MEASUREMENT OF THERMAL DECOMPOSITION AND VALIDATION OF KINETIC MODEL TO DESCRIBING THE COOK-OFF OF PBX RH8515

F. Chaves^{*}, J. C. Góis^{**}

*Mech. Eng. Dep. – E.S.T.A. – I.P.T., 2200 Abrantes, Portugal, flaviochaves@ipt.pt **Mech. Eng. Dep. – F.C.T.U.C., Pinhal de Marrocos, 3030-201 Coimbra, Portugal, jose.gois@dem.uc.pt

ABSTRACT

Measurements of thermal decomposition of PBX RH8515 [RDX(85)/HTPB(15)] under slow and fast cook-off were performed to determine the ignition temperature of runaway and time-to-explosion. The experiments of cook-off are carried out with a charge of 1.57 cm³ inside a small cylinder test vehicle (SCTV) for a heating rate (HR) near 3.3 °C.h⁻¹, describing slow cook-off and for a HR near 3.3 °C.min⁻¹ reproducing fast cook-off. The temperature increasing on the external wall of the test vehicle was provided by convection and radiation from the internal wall of a concentric metallic tube wrapped with a resistance wire. A PID control system assures an almost constant increase of temperature on the external wall of the cylinder test vehicle. The temperature of PBX RH8515 was measured using a thermocouple at the center of the explosive charge. The results obtained are compared with the prediction achieved using *ABAQUS 2D* computer model for both HR refereed above and assuming so much a single-step kinetic model, based on the Friedman analysis, as the 3-steps McGuire-Tarver kinetic model.

Keyboards: thermal decomposition, slow cook-off, fast cook-off, ignition temperature of runaway, small cylinder test vehicle.

1. INTRODUCTION

The knowledge of the response of energetic material (EM) to the perceived of threats of slow and fast cook-off and the effects on the environment is extremely important to prevent potential accidents during manufacture, storage, transport and use.

The high costs of large scale tests with EM and maintenance of required capabilities for that make the small scale tests particular important as preliminary tests so much to generate input data to simulation as to evaluate the risks. The scale of tests used for thermal characterisation of EM could be influenced by the failure size and kinetic mechanisms, which govern the thermal decomposition of EM. The geometry and material of the case that confine the charge and the composition of the EM have also a large influence on the thermal behaviour of EM. Both civil and military explosives charges commonly have cylinder geometry. Munitions are produced normally in metallic confinement and the new generation of insensitive munitions (IM) is based in PBX.

The reasons presented above demand to coupling small scale tests with the simulation of the thermal behaviour under slow and fast cook-off regimes. The approach between experiments and simulation will be a helpful contribution to developing a new philosophy of IM.

With the purpose to validate the kinetic model that better describes the thermal behaviour of the PBX RH8515 under cook-off regimes, a small cylinder test vehicle (SCTV) with 1.57 cm³ size was submitted to slow and fast cook-off. The results are compared with its obtained by simulation [1] using a numerical code implemented in *ABAQUS 2D* computer model [2].

2. EXPLOSIVE COMPOSITIONS AND EXPERIMENTAL SETUP

The PBX RH8515 is based on a bimodal particle size distribution of RDX. The solid load charge was composed by 70 wt% of RDX class A type II and 30 wt% of RDX class E type II, supplied by DYNO, Norway. The PBX RH8515 is a mixture of the load charge of RDX and HTPB for a mass fraction relationship of 85/15. The density of PBX RH8515 is 1564 kg.m⁻³, which represents 98% of theoretical maximum density.

The measurements of the thermal decomposition of PBX RH8515 under slow and fast cook-off were performed inside a 42CrMo4 SCTV with 1.57 cm³ (Fig. 1). Two caps close the SCTV: one to fix the thermocouple inside the explosive charge and the other one to close the opening used for filling the SCTV with the PBX. The thermocouple that controls the temperature of external wall of SCTV is fixed at the middle of cylinder test.



Figure 1. Small Scale Test Vehicle (SCTV).

The increase of temperature on the external wall of the SCTV is reached by convection and radiation from the internal surface of the steel tube wrapped with a resistance wire band with 28 Ohms (Fig 2). The temperature on the external wall of the SCTV was controlled by a programmable increment differential (PID) control system that assures an almost constant increasing of temperature. An electric power supply provides the current to the resistance wire. The SCTV is fixed inside the metallic cylinder heating tube (Fig. 2). Figure 3 shows the main components part of the experimental setup. The temperature of external wall of the SCTV (T_{ext}) and the temperature of the PBX at the center charge (T_{int}) are measured in real time using a specific board and software.



