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Extended multi-physics model for slow-cook off events of warheads

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Abstract

Among the Insensitive Munition hazards listed in STANAG 4439, thermal stimuli through slow cook-off heating are particularly interesting, since underlying phenomena are very complex, responses depend on various parameters and they may have a significant impact on warhead system design. A standardized test device with cast-cured or pressed plastic-bonded high explosive charges is used at TDW for investigating slow thermal stimuli that allows evaluating reaction levels and decomposition temperatures of high explosives. It provides a confined environment and also permits temperature measurements inside the HE charge. Experimental tests results varied between burn and deflagration reactions depending on the high explosive charge and the charge confinement.

Such experimental data provide a profound basis for thermal modeling of slow cook-off responses. Multi-physics coupling of transient heat conduction with Arrhenius reaction kinetics form a system of coupled partial differential equations solved numerically with MATLAB. AKTS-Thermokinetics software deliver corresponding input functions that were determined through differential scanning calorimetry tests of small explosive samples. Predicted self-heating times, rates, and partly peak temperatures approach well experimental data. Observed events of heat loss and self-heating slow-downs probably result from venting. Models for calculating internal pressures are now included in the simulation to evaluate these effects. This supports the design of venting measures for specific applications including full-scale warheads.

1 Introduction

Insensitive Munitions (IM) requirements are very relevant for today's and future munitions. Among all IM hazards listed in STANAG 4439 [1], thermal stimuli such as slow and fast cook-off (SCO / FCO) heating are particularly interesting, since they may have a significant impact on the design of warheads using large and / or strongly confined high explosive (HE) charges.

A number of experimental studies using confined, small-scale test vessels investigated effects of HE charges, binder systems, heating rates, etc. on self-heating characteristics, venting characteristics as well as on time to ignition, temperature of ignition, and reaction violence [2, 3]. Recent thermal analysis and modeling efforts apply single-phase or multi-physics finite element (FE) models. Hunter et al. [4] couple an Arrhenius rate equation for self-heating with convection as primary heat transfer mechanism. A universal cook-off model is presented in [5] for predicting ignition time, spatial temperatures, and pressurization rates and applying it to four explosives.

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TDWs IM assessment approach for thermal stimuli as outlined in Fig. 1 is based on AOP-39 [6] and starts with material tests for small HE charge samples followed by small-scale thermal testing, and a modeling & simulation phase. This helps to mitigate technical risks early in development programs and reduce both time and costs before full-scale IM tests are eventually performed on subsystem or system level for demonstrating IM compliance. [7]

This paper continues an experimental and modeling study of a confined slow cook-off vessel filled with various high explosive (HE) charges tested in heating ovens under standard slow-cook off conditions with results published in [8, 9]. Slow cook-off responses are modeled through a multi-physics system of transient heat conduction coupled with reaction kinetics applying MATLAB [10]. The model is extended to include a prediction of pressures inside the test vessel. Pressures values at distinct events of end cap venting and casing failure are analytically estimated and used to trigger model parameters. Results of simulated temperature and pressure over the entire time regime are plotted and compared to experimental data of a KS22 charge.

2 Experiments with TDWs slow cook-off vessel

A standardized, confined slow cook-off vessel is used at TDW with different cast-cured or pressed HE charges. It allows evaluating SCO responses along with thermal sensitivities, reaction temperatures and reaction times of high explosives independently of completely designed and built full-scale munitions. A thick tube casing with heavy end caps made of mild steel and a free-cutting steel, respectively, provides a confined environment. The overall charge dimensions are 70 mm in diameter and 122 mm in length. Depending on density, the high explosive charge weighs approx. 350 g with an L/D of 2. Table 1 gives further HE data for tests reported here. Two thermocouples integrated into the HE charge through an end cap hole finally closed with glue permit internal temperature measurements: one is located at the center and one close to the casing. This hole located at the vessel's centerline also serves as a built-in venting mechanism after self-heating reactions have started and it allows hot gases to escape. A picture drawing is shown in Fig. 2a.

