Insensitive Munitions & Energetic Materials Technology Symposium
April 23 - 26, 2018
Portland, OR

Thermal modeling of fast cook-offs

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Abstract

Being fully compliant to Insensitive Munitions (IM) requirements is of utmost importance for today's and future munitions. The IM approach as defined in AOP-39 is typically performed by using insensitive plastic-bonded high explosives (PBX) and assessing IM states and mitigation technologies on warhead system, munition, and, if necessary, munition packing level. Among other IM hazards listed in STANAG 4439, thermal stimuli through fast cook-off heating are usually of particular interest for large warheads and bombs, since they may strongly drive the warhead system design and shall be evaluated at the earliest opportunity.

A simplified approach applies a transient FE model in ANSYS with a typical flame temperature profile that allows predicting temperatures and times during a fast cook-off. Such investigations are used to evaluate potential areas of hot spot forming and critical components that may indicate the need for specific mitigation measures.

In a new approach, a reaction kinetic model originally developed for modeling self-heating of explosive charges at slow cook-offs and implemented into COMSOL is adapted for fast cook-off simulations. Differential scanning calorimetry (DSC) tests of small explosive samples at fast heating rates provide input data required. Parameters for self-heating of the explosive charge are derived with AKTS-Thermokinetics software fitted to such experimentally determined heating curves. This data is eventually implemented into COMSOL simulating fast cook-off behavior of full-scale warheads. This results in an accurate prediction of spatial temperature profiles as well as reaction times and temperatures. In addition, mitigation potential through intumescent coatings on the casing are assessed that provide an effective insulation layer and lead to significant reaction time delays.

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 fast cook-off studies investigate the heat transfer of a fire on test vessels through both experimental and modeling means, e.g. [2, 3, 4]. The influence of wind on flame temperatures in a large-scale experiment of a truck-sized nuclear waste transport package are reported in [5]. Recent thermal analysis and modeling efforts apply

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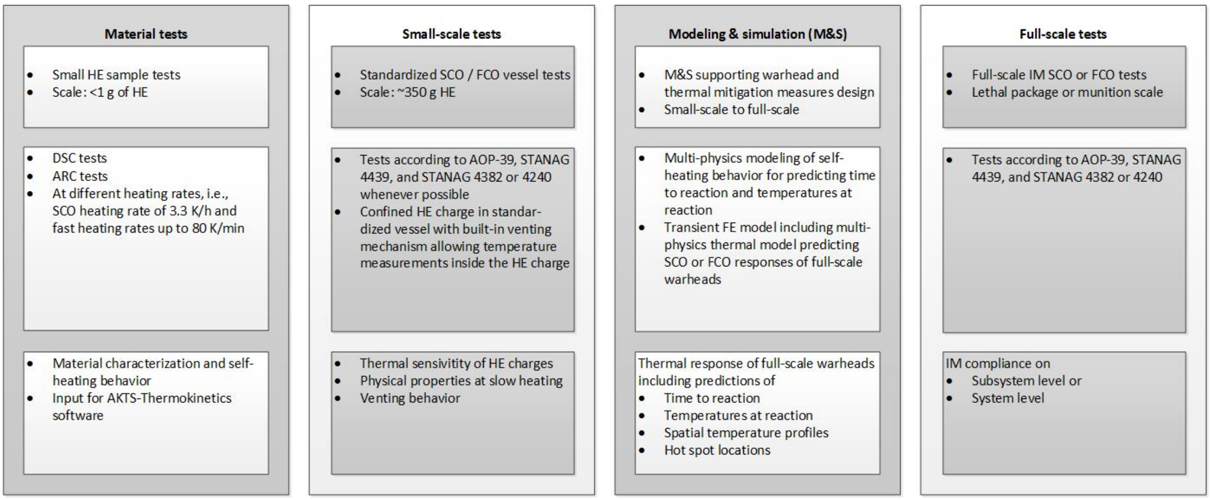
single-phase or multi-physics finite element (FE) models. Hunter et al. [6] couple an Arrhenius rate equation for self-heating with convection as primary heat transfer mechanism. In a multi-physics finite element (FE) approach using COMSOL [7], time-dependent temperature profiles of experiments with variable confinement cook-off tests (VCCT) and a 105 mm artillery projectile using melt-cast Comp B charges are predicted.

TDWs IM assessment approach for thermal stimuli as outlined in Fig. 1 is based on AOP-39 [8] 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. [9] Results of an experimental and modeling slow-cook off study using confined small-scale test vessels filled with various high explosive (HE) charges have been published in [10, 11].

