Determination of SADT and Cook-off Ignition Temperature by Advanced Kinetic Elaboration of DSC Data

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ABSTRACT

The exothermic decomposition parameters of a single-base propellant were obtained using differential scanning calorimeter (DSC) tests conducted at various heating rates. The DSC signals were processed using the Friedman isoconversional method to compute activation energy as a function of conversion. There was excellent agreement between the experimental and the simulation plots, which confirms the validity of the kinetic model used to describe the propellant's exothermic decomposition. The kinetic parameters and heat balance were subsequently analyzed and used for a simulation of cook-off experiments conducted at different experimental rates (heating rates 3.3 - 1.0 K/h and a heat-wait-search mode). This study presents a simulation of the propellant's adiabatic behaviour Time to Maximum Rate (TMR) under adiabatic conditions (TMRad) and self-accelerating decomposition temperature (SADT). This study also illustrates and discusses the effect of a material's thermal conductivity on the time to ignition at various heating modes.

INTRODUCTION

The method of the prediction of the thermal behaviour of the energetic materials such as temperature and time to the ignition during cook-off experiments or simulation of SADT strongly depends on the sample mass due to the significant influence of the heat generated during the reaction course. At the mg-scale, all the evolved heat dissipates to the surroundings and does not affect the temperature of the heated material. Whereas at the ton-scale, the system can be considered adiabatic, because almost all generated heat remains in the sample and there is the potential for a thermal runaway decomposition. From a practical perspective for the kg-scale, the temperature change of the test material results from two different processes that together determine the heat balance, which is defined by the heat generated during the thermal decomposition and heat loss to the environment. The rate of heat generated during an exothermic decomposition increases exponentially as the temperature rises but the rate of the heat loss occurs in a linear manner. Therefore, in order to properly predict the thermal decomposition behaviour of an energetic material, there must be a precise understanding of the kinetic parameters because their knowledge is the prerequisite for the correct description of the heat generation rate and heat balance of the system.

There are two critical factors which have to be considered during the simulations:

(i) The intrinsic properties of the test material, i.e., the kinetic parameters of the decomposition (activation energy, pre-exponential factor in the Arrhenius equation) and the physical-chemical properties such as the thermal conductivity, specific heat and density which cannot be changed.

(ii) The external properties of the sample, i.e., the sample mass, the geometry of the sample holder, container or the reactor, and, finally, the heating mode applied during the experiment or simulation (slow or fast cook-off, heat-wait-search mode, isothermal or adiabatic run) which can be changed arbitrarily.

It is known that changes to the external properties or experimental conditions can significantly influence the course of the decomposition process. For example it was reported that the change of the heating rate during cook-off experiment changes the location of the ignition point in the sample. By increasing the heating rate the decomposition moves from the inner to outer shell of the material (1, 2). It is also known (3) that accurate simulation of time/temperature of cook-off for low temperatures and slow heating rates are more difficult than for higher temperatures and heating rates. One of the main factors responsible for these complications is the thermal conductivity of the material.

The objective of this paper was to determine how the simulation of the cook-off parameters (time and temperature of the ignition) can be influenced by the thermal conductivity (λ) of the sample for the heating mode applied. Preliminary experiments show that lowering the heating rate has more of an impact of the λ on the cook-off ignition time. Therefore additional simulations were performed to determine the influence of λ during boundary conditions when the heating rate is = 0, i.e., under the isothermal conditions required for the simulation of SADT. Finally, the simulations of the material properties under adiabatic conditions (Time to Maximum Rate, TMRad) were performed.

EXPERIMENTAL

The present study contains the experimental results and simulations of the properties of the single-base propellant. The kinetic parameters required for the simulation were calculated from the DSC traces applying AKTS-Thermokinetics Software (4). The DSC experiments were carried out in sealed crucibles (5) from room temperature till 260°C with various heating rates. The cook-off experiments were carried out in cylindrical steel tube with: ID 47 mm, length 200 mm, wall thickness 4 mm and the volume of 0.35L (armasuisse in-house construction) equipped with three thermo elements. Three temperature modes were chosen for experiments and simulations:

- hold temperature 40°C, hold time 7h followed by the temperature ramp of 3.3 K/h according to STANAG 4383,

- hold temperature 100°C, hold time 9h followed by the 1 K/h temperature ramp,

- heat-wait-search mode (H-W-S) similar to those applied in Accelerating Rate Calorimetry. In this mode the sample was heated to the pre-selected initial temperature 109°C, slightly lower than the ignition temperature recorded during the slower cook-off (1K/h) experiment, and held a period of time (1.8 days) to achieve thermal equilibrium. A search was than conducted to measure the rate of heat gain (self-heating) of the sample. If the rate of self heating was so slow that the temperature of the sample stayed constant, the temperature was increased by 4K and the heat-wait-search sequence was repeated. This routine was continued until the significant temperature jump was observed.