Moreover, a high performance shaped charge using a molybdenum liner and a pressed P31 charge was detonated investing confinement influences, see Fig. 2b. An aluminum casing and end cap provide only a soft confinement. The HE charge weighs approx. 3,000 g and does not contain thermocouples.

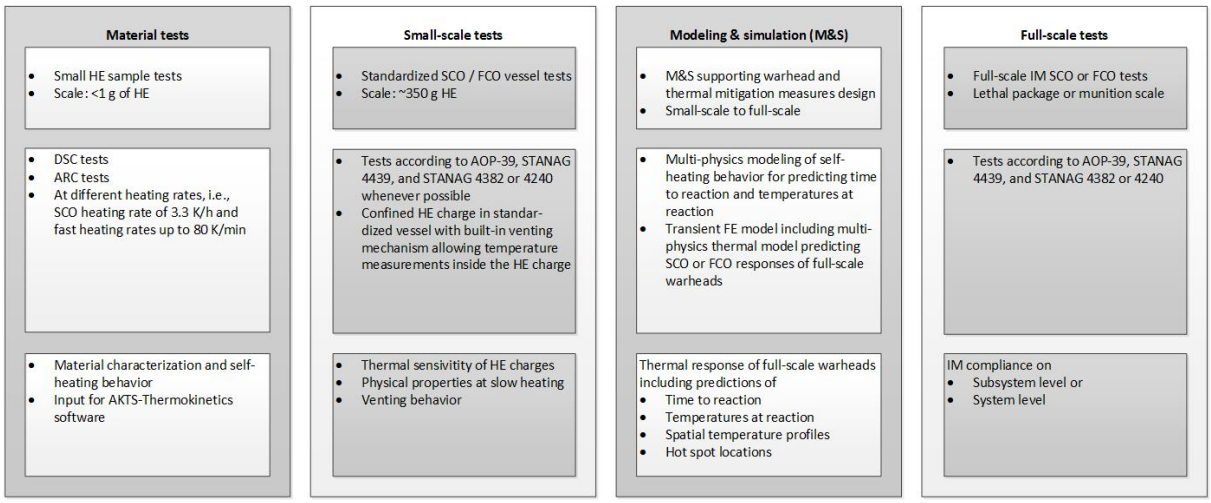


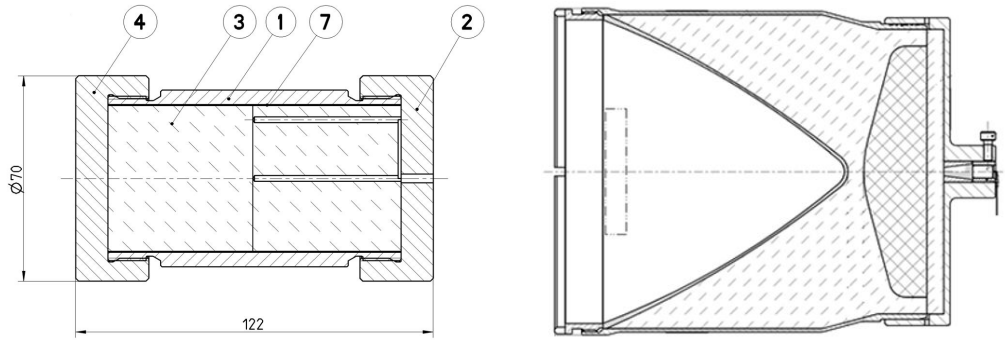
Figure 1. TDWs IM assessment approach for thermal stimuli.

