



Numerical Modeling of Self-Ignition of Energetic Materials

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Abstract: Thermal decomposition of energetic materials is accompanied by generation of heat, and under certain conditions may lead to the well-known phenomenon of the self-ignition (or thermal explosion). Therefore, it is of great concern of explosive community to predict whether or not a specimen of energetic material will ignite or not under given conditions (defined primarily by a specimen mass and shape, surrounding temperature, etc.). In order to describe the reactive heat conduction phenomena in an infinite slab, cylindrical, and spherical geometry of an explosive material, an own computer program, based on the thermal explosion theory and the finite difference method, was developed.

The program was tested by the comparison of calculated times to ignition for some standard high explosives with times to ignition determined experimentally, as well as with times to ignitions calculated by some other authors. The results of calculations were also compared with the results of calculation according to an analytical solution of the heat balance equation derived by Frank-Kamenetskii.

It was found out that not only values of the activation energy and pre-exponential factor, but also the kinetic model of thermal decomposition used in the calculation, have a crucial influence on the results of calculation. It was also shown that the Frank-Kamenetskii equation gives considerably lower values of the times to ignition, and higher values of the critical temperatures for explosives studied.

Keywords: energetic materials, self-ignition, thermal explosion, numerical modeling

Introduction

If specimen of an explosive material is heated, and if it decomposes with the rate given by the equation [1]:

$$\frac{d\alpha}{dt} = k_T f(\alpha) = eA^{(-E/RT)} f(\alpha) \quad , \quad (1)$$

where: α – conversion; t – time; da/dt – rate of conversion; k_T – temperature dependent rate constant, $f(\alpha)$ – function which represents the hypothetical model of the reaction mechanism (so-called reaction model); E – activation energy; A – pre-exponential factor, and R – universal gas constant, than the specimen heat balance can be described by the following equation [1, 2]:

$$\rho c \frac{\partial T}{\partial t} = \lambda \nabla^2 T + \rho Q A e^{(-E/RT)} f(\alpha) \quad , \quad (2)$$

where: T is temperature; c – specific heat capacity; ρ – density; λ – thermal conductivity; ∇^2 – Laplacian operator; Q – heat of decomposition.

The left-hand side of Eq. 2 gives the rate of the heat build-up in an explosive material specimen; the first term in the right side is the rate of heat loss into the surroundings; while the last right-hand term is the rate of heat generation due to exothermic reactions.

Since thermal ignition of explosive components in ammunition is always a problem of concern, the explosive community is permanently searching for an efficient method for solving reactive heat conduction problem in propellants and explosives. Since an analytical solution of the heat conduction equation with chemical reaction, the so-called reactive heat conduction is out of question; the approximate techniques and numerical methods are subjects of many investigations in this field.

Different simplifications of the Eq. 2 have been proposed in order to calculate the critical conditions of self-ignition. N. N. Semenov, for example, allowed the temperature to be uniform through a sample, and reaction to follow the zero-order kinetic law. He was than able to compare the heat generation and the heat loss

rates, and to derive the critical conditions of self-ignition [1, 3]. D. A. Frank-Kamanetskii tried to find steady state solution of Eq. 2 in the case of the zero-order kinetic law, but without assuming the temperature to be spatially uniform through a specimen [1, 3]. In this way he derived the critical conditions for thermal explosion in the following way [3]:

$$\frac{Q\rho}{4\lambda} \frac{E}{RT_e^2} d_c e^{-E/RT_e} = \delta_c \quad , \quad (3)$$

where: T_e is surrounding temperature, d_c characteristic dimension of the sample (thickness of the slab, or diameter of cylinder and sphere), δ_c is Frank-Kamanetskii parameter, or form factor ($\delta = 0.88$ for infinite slab, 2.00 for infinite cylinder, 3.32 for sphere, etc.).