The experimental setup is presented in Figure 1. Figure 2 shows the damaged tubes after cook-off experiments, the fragment size and number give the qualitative information on the violence level.
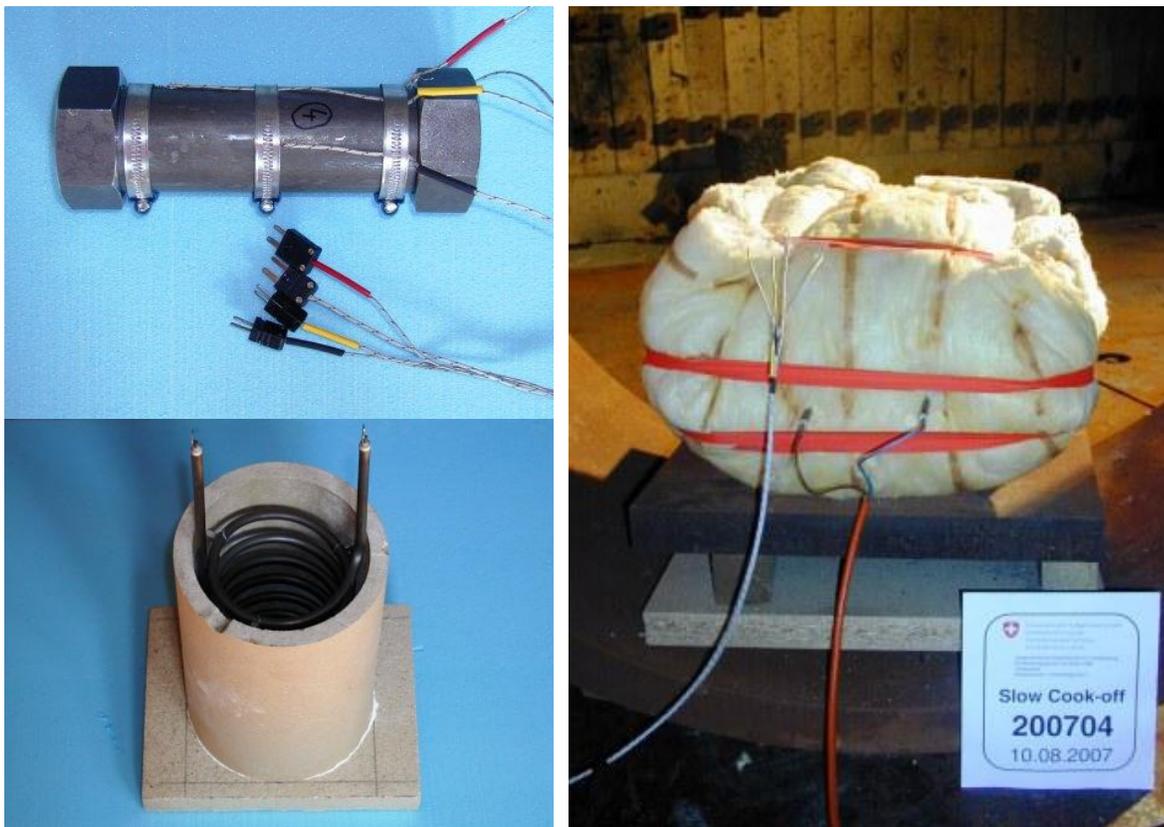
Fig. 1 Experimental setup of the cook-off experiment

Fig. 2 Cook-off steel tubes after the experiments carried out with three temperature modes described above. From left to right: temperature ramp 3.3 K/h, temperature ramp 1.0 K/h and heat-wait-search mode.

EVALUATION OF THE DECOMPOSITION KINETICS

The evaluation of the kinetics of the decomposition of energetic materials is one of the main prerequisites necessary for the correct modelling of their properties. Generally, the kinetic parameters are calculated from the experimental data obtained by means of thermoanalyzers or calorimeters such as e.g. TG, DTA or DSC signals. In DSC, the most commonly applied thermal analysis technique for examining energetic materials, the determination of the kinetic parameters from the recorded signal requires its integration in order to obtain the α-time or -temperature relationship necessary for kinetic calculations. The course of the baseline can significantly influence the determination of the heat of the reaction and the estimation of the α-T dependence. The very important feature of the AKTS-Thermokinetics Software (4) is the possibility of the optimization of the baseline for all experiments collected by different heating rates (or temperatures) so that the random errors in the various baseline constructions for all heating rates will "average themselves out".

If the decomposition follows a single kinetic model then the reaction can be described in terms of a single pair of Arrhenius parameters and the commonly used set of functions $f(\alpha)$ reflecting the mechanism of the process. In such a case the dependence of the logarithm of the reaction rate over $1/T$ is linear with the constant slope $m = E/R$ in full range of conversion degree α. The reaction rate can be described by only one value of the activation energy E and one value of the pre-exponential factor A by the following expression:

$$\frac{d\alpha}{dt} = A \, exp\left(-\frac{E}{RT(t)}\right) f(\alpha) \tag{1}$$

where t is time, T - temperature, R- the gas constant, E - the activation energy, A- the pre-exponential factor, α is the fraction converted and $f(\alpha)$ is a differential form of the conversion function depending on the reaction model.

However, the decomposition reactions are generally too complex to be described in terms of a single pair of Arrhenius parameters (A and E) and the commonly applied set of reaction models $f(\alpha)$. In general, decomposition reactions demonstrate profound multi-step characteristics. The assumption that the decomposition of an energetic material will obey a simple rate law is very rarely true. Moreover, the determination of the kinetic parameters from the single run recorded with one heating rate only (so called 'single curve' method) leads to erroneous results and according to the recent recommendations should not be applied anymore (6,7).

In the present paper the kinetic parameters have been calculated by the isoconversional method of Friedman (8) based on the calculation of E and A values at different degrees of conversion α without assuming the form of $f(\alpha)$ function, i.e. applying logarithmic form of the following reaction rate expression :

$$\frac{d\alpha}{dt}_{\alpha} = \{A_{\alpha} \, f(\alpha)\} \, exp\left(-\frac{E_{\alpha}}{RT(t_{\alpha})}\right) \tag{2}$$

according to Friedman we obtain

$$ln\left(\frac{d\alpha}{dt}_{\alpha}\right) = ln\{A_{\alpha}f(\alpha)\} - \frac{E_{\alpha}}{R}\frac{1}{T_{\alpha}} \tag{3}$$

where t_{α}, T_{α}, E_{α} and A_{α} are the time, temperature, apparent activation energy and preexponential factor, at conversion α, respectively, and $-E_{\alpha}/R$ and $ln\{A_{\alpha}f(\alpha)\}$ are the slope and the intercept with the vertical axis of the plot of $ln(d\alpha/dt_{\alpha})$ vs. $1/T_{\alpha}$.

It is then possible to the make kinetic predictions at any temperature profile $T(t)$, from the values of E_{α} and $\{A_{\alpha}f(\alpha)\}$ extracted directly from the Friedman method by the separation of the terms followed by integration:

$$t_\alpha = \int_0^{t_\alpha} dt = \int_0^\alpha \frac{d\alpha}{\{A_\alpha f(\alpha)\} e^{-\frac{E_\alpha}{RT_\alpha}}} \tag{4}$$