Test setups consisted of commercially available heating ovens adopted with a special temperature control. As depicted in Fig. 3, test samples mounted on steel racks were contained in the oven center and exposed to the heat flow from the back side. Due to compactly built ovens and slow heating rates, no practical differences to requirements stated in STANAG 4382 [11] were expected. The following diagnostics were typically used mostly according to STANAG 4382:

- A horizontal, 10 mm thick witness panel at the oven's bottom
- One thermocouple as oven reference temperature
- Four thermocouples besides, in front and behind the test vessel
- Two thermocouples attached onto the casing skin of the vessel
- Two thermocouples applied within the vessel's HE charge (except of the shaped charge vessel)
- Two high speed video cameras providing a close-up view and an overview from a greater distance

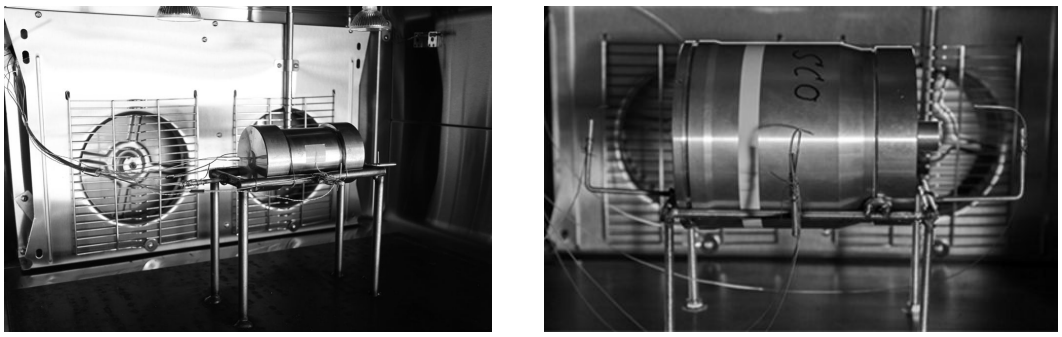
Gauges for measuring blast overpressures were not used since bunkers and additional fragment shielding do not allow undisturbed measurements without intense reflections.

Table 2 provides an overview on the test results. Basically all SCO vessels with HE charges reported here responded in a Type IV, i.e., deflagration reaction according to AOP-39. This is proven by recovered witness panels showing distortions and fragment hits but no perforations, medium-to-large casing fragments with shear fractures, and end caps mostly showing thread fractures (#3). All ovens were completely destroyed, see Fig. 4. Reaction violence is hard to discriminate between these tests, but test #1 with a KS57 charge seem less violent as suggested by SCO vessel fragments.



(a) Standardized SCO vessel. (b) Shaped charge vessel.

Figure 2. Drawings of test samples (SCO vessel parts: 1 – casing, 2, 4 – end caps, and 3 – HE charge glued (7) into the casing).



(a) Standardized SCO vessel. (b) Shaped charge vessel.

Figure 3. Oven front views with instrumented test vessels.

Table 1. Data on high explosives used in SCO vessels.

HE charge	Composition	Density TMD in g/cc	Porosity Estimate in %
KS57	RDX/AP/Al/HTPB (24/40/24/12)	1.82	2.1
KS22d	RDX/Al/HTPB (67/18/15)	1.68	1.6
P31	HMX/Si (96/4)	1.83	1.0

Table 2. Overview on experimental test results and measured temperatures at reaction and time to reaction (based on oven reference temperature).

#	HE charge	ERL AOP-39	Temp θ in °C	Time in 10^5 s	Events observed by high speed video recordings
1	KS57	IV	170	1.67	Two gas flows associated with HE material evacuations observed, followed by temp drop
2	KS22d	IV	158	1.54	Significant self-heating until gases escape followed by sudden temp drop, short second self-heating until reaction
3	P31	IV	195	1.95	Several gas and HE material evacuations, vessel moved finally sideways
4	P31 (SC)	V	196	1.95	Bubbles at end cap before it moved off the charge

Temperature measurements plotted in Fig. 5a deliver time to reaction and temperature at reaction results, see also Tab. 2. SCO vessels with RDX charges (KS22d and KS57) reacted several hours earlier and at lower temperatures compared to P31 charges containing HMX that is also confirmed by literature: approx. 160 to 170°C vs. approx. 200°C temperature regimes (according to oven reference temperature).

