

文章编号: 1006-9941(2011)02-0132-06

Analysis of Overall Standard Deviation of Thermal Safety Criteria for Small-scale Energetic Materials

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Abstract: Twenty expressions describing the overall standard deviation (σ) of thermal safety criteria of small-scale energetic materials were presented. The values of σ and relative standard deviation of thermal safety criteria for 1, 1'-dimethyl-5, 5'-azotetrazol monohydrate, 3-nitro-1, 2, 4-triazol-5-one, bis(2,2,2-trinitroethyl) formal and double-base propellant composed (56 ± 1) wt% of NC, (27 ± 0.5) wt% of NG, (8.5 ± 0.15) wt% of DNT, (2.5 ± 0.1) wt% of methyl centralite, (5.0 ± 0.15) wt% of catalyts and (1.0 ± 0.1) wt% of other were reported.

Key words: physical chemistry; thermal safety; criteria; overall standard deviation; energetic materials

CLC number: TJ55; O642

Document code: A

DOI: 10.3969/j.issn.1006-9941.2011.02.003

1 Introduction

The adiabatic time-to-explosion (t_c), critical half-thickness (r), critical temperature (T_c), adiabatic decomposition temperature (T_a), explosion potential (E_p), shock sensitivity relative to *m*-dinitrobenzene (S_s), instantaneous power density (I_{pd}), characteristic decomposition temperature corresponding to certain heating rate (T_{e0} or p_0), critical temperature of thermal explosion based on Berthelot's equation (T_b), critical temperature of thermal explosion based on Arrhenius equation (T_{be0} or bp_0), critical temperature of thermal explosion based on Harcourt-Esson's equation (T_{be0} or bp_0), free energy of activation (ΔG^\ddagger), enthalpy of activation (ΔH^\ddagger), entropy of activation (ΔS^\ddagger), safe storage life (t), reaction rate constant (k), self-accelerating decomposition temperature (T_{e0} or p_0), time lag prior to explosion (t_{5s} or $1000s$), explosion temperature (T_E) and 50% drop height of impact sensitivity (H_{50}) are twenty criteria of evaluating the thermal safety of small-scale energetic materials. The overall standard deviation ($\sigma_{\text{criterion}}$), relative standard deviation ($\sigma_{\text{criterion}}/\text{criterion value}$) and percentage that the percentage error of measurement quantity or calculation quantity accounts for the overall error,

$\frac{\text{partial differential of criterion}}{\text{partial differential of measurement quantity or calculation quantity}}$ are three important parameters of

analyzing the magnitude of error of the criterion and exposing the order of principal factors affecting the criterion. The aim of this work is to derive the expressions describing the overall standard deviation (σ) of thermal safety criteria of small-scale energetic materials and to report the values of σ and relative standard deviation of thermal safety criteria for 1, 1'-dimethyl-5, 5'-azotetrazol monohydrate, 3-nitro-1, 2, 4-triazol-5-one, bis(2,2,2-trinitroethyl) formal and double-base propellant composed (56 ± 1) wt% of NC, (27 ± 0.5) wt% of NG,

Received Date: 2010-05-19; **Revised Date:** 2010-07-18

Project Supported: Science and Technology Foundation of National Defence Key Laboratory of Propellant and Explosive Combustion of China(9140C3501010601)

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(8.5 ± 0.15) wt% of DNT, (2.5 ± 0.1) wt% of methyl centralite, (5.0 ± 0.15) wt% of catalyts and (1.0 ± 0.1) wt% of other obtained with the derived expressions.

2 Criteria for thermal safety of EM and derivation of expressions of the overall standard deviation of the criteria

(1) Adiabatic time-to-explosion is defined by:

$$t_c = \frac{C_p R T_i^2 \exp(E/RT_i)}{EAQ_d} \quad (1)$$

where: t_c = adiabatic time-to-explosion, s

C_p = specific heat capacity, $J \cdot g^{-1} \cdot K^{-1}$

R = gas constant = $8.314 J \cdot g^{-1} \cdot mol^{-1}$

T = initial (or environmental) temperature, K

E = activation energy, $J \cdot mol^{-1}$

A = per-exponential constant, s^{-1}

Q_d = heat of reaction, $J \cdot g^{-1}$.

The function equation (2), overall standard deviation formula (3), error propagation coefficient Eqs. (4) - (8) and standard deviation Eqs. (9) and (10) are used to analyze and gain the value of overall standard deviation σ_{t_c}

$$t_c = f(C_p, T_i, E, A, Q_d) \quad (2)$$

$$\sigma_{t_c} = \left[\left(\frac{\partial t_c}{\partial C_p} \right)^2 \sigma_{C_p}^2 + \left(\frac{\partial t_c}{\partial T_i} \right)^2 \sigma_{T_i}^2 + \left(\frac{\partial t_c}{\partial E} \right)^2 \sigma_E^2 + \left(\frac{\partial t_c}{\partial A} \right)^2 \sigma_A^2 + \left(\frac{\partial t_c}{\partial Q_d} \right)^2 \sigma_{Q_d}^2 \right]^{1/2} \quad (3)$$

$$\frac{\partial t_c}{\partial C_p} = \frac{RT_i^2 \exp(E/RT_i)}{EAQ_d} = \frac{C_p RT_i^2 \exp(E/RT_i)}{C_p EAQ_d} = \frac{t_c}{C_p} \quad (4)$$

$$\begin{aligned} \frac{\partial t_c}{\partial T_i} &= \frac{C_p R}{EAQ_d} \left[2T_i \exp(E/RT_i) + T_i^2 \exp(E/RT_i) \left(-\frac{E}{RT_i^2} \right) \right] \\ &= \frac{C_p RT_i^2 \exp(E/RT_i)}{EAQ_d} \left[\frac{2}{T_i} - \frac{E}{RT_i^2} \right] = t_c \left(\frac{2}{T_i} - \frac{E}{RT_i^2} \right) \end{aligned} \quad (5)$$

$$\begin{aligned} \frac{\partial t_c}{\partial E} &= \left(\frac{C_p RT_i^2 \exp(E/RT_i)}{EAQ_d} \right)' = \frac{C_p RT_i^2 \exp(E/RT_i)}{AQ_d} \cdot \frac{1}{RT_i} \cdot E - \exp(E/RT_i) \\ &= \frac{C_p RT_i^2 e^{E/RT}}{AQ_d} \cdot \frac{1}{RT_i} \cdot E - 1 = t_c \left(\frac{1}{RT_i} - \frac{1}{E} \right) \end{aligned} \quad (6)$$

$$\frac{\partial t_c}{\partial A} = \frac{C_p RT_i^2 \exp(E/RT_i)}{EQ_d} \cdot \left(-\frac{1}{A^2}\right) = -\frac{t_c}{A} \quad (7)$$

$$\frac{\partial t_c}{\partial Q_d} = \frac{C_p RT_i^2 \exp(E/RT_i)}{EA} \cdot \left(-\frac{1}{Q_d^2}\right) = -\frac{t_c}{Q_d} \quad (8)$$

$$\sigma_x = \Delta d/\sqrt{3}, \quad x = T_i, r, t_{5s}, t_{1000s}, \rho \quad (9)$$

where Δd is the value of the minimal scale division of measuring equipment, for the single measurement quantities, $T_i, r, t_{5s}, t_{1000s}, \rho$.

$$\sigma_x = \sqrt{\frac{\sum (x_i - \bar{x})^2}{n-1}}, x = C_p, E, A, Q_d, \lambda \quad (10)$$

for the repeatable measurement quantities, C_p, E, A, Q_d and λ .