The results of the determination of the kinetic parameters of the decomposition process of the single-base propellant are presented in Figure 3 containing the Friedman analysis applied for four heating rates (A), the dependence of activation energy (left axis) and pre-exponential factor (right axis) on the reaction progress α (B) and the plot depicting the simulation of the experimental DSC signals by means of the determined kinetic parameters E_α and $\{A_\alpha f(\alpha)\}$ (C).
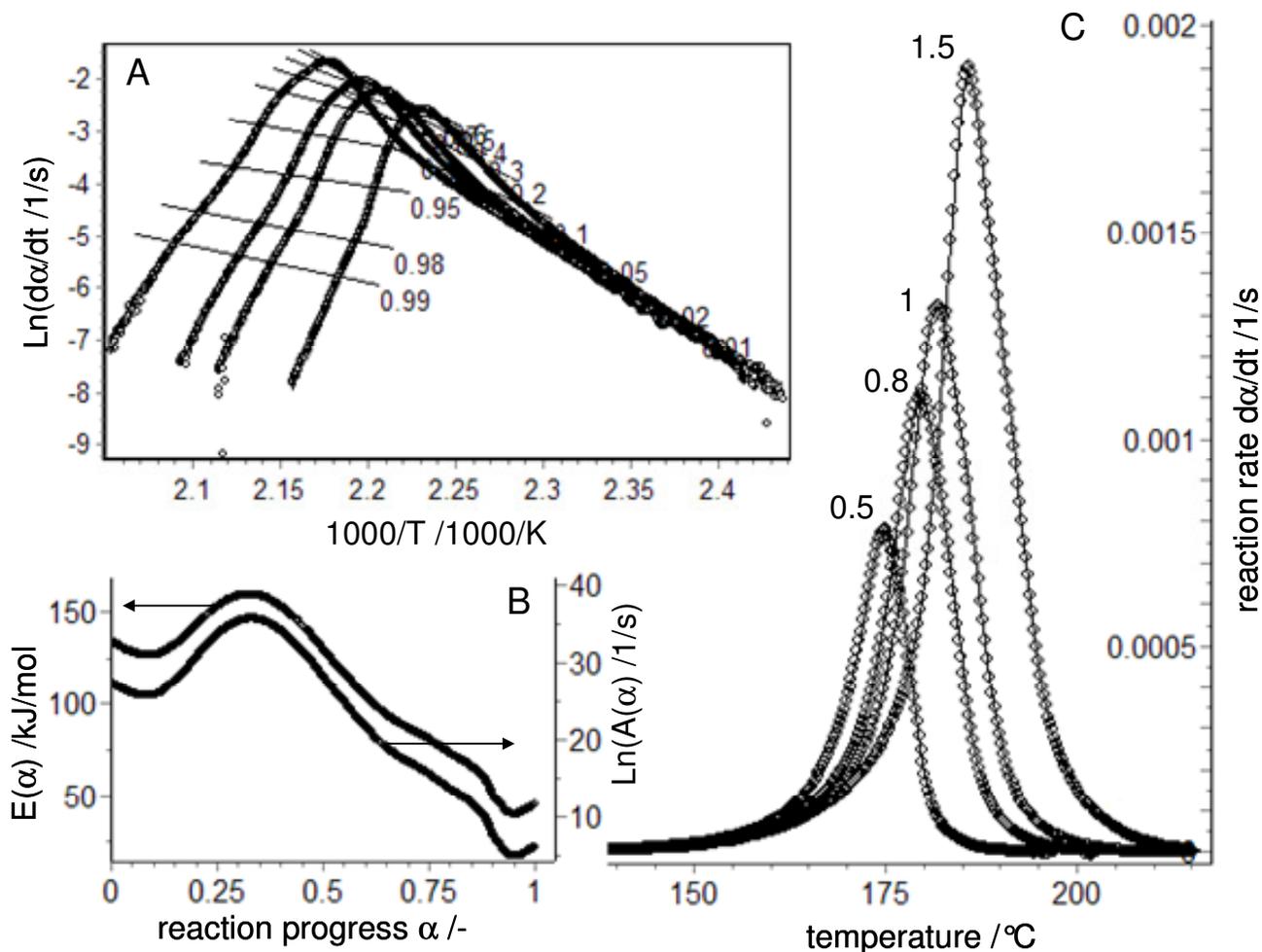

Fig. 3 Results of the kinetic analysis of the propellant decomposition.
(A) Friedman analysis based on the DSC signals recorded with four heating rates, (B) Activation energy E and the pre-exponential factor A as a function of the reaction progress, (C) Comparison of the experimental (symbols) and simulated (lines) DSC signals. The kinetic parameters depicted in fig. (B) were used during the simulation. The values of the heating rates in K/min are marked on the curves.

There was excellent correlation between the experimental data and the simulated plots using our advanced kinetic modelling approach. It can be shown that a much weaker correlation is observed if one used a very simple kinetic model (e.g., "zero" or "first" order for the decomposition reaction) (9). The weak correlation occurs because of the assumption that the reaction mechanism and values of E and A are assumed to be constant during the course of the decomposition.

HEAT BALANCE

To carry out an accurate heat balance, numerical techniques such as finite element analysis or finite differences or volumes can be used. This simulation requires the solution of partial differential equations as they are encountered in the heat conduction problem, especially when analyzing the heat accumulation conditions. The sample data is virtually divided into a set of adjoining elements (see Fig. 4). These elements are organized in a virtual matrix and described by advanced thermokinetics that is based on the Friedman analysis of each node of the time and space. This procedure enables the calculation of the heat transfer and temperature profiles at any time and any point in the space of investigated energetic material. In fact, if we consider 1 kg of substance compared with 1 mg of substance measured with the DSC, the approach is 'like' performing 1 million DSC measurements at the same time and interrelating them using the thermal conductivity of the examined substance and applying the correct boundary conditions.
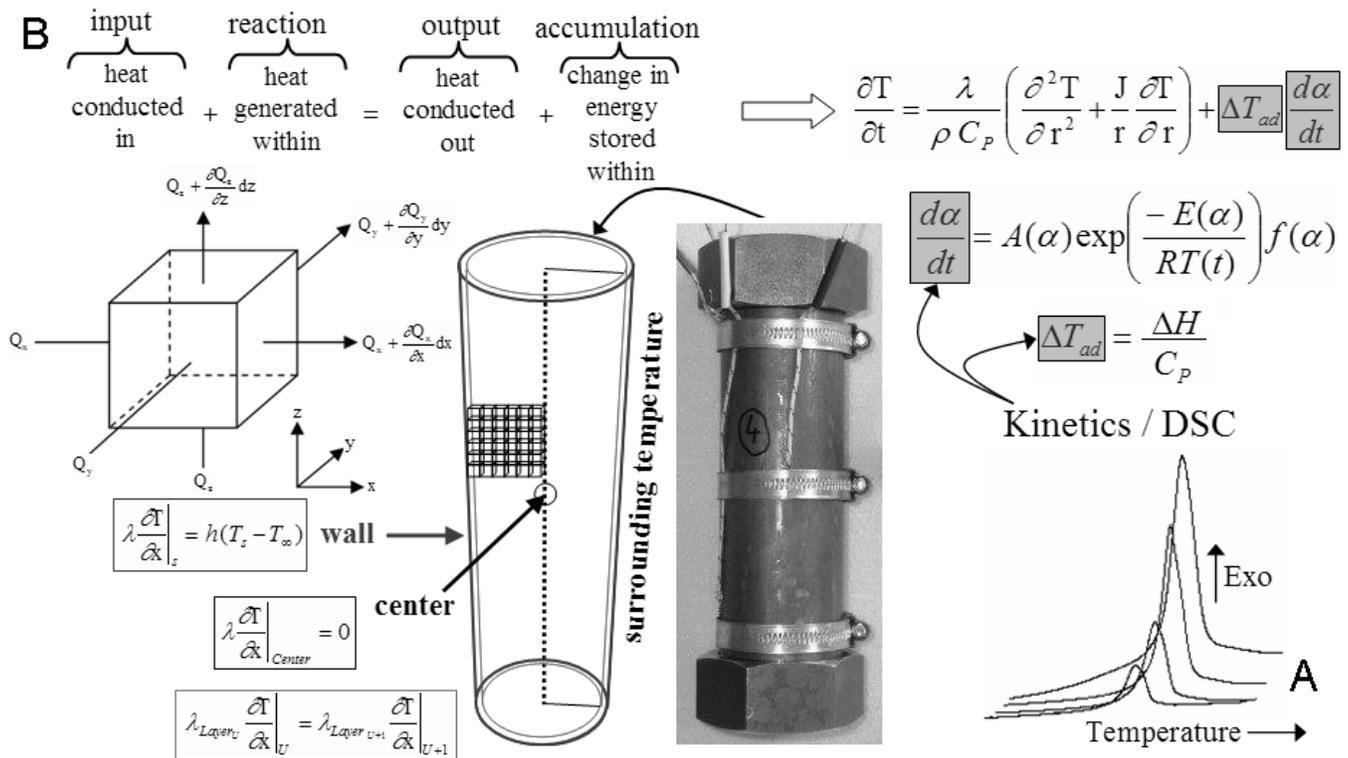