Self-heating can be observed when thermocouples inside the HE charge provide higher temperatures than those mounted on the vessel's casing as visualized in Fig. 5b. All HE charges reported show at least one significant self-heating process with hot spots forming at the vessel's centerline. These self-heating processes are typically interrupted by escapes of hot gases through the vessel's built-in venting hole leading to sudden temperature drops. This is supported by high-speed video recordings showing gas and also HE material evacuations as summarized in Tab. 2. Figure 6 shows such effects for test #3 with a P31 charge: HE material is evacuated and hot gases escape before the vessel moves suddenly sideways (except at this test, all other vessels were fixed to the steel rack). Shortly after, the P31 vessel reacted violently with a type IV response.

The confinement influence can be well observed through test #4 of the shaped charge resulting in Type V, a burning response. It is proven by inert parts such as liner and end cap that remained intact and an oven only slightly damaged. Temperatures measured inside the oven and on the casing were, nevertheless, close to those of test #3. That means that self-heating and an initial thermal reaction is triggered by HE charge properties, dimensions, and heating rate, while the final response depends strongly on confinement and venting.

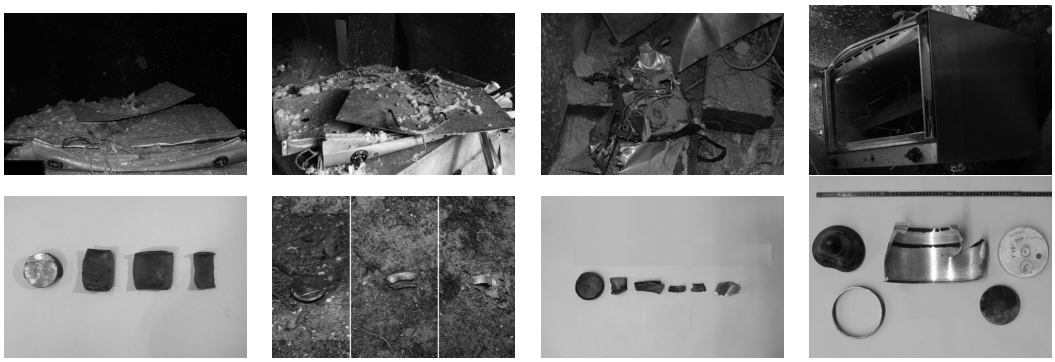
3 Modeling SCO responses

Such experimental data provide a sound basis for creating self-heating models to predict slow cook-off responses. These thermal models can be mathematically described by coupling heat conduction with Arrhenius reaction kinetics [12]. The heat transfer for SCO reactions within the test vessel can be modeled through a transient heat transfer equation in cylindrical coordinates r [13]:

$$\rho c_p \frac{\partial \theta}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rk\frac{\partial \theta}{\partial r}\right) + Q\left(r,t\right) \tag{1}$$

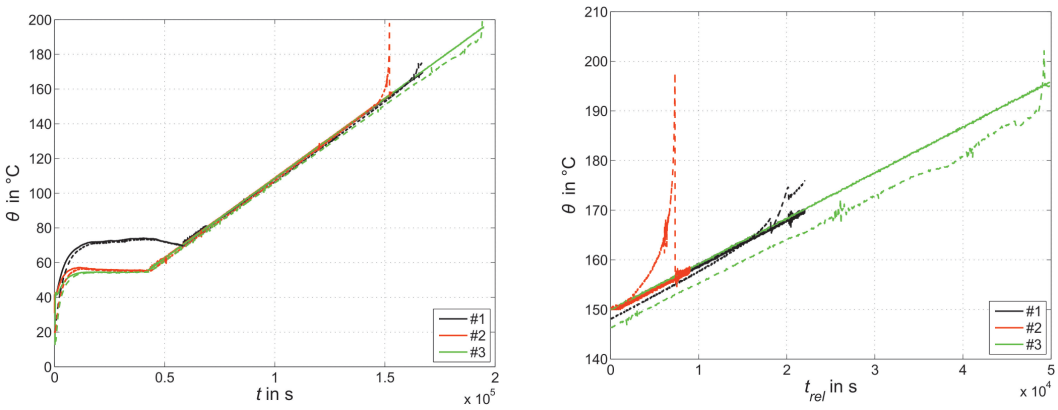
where ρ is the density, c_p is specific heat capacity, k is thermal conductivity, Q is the volumetric heat term, t is the time, and θ is the temperature.