(2) Critical half-thickness is defined by:

$$r = \left(\frac{\delta \lambda RT_{env}^2 \exp(E/RT_{env})}{Q_d A E \rho}\right)^{\frac{1}{2}} \quad (11)$$

where: r = critical half-thickness, cm

T_{env} = environment temperature, K

δ = form factor (dimensionless):

0.88 for infinite slab

2.00 for infinite cylinder

2.53 for a cube

2.78 for a square cylinder

3.32 for sphere

λ = thermal conductivity, $J \cdot (cm \cdot s \cdot K)^{-1}$

ρ = density or concentration, $g \cdot cm^{-3}$

Similarly, Eqs. (9), (10) and (11) – (19) are used to obtain the value of σ_r .

$$r = f(\lambda, T_{env}, E, A, Q_d, \rho) \quad (12)$$

$$\sigma_r = \left[\left(\frac{\partial r}{\partial \lambda}\right)^2 \sigma_\lambda^2 + \left(\frac{\partial r}{\partial T_{env}}\right)^2 \sigma_{T_{env}}^2 + \left(\frac{\partial r}{\partial E}\right)^2 \sigma_E^2 + \left(\frac{\partial r}{\partial Q_d}\right)^2 \sigma_{Q_d}^2 + \left(\frac{\partial r}{\partial A}\right)^2 \sigma_A^2 + \left(\frac{\partial r}{\partial \rho}\right)^2 \sigma_\rho^2 \right]^{\frac{1}{2}} \quad (13)$$

$$\frac{\partial r}{\partial \lambda} = \frac{1}{2} \left(\frac{\delta \lambda RT_{env}^2 \exp(E/RT_{env})}{Q_d A E \rho}\right)^{\frac{1}{2}} \cdot \frac{\delta RT_{env}^2 \exp(E/RT_{env})}{Q_d A E \rho} = \frac{1}{2} \cdot \frac{1}{r} \cdot \frac{1}{\lambda} \cdot r^2 = \frac{r}{2\lambda} \quad (14)$$

$$\begin{aligned} \frac{\partial r}{\partial T_{env}} &= \frac{1}{2} \left(\frac{\delta \lambda RT_{env}^2 \exp(E/RT_{env})}{Q_d A E \rho}\right)^{\frac{1}{2}} \cdot \frac{\delta \lambda R}{Q_d A E \rho} \times \\ &\quad \left[2 T_{env} \exp(E/RT_{env}) + T_{env}^2 \exp(E/RT_{env}) \left(-\frac{E}{RT_{env}^2}\right) \right] \\ &= \frac{1}{2r} \frac{\delta \lambda RT_{env}^2 \exp(E/RT_{env})}{Q_d A E \rho} \left(\frac{2}{T} - \frac{E}{RT_{env}^2}\right) \\ &= \frac{r}{2} \left(\frac{2}{T_{env}} - \frac{E}{RT_{env}^2}\right) \end{aligned} \quad (15)$$

$$\begin{aligned} \frac{\partial r}{\partial E} &= \frac{1}{2} \left[\frac{\delta \lambda RT_{env}^2 \exp(E/RT_{env})}{Q_d A E \rho}\right]^{\frac{1}{2}} \cdot \frac{\delta \lambda RT_{env}^2}{Q_d A \rho} \times \\ &\quad \frac{\exp(E/RT_{env}) \cdot \frac{E}{RT_{env}} - \exp(E/RT_{env})}{E^2} \\ &= \frac{1}{2r} \frac{\delta \lambda RT_{env}^2 \exp(E/RT_{env})}{Q_d A E \rho} \left(\frac{E}{RT_{env}} - 1\right) = \frac{r}{2} \left(\frac{1}{RT_{env}} - \frac{1}{E}\right) \end{aligned} \quad (16)$$

$$\begin{aligned} \frac{\partial r}{\partial Q_d} &= \frac{1}{2} \left[\frac{\delta \lambda RT_{env}^2 \exp(E/RT_{env})}{Q_d A E \rho}\right]^{\frac{1}{2}} \cdot \frac{\delta \lambda RT_{env}^2 \exp(E/RT_{env})}{A E \rho} \cdot \left(-\frac{1}{Q_d}\right) \\ &= \frac{1}{2r} (-r^2) \cdot \frac{1}{Q_d} = -\frac{r}{2Q_d} \end{aligned} \quad (17)$$

$$\frac{\partial r}{\partial A} = -\frac{r}{2A} \quad (18)$$

$$\frac{\partial r}{\partial \rho} = -\frac{r}{2\rho} \quad (19)$$

(3) Critical temperature is defined by:

$$T_c = \left(\frac{R}{E} \ln\left(\frac{r_1^2 \rho Q_d A E}{T_c^2 \lambda \delta R}\right)\right)^{-1} \quad (20)$$

where: T_c = critical temperature, K

r_1 = shortest semi-thickness, cm

Similarly, for Eq. (20), we have Eqs. (21) – (28)

$$T_c = f(\rho, Q_d, A, E, r_1, \lambda) \quad (21)$$

$$\begin{aligned} \sigma_{T_c} &= \left[\left(\frac{\partial T_c}{\partial \rho}\right)^2 \sigma_\rho^2 + \left(\frac{\partial T_c}{\partial Q_d}\right)^2 \sigma_{Q_d}^2 + \left(\frac{\partial T_c}{\partial A}\right)^2 \sigma_A^2 + \right. \\ &\quad \left. \left(\frac{\partial T_c}{\partial E}\right)^2 \sigma_E^2 + \left(\frac{\partial T_c}{\partial r_1}\right)^2 \sigma_{r_1}^2 + \left(\frac{\partial T_c}{\partial \lambda}\right)^2 \sigma_\lambda^2 \right]^{\frac{1}{2}} \end{aligned} \quad (22)$$

$$\begin{aligned} \frac{\partial T_c}{\partial \rho} &= (-1) \left[\frac{R}{E} \ln\left(\frac{r_1^2 \rho Q_d A E}{T_c^2 \lambda \delta R}\right)\right]^{-2} \cdot \frac{R}{E} \cdot \frac{T_c^2 \lambda \delta R}{r_1^2 \rho Q_d A E} \cdot \frac{r_1^2 Q_d A E}{T_c^2 \lambda \delta R} \\ &= -T_c^2 \cdot \frac{R}{E} \cdot \frac{1}{\rho} \end{aligned} \quad (23)$$