According to the Frank-Kamanetskii solution of Eq. 2 equations for the calculation of the critical temperature (T_c), critical sample half-thickness (a_c), and time to ignition (t_c), are derived [4]. The time to ignition (t_c), *i.e.* time required for an exothermic reaction, in an adiabatic container, to reach the point of thermal ignition can be calculated by equation:

$$t_c = \frac{cRT_e^2 e^{E/RT_e}}{EAQ} \quad . \quad (4)$$

The critical half-thickness (a_c), *i.e.* half thickness of a sample in an unstirred container in which the heat losses to the environment are less than the retained heat:

$$a_c = \left[\frac{\delta\lambda RT_e^2 e^{E/RT_e}}{QAE\rho} \right]^{1/2} \quad . \quad (5)$$

The critical temperature (T_c), *i.e.* the lowest temperature of an unstirred container at which the heat losses to the environment are less than the retained heat leading to a build-up of internal temperature:

$$T_c = \left[\frac{R}{E} \ln \left(\frac{a_c^2 \rho QAE}{T_c^2 \delta \lambda R} \right) \right]^{-1} \quad . \quad (6)$$

To obtain time-dependent solution of the heat of equation different numerical techniques have to be applied. J. Zinn and C. Mader used numerical method based on a Fourier series spatial representation of solutions to obtain the ignition times for slabs, cylinders, and spheres of explosive material [2, 5]. A. Merzhanov and co-workers were the first that applied the finite difference method to solve the heat conduction equation with the zero-order kinetic reaction model. C. A. Anderson developed the finite difference code for one-dimensional heat conduction, based on zero-order kinetic model and the Crank-Nicolson method. This code treats the problems of layered media in slabs, cylindrical, or spherical geometry, and incorporates temperature dependent thermal properties and phase transitions [6].

Since thermal decomposition model plays a crucial role in each numerical method, some authors have tried to incorporate more complex kinetic model into computer codes based on the finite difference method. For example, J. Isler used the power law kinetic model to describe thermal ignition of a nitrocellulose propellant [1, 7]. R. McGuire and C. Tarver used 2-3 steps chemical decomposition models and incorporated them to a thermal conduction code based on the finite difference method, obtaining a good agreement with experimental results [8].

Numerical technique applied in the program

In the case of infinite long cylinders, infinite slabs, and sphere, the Laplacian operator (∇^2) in the general heat conduction equation (Eq. 2) reduces in one dimension [5]:

$$\nabla^2 = \lambda \left(\frac{\partial^2}{\partial r^2} + \frac{m}{r} \frac{\partial}{\partial r} \right) , \quad (7)$$

where r is radius of cylinder (or sphere). The integer m has a value 0 for slabs, 1 for cylinders, and 2 for spheres). In the case of an infinite slab r is replaced by slab thickness (x). Thus, for example, Eq. 2 for an infinitely long cylinder will have the form:

$$\rho c \frac{\partial T}{\partial t} = \lambda \left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} \right) + \rho Q A e^{(-E/RT)} f(\alpha) \quad (8)$$

Time dependent solution of Eq. 8 can be obtained by applying the finite difference method, *i.e.* by approximating partial derivatives with finite differences. The finite difference scheme of an infinitely long cylinder whose time-dependent temperature field we wish to compute from an initial temperature distribution, surrounding temperature, and boundary conditions may be represented by Figure 1.

The radius of an infinitely long cylinder (r_c) is divided into k cells, thickness of which is Δr ($\Delta r = r_c/k$). The initial temperature (at $t = 0$, *i.e.* $j = 0$, where j is time index) is specified at individual mesh points ($T_{0,i}^{j=0}$, $i = 0$ to $k-1$, where i is space index), while the temperature at the cylinder surface (T_s^j) is specified by the boundary conditions (Eqs. 16 and 17).

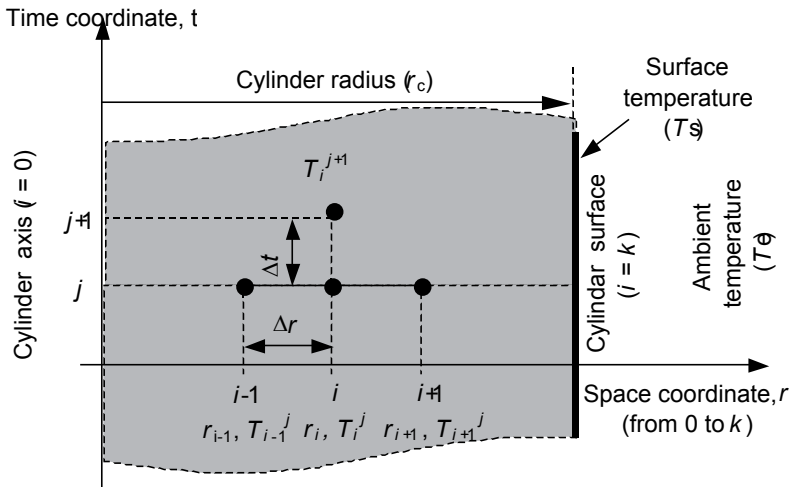


Figure 1. Finite difference scheme of an infinitely long cylinder.