The system is modeled as a cylinder with Neumann boundary condition using the heat flux h. Adiabatic boundary conditions are assumed at top and bottom of the cylinder. Self-heating of the



(a) #1: KS57. (b) #2: KS22d. (c) #3: P31. (d) #4:P31/SC.

Figure 4. Test results showing oven remnants and test vessel fragments.



(a) Plot for entire time regime.

(b) Data shown above 150°C oven ref threshold.

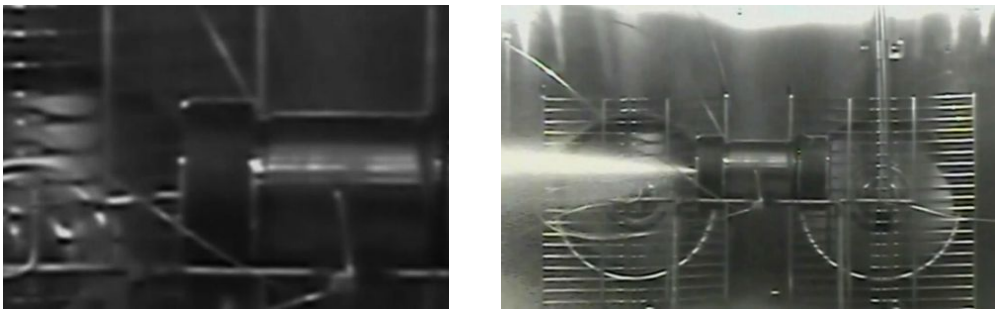
Figure 5. Measured temperature curves plotted for three high explosives: oven reference (solid line) and thermocouple (dashed line) located at charge's center for each test.

system is reproduced through internal heat generation from the SCO reaction realized by a multi-physics coupling of a model-free reaction kinetics with heat generation Q:

$$Q\left(r,t\right) = q\frac{\partial \alpha}{\partial t} = qA_{\alpha}f(\alpha)e^{-\frac{E_{\alpha}(\alpha)}{R\theta}} \tag{2}$$

where q is the heat of reaction, $A_{\alpha}f(\alpha)$ is a pre-exponential factor, $E_{\alpha}(\alpha)$ is an activation energy function for model-free reaction kinetics, R is the universal gas constant, and α describes the reaction progress.

Equations (1) and (2) form a system of coupled partial differential equations for $\theta(t,r)$ and $\alpha(t,r)$ transformed into an ordinary difference equation and eventually solved numerically in MATLAB [10]. The AKTS-Thermokinetics software [14] was used to determine the corresponding functions for $A_{\alpha}f(\alpha)$



(a) HE material pressed out at the left side.

(b) Sample driven by escaping gases to the right.

Figure 6. Slow cook-off test #3 of a P31 charge sample: evacuation of material and gas during self-heating.

and $E_\alpha(\alpha)$ through differential scanning calorimetry (DSC) tests of small explosive samples with different heating rates. Figure 7 shows these (normalized) curves for KS22 and KS57 HE charges. Further input data can be found in Tab. 3.

The original model reported in [8] is further enhanced using a modular design for routines of data input, preprocessing, ODE solving, and postprocessing. Additional boundary conditions implemented into this MATLAB model are

- Casing wall conduction by thermal diffusivity $\frac{k_c}{\rho_c c_{p,c}}$ of steel
- Temperature dependent heat transfer coefficient $h(\theta)$ representing forced convection by turbulent heat flows in the oven

These conditions allows starting the model at initial oven temperatures θ_0 when the constant heating rate of 3.3 K/h is applied.