This paper presents a modeling and simulation study of a full-scale MK-82 warhead filled with TDWs insensitive and blast-enhanced KS22 (RDX/Al/Binder 67/18/15) high explosive charge. The fast-cook off modeling approach with heat transfer from the fire into the warhead and Arrhenius reaction kinetics for the HE charge is described in detail. A simplified approach of transient FCO simulations without reaction kinetics using ANSYS Mechanical provides initial results of critical parts and components. In a new approach, a reaction kinetic model is implemented into COMSOL and adapted for fast cook-off simulations. It provides an accurate prediction of reaction times, temperatures, and spatial temperature profiles and allows assessments of potential mitigation technologies.

2 Thermal modeling approach

Heat transfer from fires into solid media takes place through by conduction, convection, and radiation. At fast cook-off tests, the test vessel needs to be fully surrounded by flames. This results in heat transfer through radiation of the gaseous-solid mixture as major part and an inward convective flux as minor part, while an outward convective flux into the atmosphere can be neglected. Within the test vessel, conduction acts as main heat transfer process. When certain conditions are met, energetic materials inside the test vessel start to react resulting in burning or even more violent reactions that depend upon the high explosive properties, as well as confinement and venting conditions. Figure 2 visualizes this general heat transfer process.



Material tests	Small-scale tests	Modeling & simulation (M&S)	Full-scale tests
• Small HE sample tests • Scale: <1 g of HE	• Standardized SCO / FCO vessel tests • Scale: ~350 g HE	• M&S supporting warhead and thermal mitigation measures design • Small-scale to full-scale	• Full-scale IM SCO or FCO tests • Lethal package or munition scale
• DSC tests • ARC tests • At different heating rates, i.e., SCO heating rate of 3.3 K/h and fast heating rates up to 80 K/min	• Tests according to AOP-39, STANAG 4439, and STANAG 4382 or 4240 whenever possible • Confined HE charge in standardized vessel with built-in venting mechanism allowing temperature measurements inside the HE charge	• Multi-physics modeling of self-heating behavior for predicting time to reaction and temperatures at reaction • Transient FE model including multi-physics thermal model predicting SCO or FCO responses of full-scale warheads	• Tests according to AOP-39, STANAG 4439, and STANAG 4382 or 4240
• Material characterization and self-heating behavior • Input for AKTS-Thermokinetics software	• Thermal sensivitity of HE charges • Physical properties at slow heating • Venting behavior	Thermal response of full-scale warheads including predictions of • Time to reaction • Temperatures at reaction • Spatial temperature profiles • Hot spot locations	IM compliance on • Subsystem level or • System level

Figure 1. TDWs IM assessment approach for thermal stimuli.

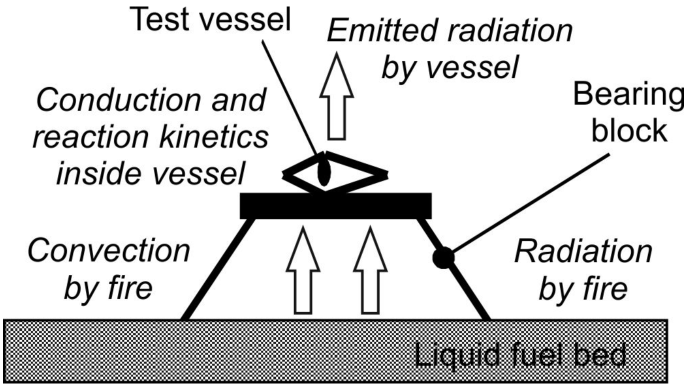


Figure 2. Schematic heat transfer process at fast cook-off tests.

Models simulating thermal responses can be mathematically described by coupling heat conduction with Arrhenius reaction kinetics via heat flux of the exothermal reaction [12]. Heat transport for thermal reactions of a high explosive charge can be modeled through a transient heat transfer equation in cylindrical coordinates r, since the test vessel is rotationally symmetric with its ends typically thermally isolated [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 heat flux, t is the time, and θ is the temperature.

Heat transfer into solid media by conduction, convection, and radiation is simulated with ANSYS Mechanical 15.0 [14] and COMSOL Multiphysics 5.3a [15]. The latter allows the use of a global equation model for implementing reaction kinetics. Quadratic shape functions are used for the Lagrangian elements. Temperature dependent thermal conductivities and specific heat capacities were used for most materials in the simulation. Various boundary conditions were applied to account for the heat exchange with the environment. The inward convective heat flux q_{con} from the atmosphere is defined by

$$q_{con} = h\left(\theta_{ext} - \theta\right) \tag{2}$$

where θ_{ext} is the ambient temperature within the atmosphere. The temperature dependent heat transfer coefficient h is determined using an analytical equation for the turbulent heat transfer through the gas media in the flame profile close to the boundary. The ambient-to-surface radiative flux is the difference between absorbed and emitted radiation and described by:

$$q_{rad} = \varepsilon\sigma\left(\theta_{ext}^4 - \theta^4\right) \tag{3}$$

where ε is the emissivity and σ is the Stefan-Boltzmann constant. Emissivity of the fire is one according to black bodies. Table 1 gives an overview on boundary conditions applied.