For the case of an infinitely long cylinder the space derivatives in Eq. 8, in a time j , may be approximated by the following finite differences [6]:

$$\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} \right) = \left(\frac{T_{i+1}^j + T_{i-1}^j - 2T_i^j}{(\Delta r^2)} + \frac{1}{r} \frac{T_{i+1}^j - T_i^j}{\Delta r} \right) . \quad (9)$$

For the case of spheres and infinite slabs the space derivatives will be [6]:

$$\left(\frac{\partial^2 T}{\partial r^2} + \frac{2}{r} \frac{\partial T}{\partial r} \right) = \left(\frac{T_{i+1}^j + T_{i-1}^j - 2T_i^j}{(\Delta r^2)} + \frac{2}{r} \frac{T_{i+1}^j - T_i^j}{\Delta r} \right) , \quad (10)$$

$$\left(\frac{\partial^2 T}{\partial x^2} \right) = \left(\frac{T_{i+1}^j + T_{i-1}^j - 2T_i^j}{(\Delta x^2)} \right) . \quad (11)$$

The time derivative in Eq. 8 may be replaced by its simplest finite difference approximation [6]:

$$\left(\frac{\partial T}{\partial t} \right) = \frac{T_i^{j+1} - T_i^j}{\Delta t} , \quad (12)$$

where Δt is time increment.

By replacing the space and time derivatives in Eq. 8 by the finite differences (Eqs. 9-12), the equation for the calculation of temperature distribution along a space co-ordinate, at time t^{j+1} , can be derived. For example, in the case of a cylinder this equation will be:

$$T_i^{j+1} = T_i^j + \frac{\lambda(\Delta t)}{c\rho} \left(\frac{T_{i+1}^j + T_{i-1}^j - 2T_i^j}{(\Delta r^2)} + \frac{1}{r} \frac{T_{i+1}^j - T_i^j}{\Delta r} \right) + \frac{(\Delta t)}{c} Q A e^{(-E/RT)} f(\alpha) \quad (13)$$

It follows from the above equation that the temperature distribution along a cylinder radius at time t^{j+1} is evaluated from temperature distribution at earlier time (t^j), where:

$$t^{j+1} = t^j + \Delta t . \quad (14)$$

By an analogous way the equations for the calculation of temperature

distribution along a sphere radius or a slab thickness can be obtained from Eqs. 10, 11, 12, and 8.

In additions to the finite difference approximation to the reactive heat conduction equation, the approximations to the initial and boundary conditions should be included in order to calculate time-temperature distribution along a specimen space co-ordinate.

The initial conditions give an initial temperature distribution (at $t = 0$) along a specimen radius. In the most usual way the initial conditions are given in the form:

$$T_i^{j=0} = T_{0,i}^{j=0} \text{ where } i = 0, 1, 2, 3, \dots, k-1 \quad . \quad (15)$$

The boundary conditions give the temperature at a specimen surface at any time (T_s^j). The simplest case is when the specimen surface temperature remains constant during the whole process. In this case the boundary conditions can be written in the form:

$$T_s^j = T_e = \text{const.} \quad , \quad (16)$$

where T_e is surrounding temperature. However, in the case of convective heat transfer from an ambient fluid to a specimen surface, the boundary conditions are given by the following equation [6, 7]:

$$\varepsilon(T_s - T_e) = -\lambda \frac{T_s - T_{k-1}}{\Delta r} \quad , \quad (17)$$

where ε is the heat transfer coefficient.

Results and discussion

Applying the numerical technique described above, the computer program named THERMEX was written. The accuracy and applicability of the program is tested in several ways: a) influence of time and space

increments on the results of calculation; b) comparison of the results of calculation with the results of calculation by similar computer programs, and c) influence of kinetic model on the results of calculation.

