velocity formula in a certain medium

\[
c = V \sqrt{\frac{dP}{d\rho}}
\]

where \(V=1/\rho\) is specific volume of the medium. So

\[
c^2 \approx \gamma PV = \frac{\alpha P}{\rho}
\]

When \(\mu=0\), equations for detonation parameters of condensational explosive is given by

\[
\begin{align*}
\mu_2 &= \sqrt{(P_2 - P_o) (V_0 - V_2)} \\
V_D &= V_o \frac{P_2 - P_o}{V_0 - V_2} \\
\frac{P_2 V_2}{\gamma - 1} - \frac{P_o V_0}{\gamma - 1} &= \frac{1}{2} (P_2 + P_o) (V_0 - V_2) + Q_0 \\
V_D - \mu_2 &= c_2 \\
P &= AV^{-\gamma}
\end{align*}
\]

From Eq.(44) one can see that, equations for solving detonation parameters are mathematically similar to that of ideal gas-Eq.(45)

\[
\begin{align*}
\mu_2 &= \sqrt{(P_2 - P_o) (V_0 - V_2)} \\
V_D &= V_o \frac{P_2 - P_o}{V_0 - V_2} \\
\frac{P_2 V_2}{k - 1} - \frac{P_o V_0}{k - 1} &= \frac{1}{2} (P_2 + P_o) (V_0 - V_2) + Q_0 \\
P_2 V_2 &= R_g T_2 \\
V_D - \mu_2 &= c_2
\end{align*}
\]
Similarly, one can obtain explicit expressions for $P_2$, $V_2$, $\rho_2$, $u_2$, $V_D$, $c_2$ when $k$ is replaced by $\gamma$. For condensational explosive, $P_0$ can be ignorable, so Eq.(45) can be reduced to

\[
\begin{align*}
P_2 &= \frac{\rho_0 V_D^2}{\gamma + 1} \\
\rho_2 &= \frac{\gamma + 1}{\gamma} \rho_0 \quad V_2 = \frac{\gamma}{\gamma + 1} V_0 \\
\mu_2 &= \frac{V_D}{\gamma + 1} \\
V_D &= \sqrt{2(\gamma^2 - 1)Q_V} \\
c_2 &= V_D - \mu_2 = \frac{\gamma V_D}{\gamma + 1}
\end{align*}
\] (46)

As shown above, detonation parameters can be determined if one know detonation speed and local isentropic value $\gamma$. Next, we will discuss determination of $\gamma$ value.

A simple power exponential relationship exists for detonation speed of many explosives and loading density

\[
V_D = b\rho_0^a
\] (47)

where $b$, $a$ are constants in correlation with explosive properties.

From the following equation

\[
\begin{align*}
P &= AV^{-\gamma} \\
P_2 &= \frac{\rho_0 V_D^2}{\gamma + 1}
\end{align*}
\] (48)

one can obtain

\[
A\rho_0^2 = \frac{\rho_0 V_D^2}{\gamma + 1}
\] (49)

Substituting of $\rho_2$, $V_2$ and Eq.(1) into Eq.(49) yields

\[
A \left(\frac{\gamma + 1}{\gamma}\right)^\gamma \rho_0^2 = \frac{b^2}{\gamma + 1} \rho_0^{2a + 1}
\] (50)

And

\[
\gamma = 2a + 1
\] (51)

One can obtain $\gamma$ value (Eq.(51)) through asymptotic method solving power exponential constant $a$ as long as experimental $V_D\rho_0$ curve is determined.

$a$ value is between 0.65 and 1.00 in that density of PETN explosive is $\rho_0>1000$ Kg∙m$^{-3}$. For denser explosive, $a=1$ ($\gamma=3$). Therefore, equations of state for products are given by

\[
P = A\rho^3
\] (52)

From Eq.(46) one can obtain

\[
\begin{align*}
P_2 &= \frac{1}{4} \rho_0 V_D^2 \\
\rho_2 &= \frac{4}{3} \rho_0 \quad V_2 = \frac{3}{4} V_0 \\
\mu_2 &= \frac{V_D}{4} \\
V_D &= 4\sqrt{Q_V} \\
c_2 &= \frac{2}{4} V_D
\end{align*}
\] (53)

As discussed above, Substituting of detonation speed $D=8325$ m$\cdot$s$^{-1}$ (namely $V_D=8325$ m$\cdot$s$^{-1}$) into Eq.(53) can obtain other detonation parameters. In fact, an empirical formula for temperature of detonation wave front is

\[
T_2 = 48P_2 V_2 (V_2 - 0.20) M_{\gamma_2}
\] (54)
where $T_2$ is product temperature on C-J surface (in K), $P_2$ pressure on C-J surface (in GPa), $V_2$ specific volume on C-J surface (in m$^3$/Kg), $M_{*2}$ average relative mass of product molecule (dimensionless).

3. Result and discussion

3.1 Influence of nuclear radiation on decomposition speed of explosive molecule

Energy depositions of n & γ particles, which are emitted from radiation source, in explosive components are calculated by GEANT4 code, and total energy deposition is substituted into Eq.(8) to obtain influence degree $\Delta k$ of n & γ radiation on decomposition speed of explosive components.

Monte Carlo calculations show that rate of energy deposition $\mu$ is at magnitude of 0.01 J·year$^{-1}$. We choose assurance coefficient to be 10 (namely safe storage of explosive components maintain at least 10 years), $\Delta k/k$ ($k$ is decomposition speed under natural conditions, usually $10^{-6}$–$10^{-7}$ year$^{-1}$) is less than $10^{-7}$, so nuclear radiation has an insignificant effect on decomposition speed.