Multi-physics coupling to global equation (1) is realized by adding a volumetric heat source term Q through the following equation:

$$Q\left(r,t\right) = q\frac{\partial \alpha}{\partial t} = qA_\alpha f(\alpha)e^{-\frac{E_\alpha(\alpha)}{R\theta}} \tag{4}$$

Table 1. Thermal properties as boundary conditions and for energy release.

Material	Parameter	–	Value
Steel	Convective heat transfer coefficient	h in W/(m^2 K)	15
Steel	Surface emissivity	ε in 1	0.7
KS22	Effective reaction rate	q_{eff} in K/s	10^4

where q is the heat of reaction ($q_{eff} = \frac{q}{\rho c_p}$), $A_\alpha f(\alpha)$ 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. This reflects the self-heating of the system which is reproduced through internal heat generation coupling with model-free reaction kinetics.

AKTS-Thermokinetics software [16] was used to determine the corresponding functions for $A_\alpha f(\alpha)$ and $E_\alpha(\alpha)$ through differential scanning calorimetry (DSC) tests of small explosive samples with fast heating rates up to 80 K/min. Figure 3 shows these (normalized) curves for a KS22 charge. Further input data for simulations can be found in Tab. 2.

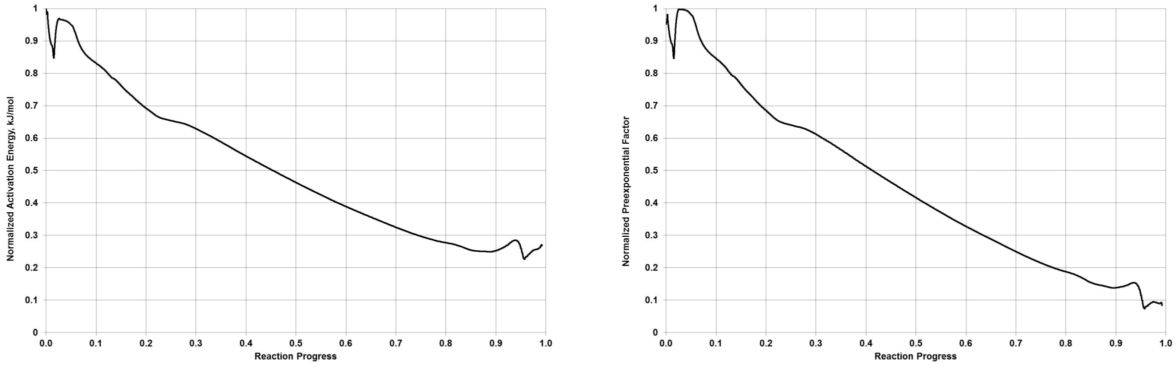
3 FCO simulations in ANSYS Mechanical

Transient FCO simulations of a MK-82 warhead were conducted in ANSYS Mechanical 15.0 [14]. A simplified approach without reaction kinetics was used assessing critical parts of such warhead designs and mitigation technologies within the scope of a prototype development phase. Figure 4 shows a simplified flame temperature profile applied for transient simulations.

Figure 5 visualizes a FCO response of the complete warhead and its high explosive charge after ten seconds. Due to the short time nature of such fast cook-offs, heat generated by the fire is absorbed primarily by the casing and the high explosive charge underneath. This high explosive charge made of KS22 features a comparably low thermal conductivity and, therefore, is effectively isolating the inner core within FCO timeframes. Maximum temperatures are, hence, observed in the HE layer directly underneath the casing. A fast cook-off reaction is expected being ignited within this layer.

4 FCO simulations in COMSOL Multiphysics

A more detailed analysis of FCO processes is possible using a multi-physics approach through COMSOL [15] with heat generation of hot spots forming and eventually inducing a chemical reaction. A flame temperature profile according to STANAG 4240 [17] as shown in Fig. 6 was applied enabling a predictive simulation capability. This temperature profiles reaches an ambient temperature of 550 degrees C after



(a) Normalized activation energy vs. reaction progress.

(b) Normalized reaction coefficient vs. reaction progress.

Figure 3. AKTS input data for a KS22a charge.