Since an explicate finite difference solution to the differential equations is often conditionally stable, the correct choice of space and time increments is of crucial importance to obtain accurate solutions. Because of that, a detailed analysis of influence of time and space increments on the results of calculation was carried out and reported in previous paper [9]. The analysis has shown that the time increment which enables the times to ignition to be calculated with a sufficiently small error, may be chosen on the basis of the stability criterion given by the equation [6]:

$$\frac{\lambda}{\rho c} \cdot \frac{\Delta t}{(\Delta r)^2} < f_s \quad . \quad (18)$$

The results have shown that, in order to obtain ignition times which differ less than 1% in the respect to ignition times obtained by the extrapolation to $\Delta t \rightarrow 0$, the value of f_s should be less than 0.01. On the other hand, the space increment has to be also very small – from some tenth of microns to some hundreds of microns, depending on the surrounding temperature and sample size.

In order to compare results of calculation obtained by THERMEX with results obtained by similar computer codes, hexogen (RDX) sphere 25.4 mm in diameter was used as a test model. The sphere, being initially at the temperature of 25 °C, was subjected instantaneously to the surrounding temperatures higher than the critical ones – in the 180-260 °C range. The same test model was used by J. Zinn and C. Mader [2, 5], and by C. Anderson [6] to study numerically the thermal ignition phenomena of RDX. The times to ignitions calculated by THERMEX and similar computer codes, as well as by the Frank-Kamenetskii equation (Eq. 4) are given in Table 1.

Table 1. Times to ignition for RDX spheres 25.4 mm in diameter calculated by different authors and different methods

Surrounding temperature [°C]	Time to ignition [s]				
	J. Zinn and C. Mader [2, 5]	C. Anderson (code TE-PLO) [6]	C. Anderson (code TE-PLO) [6]*	This work (code THER-MEX)	Calculated by Frank-Kamenetskii equation
180	1000	1030	1200	1051.8	236.3
200	420	458	593	466.9	27.6
220	120	162	183	166.1	3.9
240	33	42.9	43.8	44.0	0.6
260	10.5	10.1	10.0	10.3	0.1

* Time to ignition is calculated taking temperature-dependent heat capacity and taking into account melting of RDX.

The values of the kinetic and thermal parameters of RDX used in the calculations were: $\rho = 1.8 \text{ g/cm}^3$; $Q = 2093 \text{ J/g}$; $E = 199 \text{ kJ/mol}$; $A = 3.16 \cdot 10^{18} \text{ 1/s}$; $c = 2.093 \text{ J/g K}$, and $\lambda = 0.293 \text{ W/m K}$ [2, 6].

It is evident from Table 1 that the agreement between the times to ignition calculated by THERMEX and by similar computer programs (*e.g.* TEPLO) is very good. At the same time, the times to ignition calculated by the Frank-Kamenetskii equation are for order of magnitude lower in all cases.

The times to ignition are also calculated for a 25.4 mm diameter RDX cylinder, and compared with the experimentally obtained values. The results of the comparison are shown in Figure 2. A reasonable good agreement was found between the experimentally obtained and calculated ignition times, as well as between the results of calculation in this work and those obtained by J. Zinn and C. Mader [2].

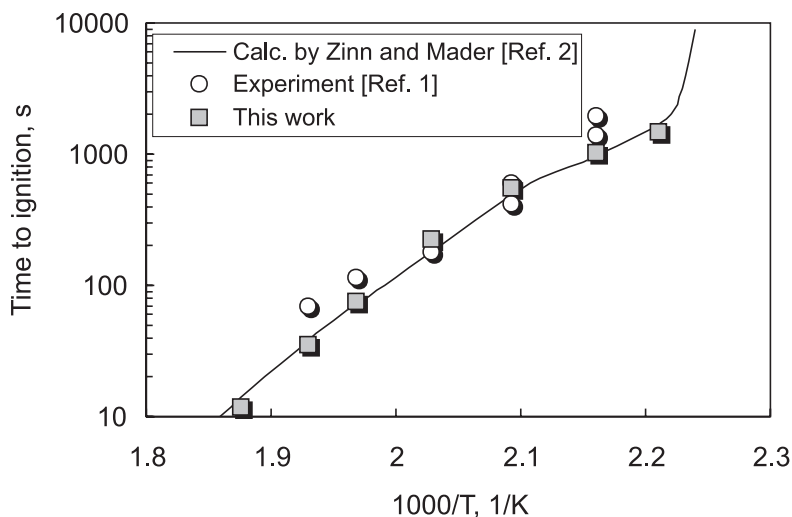


Figure 2. Comparison of experimentally obtained and calculated times to ignition for an RDX cylinder 25.4 mm in diameter.