Fig. 4 Generalized heat balance over a container and a volume element.
(A) Kinetic parameters calculated from the DSC measurements enable the determination of the reaction rate required for the heat balance. (B) Heat balance, depending on the sample mass, must be calculated using numerical techniques.

When heat is transferred to the surrounding environment, the temperature profile within a body depends upon the rate of heat generation, its capacity to store part of this heat, and the rate of heat conduction to its boundaries. This can be described mathematically, using Fourier's law of heat conduction, which we can derive from the heat equation:

$$\frac{\partial T}{\partial t} = \frac{\lambda}{\rho C_P} \nabla^2 T + \frac{1}{\rho C_P} q_r \tag{5}$$

where λ, ρ, C_P, T, q_r mean: thermal conductivity, density, specific heat, temperature and the power generated per unit volume by the decomposition reaction, respectively. With

$$q_r = \rho \, \Delta H_r \, \frac{d\alpha}{dt} \tag{6}$$

after considering cylindrical coordinates and additional simplifications,

$$\frac{\partial T}{\partial r} \gg \frac{\partial T}{\partial z} \Rightarrow \frac{\partial^2 T}{\partial r^2} \gg \frac{\partial^2 T}{\partial z^2} \tag{7}$$

one can write

$$\frac{\partial T}{\partial t} = \frac{\lambda}{\rho \, C_P} \left(\frac{\partial^2 T}{\partial r^2} + \frac{J}{r} \frac{\partial T}{\partial r} \right) + \Delta T_{ad} \frac{d\alpha}{dt} \tag{8}$$

where: J is a geometry factor dependent on the type of the container: $J=0$ for the infinite plate, $J=1$ for the infinite cylinder and $J=2$ for the sphere, $d\alpha/dt$ is the rate of the decomposition reaction expressed by the Arrhenius type equation as those applied in Friedman analysis (eq.2) and ΔT_{ad} is the adiabatic temperature rise expressed by the heat release ΔH and the specific heat C_P : $\Delta T_{ad} = \Delta H/C_P$.

ADIABATIC CONDITIONS: PREDICTION OF THE THERMAL BEHAVIOUR (TMR$_{ad}$)
Under adiabatic conditions, all the heat generated during the decomposition reaction is accumulated in the system. Initially the reaction rate may be low but increases rapidly resulting in an increase in the sample temperature, which can eventually lead to a thermal runaway reaction condition. The main parameters used to characterize the adiabatic process are: the adiabatic temperature rise ΔT_{ad}; time to maximum rate TMR_{ad}; and maximum self-heat rate $Max\ SHR$. Heat balance over the sample inside the vessel may be expressed by the equation:

$$M_s C_{p,s} \frac{dT_s}{dt} + M_c C_{p,c} \frac{dT_c}{dt} + M_x C_{p,x} \frac{dT_x}{dt} = UA(T_{env} - T_c) + M_s \Delta H \frac{d\alpha}{dt} \tag{9}$$

with M: mass, Cp: specific heat, T: temperature, U: heat transfer coefficient, A: contact surface between the sample and the container, ΔH : total heat release, indices c, s, x and env: container (or bomb in the adiabatic calorimeter experiment), sample, solvent (in the case of the presence of the liquid phase) and environment, respectively. In a fully operational adiabatic environment all the heat release goes to the sample and the container (this is the case when $T_{env} = T_c$ or $U = 0$). If there is thermal equilibrium within the sample and the container then the whole system will have the same temperature rise and we can simplify equation (9) to

$$\frac{dT}{dt} = \frac{1}{\Phi} \Delta T_{ad,real} \frac{d\alpha}{dt} \tag{10}$$

with:

- the adiabatic temperature rise: $\Delta T_{ad,real} = \dfrac{\Delta H}{C_{p,s}}$ \hfill (11)

- the thermal inertia factor: $\Phi = \dfrac{M_c C_{p,c} + M_s C_{p,s} + M_x C_{p,x}}{M_s C_{p,s}}$ (12)

- the: reaction rate $\dfrac{d\alpha}{dt}_\alpha = \{A_\alpha\, f(\alpha)\} exp\left(-\dfrac{E_\alpha}{RT(t_\alpha)}\right)$ (13)