$$\frac{\partial T_c}{\partial Q_d} = -T_c^2 \cdot \frac{R}{E} \cdot \frac{1}{Q_d} \quad (24)$$

$$\frac{\partial T_c}{\partial A} = -T_c^2 \cdot \frac{R}{E} \cdot \frac{1}{A} \quad (25)$$

$$\begin{aligned} \frac{\partial T_c}{\partial E} &= (-1) \left[\frac{R}{E} \ln\left(\frac{r_1^2 \rho Q_d A E}{T_c^2 \lambda \delta R}\right)\right]^{-2} \cdot \left[\left(-\frac{R}{E^2}\right) \times \right. \\ &\quad \left. \ln\left(\frac{r_1^2 \rho Q_d A E}{T_c^2 \lambda \delta R}\right) + \frac{R}{E} \cdot \frac{T_c^2 \lambda \delta R}{r_1^2 \rho Q_d A E} \cdot \frac{r_1^2 \rho Q_d A E}{T_c^2 \lambda \delta R}\right] \\ &= -T_c^2 \left[-\frac{1}{E} \cdot \frac{1}{T_c} + \frac{R}{E} \cdot \frac{1}{E}\right] = T_c^2 \frac{1}{E} \left(\frac{R}{E} - \frac{1}{T_c}\right) \end{aligned} \quad (26)$$

$$\frac{\partial T_c}{\partial r_1} = -T_c^2 \cdot \frac{R}{E} \cdot \frac{1}{r_1} \cdot 2r_1 = -T_c^2 \cdot \frac{R}{E} \cdot \frac{2}{r_1} \quad (27)$$

$$\begin{aligned} \frac{\partial T_c}{\partial \lambda} &= (-1) \left[\frac{R}{E} \ln\left(\frac{r_1^2 \rho Q_d A E}{T_c^2 \lambda \delta R}\right)\right]^{-2} \cdot \frac{R}{E} \cdot \frac{T_c^2 \lambda \delta R}{r_1^2 \rho Q_d A E} \cdot \frac{r_1^2 \rho Q_d A E}{T_c^2 \lambda \delta R} \cdot \left(-\frac{1}{\lambda^2}\right) \\ &= -T_c^2 \cdot \frac{R}{E} \cdot \left(-\frac{1}{\lambda}\right) = T_c^2 \cdot \frac{R}{E} \cdot \frac{1}{\lambda} \end{aligned} \quad (28)$$

(4) Adiabatic decomposition temperature rise is defined by:

$$T_a = \frac{Q_d}{C_p} \quad (29)$$

where:

T_a = adiabatic decomposition temperature rise, K.

Similarly, for Eq. (29), we have Eqs. (30) – (33)

$$T_a = f(Q_d, C_p) \quad (30)$$

$$\sigma_{T_a} = \left[\left(\frac{\partial T_a}{\partial Q_d}\right)^2 \sigma_{Q_d}^2 + \left(\frac{\partial T_a}{\partial C_p}\right)^2 \sigma_{C_p}^2 \right]^{\frac{1}{2}} \quad (31)$$

$$\frac{\partial T_a}{\partial Q_d} = \frac{1}{C_p} = \frac{T_a}{Q_d} \quad (32)$$

$$\frac{\partial T_a}{\partial C_p} = -\frac{Q_d}{C_p^2} = -\frac{T_a}{C_p} \quad (33)$$

(5) Explosion potential is defined by:

$$E_p = \lg[Q_d] - 0.38 \lg[T_{onset} - 298 \text{ K}] - 1.05 \quad (34)$$

where: E_p = explosion potential, and T_{onset} = onset temperature by DSC curve at a heating rate of $10 \text{ K} \cdot \text{min}^{-1}$

Similarly, for Eq. (34), we have Eqs. (35) – (38)

$$E_p = f(Q_d, T) \quad (35)$$

$$\sigma_{E_p} = \left[\left(\frac{\partial E_p}{\partial Q_d}\right)^2 \sigma_{Q_d}^2 + \left(\frac{\partial E_p}{\partial T_{onset}}\right)^2 \sigma_{T_{onset}}^2 \right]^{\frac{1}{2}} \quad (36)$$

$$\frac{\partial E_p}{\partial Q_d} = \frac{1}{Q_d} \cdot \frac{1}{\ln 10} = \frac{0.4342945}{Q_d} \quad (37)$$

$$\frac{\partial E_p}{\partial T_{\text{onset}}} = -0.38 \frac{1}{T_{\text{onset}} - 298 \text{ K}} \cdot \frac{1}{\ln 10} = \frac{-0.165032}{T_{\text{onset}} - 298 \text{ K}} \quad (38)$$

(6) Shock sensitivity relative to *m*-dinitrobenzene is defined by:

$$S_s = \lg[Q_d] - 0.72 \lg[T_{\text{onset}} - 298 \text{ K}] - 0.36 \quad (39)$$

where: S_s = shock sensitivity relative to *m*-dinitrobenzene.

Similarly, for Eq. (39), we have Eqs. (40) – (43)

$$S_s = f(Q_d, T_{\text{onset}}) \quad (40)$$

$$\sigma_{S_s} = \left[\left(\frac{\partial S_s}{\partial Q_d} \right)^2 \sigma_{Q_d}^2 + \left(\frac{\partial S_s}{\partial T_{\text{onset}}} \right)^2 \sigma_{T_{\text{onset}}}^2 \right]^{\frac{1}{2}} \quad (41)$$

$$\frac{\partial S_s}{\partial Q_d} = \frac{1}{Q_d} \cdot \frac{1}{\ln 10} = \frac{0.4342945}{Q_d} \quad (42)$$

$$\frac{\partial S_s}{\partial T_{\text{onset}}} = -0.72 \frac{1}{T_{\text{onset}} - 298 \text{ K}} \cdot \frac{1}{\ln 10} = \frac{-0.31269}{T_{\text{onset}} - 298 \text{ K}} \quad (43)$$

(7) Instantaneous power density at 250 °C is defined by:

$$I_{\text{pd}} = Q_d A \rho \exp[-E/523R] \quad (44)$$

where: I_{pd} = instantaneous power density at 250 °C.