An analysis given in Table 2 has shown that the critical temperatures for some standard high explosives calculated by the Frank-Kamenetskii equation (Eq. 6) are up to 20% higher in respect to the critical temperatures determined experimentally [5]. At the same time THERMEX gives values that differ less than 10% from the experimental ones, except in the case of NQ for which the difference is 13%.

Table 2. Comparison of calculated and experimental critical temperatures for some standard high explosives

Explosive	a_c mm	T_c (Experim. [5]) °C	T_c (THER- MEX) °C	T_c (Frank- Kamenetskii Eq.) °C	ρ g/cm ³	Q J/g	E kJ/mol	A 1/s	λ W/ m K
HMX	0.33	253-255	254	269	1.81	2093	221	$5.0 \cdot 10^{19}$	0.29
RDX	0.35	215-217	224	231	1.72	2093	197	$2.0 \cdot 10^{18}$	0.10
TNT	0.38	287-289	306	319	1.57	1256	144	$2.5 \cdot 10^{11}$	0.21
PETN	0.34	200-203	198	210	1.74	1256	197	$6.3 \cdot 10^{19}$	0.25
NQ	0.39	200-204	227	242	1.63	2093	88	$2.8 \cdot 10^7$	0.21
HNS	0.37	320-321	342	352	1.65	2093	127	$1.5 \cdot 10^9$	0.21

The critical temperatures are calculated by THERMEX in convenient way – from the plot of logarithms of the calculated times to ignition *vs* the reciprocal surrounding temperature (Figure 3). These plots are linear over quite a large region but bend upward sharply near the critical temperature. At the critical temperature the plot becomes vertical, indicating an infinitely long induction period.

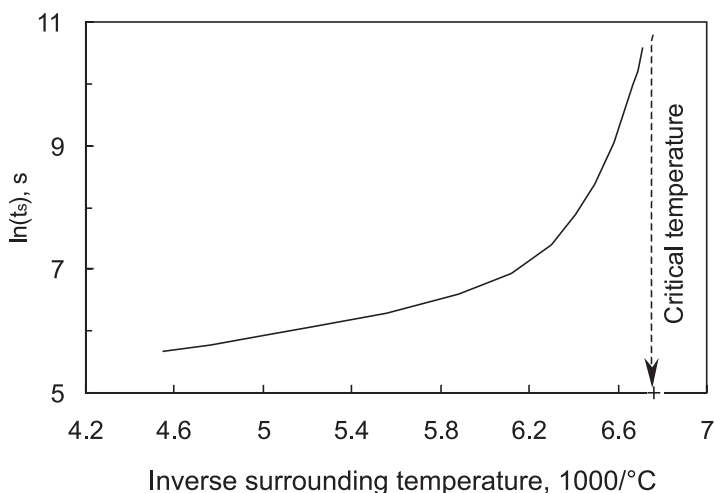


Figure 3. Determination of critical temperature.

Space- and time-temperature profiles

Although the time to ignition and the critical temperature are the essential parameters for the prediction of self-ignition possibility of an explosive specimen, it was also interesting to have details of the heat flow, *i.e.* to have the temperature-time profile at a given position within a specimen, and the temperature-radius profile at a given time.

It is known that the time to ignition decreases with the surrounding temperature increase (Table 1), as well as that the ignition of the specimen occurs at a position closer to the specimen surface with the increase of the surrounding temperature. The last is visible in Figures 4 and 5, which shows calculated spatial distribution of the temperature at different times

for RDX spheres subjected to different surrounding temperatures (180 and 190 °C).