Using equations (10) and (13) that describe the heat balance under experimental conditions and kinetic description of the process one can now predict the reaction progress $\alpha(t)$ and the rate $d\alpha/dt$. Knowing the value of heat release of the exothermic decomposition determined from the DSC experiment (ΔH) and the value of the specific heat (C_p), one can calculate the development of temperature $T(t)$ and dT/dt due to the self-heating ΔT_{ad} (with $\Delta T_{ad} = \Delta H/ C_p$) and the adiabatic inductions times at any selected starting temperature. The results of these simulations are presented in Figure 5A, which describe the simulated T-time relationship for the starting temperature of 90°C ($\Delta T_{ad} = 1866 \pm 115.2°C$). Figure 5B shows the dependence of the adiabatic induction time on the starting temperature with the confidence interval determined at 95% probability. The inset (Fig. 5C) presents the simulation of the heat rate curves for a starting temperature of 90°C.
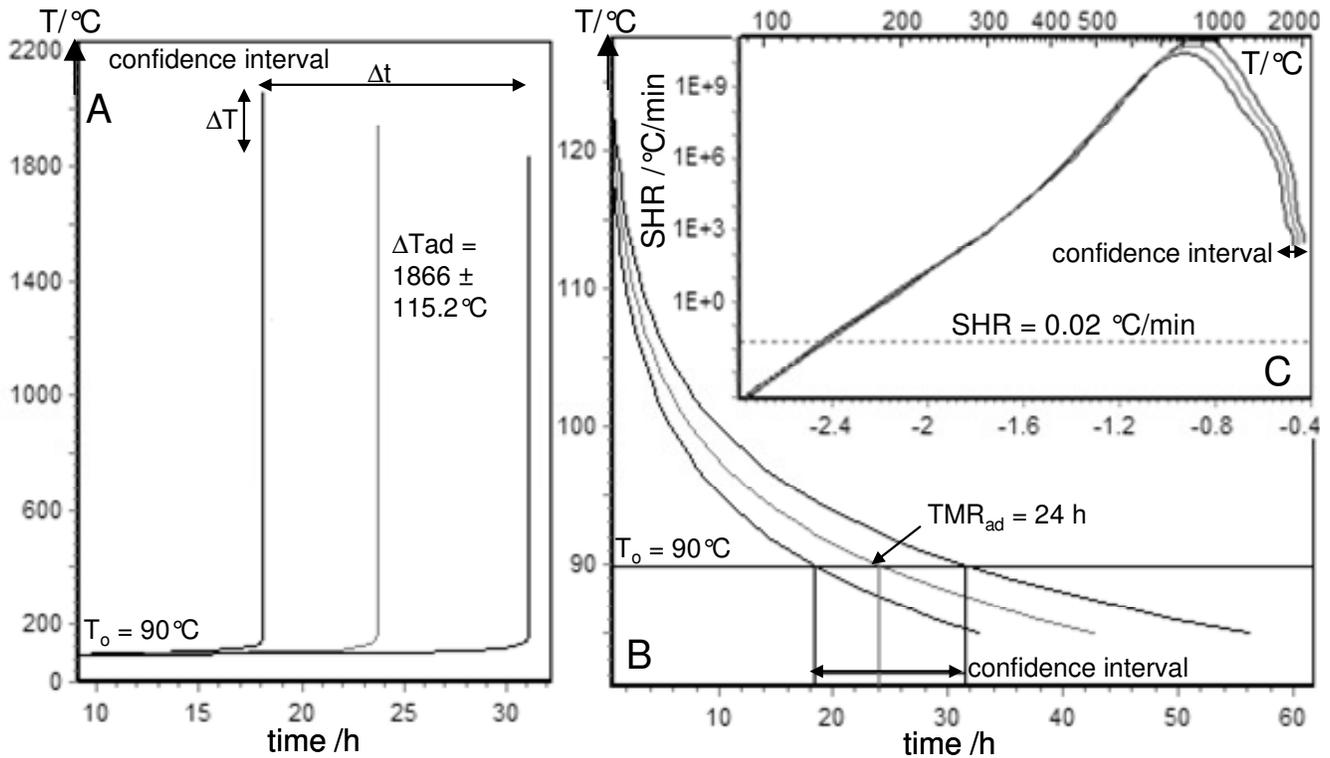

Fig. 5 (A) Adiabatic runaway curves for a single-base propellant showing the confidence interval for the prediction (T_{begin}=90°C and $\Delta T_{ad}=\Delta H/C_p$=1866±115.2°C). The confidence interval was determined for 95% probability. (B) Starting temperature and corresponding adiabatic induction time TMR$_{ad}$ relationship of the propellant under isochoric conditions. The choice of the starting temperatures strongly influences the adiabatic induction time (confidence interval: 95% probability). (C) Dependence of the heat rate curves on the temperature under isochoric conditions.
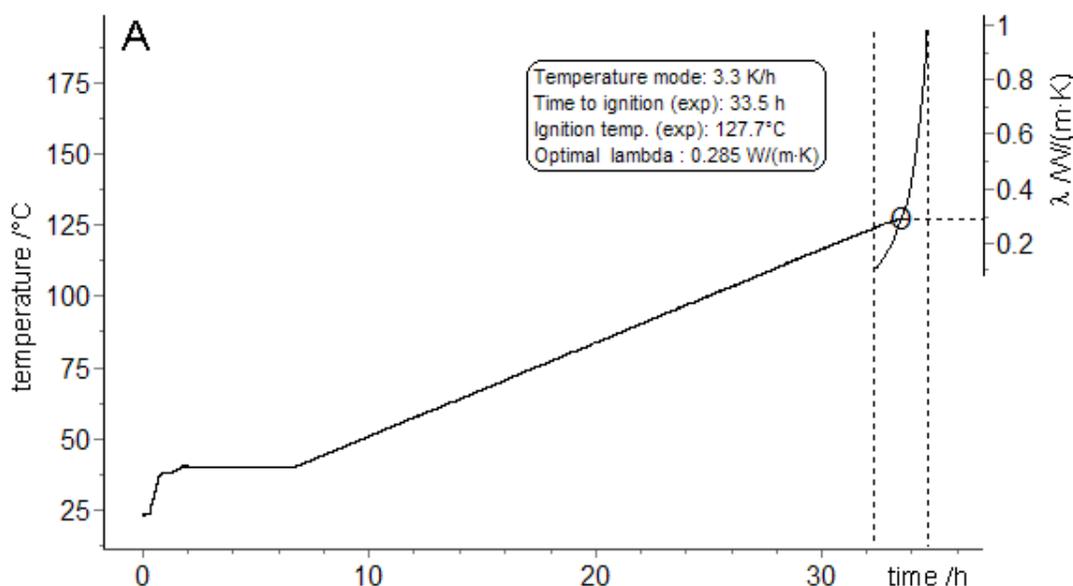
SIMULATION OF COOK-OFF

Applying the kinetic parameters determined by Friedman method and the heat balance, as described in the Section 4, we can now simulate two cook-off experiments carried out with different settings (see Experimental) and in H-W-S mode. The simulations were compared with the experimental data and were done by varying the value of the thermal conductivity λ to achieve the best fit for the experimental cook-off values. Results of these simulations are presented in Figure 6. The values of λ which provided the best fit are presented in the Table 1.