Similarly, for Eq. (44), we have Eqs. (45) – (50)

$$I_{\text{pd}} = f(Q_d, A, \rho, E) \quad (45)$$

$$\sigma_{I_{\text{pd}}} = \left[\left(\frac{\partial I_{\text{pd}}}{\partial Q_d} \right)^2 \sigma_{Q_d}^2 + \left(\frac{\partial I_{\text{pd}}}{\partial A} \right)^2 \sigma_A^2 + \left(\frac{\partial I_{\text{pd}}}{\partial \rho} \right)^2 \sigma_\rho^2 + \left(\frac{\partial I_{\text{pd}}}{\partial E} \right)^2 \sigma_E^2 \right]^{\frac{1}{2}} \quad (46)$$

$$\frac{\partial I_{\text{pd}}}{\partial Q_d} = A \rho e^{-E/523R} = \frac{I_{\text{pd}}}{Q_d} \quad (47)$$

$$\frac{\partial I_{\text{pd}}}{\partial A} = \frac{I_{\text{pd}}}{A} \quad (48)$$

$$\frac{\partial I_{\text{pd}}}{\partial \rho} = \frac{I_{\text{pd}}}{\rho} \quad (49)$$

$$\frac{\partial I_{\text{pd}}}{\partial E} = Q_d A \rho e^{-E/523R} \cdot \left(-\frac{1}{523R} \right) = -\frac{I_{\text{pd}}}{523R} \quad (50)$$

(8) Characteristic decomposition temperature corresponding to certain heating rate is defined by:

$$T_{(o,e, \text{ or } p)i} = T_{(a0, e0, \text{ or } p0)i} + a_1 \beta_i + a_2 \beta_i^2 + \dots + a_{L-2} \beta_i^{L-2}, \quad (51)$$

$i = 1, 2, \dots, L$

$$\text{and} \quad T_{\text{SADT}} = T_{e0 \text{ or } p0} \quad (52)$$

where: a_1, a_2, a_3 and a_4 are coefficients, and β is the heating rate, $\text{K} \cdot \text{min}^{-1}$.

Similarly, for Eqs. (51) and (52), we have Eqs. (53) – (55)

$$T_{(o,e, \text{ or } p)i} = f(\beta) \quad (53)$$

$$\sigma_{T_{(o,e, \text{ or } p)i}} = \left[\left(\frac{\partial T_{(o,e, \text{ or } p)i}}{\partial \beta_i} \right)^2 \sigma_{\beta_i}^2 \right]^{\frac{1}{2}} \quad (54)$$

$$\begin{aligned} \frac{\partial T_{(o,e, \text{ or } p)i}}{\partial \beta_i} &= a_1 + 2a_2 \beta_i + 3a_3 \beta_i^2 + \dots + (L-2)a_{L-2} \beta_i^{L-3} \\ &= \sum_{n=1}^{L-2} n a_n \beta_i^{n-1} \end{aligned} \quad (55)$$

(9) Critical temperature of thermal explosion based on Berthelot's equation is defined by:

$$T_b = T_{e0} + \frac{1}{b} \quad (56)$$

where: T_b = critical temperature of thermal explosion based on Berthelot's equation, K

T_{e0} = onset temperature (T_e) corresponding to $\beta \rightarrow 0$, K, and

b = coefficient in Berthelot's equation, $k = A_0 e^{bT}$, K^{-1} .

Similarly, for Eq. (56), we have Eqs. (57) – (60)

$$T_b = f(T_{e0}, b) \quad (57)$$

$$\sigma_{T_b} = \left[\left(\frac{\partial T_b}{\partial T_{e0}} \right)^2 \sigma_{T_{e0}}^2 + \left(\frac{\partial T_b}{\partial b} \right)^2 \sigma_b^2 \right]^{\frac{1}{2}} \quad (58)$$

$$\frac{\partial T_b}{\partial T_{e0}} = 1 \quad (59)$$

$$\frac{\partial T_b}{\partial b} = -\frac{1}{b^2} \quad (60)$$

(10) Critical temperature of thermal explosion based on Arrhenius equation is defined by:

$$T_{\text{be0 or bp0}} = \frac{E_{\text{oe or op}} - \sqrt{E_{\text{oe or op}}^2 - 4E_{\text{oe or op}} RT_{\text{e0 or p0}}}}{2R} \quad (61)$$

where: $T_{\text{be0 or bp0}}$ = critical temperature of thermal explosion based on Arrhenius equation, K

$E_{\text{oe or op}}$ = activation energy calculated from the relationship of $\lg \beta_i$ vs. $1/T_{ei}$ or $1/T_{pi}$, $\text{J} \cdot \text{mol}^{-1}$, and

$T_{\text{e0 or p0}}$ = onset temperature (T_e) or peak temperature (T_p) corresponding to $\beta \rightarrow 0$, K.

Similarly, for Eq. (61), we have Eqs. (62) – (65)

$$T_{\text{be0 or bp0}} = f(E_{\text{oe or op}}, T_{\text{e0 or p0}}) \quad (62)$$

$$\sigma_{T_{\text{be0 or bp0}}} = \left[\left(\frac{\partial T_{\text{be0 or bp0}}}{\partial E_{\text{oe or op}}} \right)^2 \sigma_{E_{\text{oe or op}}}^2 + \left(\frac{\partial T_{\text{be0 or bp0}}}{\partial T_{\text{e0 or p0}}} \right)^2 \sigma_{T_{\text{e0 or p0}}}^2 \right]^{\frac{1}{2}} \quad (63)$$

$$\begin{aligned} \frac{\partial T_{\text{be0 or bp0}}}{\partial E_{\text{oe or op}}} &= \frac{1}{2R} \cdot \frac{1}{2R} \cdot \frac{1}{2} (E_{\text{oe or op}}^2 - 4E_{\text{oe or op}} RT_{\text{e0 or p0}})^{-\frac{1}{2}} (2E_{\text{oe or op}} - 4RT_{\text{e0 or p0}}) \\ &= \frac{1}{2R} [1 - (E_{\text{oe or op}}^2 - 4E_{\text{oe or op}} RT_{\text{e0 or p0}})^{-\frac{1}{2}} (E_{\text{oe or op}} - 2RT_{\text{e0 or p0}})] \end{aligned} \quad (64)$$

$$\begin{aligned} \frac{\partial T_{\text{be0 or bp0}}}{\partial T_{\text{e0 or p0}}} &= 0 - \frac{1}{2R} \cdot \frac{1}{2} (E_{\text{oe or op}}^2 - 4E_{\text{oe or op}} RT_{\text{e0 or p0}})^{-\frac{1}{2}} \cdot (-4RE_{\text{oe or op}}) \\ &= E_{\text{oe or op}} (E_{\text{oe or op}}^2 - 4E_{\text{oe or op}} RT_{\text{e0 or p0}})^{-\frac{1}{2}} \end{aligned} \quad (65)$$

(11) Critical temperature of thermal explosion based on Harcourt-Esson's equation is defined by:

$$T_{\text{be0 or bp0}} = \left(\frac{a_{e0 \text{ or } p0}}{a_{e0 \text{ or } p0} - 1} \right) T_{e0 \text{ or } p0} \quad (66)$$

where: $T_{\text{be0 or bp0}}$ = critical temperature of thermal explosion based on Harcourt-Esson's equation, K, and