Table 2. Further input data for thermal simulations.

Material	Density ρ in kg/m^3	Thermal conductivity k in W/(m K)	Specific heat capacity c_p in J/(kg K)
Steel	7850	60.50	434
KS22	1650	0.40	1140
Coating A	270	0.25	840
Coating B	270	0.10	840

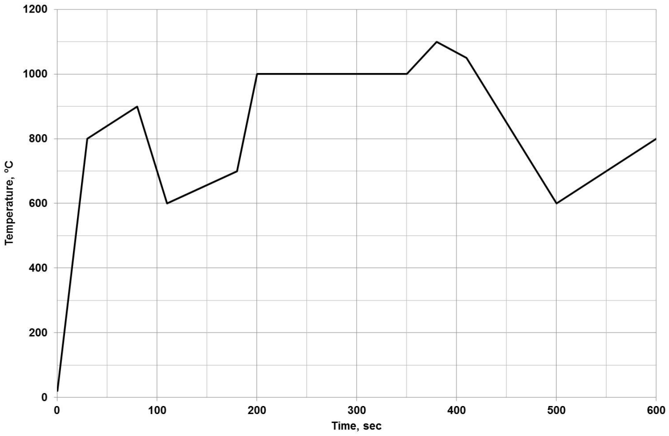
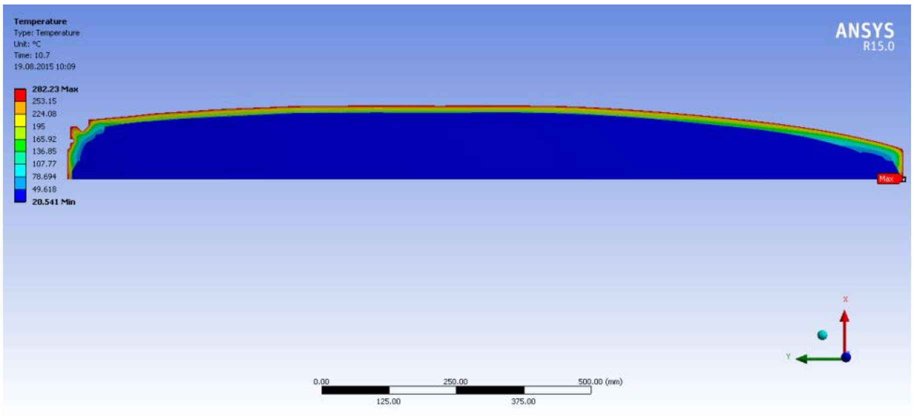
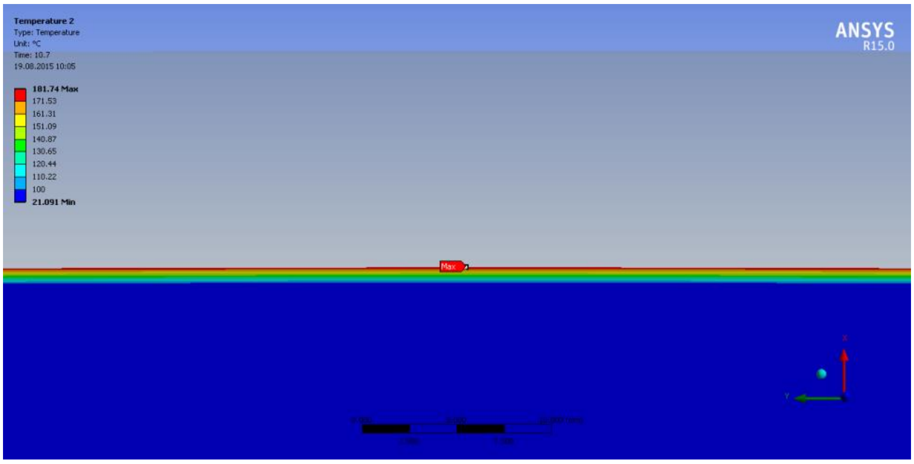


Figure 4. Flame temperature profile for transient simulations.



(a) Complete warhead.



(b) HE charge.

Figure 5. Resulting thermal FCO response of a MK-82 warhead after 10 seconds.

30 s and provides an average ambient temperature of 800 degrees C for the remaining test period as required.