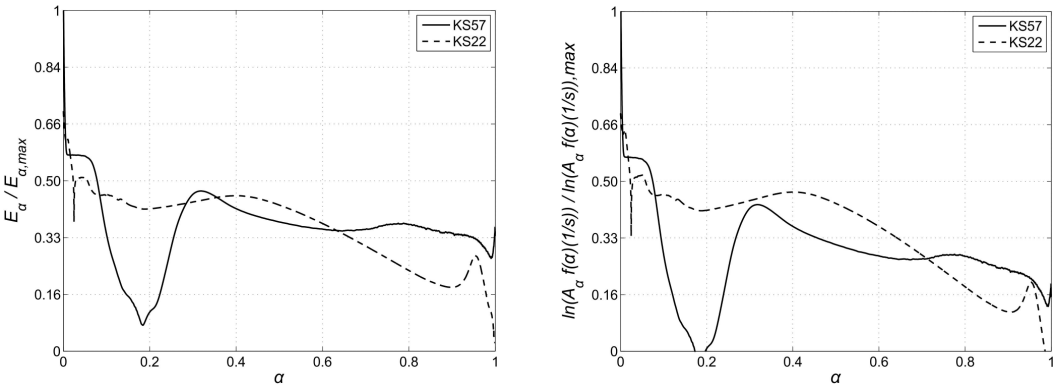
Such simulations were performed for KS22 charges. Figure 8a shows the complete heating cycle simulated by MATLAB starting with an initial temperature of 57°C after a uniform spatial temperature distribution is reached within the KS22 charge. A detailed view above 150°C is provided with Fig. 8b. Simulated self-heating curves are generally close to measured temperatures at the vessel charge's border and center. Differences can be observed shortly before thermal ignition resulting from heat loss effects attributed to the dedicated venting mechanism integrated into the vessel's end cap that are not considered here. Casing temperatures are slightly underpredicted with less than two Kelvin that may be attributed to radiation (not included in this model) and / or thermal coupling of sensors with casing.

4 Extending the MATLAB model

The MATLAB model described before was extended for simulating pressures resulting from self-heating inside the HE charge. At first, pressures because of failure of various test vessel's components were evaluated analytically:

Table 3. Input data for thermal simulations.

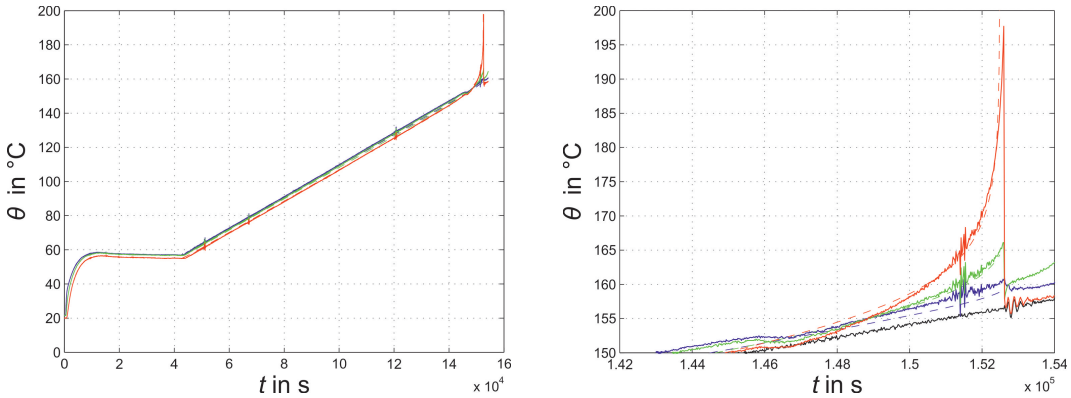
Test vessel	Convection heat transfer coefficient h in W/(K m^2)	Casing's thermal diffusivity $\frac{k_c}{\rho_c c_{p,c}}$ in mm^2/s	HE charge's thermal diffusivity $\frac{k}{\rho c_p}$ in mm^2/s	Reaction heating term $\frac{q}{\rho c_p}$ in K/s	Start temperature θ_0 in deg C
KS22	19	11.14	0.09	6.50 10^4	57



(a) Normalized activation energy vs. reaction progress.

(b) Normalized reaction coefficient vs. reaction progress.

Figure 7. AKTS input data for KS22 and KS57 HE charges.