$a_{e0 \text{ or } p0}$ = coefficient in Harcourt-Esson's equation,

$$k = A_0 T^3.$$

Similarly, for Eq. (66), we have Eqs. (67) – (70)

$$T_{\text{be0 or bp0}} = f(a_{e0 \text{ or } p0}, T_{e0 \text{ or } p0}) \quad (67)$$

$$\sigma_{T_{\text{be0 or bp0}}} = \left[\left(\frac{\partial T_{\text{be0 or bp0}}}{\partial a_{e0 \text{ or } p0}} \right)^2 \sigma_{a_{e0 \text{ or } p0}}^2 + \left(\frac{\partial T_{\text{be0 or bp0}}}{\partial T_{e0 \text{ or } p0}} \right)^2 \sigma_{T_{e0 \text{ or } p0}}^2 \right]^{\frac{1}{2}} \quad (68)$$

$$\frac{\partial T_{\text{be0 or bp0}}}{\partial a_{e0 \text{ or } p0}} = \frac{(a_{e0 \text{ or } p0} - 1) - a_{e0 \text{ or } p0} T_{e0 \text{ or } p0}}{(a_{e0 \text{ or } p0} - 1)^2} T_{e0 \text{ or } p0} = \frac{-T_{e0 \text{ or } p0}}{(a_{e0 \text{ or } p0} - 1)^2} \quad (69)$$

$$\frac{\partial T_{\text{be0 or bp0}}}{\partial T_{e0 \text{ or } p0}} = \frac{a_{e0 \text{ or } p0}}{a_{e0 \text{ or } p0} - 1} \quad (70)$$

(12) Free energy of activation is defined by:

$$\Delta G^\ddagger = E - RT \ln \left(\frac{Ah}{k_B T} \right) \quad (71)$$

where: ΔG^\ddagger = free energy of activation, $\text{J} \cdot \text{mol}^{-1}$

h = Planck constant = $6.626 \times 10^{-34} \text{ J} \cdot \text{s}$, and

k_B = Boltzmann constant = $1.3807 \times 10^{-23} \text{ J} \cdot \text{K}^{-1}$.

Similarly, for Eq. (71), we have Eqs. (72) – (76)

$$\Delta G^\ddagger = f(E, T_{p0}, A) \quad (72)$$

$$\sigma_{\Delta G^\ddagger} = \left[\left(\frac{\partial \Delta G^\ddagger}{\partial E} \right)^2 \sigma_E^2 + \left(\frac{\partial \Delta G^\ddagger}{\partial T_{p0}} \right)^2 \sigma_{T_{p0}}^2 + \left(\frac{\partial \Delta G^\ddagger}{\partial A} \right)^2 \sigma_A^2 \right]^{\frac{1}{2}} \quad (73)$$

$$\frac{\partial \Delta G^\ddagger}{\partial E} = 1 \quad (74)$$

$$\begin{aligned} \frac{\partial \Delta G^\circ}{\partial T_{p0}} &= -R \left[\ln \left(\frac{Ah}{k_B T_{p0}} \right) + T_{p0} \cdot \frac{k_B T_{p0}}{Ah} \cdot \frac{Ah}{k_B} \cdot \left(-\frac{1}{T_{p0}^2} \right) \right] \\ &= -R \left[\ln \left(\frac{Ah}{k_B T_{p0}} \right) - 1 \right] = R \left[1 - \ln \left(\frac{Ah}{k_B T_{p0}} \right) \right] \end{aligned} \quad (75)$$

$$\frac{\partial \Delta G^\circ}{\partial A} = -RT_{p0} \cdot \frac{k_B T_{p0}}{Ah} \cdot \frac{h}{k_B T_{p0}} = -\frac{RT_{p0}}{A} \quad (76)$$

(13) Enthalpy of activation is defined by:

$$\Delta H^\circ = E - RT_{p0} \quad (77)$$

where: ΔH° = enthalpy of activation, $J \cdot mol^{-1}$.

Similarly, for Eq. (77), we have Eqs. (78) - (81)

$$\Delta H^\circ = f(E, T_{p0}) \quad (78)$$

$$\sigma_{\Delta H^\circ} = \left[\left(\frac{\partial \Delta H^\circ}{\partial E} \right)^2 \sigma_E^2 + \left(\frac{\partial \Delta H^\circ}{\partial T_{p0}} \right)^2 \sigma_{T_{p0}}^2 \right]^{\frac{1}{2}} \quad (79)$$

$$\frac{\partial \Delta H^\circ}{\partial E} = 1 \quad (80)$$

$$\frac{\partial \Delta H^\circ}{\partial T_{p0}} = -R \quad (81)$$

(14) Entropy of activation is defined by:

$$\Delta S^\circ = \frac{\Delta H^\circ - \Delta G^\circ}{T_{p0}} \quad (82)$$

where: ΔS° = entropy of activation, $J \cdot mol^{-1} \cdot K^{-1}$.

Similarly, for Eq. (82), we have Eqs. (83) - (87)

$$\Delta S^\circ = f(\Delta H^\circ, \Delta G^\circ, T_{p0}) \quad (83)$$

$$\sigma_{\Delta S^\circ} = \left[\left(\frac{\partial \Delta S^\circ}{\partial \Delta H^\circ} \right)^2 \sigma_{\Delta H^\circ}^2 + \left(\frac{\partial \Delta S^\circ}{\partial \Delta G^\circ} \right)^2 \sigma_{\Delta G^\circ}^2 + \left(\frac{\partial \Delta S^\circ}{\partial T_{p0}} \right)^2 \sigma_{T_{p0}}^2 \right]^{\frac{1}{2}} \quad (84)$$

$$\frac{\partial \Delta S^\circ}{\partial \Delta H^\circ} = \frac{1}{T_{p0}} \quad (85)$$

$$\frac{\partial \Delta S^\circ}{\partial \Delta G^\circ} = -\frac{1}{T_{p0}} \quad (86)$$

$$\frac{\partial \Delta S^\circ}{\partial T_{p0}} = -\frac{1}{T_{p0}^2} (\Delta H^\circ - \Delta G^\circ) = \frac{1}{T_{p0}^2} (\Delta G^\circ - \Delta H^\circ) \quad (87)$$

(15) Safe storage life is defined by:

$$t = 10^{a_1 + b_1 T} \quad (88)$$

where: t = safe storage life, y , and a_1 and b_1 are parameters of the correlation.

Similarly, for Eq. (88), we have Eqs. (89) - (93)

$$t = f(a_1, b_1, T) \quad (89)$$

$$\sigma_t = \left[\left(\frac{\partial t}{\partial a_1} \right)^2 \sigma_{a_1}^2 + \left(\frac{\partial t}{\partial b_1} \right)^2 \sigma_{b_1}^2 + \left(\frac{\partial t}{\partial T} \right)^2 \sigma_T^2 \right]^{\frac{1}{2}} \quad (90)$$

$$\frac{\partial t}{\partial a_1} = 10^{a_1 + b_1 T} \cdot \ln 10 = t \ln 10 \quad (91)$$

$$\frac{\partial t}{\partial b_1} = 10^{a_1 + b_1 T} \cdot \ln 10 \cdot T = t T \ln 10 \quad (92)$$

$$\frac{\partial t}{\partial T} = 10^{a_1 + b_1 T} \cdot \ln 10 \cdot b_1 = t b_1 \ln 10 \quad (93)$$

(16) Reaction rate constant is defined by:

$$k = Ae^{-\frac{E}{RT_{p0}}} \quad (94)$$

where: k = reaction rate constant, s^{-1} .