Table 1. Optimal λ values securing the best fit of the simulation to the experimental cook-off parameters obtained at different temperature modes.

Heating rate (K/h)	Time to ignition (exp) (h)	Ignition temperature (exp) (°C)	Optimal λ (W/(m·K))
3.3	33.5	127.7	0.285
1.0	31.4	123.0	0.459
H-W-S	110.4	116.4	0.320

The data presented in Table 1 and shown in Figure 6 indicate that for each temperature mode (different temperature ramps during conventional cook-off settings or pseudo-isothermal ramps in the H-W-S mode) slightly different values of λ have to be applied during the simulations in order to conform to the experimental results. On closer inspection, the dependence of the cook-off parameters on the λ values indicates that the influence of thermal conductivity on the time to ignition and temperature of the thermal event is less apparent at higher heating rate (Fig. 6A) and most pronounced by the pseudo-isothermal ramp used in H-W-S experiment (Fig. 6C). In the experiment carried out at a rate of 3.3 K/h (Fig.6A) the change of the λ value from 0.1 to 1.0 W/(m·K) leads to the change of the time to ignition from 32.2h to 34.3 h, at a heating rate of 1.0 K/h from 25.2h to 33.4 h and in H-W-S experiment from 49 to 120h. Obviously, the influence of the thermal conductivity on the time to ignition is the most significant under pseudo-isothermal conditions and significantly decreases when the heating rate increases. This observation indicates that parameters of the model derived from the conventionally applied cook-off setup with heating rate of 3.3 K/h, as being the less sensitive on λ, can lead to significant errors when applied to simulation of the events at slower heating rates or, in extreme case, isothermally as during the simulation of SADT.
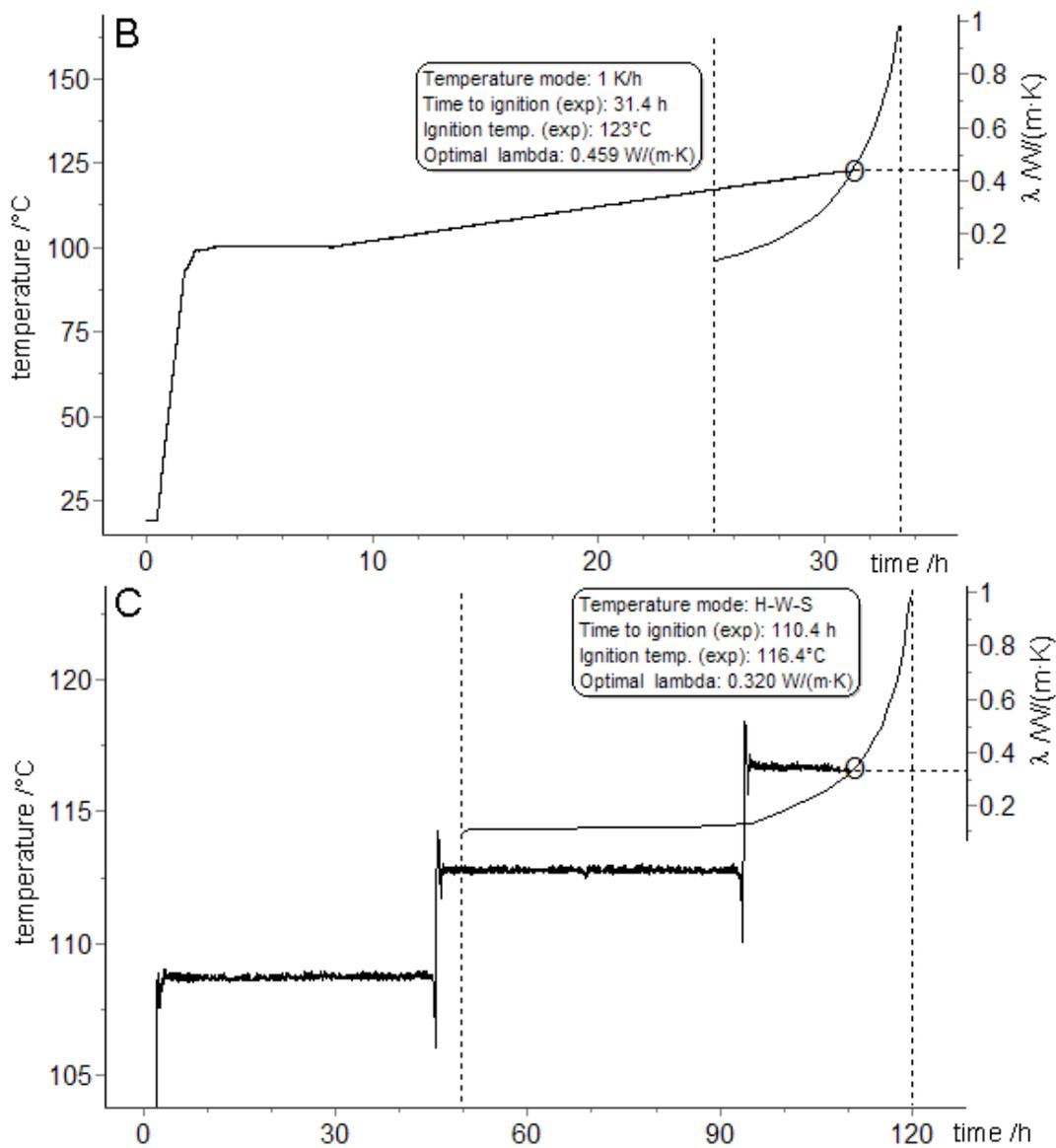

A — Temperature mode: 3.3 K/h; Time to ignition (exp): 33.5 h; Ignition temp. (exp): 127.7°C; Optimal lambda : 0.285 W/(m·K)

Fig. 6 Influence of λ on the time to ignition for: (A) cook-off experiment with heating rate of 3.3 K/h, (B) heating rate 1.0 K/h and (C) heat-wait-search mode. The values of λ that provide for the best fit to the experimental values are summarized in the Table 1. Note the increasing influence of the λ value on the time to ignition during decreasing heating rate.