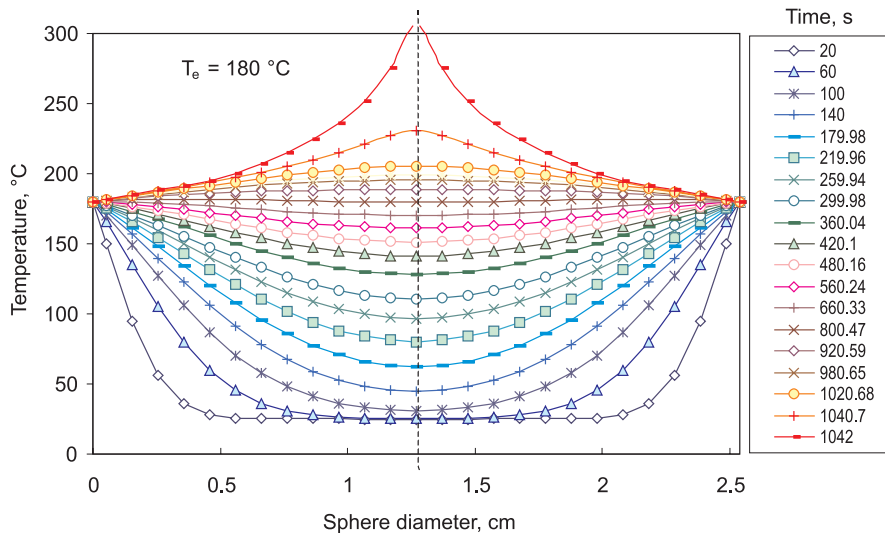


Figure 4. Calculated temperature-diameter profiles at different times for RDX sphere 25.4 mm in diameter subjected to 180 °C (sphere initial temperature is 25 °C; boundary conditions according to Eq. 16).

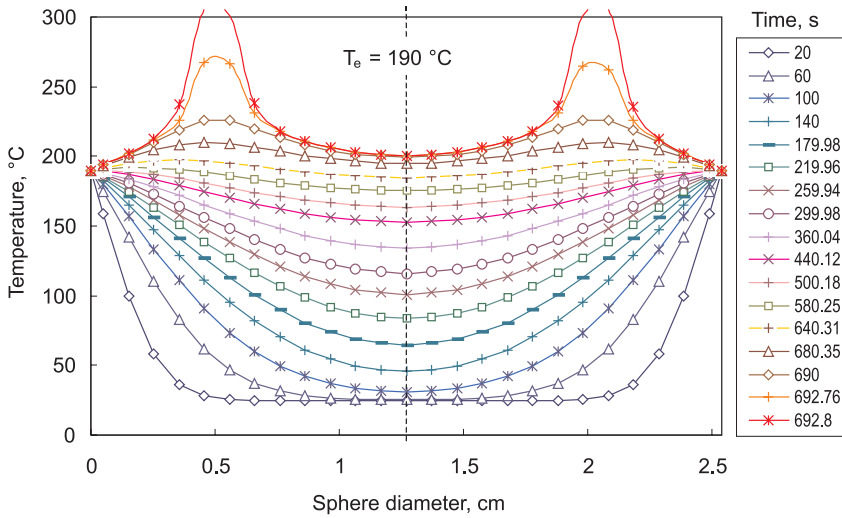


Figure 5. Calculated temperature-diameter profiles at different times for RDX sphere 25.4 mm in diameter subjected to 190 °C (sphere initial temperature is 25 °C; boundary conditions according to Eq. 16).

For low surrounding temperatures, *e.g.* 180 °C, the ignition occurs at the centre of sphere. At the same time the surface of the sphere remains at the surrounding temperature. For 190 °C surrounding temperatures the ignition occurs at the position between sphere centre and surface ($r/r_s \approx 0.85$). For the surrounding temperature higher than 190 °C the ignition will occur at the position near cylinder surface, while at the same time in this case the centre of sphere will remain relatively cool during the whole induction period.

The above mentioned is also visible in Figure 6, showing the time-temperature distribution at several locations within the RDX sphere subjected to 190 °C surrounding temperature. At the location $r/r_s \approx 0.96$ (near sphere surface) the temperature increases quickly, while at the centre of sphere the temperature reaches the same value only at the end of the induction period.

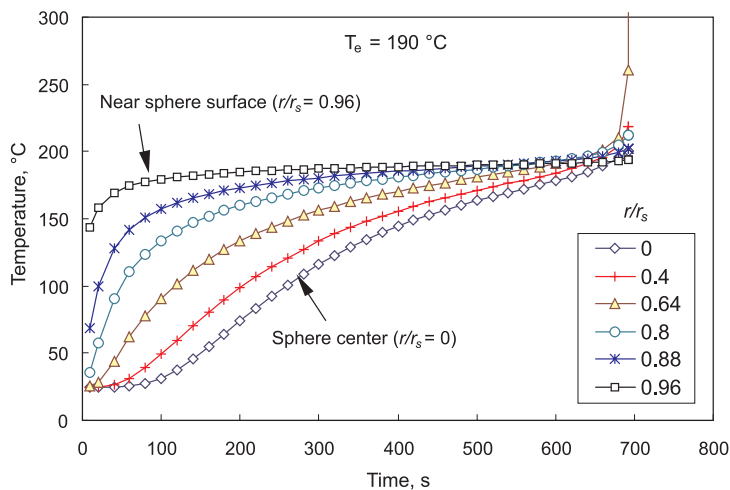


Figure 6. Calculated temperature-time profiles at different locations inside a 25.4 mm diameter sphere of RDX subjected to the 190 °C surrounding temperature.