Similarly, for Eq. (94), we have Eqs. (95) - (99)

$$k = f(A, E, T_{p0}) \quad (95)$$

$$\sigma_k = \left[\left(\frac{\partial k}{\partial A} \right)^2 \sigma_A^2 + \left(\frac{\partial k}{\partial E} \right)^2 \sigma_E^2 + \left(\frac{\partial k}{\partial T_{p0}} \right)^2 \sigma_{T_{p0}}^2 \right]^{\frac{1}{2}} \quad (96)$$

$$\frac{\partial k}{\partial A} = e^{-\frac{E}{RT_{p0}}} \quad (97)$$

$$\frac{\partial k}{\partial E} = Ae^{-\frac{E}{RT_{p0}}} \cdot \left(-\frac{1}{RT_{p0}} \right) = k \left(-\frac{1}{RT_{p0}} \right) = -\frac{k}{RT_{p0}} \quad (98)$$

$$\frac{\partial k}{\partial T_{p0}} = Ae^{-\frac{E}{RT_{p0}}} \cdot \left(-\frac{E}{R} \right) \cdot \left(-\frac{1}{T_{p0}^2} \right) = \frac{kE}{RT_{p0}^2} \quad (99)$$

(17) Self-accelerating decomposition temperature is defined by:

$$T_{00, e0, \text{ or } p0} = T_{0, e, \text{ or } p} - a_1 \beta - a_2 \beta^2 - a_3 \beta^3 - a_4 \beta^4 \quad (100)$$

and

$$T_{\text{SADT}} = T_{e0 \text{ or } p0} \quad (101)$$

where: a_1 , a_2 , a_3 and a_4 are coefficients, and β is the heating rate, $K \cdot \text{min}^{-1}$.

Similarly, for Eqs. (100) and (101), we have Eqs. (101) - (104)

$$T_{00, e0, \text{ or } p0} = f(T_{0, e, \text{ or } p}, \beta) \quad (101)$$

$$\sigma_{T_{00, e0, \text{ or } p0}} = \left[\left(\frac{\partial T_{00, e0, \text{ or } p0}}{\partial T_{0, e, \text{ or } p}} \right)^2 \sigma_{T_{0, e, \text{ or } p}}^2 + \left(\frac{\partial T_{00, e0, \text{ or } p0}}{\partial \beta} \right)^2 \sigma_\beta^2 \right]^{\frac{1}{2}} \quad (102)$$

$$\frac{\partial T_{00, e0, \text{ or } p0}}{\partial T_{0, e, \text{ or } p}} = 1 \quad (103)$$

$$\frac{\partial T_{00, e0, \text{ or } p0}}{\partial \beta} = -a_1 - 2a_2 \beta - 3a_3 \beta^2 - 4a_4 \beta^3 \quad (104)$$

(18) Time lag prior to explosion is defined by:

$$t_{5 \text{ s or } 1000 \text{ s}} = e^{-\ln A + \frac{E}{RT_E}} \quad (105)$$

where: $t_{5 \text{ s or } 1000 \text{ s}}$ = time lag prior to explosion, s , and

T_E = explosion temperature corresponding to $t = 5 \text{ s}$ or $t = 1000 \text{ s}$, K .

Similarly, for Eq. (105), we have Eqs. (106) - (111)

$$t_{5 \text{ s or } 1000 \text{ s}} = f(A_E, E_E, T_E) \quad (106)$$

$$\sigma_{t_{5 \text{ s or } 1000 \text{ s}}} = \left[\left(\frac{\partial t_{5 \text{ s or } 1000 \text{ s}}}{\partial A_E} \right)^2 \sigma_{A_E}^2 + \left(\frac{\partial t_{5 \text{ s or } 1000 \text{ s}}}{\partial E_E} \right)^2 \sigma_{E_E}^2 + \left(\frac{\partial t_{5 \text{ s or } 1000 \text{ s}}}{\partial T_E} \right)^2 \sigma_{T_E}^2 \right]^{\frac{1}{2}} \quad (107)$$

$$\frac{\partial t_{5 \text{ s or } 1000 \text{ s}}}{\partial A_E} = e^{-\ln A_E + \frac{E_E}{RT_E}} \cdot \left(-\frac{1}{A_E} \right) = t_{5 \text{ s or } 1000 \text{ s}} \cdot \left(-\frac{1}{A_E} \right) \quad (108)$$

$$\frac{\partial t_{5 \text{ s or } 1000 \text{ s}}}{\partial E_E} = e^{-\ln A_E + \frac{E_E}{RT_E}} \cdot \frac{1}{RT_E} = t_{5 \text{ s or } 1000 \text{ s}} \cdot \frac{1}{RT_E} \quad (109)$$

$$\frac{\partial t_{5 \text{ s or } 1000 \text{ s}}}{\partial T_E} = e^{-\ln A_E + \frac{E_E}{RT_E}} \cdot \frac{E_E}{R} \cdot \left(-\frac{1}{T_E^2} \right) = t_{5 \text{ s or } 1000 \text{ s}} \cdot \left(-\frac{E_E}{RT_E^2} \right) \quad (110)$$

(19) Explosion temperature is defined by:

$$T_E = \frac{E}{R} [\ln t_{5 \text{ s or } 1000 \text{ s}} + \ln A]^{-1} \quad (111)$$

where: T_E = explosion temperature corresponding to $t = 5 \text{ s}$ or $t = 1000 \text{ s}$, K .

Similarly, for Eq. (111), we have Eqs. (112) - (116)

$$T_E = f(E_E, t_{5 \text{ s or } 1000 \text{ s}}, A_E) \quad (112)$$

$$\sigma_{T_E} = \left[\left(\frac{\partial T_E}{\partial E_E} \right)^2 \sigma_{E_E}^2 + \left(\frac{\partial T_E}{\partial t_{5 \text{ s or } 1000 \text{ s}}} \right)^2 \sigma_{t_{5 \text{ s or } 1000 \text{ s}}}^2 + \left(\frac{\partial T_E}{\partial A_E} \right)^2 \sigma_{A_E}^2 \right]^{\frac{1}{2}} \quad (113)$$

$$\frac{\partial T_E}{\partial E_E} = \frac{1}{R} [\ln t_{5 \text{ s or } 1000 \text{ s}} + \ln A_E]^{-1} = \frac{T_E}{E_E} \quad (114)$$

$$\frac{\partial T_E}{\partial t_{5 \text{ s or } 1000 \text{ s}}} = \frac{E_E}{R} (-1) [\ln t_{5 \text{ s or } 1000 \text{ s}} + \ln A_E]^{-2} \cdot \left(\frac{1}{t_{5 \text{ s or } 1000 \text{ s}}} \right) \quad (115)$$

$$= T_E^2 \cdot \frac{R}{E_E} \cdot \left(-\frac{1}{t_{5 \text{ s or } 1000 \text{ s}}} \right) \quad (115)$$

$$\frac{\partial T_E}{\partial A_E} = T_E^2 \cdot \frac{R}{E_E} \cdot \left(-\frac{1}{A_E} \right) \quad (116)$$

(20) 50% drop height of impact sensitivity is defined by:

$$c_1 \lg(H_{50}) + \lg \sqrt{\frac{\lambda}{A \rho Q_d}} - c_2 + \frac{c_5 E}{T_1 + c_3 H_{50}^4} = 0 \quad (117)$$

where: H_{50} = 50% drop height of impact sensitivity, cm ;

c_1 , c_2 , c_3 and c_4 are parameters of correlation, and c_5 = constant = 0.02612.