(a) Complete heating cycle.

(b) Curves above 150°C.

Figure 8. Comparing measured (solid lines) and MATLAB simulated (dashed lines) temperature curves for a KS22 charge: oven reference (black) and thermocouples located at casing (blue), HE border (green), and HE center (red).

- End cap's hole closed with a glue will fail at approx. 46 bar after exceeding the lap shear strength of the glue. Lap shear strength was reduced to a quarter of its original value accounting for a strength reduction by heat effects.
- Failure of the cylindrical casing was calculated to 760 bar using Barlow's formula. It relates the internal pressure a pipe can withstand to its material strength and dimensions.
- Threads between casing and end caps will fail at approx. 2500 bar considering surface pressures of thread flanks of drive screws.

A slow cook-off trial can be differentiated into three distinct periods starting with heating to and holding at a specific temperature for several hours followed by heating with a rate of 3.3 K/h until first venting occurs, and the following period to the final chemical reaction. Each portion is modeled differently and concentrated on the center of the high explosive charge, i.e., micro damages or phase changes caused by thermal effects leading to different densities and porosities over time and vessel's radial dimensions are currently not considered. For the first period, an isochoric heating of the air inside the completely closed test vessel is assumed leading to a slightly increased pressure compared to ambient conditions. The ideal gas law is obeyed

$$p\left(t\right) = \frac{\theta\left(t\right)}{\theta_a} p_a \tag{3}$$

where θ_a and p_a are ambient temperature and pressure, respectively.

A pyrolytic model is applied accounting for the second period with increasing pressures resulting from gases produced by heat transfer in the oven and and self-heating of the explosive charge

$$\frac{\partial p}{\partial t} = \frac{R}{V}\left(\frac{\partial n}{\partial t}\theta + n\frac{\partial \theta}{\partial t}\right) \tag{4}$$

and

$$\frac{\partial n}{\partial t} = \beta \frac{\partial \alpha}{\partial t} \tag{5}$$

where n is the number of particles, p is the pressure, t is the time, R is the universal gas constant, V is the volume, α describes the reaction progress, β is a charge specific constant, and θ is the temperature. Parameter β is chosen such that the both temperature and pressure are reached at the time the glue fails and first venting starts.

For the third and last period it is assumed that temperature and pressure are relieved to ambient conditions as a result of gas venting through the vessel's end cap hole. Self-heating and chemical reactions

in the HE charge are ongoing, but slowed down due to lower temperatures and pressures. Equation (1) can be, therefore, applied for simulating temperatures while the following heat dissipation term is subtracted on its right side

$$Q_v\left(r,t\right)=\frac{A_v\Delta p\left(r,t\right)}{c}\frac{c_p}{V}\gamma\theta\left(r,t\right) \tag{6}$$

where A_v is the venting area, c is a characteristic velocity of the vented gases, Δp is the pressure difference between charge and ambient pressures, c_p is the specific heat capacity, V is the charge volume, γ is a simulation constant, and θ is the temperature.

Calculating pressures, Equation (4) is used again with a pressure dissipation term subtracted on its right side

$$p_v\left(r,t\right)=\frac{A_v\Delta p\left(r,t\right)}{c}\frac{c_p}{V}\theta\left(r,t\right) \tag{7}$$

Figure 9 displays simulation results of temperature and pressure curves in the center of a KS22 charge for the entire period of the trial. It shows a simulated temperature curve approximating well the measured one most of the time, while differences are observed after venting occurs. The measured temperature remains basically at ambient condition and is increased slowly only until a final chemical reaction is observed. The pressure simulation of the extended model provides a slight pressure increase compared to ambient conditions until self-heating starts. Self-heating of the charge leads to a temperature increase, gas generation, and an eventual pressure increase until the glue fails and venting through the end cap's hole starts. After a significant pressure drop to ambient conditions, is is increased rapidly until the casing fails as a result of the charge's chemical reaction. Constant β is chosen in a way such that temperature and pressures meet measured or expected values at this first venting event. Following temperature values are, however, overestimated, since a parameter γ could not be found for meeting both pressure and temperatures curves. This may be caused by thermal decomposition, subsequent ignition, and violent response to a burning or deflagration reaction of the explosive charge leading to a very sharp temperature and pressure increase or a temperature sensor that failed as a result of venting and / or such a chemical reaction.