3.2 Influence of nuclear radiation on detonation parameters of inert explosive

Parameters for equation of states for H$_2$O, CO$_2$, CO and N$_2$ individual gas products are listed in Table 1, and various $C_v$ values at average constant-volume are shown in Table 2.

| Table 1. Parameters for equation of states for individual gas products |
|--------------------------|-----------------|-----------------|-----------------|-----------------|
| product                 | H$_2$O | CO$_2$ | CO   | N$_2$   |
| $S_{g0K}^i$ (in J·mol$^{-1}$·K$^{-1}$) | 45.106 | 51.07 | 47.214 | 45.77 |

| Table 2. $C_v$ values at average constant volume |
|-----------------------------------------------|
| coefficient | $a_i$ | $b_i\times10^{-3}$ |
| double-atom gas | 20.08 | 1.883 |
| triple-atom gas | 37.66 | 2.427 |
| vapor | 16.74 | 8.996 |

We substitute $T=300$K, $R=8.314$J·mol$^{-1}$·K$^{-1}$ into Eq.(21) to obtain Gibbs free energy of various gases, as shown in Table 3.

| Table 3. Gibbs free energy for individual gas products |
|----------------|----------------|----------------|----------------|
| Product                  | H$_2$O | CO$_2$ | CO   | N$_2$   |
| $G$ (in J·mol$^{-1}$)  | -105.4893 | -106.4515 | 7.85E+03 | -105.4893 |

A set of appropriate equilibrium initial values $n_i^0$ ($i=1,...,t$) for PETN explosive are listed in Table 4.

| Table 4. Equilibrium initial values for individual product |
|----------------|----------------|----------------|----------------|
| Product            | $n_{H,O}^0$ | $n_{CO_2}^0$ | $n_{CO}^0$ | $n_{N_2}^0$ |
| Initial value (in mol) | 4 | 3 | 2 | 2 |

The iteration results (through Eqs.(13)-(19)) for various equilibrium products with n & γ energy deposition are shown in Table 5.

| Table 5. Equilibrium product amount of various product with energy deposition |
|----------------|----------------|----------------|----------------|
| Product            | $n_{H,O}^0$ | $n_{CO_2}^0$ | $n_{CO}^0$ | $n_{N_2}^0$ |
| Amount (in mol)    | 3.562 | 3.1034 | 0.1700 | 1.5664 |
Detonation speed calculation is $D=8330 \text{ m}\cdot\text{s}^{-1}$ when $P=21.08 \text{ GPa}$, $T=3000\text{ K}$. Substituting these results into Eq.(53) yields other detonation parameters are listed in Table 6.

| Detonation parameter | $V_0$ (in m/s) | $T_z$ (in K) | $P_z$ (in GPa) |
|----------------------|----------------|-------------|---------------|
| Without energy deposition | 8325           | 3917        | 30.67         |
| With energy deposition    | 8330           | 4193        | 30.70         |

From Table 6 one can see that long-term small dose has an ignorable influence on detonation speed and detonation pressure of inert explosive, however, remarkably increases detonation temperature, three reasons for these results include:

1. We consider molecular structure and loading density of explosive to be constant in this work, so a single influencing factor for detonation speed is detonation heat. In fact, detonation speed is scaled with square root of detonation heat $Q_{2,3}$, where $Q_{2,3}=Q_{1,3}-Q_{1,2}$. As discussed above, energy deposition of nuclear radiation has a neglectable effect on $Q_{1,3}$ and $Q_{1,2}$ (thereby detonation speed).

2. From Eq.(53) one can see that important influencing factors of detonation pressure are density and detonation speed of explosive. In this work, density keeps constant in all calculations, and influence of nuclear radiation on detonation speed can be negligible, so energy deposition has an ignorable effect on detonation pressure.

3. As a matter of fact, two manners can be used to increase detonation temperature of explosive: increasing formation heat of explosive product (thereby reducing heat generation of explosive) or decreasing heat capacity of explosive product. Therefore, the more generation amount for $\text{H}_2\text{O}$, CO in products, the more detonation temperature will be. While nuclear radiation notably increases $\text{H}_2\text{O}$ and CO amount in explosive product, so energy deposition of nuclear radiation has a relatively large impact on detonation temperature. From above analysis we can conclude that theoretical calculations for influences of nuclear radiation on detonation parameters are reasonable.

4. Conclusion
Influences of energy deposition of n & $\gamma$ mixing radiation field on decomposition speed and detonation parameters of long-term storage explosive have been studied in this work. The results show that energy deposition has a negligible effect on the decomposition speed, detonation speed and detonation pressure, however, remarkably increases the detonation temperature. Our main quantitative or qualitative results may not remarkably change although more aspects are taken into account during calculations for detonation parameters and influences of energy deposition. In the future work, we plan to investigate influences of nuclear radiation on detonation parameters of mixing explosive or physicochemical properties (such as molecular structure, elastic modulus, shear modulus) of explosive molecule. At the same time, more products will be included in future calculations. Moreover, only a set of $(P, T)$ is considered in this work, this simple choice may affect universality of calculation results, so it is essential to increase parameter sets and iteration steps for detonation parameters aiming at improving generality and transportability of calculation method.

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