Similarly, for Eq. (117), we have Eqs. (118) - (124)

$$H_{50} = f(\lambda, \rho, Q_d, E, A) \quad (118)$$

$$\sigma_{H_{50}} = \left[\left(\frac{\partial H_{50}}{\partial \lambda} \right)^2 \sigma_\lambda^2 + \left(\frac{\partial H_{50}}{\partial \rho} \right)^2 \sigma_\rho^2 + \left(\frac{\partial H_{50}}{\partial Q_d} \right)^2 \sigma_{Q_d}^2 + \right]$$

$$\left(\frac{\partial H_{50}}{\partial E}\right)^2 \sigma_E^2 + \left(\frac{\partial H_{50}}{\partial A}\right)^2 \sigma_A^2 \Bigg]^{\frac{1}{2}} \quad (119)$$

$$\frac{\partial H_{50}}{\partial \lambda} = -\frac{\frac{1}{2 \ln 10} \cdot \lambda^{-1}}{c_1 \frac{1}{H_{50}} \cdot \frac{1}{\ln 10} + \frac{-c_3 c_4 H_{50}^{c_4-1} c_5 E}{(T_1 + c_3 H_{50}^{c_4})^2}} \quad (120)$$

$$\frac{\partial H_{50}}{\partial \rho} = -\frac{\frac{1}{2 \ln 10} \cdot \left(-\frac{1}{\rho}\right)}{c_1 \frac{1}{H_{50}} \cdot \frac{1}{\ln 10} + \frac{-c_3 c_4 H_{50}^{c_4-1} c_5 E}{(T_1 + c_3 H_{50}^{c_4})^2}} \quad (121)$$

$$\frac{\partial H_{50}}{\partial Q_d} = -\frac{\frac{1}{2 \ln 10} \cdot \left(-\frac{1}{Q_d}\right)}{c_1 \frac{1}{H_{50}} \cdot \frac{1}{\ln 10} + \frac{-c_3 c_4 H_{50}^{c_4-1} c_5 E}{(T_1 + c_3 H_{50}^{c_4})^2}} \quad (122)$$

$$\frac{\partial H_{50}}{\partial E} = -\frac{\frac{c_5}{T_1 + c_3 H_{50}^{c_4}}}{c_1 \frac{1}{H_{50}} \cdot \frac{1}{\ln 10} + \frac{-c_3 c_4 H_{50}^{c_4-1} c_5 E}{(T_1 + c_3 H_{50}^{c_4})^2}} \quad (123)$$

$$\frac{\partial H_{50}}{\partial A} = -\frac{\frac{1}{2 \ln 10} \cdot \left(-\frac{1}{A}\right)}{c_1 \frac{1}{H_{50}} \cdot \frac{1}{\ln 10} + \frac{-c_3 c_4 H_{50}^{c_4-1} c_5 E}{(T_1 + c_3 H_{50}^{c_4})^2}} \quad (124)$$

3 Rating of thermal safety criteria

(1) The higher the temperatures, T_c , $T_{0,e,or p}$, $T_{00,e0,or p0}$, T_b , $T_{be0,or bp0}$, $T_{5s,or 1000s}$, T_E , and 50% drop height of impact sensitivity (H_{50}), the better the thermal safety of EM.

(2) The smaller the critical half-thickness (r) and the greater the reaction rate constant at same temperature, the poorer the heat-resistance ability of EM.

(3) The greater the values of $\Delta G^\#$ and $\Delta H^\#$, the smaller the values of $\Delta S^\#$, the better the heat-resistance ability of EM.

(4) The shorter the adiabatic time-to-explosion (t_c) and time lag prior to explosion at same temperature, the poorer the thermal safety of EM.

(5) For E_p , positive values indicate likelihood and negative values indicate unlikelihood. The greater the magnitude of E_p values, the more reliable to go-no-go indication^[1].

(6) Instability rating is defined by Table 1.

Table 1 Instability rating^[2]

instability rating	instantaneous power density at 523 K
4	1000 WmL ⁻¹ or greater
3	at or greater than 100 WmL ⁻¹ and below 1000 W mL ⁻¹
2	at or greater than 10 WmL ⁻¹ and below 100 WmL ⁻¹
1	at or greater than 0.01 WmL ⁻¹ and below 10 WmL ⁻¹
0	below 0.01 WmL ⁻¹

4 Calculation examples

Assuming:

for 1,1'-dimethyl-5, 5'-azotelrazol^[3],

$t_c = 4.90$ s

$C_p = 1.16$ J · g⁻¹ · K⁻¹

$T_i = 468.92$ K

$R = 8.314$ J · mol⁻¹ · K⁻¹

$E = 127520$ J · mol⁻¹

$A = 10^{11.05}$ s⁻¹

$Q_d = 3188$ J · g⁻¹

$r = r_1 = 50$ cm

$\lambda = 32.44 \times 10^{-4}$ J · cm⁻¹ · s⁻¹ · K⁻¹

$T_{env} = 323$ K

$\rho = 1.62$ g · cm⁻³

$T_c = 342.20$ K

$T_a = 2870$ K

$T_{onset} = 500.05$ K

$E_p = 1.58$

$S_s = 1.48$

$I_{pd} = 106.3$ W · cm⁻³

$T_{ei} = 468.92 + 5.8101\beta - 0.2452\beta^2 + 0.00385\beta^3$

$T_{e0} = 468.92$ K

$\beta = 10$ K · min⁻¹

$b = 0.05992$

$T_b = 485.61$ K

$E_{oe} = 126840$ J · mol⁻¹

$a_{e0} = 32.320$

$T_{p0} = 473.25$ K

$\Delta G^\# = 145130$ J · mol⁻¹

$\Delta H^\# = 123580$ J · mol⁻¹

$\Delta S^\# = -45.53$ J · K⁻¹ · mol⁻¹

for double-base propellant^[4],

$t = 18030$ d

$a_1 = 32.2531$

$b_1 = -6.0664$

$T = 313.15$ K

$k_{Tp0} = 10^{-3.03}$ s⁻¹ = 9.33×10^{-4} s⁻¹

$H_{50} = 24.49$ cm

$T_1 = 300$ K

$C_1 = 0.282312$

$C_2 = 0.347174$

$C_3 = 33.8765$

$C_4 = 0.564623$

$C_5 = 0.02612$

$\sigma_{cp} = 0.0142$ J · g⁻¹ · K⁻¹

$\sigma_T = 3$ K

$\sigma_E = \sigma_{E_{oe}} = 3000$ J · mol⁻¹

$\sigma_A = 0.030 \times 10^{11.05}$ s⁻¹

$\sigma_{Q_d} = 30$ J · g⁻¹

$\sigma_\lambda = 0.0002$ J · cm⁻¹ · s⁻¹ · K⁻¹

$\sigma_\rho = 0.0013$ g · cm⁻³

$\sigma_{T_{onset}} = \sigma_{T_{env}} = 3$ K

$\sigma_\beta = 0.1$ K · min⁻¹

$\sigma_{T_{e0}} = 3$ K

$\sigma_b = 0.0025$ K⁻¹

$\sigma_{a_{e0}} = 0.50$

$\sigma_{\Delta H^\#} = 30$ J · mol⁻¹

$\sigma_{\Delta G^\#} = 30$ J · mol⁻¹

$\sigma_{a1} = 10^{-9}$

$\sigma_{b1} = 10^{-9}$

$\sigma_{T_{p0}} = 3$ K

for 3-nitro-1, 2, 4-triazol-5-one^[5]