Influence of kinetic model on the results of calculation

In order to test influence of kinetic model on the results of calculations, the thermal decomposition and the self-ignition data obtained experimentally by J. Isler and D. Kayser are used in the paper [1]. The authors have carried out the thermal decomposition experiments in air by both manual (130-150 °C) and by thermogravimetry technique (150-170 °C), using nitrocellulose (NC) propellant samples being ~5 mg in mass.

The self-ignitions experiments the authors have performed with cylindrical samples of NC propellant having 7 mm in diameter, 26 mm in length, and 1.3 g in mass. The central temperature of samples was measured by 0.5 mm wide thermocouple inserted into a hole made along the cylinder axis.

On the basis of the thermal decomposition experiments they have obtained degree of conversion-time dependency given in Figure 7. It is evident from Figure 7 that all $\alpha-t$ curves are of sigmoid shape, with the inflexion at about 0.25 conversion (25% decomposition). That means

that the rate of conversion (Figure 8), and consequently the rate of heat generation, increase up to this point, and decreases gradually above it.

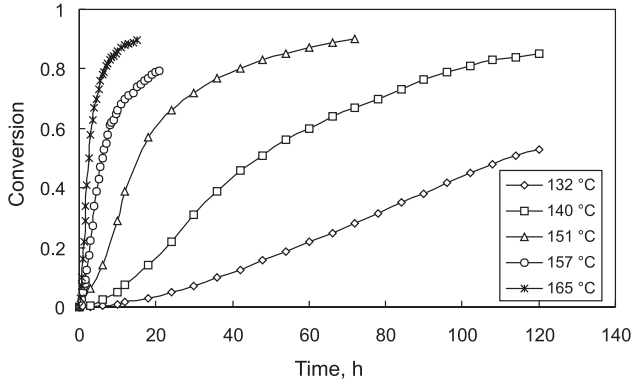


Figure 7. NC propellant conversion as a function of time at different environmental temperatures.

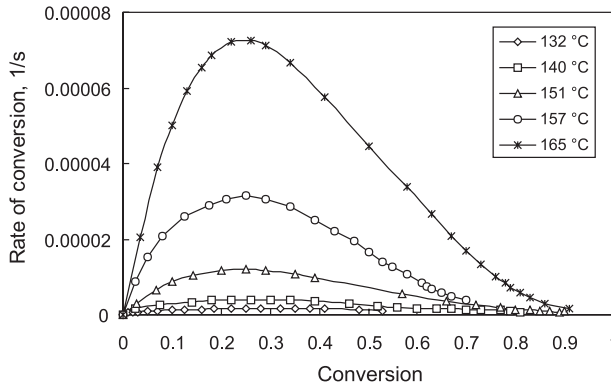


Figure 8. Dependence of rate of NC propellant conversion on degree of conversion for several different environmental temperatures.

The shape of $(d\alpha / dt) = f(\alpha)$ dependency shown in Figure 8 is typical for autocatalytic reactions and may be described mathematically by the equation:

$$\frac{d\alpha}{dt} = k_T f(\alpha) = k_T \alpha^n (1 - \alpha)^m \quad (19)$$

Since the rate of heat generation decreases above 0.25 conversions it is reasonable to suppose that the self-ignition of NC propellant may occur only below that conversion. This means that, in order to study the self-ignition phenomena, the kinetic study may be limited to the early stage of NC propellant decomposition: $0 < \alpha < 0.25$. It was shown in the previous paper [10] that for conversions lying between 0 and 0.25, the power law kinetic model (Eq. 20) fits the best experimental $(d\alpha/dt) = f(\alpha)$ dependency:

$$\frac{d\alpha}{dt} = k_T f(\alpha) = k_T \alpha^n \quad (20)$$

Because of its simplicity (since $f(\alpha) = 1$) the zero-order kinetic model is often used to describe the thermal decomposition of energetic materials. One note from Figure 7 that $\alpha-t$ dependency is almost linear for conversions up to 0.10. That means that the zero-order kinetic model (Eq. 21) may be used to describe (roughly) early stage of NC propellant decomposition.

$$\alpha = k_T t, \text{ or in differential form: } \frac{d\alpha}{dt} = k_T f(\alpha) = k_T \quad (21)$$

By the non-linear curve fitting procedure of experimentally obtained data in accordance with the above mentioned given kinetic models, the rate constants (k_T in Eq. 19-21) are evaluated for each temperature. The activation energy and the pre-exponential factor are then calculated from $\ln k_T - 1/T$ dependency, according to the Arrhenius equation [10]. The values of kinetic parameters obtained in this way are given in Table 3.