Figure 7 shows the simulated temperature distribution in the sample during cook-off experiment carried out in the H-W-S mode. The plot depicts the average temperature recorded by three thermo elements and temperatures of the material from the surface (bottom line) to its center (top line).
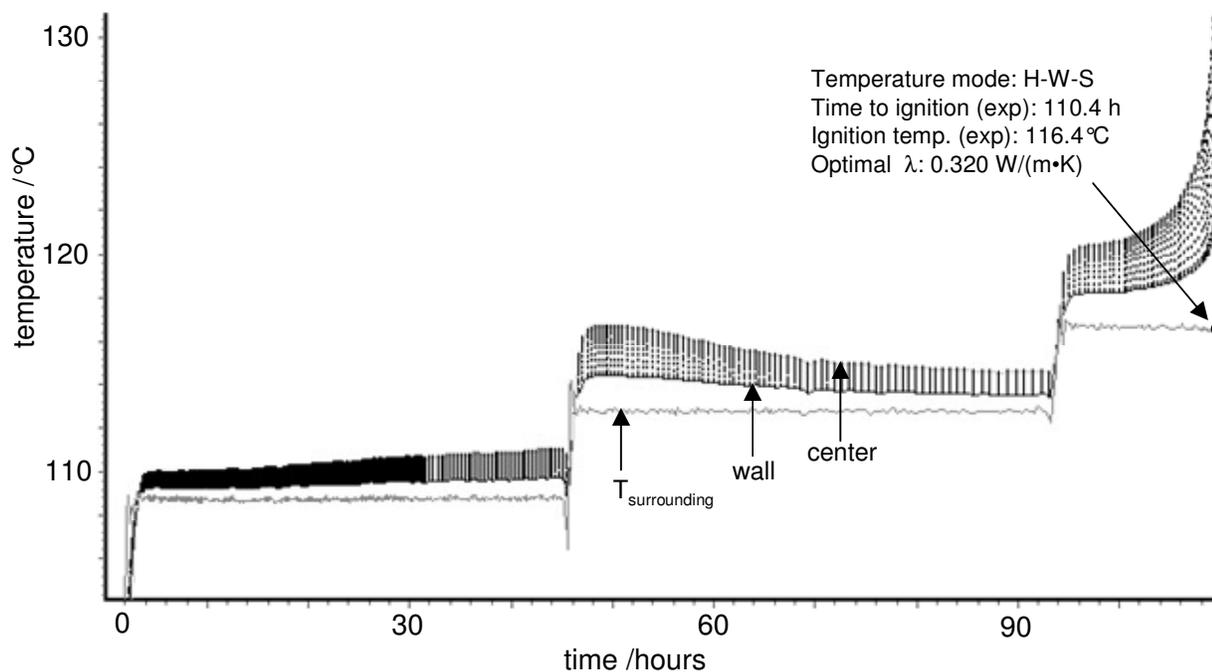
Fig. 7 Simulation of the single-base propellant cook-off ignition under H-W-S temperature mode applying $\lambda = 0.32$ W/(m·K) (see last row in Table 1 and Fig. 6C).

SELF-ACCELERATING DECOMPOSITION TEMPERATURE (SADT)

The DSC signals of a material's decomposition are processed using AKTS Thermokinetics software's unique numerical techniques to create an accurate kinetic model. Subsequently, this kinetic model is used by the AKTS-Thermal Safety Software to predict the material's thermal conductivity properties for a specific container type and size under any global temperature environment.

The results presented in the previous sections indicate that at very low heating rates the influence of the thermal conductivity on the heat conduction are more significant than at higher heating rates, therefore we decided to check how a change of λ will influence the value of SADT which is determined under isothermal conditions.

The Self-Accelerating Decomposition Temperature (SADT) is an important parameter that characterizes thermal hazard under transport conditions of self-reactive substances. The SADT is used in international transportation regulations and is referenced in the United Nations presented in "*Recommendations on the Transport of Dangerous Goods*, *Manual of Tests and Criteria*" (TDG) (10). The Globally Harmonized System (GHS) (11) has inherited the SADT as a classification criterion for self-reactive substances. According to the Recommendations on TDG the SADT is defined as "the lowest temperature at which self-accelerating decomposition may occur with a substance in the packaging as used in transport". An important feature of the SADT is that it is not an intrinsic property of a substance but "…a measure of the combined effect of the ambient temperature, decomposition kinetics, packaging size and the heat transfer properties of the substance and its packaging" (10).

The Manual of Tests and Criteria of the United Nations of the transport of dangerous goods and on the globally harmonized system of classification and labelling of chemicals indicates that the characterization of the materials is based on the heat accumulation storage tests. The regulatory compliance definitions are:

(i) SADT is the lowest environment temperature at which overheat in the middle of the specific commercial packaging exceeds 6 °C (ΔT_6) after a lapse of the period of seven days (168 hours) or less. This period is measured from the time when the packaging center temperature reaches 2°C below the surrounding temperature.

(ii) SADT is the critical ambient temperature rounded to the next higher multiple of 5 °C.

The first definition is based on two essential parameters – maximal permissible overheating temperature and minimal acceptable induction period. The second definition considers only one parameter: the critical ambient temperature of thermal runaway rounded to the next higher multiple of 5 °C without any fixed transportation time in the definition.

The results of the simulation of SADT when applying the λ value taken from the H-W-S-mode simulation (see last row in Table 1 and Fig. 6C) are presented in Figure 8. This simulation was carried out for the same amount of propellant as those being used during cook-off experiments (0.35L).
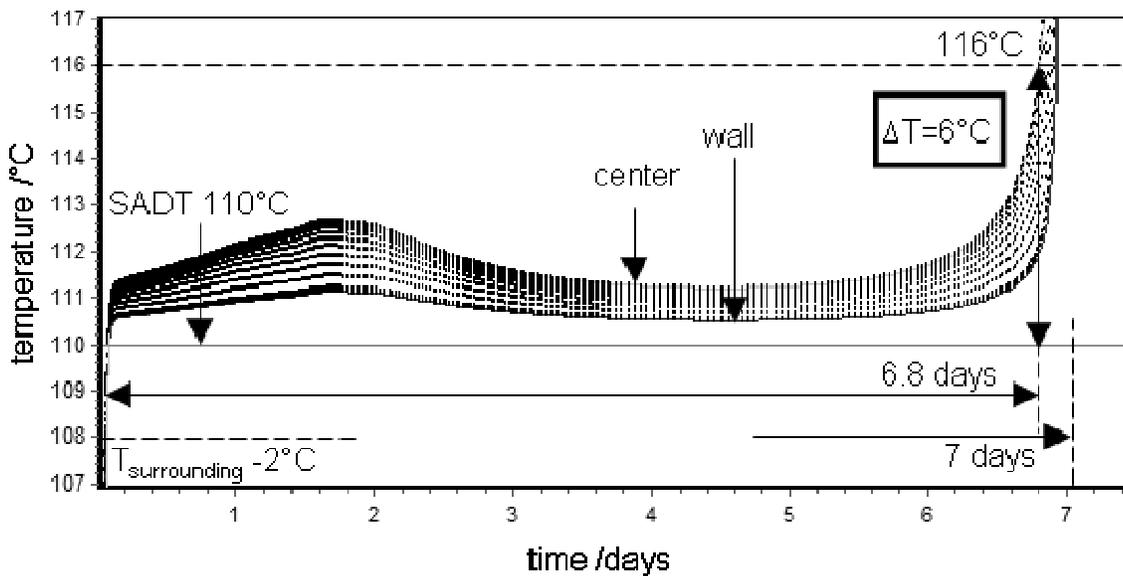