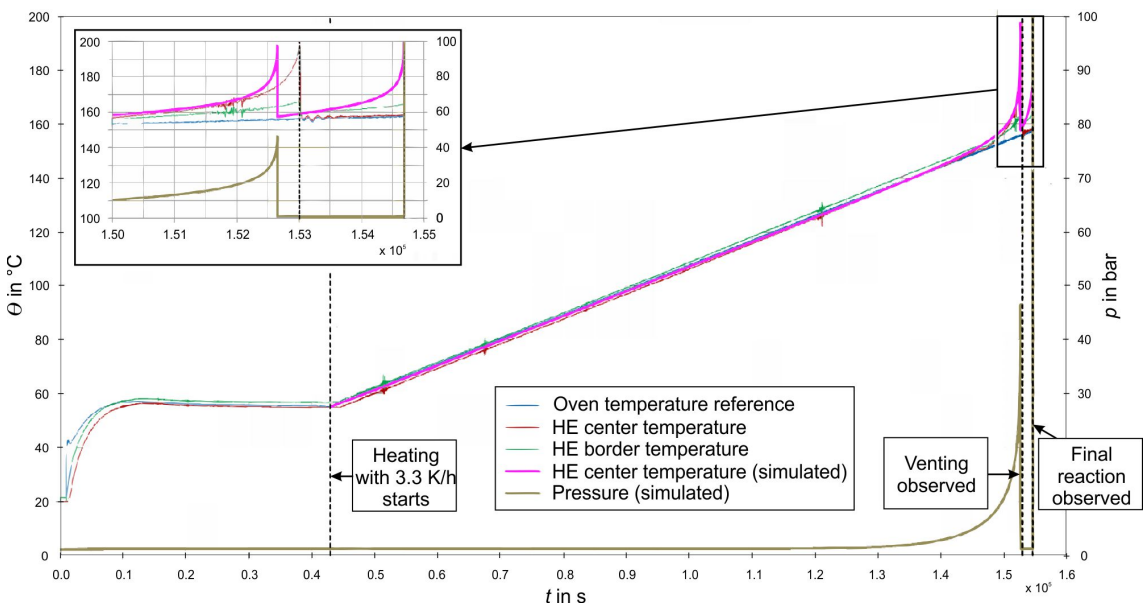


Figure 9. Simulating temperatures (magenta) and pressures (brown) in the center of a KS22 high explosive charge for the complete heating cycle. Measured curves are plotted for sensors located at oven, HE center, and HE border.

5 Conclusions

Results of this continued experimental and modeling slow cook-off study can be summarized to:

- TDWs standardized, confined SCO vessel allows small-scale tests to experimentally investigate the thermal sensitivity of HE charges and provide valuable temperature data for evaluating self-heating phenomena and supporting thermal modeling.
- Self-heating rates and times predicted with a multi-physics thermal model implemented into MATLAB (and COMSOL as well) match measured data of a KS22 charge.
- The model is extended to include a pressure simulation for the entire trial period. Simulated pressure curves meet approximated values at the events of gas venting through the end cap's hole and casing failure. This simplified approach can support the design of a warhead system and pressure mitigation measures for meeting IM requirements.

In future, it will be necessary to confirm these pressure simulations by applying pressure gauges inside and outside the HE charge and measuring spatial pressure distributions over time. It might also be helpful to measure the flow of reaction gases venting through the end cap's hole with a Prandtl tube. This will support verifying simulation models and adapting material specific properties. One interesting aspect in this field are micro damages, phase changes, or dissolution of the explosive charge caused by increasing temperatures and pressures and leading to increased porosities or changed material properties that may accelerate ongoing reactions. Another aspect may be to model the reaction progress also as a function of pressure since rate of decomposition is typically strongly dependent on pressure.

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