$$t_{1000\text{ s}} = 1000\text{ s}$$

$$T_E = t_{1000} = 526.45\text{ K}$$

$$E_E = 129160\text{ J} \cdot \text{mol}^{-1}$$

$$A_E = 10^{10.65}\text{ s}^{-1}$$

$$\sigma_{E_E} = 3000\text{ J} \cdot \text{mol}^{-1}$$

$$\sigma_{A_E} = 0.030 \times 10^{10.65}\text{ s}^{-1}$$

$$\sigma_{1000\text{ s}} = 0.006\text{ s}$$

for bis(2,2,2-trinitroethyl) formal^[6]

$$t_{5\text{ s}} = 5\text{ s}$$

$$T_E = t_{5\text{ s}} = 508.96\text{ K}$$

$$E_E = 102490\text{ J} \cdot \text{mol}^{-1}$$

$$A_E = 10^{9.82}\text{ s}^{-1}$$

$$\sigma_{E_{E,5\text{ s}}} = 3000\text{ J} \cdot \text{mol}^{-1}$$

$$\sigma_{A_{E,5\text{ s}}} = 0.030 \times 10^{9.82}\text{ s}^{-1}$$

$$\sigma_{a1} = 0.005$$

$$\sigma_{b1} = 0.005$$

Then:

$$(1) \sigma_{t_c} = 3.73\text{ s}, \sigma_{t_c}/t_c = 76.1\% \text{ (when } T_i = \text{constant, } \sigma_{t_c} = 3.60\text{ s, } \sigma_{t_c}/t_c = 73.5\%);$$

$$(2) \sigma_r = 29.44\text{ cm}, \sigma_r/r = 58.9\% \text{ (when } T_{\text{env}} = \text{constant, } \sigma_r = 27.48\text{ cm, } \sigma_r/r = 55.0\%);$$

$$(3) \sigma_{T_c} = 17.18\text{ K}, \sigma_{T_c}/T_c = 5.02\%;$$

$$(4) \sigma_{T_a} = 44.31\text{ K}, \sigma_{T_a}/T_a = 1.54\%;$$

$$(5) \sigma_{E_p} = 0.00476, \sigma_{E_p}/E_p = 0.30\%;$$

$$(6) \sigma_{s_s} = 0.00616, \sigma_{s_s} = 0.42\%;$$

$$(7) \sigma_{I_{pd}} = 3.706, \sigma_{I_{pd}}/I_{pd} = 3.48\%;$$

$$(8) \sigma_{T_e} = 0.01\text{ K}, \sigma_{T_e}/T_e = 0.002\%;$$

$$(9) \sigma_{T_b} = 3.08\text{ K}, \sigma_{T_b}/T_b = 0.63\%;$$

$$(10) \sigma_{T_{be0}} = 180.92\text{ K}, \sigma_{T_{be0}}/T_{be0} = 38.6\%;$$

$$(11) \sigma_{T_{be0}} = 3.11\text{ K}, \sigma_{T_{be0}}/T_{be0} = 0.66\%;$$

$$(12) \sigma_{\Delta G^\#} = 3004.4\text{ J} \cdot \text{mol}^{-1}, \sigma_{\Delta G^\#}/\Delta G^\# = 20.7\%;$$

$$(13) \sigma_{\Delta H^\#} = 3000.1\text{ J} \cdot \text{mol}^{-1}, \sigma_{\Delta H^\#}/\Delta H^\# = 24.3\%;$$

$$(14) \sigma_{\Delta S^\#} = 0.302\text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}, \sigma_{\Delta S^\#}/\Delta S^\# = 0.66\%;$$

$$(15) \sigma_t = 7555.5\text{ s}, \sigma_t/t = 42.0\% \text{ (when } a \text{ and } b \text{ are constant, } \sigma_t = 0.182\text{ d, } \sigma_t/t = 0.001\%);$$

$$(16) \sigma_k = 0.000737\text{ s}^{-1}, \sigma_k/k = 79\% \text{ (when } E \text{ and } A \text{ are constant, } \partial k/\partial E = 0, \partial k/\partial A = 0, \sigma_k = 0.000192\text{ d, } \sigma_k/k = 20.6\%);$$

$$(17) \sigma_{T_{e0}} = 52.63\text{ K}, \sigma_{T_{e0}}/T_{e0} = 11.2\%;$$

$$(18) \sigma_{5\text{ s}} = 0.73\text{ s}, \sigma_{5\text{ s}}/5 = 14.6\%; \sigma_{1000\text{ s}} = 170.83\text{ s}, \sigma_{1000\text{ s}}/1000 = 17.1\%;$$

$$(19) \sigma_{T_{E,5\text{ s}}} = 14.89\text{ K}, \sigma_{T_{E,5\text{ s}}} = 2.93\%; \sigma_{T_{E,1000\text{ s}}} = 12.31\text{ K},$$

$$\sigma_{T_{E,1000\text{ s}}}/T_{E,1000\text{ s}} = 2.34\%;$$

$$(20) \sigma_{H_{50}} = 2.74\text{ cm}, \sigma_{H_{50}}/H_{50} = 11.2\%.$$

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小药量含能材料热安全性判据总标准偏差的分析

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摘要: 提出了描述小药量含能材料热安全性判据总标准偏差(σ)的20个表达式。报道了1,1'-二甲基-5,5'-偶氮四唑一水合物、3-硝基-1,2,4-三唑-5-酮、二(2,2,2-三硝基乙醇)缩甲醛和双基推进剂($56 \pm 1/27 \pm 0.5/8.5 \pm 0.15/2.5 \pm 0.1/5.0 \pm 0.15/1.0 \pm 0.1$ -NC/NG/DNT/甲基中定剂/催化剂/其它添加剂)热安全性判据的 σ 值和相对偏差值。

关键词: 物理化学; 热安全性; 判据; 总标准偏差; 含能材料

中图分类号: TJ55; O642

文献标识码: A

DOI: 10.3969/j.issn.1006-9941.2011.02.003