Figure 2. Scheme of experimental setup.



Figure 3. Main components parts of experimental setup.

Legend:

- 1 Transformer (converts power of 220Vac to 110Vac)
- 2 Electrical power supply
- $3-PID\;30880$
- 4 Interface RS232
- 5 Interface CIO-DAS-TC

3. RESULTS AND DISCUSSION

For slow cook-off experiments carried out at quasi-constant heating rate (HR) of $3.1 \, {}^{\circ}\text{C.h}^{-1}$ was obtained an ignition temperature of runaway of PBX RH8515 near 175.0 °C, being the time-to-explosion of 2900 minutes (Fig. 4). Due to the large time required performing slow cook-off experiments we also conducted some tests submitting the SCTV to a preliminary fast HR of $3.4 \, {}^{\circ}\text{C.min}^{-1}$ until a temperature of 140 °C. After the time for the stabilisation of the temperature of the SCTV and the PBX (about 26.5 minutes), was restarted the increasing of temperature for a HR of $4.75 \, {}^{\circ}\text{C.h}^{-1*}$. The ignition temperature of runaway of PBX RH8515 obtained under this heating process is closed to 179.9 °C (Fig. 5).



Figure 4. Temperatures records under slow cook-off regime: external wall temperature of SCTV – T_{ext} , and center temperature of PBX – T_{int}).

In figure 4 the temperature oscillation at the beginning of slow cook-off process is caused by the thermal inertia of the steel tube, due to the large mass of it. From 56 °C the external wall of SCTV and the PBX RH8515 are submitted to a quasi-linear temperature rise.

^{*} The thermal inertia of metallic tube has not allowed keeping the HR near 3.3 °C.h⁻¹.



Figure 5. Temperatures records under fast cook-off regime (until about 140 °C) followed by slow cook-off regime: external wall temperature of SCTV – T_{ext} , and center temperature of PBX – T_{int}).

Under slow cook-off regime the temperature of SCTV and PBX (see Fig. 4 and 5) are very closed. Near the ignition temperature of PBX RH8515 was verified a significant increase of the temperature at the center of PBX RH8515, while the temperature of external wall of the SCTV is maintained in agreement with the pre-established HR. Table 1 resumes some details about temperatures and HR verified for both slow cook-off processes tested for the PBX RH8515. In table 1 the numbers in bold represent the ignition temperature of runaway and time-to-explosion.

Test Nº	Ramp temperature process	PBX RH8515	Temperature Range	
	Time range [min]	Heating rate [°C.h ⁻¹]	T_{int} [°C]	T_{ext} [°C]
1	Single ramp of temperature $0 - 801.8$	2.65	20.5 - 56.0	20.5 - 55.8
	Single ramp of temperature 801.8 – 2900.7	3.1	56.0 – 175.0	55.8 - 161.0
	First ramp of temperature $0 - 34$	204.6	20.9 - 131.4	20.9 - 140.1
2	Stage of temperature 34 – 60.5	_	131.4 - 142.2	140.1 – 139.6
2	Second ramp of temperature 60.5 – 260.5	4.75	142.2 - 157.0	139.6 – 159.1
	Second ramp of temperature 260.5 – 380.5	9.34	157.0 – 179.9	159.1 – 168.7

Table 1. Experimental results obtained for PBX RH8515 under slow cook-off regime.

When compared the ignition temperature of runaway (and time-to-explosion for the experiment with a single ramp of temperature), for both experiments, with its predicted using *ABAQUS 2D* computer model for a HR of $3.3 \, {}^{\circ}\text{C.h}^{-1}$ we observe a good agreement with the results obtained when the 3-steps McGuire-Tarver kinetic model is

assuming (Tab. 2). Assuming the 3-steps McGuire-Tarver kinetic model the ignition temperature of runaway of PBX RH8515 is reached near the center of the charge for a temperature of 164.6 °C (when the minimum temperature in the charge is 159.7 °C) and the time to ignition, from 20 °C, is 2912.7 minutes.

Kinetic model	Time to ignition [min]	Maximum temperature achieved in the EM [°C]	Minimum temperature achieved in the EM [°C]	Ignition location
Single-step (Friedman analysis)	3445.9	193.5	188.9	Center
3-steps (McGuire and Tarver analysis)	2912.7	164.6	159.7	Center

Table 2. Prediction results of PBX RH8515 under slow cook-off regime for HR=3.3 °C.h⁻¹.