Table 3. Values of kinetic parameters derived applying different kinetic models

Kinetic model	Differential kinetic equation	Function $f(\alpha)$	Values of kinetic parameters
Zero order ($0 < \alpha < 0.10$)	$\alpha = k_T \alpha$	$f(\alpha) = 1$	$E = 189.14$ kJ/mol; $A = 1.40 \times 10^{18}$ 1/s
Power law ($0 < \alpha < 0.25$)	$\frac{d\alpha}{dt} = k_T \alpha^n$	$f(\alpha) = \alpha^n$	$E = 182.20$ kJ/mol; $A = 4.20 \times 10^{17}$ 1/s $n = 0.29$
Autocatalytic ($0 < \alpha < 0.95$)	$\frac{d\alpha}{dt} = k_T \alpha^n (1 - \alpha)^m$	$f(\alpha) = \alpha^n (1 - \alpha)^m$	$E = 170.60$ kJ/mol; $A = 7.57 \times 10^{16}$ 1/s $n = 0.67$; $m = 2.27$

Using the above mentioned kinetic models and the values of kinetic parameters given in Table 3, the self-ignition calculations for cylindrical NC propellant specimen 7 mm in diameter was carried out. The following values of thermokinetic parameters of NC propellant are used in the calculations:

- specific heat capacity (c) = 1.254 J/g K
- heat of decomposition (Q) = 3970 kJ/kg
- thermal conductivity (λ) = 0.16 W/m K
- heat transfer coefficient (ε) = 0.22 W/m² K
- density (ρ) = 1.6 g/cm³

The influence of kinetic model on the calculated times to ignition for tested NC propellant subjected to 156 °C environmental temperature is illustrated in Figure 9. The results show that the influence of kinetic model on the calculated values of times to ignition is very pronounced – difference is almost 6 times. At the same time the results show that power law kinetic model gives the best agreement between experimentally obtained and calculated times to ignitions for 156 °C surrounding temperature.

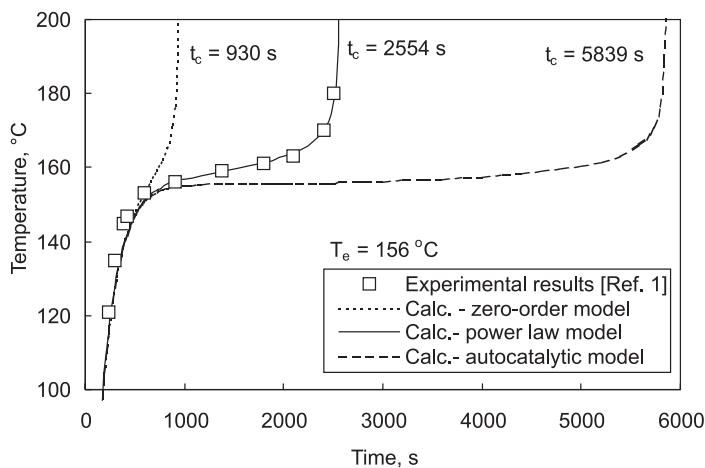


Figure 9. Times to ignition of cylindrical NC propellant specimen 7 mm in diameter at 156 °C surrounding temperature calculated using different kinetic models.

Conclusions

The presented numerical model for the studying self-ignition phenomena of explosives, based on the finite difference method, can be used to predict the time to ignition, the critical temperature, as well as to obtain temperature-time, and temperature-space co-ordinate profiles of an explosive material specimen.

However, because of complexity of the self-ignition phenomena, a number of parameters may affect results of calculation; *e.g.* values of space and time increments, boundary conditions, kinetic model used in the calculations, thermochemical and thermokinetic constants of an energetic material (heat capacity, heat of decomposition, heat conductivity, heat transfer coefficient etc.).

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