Fig. 8 Determination of SADT of the single-base propellant. Based on *the first definition (i)* we obtain a SADT of 110°C. This temperature is the lowest environment temperature at which the overheat in the middle of the specific packaging exceeds 6 °C (ΔT_6) after a lapse of the period of seven days (168 hours) or less. This period is measured from the time when the packaging centre temperature reaches 2°C below the surrounding temperature. This overheat of 6°C occurs after about 6.8 days.

Table 2. Dependence of the SADT (°C) on the thermal conductivity λ and the amount of the propellant expressed by the sample volume (L) or the equivalent spherical radius (cm).

λ W/(m·K)	SADT /°C						
	Equivalent spherical radius (cm) / volume of the sample (L)						
	4.35/0.35	6.2/1	10.61/ 5	13.36/10	18.14/ 25	22.85/50	28.79/100
0.10	102	96	89	86	82	79	76
0.32	**109**	**105**	**96**	**93**	**89**	**86**	**84**
1.00	110	109	103	100	95	92	90
10.00	111	110	109	107	104	101	99
100.00	111	110	109	108	105	103	101

It seems to be obvious that the influence of the change of the thermal conductivity on SADT will be larger for the larger mass of the energetic material. The Table 2 and Figure 9 contain the results of these simulations. The change of the thermal conductivity from 0.1 to 1.0 W/(m·K) for the 0.35L sample will increase the SADT from 102 to 110°C (ΔT = 8°C) whereas for the larger, 100L sample, the increase of the SADT will be almost twice as large (from 76° to 90°C, ΔT =14°C). These results clearly indicate the importance of an accurate value of λ that is used in the simulations. Our results show that the best way is to apply the thermal conductivity value that was obtained during the simulation of the H-W-S experiments.
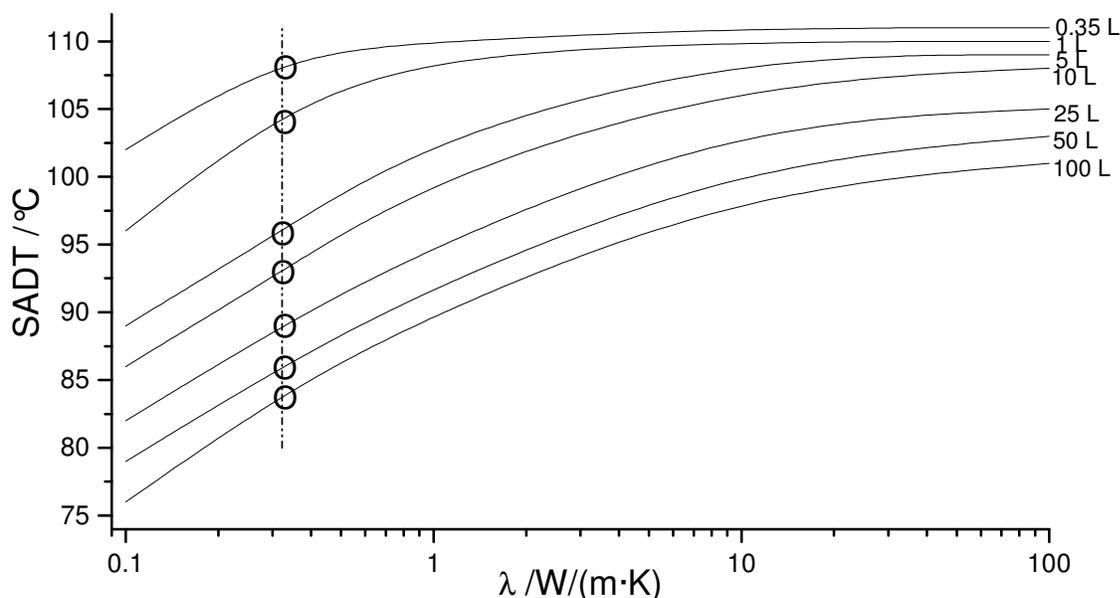

Fig.9 SADT as a function of the thermal conductivity λ and sample volume expressed in L. The open circles represent the simulation of SADT when applying the λ value taken from the H-W-S-mode simulation (see last row in Table 1 and Fig. 6C).

CONCLUSIONS

A precise prediction for the decomposition behaviour of a highly energetic material (single-base propellant) can be obtained from DSC data, an accurate kinetic model and an overall heat balance of the system.

It is possible to simulate the behaviour in mg-scale (see results presented in Fig. 3C), during cook-off experiments (kg-scale, see Figs. 6, 7) and to use the DSC data for the simulation of the adiabatic behaviour as depicted in Fig.5, which demonstrates the dependence of the adiabatic induction time on the starting temperature. The prediction of a sample's thermal behaviour can be carried out for any temperature mode (different heating rates or H-W-S mode) as presented in Fig.6. Moreover, one can also simulate the SADT values i.e., the behaviour of the material under isothermal conditions as depicted in the Figs.8 and 9.

The results presented in this study indicate that the temperature ramps applied during experiment and simulation significantly influence the impact of the thermal conductivity on the time to ignition (see Fig.6). The influence of λ on the time to ignition is the most significant at pseudo-isothermal conditions and decreases when the heat rate increases. This indicates that the results of the simulation of the cook-off experiment carried out with the heating rate of 3.3 K/h may introduce significant errors when applied

to simulation of the processes occurring at lower heating rates or isothermally (simulation of SADT). The results of the simulation of SADT presented in Fig. 9 indicate that the influence of λ significantly rises by increasing the mass of the energetic material.

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