However the similarity of temperature growing in the PBX RH8515 for both kinetic models, the results using the single-step kinetic model, based on the Friedman analysis [4–7], gives higher values that its from the experiments, being 10.6% for ignition temperature of runaway and 18.8% for the time to ignition. The temperature contour plot (Celsius degrees) inside the SCTV and the explosive charge, just before the ignition temperature of runaway, is shown in figures 6 and 7 for each of the kinetic models described above.



Figure 6. Temperature contour plot just before ignition, under slow cook-off, when 3-steps kinetic McGuire-Tarver model is used.

Figure 7. Temperature contour plot just before ignition, under slow cook-off, when the single-step kinetic model (Friedman analysis) is used.

Fast cook-off experiments were performed applying a HR of 3.3 °C.min⁻¹. Figure 8 shows the temperature profiles of the external wall of SCTV and PBX RH8515 at the center submitted to a HR = 3.3 °C.min⁻¹, from the ambient temperature until the ignition temperature of runaway. For both HR, table 3 shows the results for fast cook-off experiments, obtained for the ignition temperature of runaway of PBX RH8515 and time-to-explosion.



Figure 8. Temperatures records under fast cook-off regime (HR=3.5 °C.min⁻¹): external wall temperature of SCTV – T_{ext}, and center temperature of PBX – T_{int}).

Under fast cook-off regimes exist a higher gap between the temperature at the center of the explosive charge and the external wall of the SCTV than its observed under slow cook-off regimes. For the HR = $3.5 \, {}^{\circ}$ C.min⁻¹ the temperature gap is maintained near 14 °C. Taking into account the higher value of thermal conductivity of steel case in comparison with the PBX RH8515 is seems us highly probable that the ignition process occurs near the interface between the PBX and inner face of the SCTV. Considering the small size of the test vehicle used to carry out the experiments, it will be credible to assume the occurrence of ignition also near the caps.

Heating rate	Time until	Temperature		
[°C.min ⁻¹]	[min]	T_{int} [°C]	T _{ext} [°C]	
3.5	51.3 ± 2.02	192.1 ± 8.96	208.7 ± 4.76	

Table 3. Experimental results obtained for PBX RH8515 under fast cook-off regime.

The experimental results obtained for fast cook-off are in good agreement with its predicted by the computer model for a HR = $3.3 \,^{\circ}$ C.min⁻¹, using the 3-steps McGuire-Tarver kinetic model, which gives an ignition temperature of 194.8 °C and a time to ignition of 59 minutes. The single-step kinetic model, based on the Friedman analysis, provides higher values for the ignition temperature of runaway and time than its obtained using the 3-steps McGuire-Tarver kinetic model (Tab. 4), increasing the difference with the experimental results.

Kinetic model	Time to ignition [min]	Maximum temperature achieved in the EM [°C]	Minimum temperature achieved in the EM [°C]	Ignition location
Single-step (Friedman analysis)	66.4	219.1	218	Almost total volume
3-steps (McGuire and Tarver analysis)	59	194.8	177.8	Ring near interface

Table 4. Prediction results of PBX RH8515 under fast cook-off regime for HR=3.3 °C.min⁻¹.

Figures 9 and 10 show for fast cook-off regime the temperature contour plot, like in figures 6 and 7 for slow cook-off regime.





Figure 9. Temperature contour plot just before ignition, under fast cook-off, when the 3-steps kinetic McGuire-Tarver model is used.



Comparing the ability of both kinetic models to describe slow and fast cook-off regimes it seems clear the high performance of the 3-steps McGuire-Tarver kinetic model when compared with the single-step Friedman kinetic model. Comparing both cook-off regimes, the 3-steps McGuire-Tarver kinetic model provides an approach with the experimental results for slow cook-off regime.

4. CONCLUSIONS

The measurement of ignition temperature of runaway and time-to-explosion of the PBX RH8515, based in RDX and HTPB (85/15 mass percent), under slow and fast cook-off regimes can be performed using a SCTV with 1.57 cm³. The small size of the SCTV only allows the measurement of temperature at the center of explosive charge. Although this limitation for the measurement of ignition temperature of runaway under fast cook-off regime, the small volume of explosive charge allows assumed an ignition temperature of runaway slight higher than the temperature at the center.

An ABAQUS 2D computer model for prediction of ignition temperature of runaway, location and time, as also the temperature distribution inside the SCTV and the PBX,

for both cook-off regimes, allows evaluating the validation of the 3-steps McGuire-Tarver kinetic model and the single-step Friedman kinetic model to describe cook-off phenomena. For slow and fast cook-off regimes the 3-steps McGuire-Tarver kinetic model has shown a higher approach with experimental results. Although the constraints of the trials, described in the paper, the approach with experimental results is very closed for slow cook-off regimes.

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