A sensitivity analysis was performed of the simulation model regarding mesh sizes and numerical solvers as well as thermal boundary conditions for radiative and convective heat flux. Significant parameters such as surface emissivity of the casing and convective heat transfer coefficient were varied between 0.2 and 0.9 [2, 5] as well as 5 and 50 W/(m^2 K) [3], respectively. In addition, a simplified calculation of burning 4000 l of jet fuel for approx. 30 min results in approx. 15 W/(m^2 K) used as an estimate. The

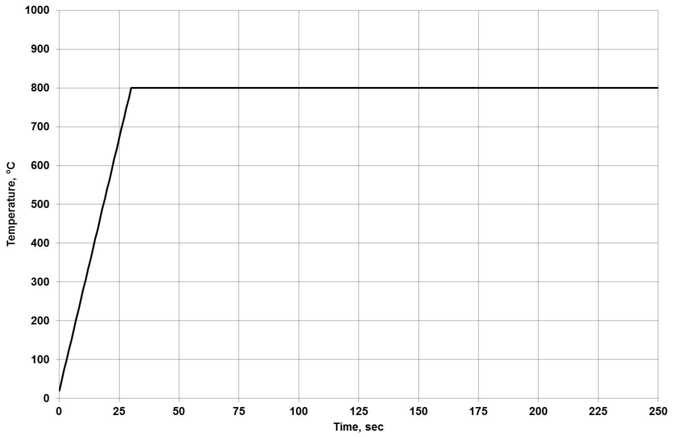
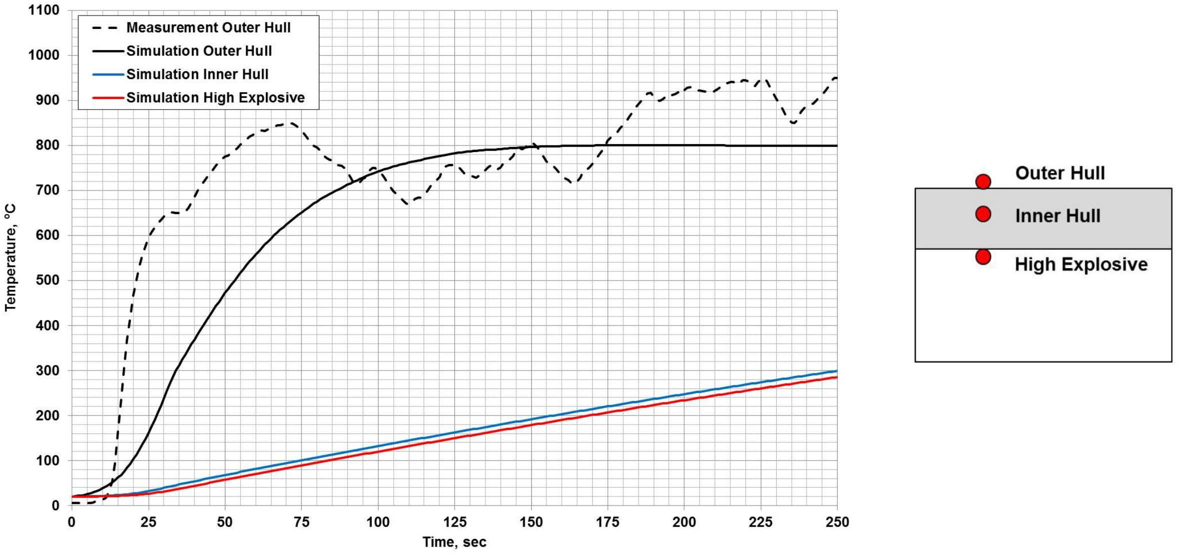


Figure 6. Flame temperature profile according to STANAG 4220 applied for COMSOL simulations.

analysis confirmed the earlier assumption with radiation as major heat transfer and revealed a significant impact of the emissivity on simulated casing temperatures, while the effect of the convective heat transfer coefficient was less significant. Last not least, values given in Tab. 1 were chosen for further simulations.

COMSOL simulation results excluding reaction kinetics are given in Fig. 7 with temperature-time profiles of gauge points located at outer casing, inner casing, and adjacent HE charge. It also includes a measured curve of a temperature sensor attached to the outer casing of a typical FCO test. Deviations between experimental and simulated data is relatively small reflecting results of the sensitivity analysis as discussed and considering random environmental conditions such as wind. Temperatures of the inner casing and inside the high explosive charge are significantly below the ambient temperature since this is based on the heat flux from gaseous to solid materials. Differences between temperatures of the inner casing and high explosive charge are small as a result of the high thermal conductivity of the steel casing compared to the HE charge.



(a) Simulated temperature-time profiles. (b) Gauge locations.

Figure 7. COMSOL simulation with temperatures at the outer casing, inner casing, and in the adjacent HE charge.

4.1 Applying reaction kinetics

An in-depth analysis of a COMSOL model including reaction kinetics was also performed. Figure 8 presents corresponding results of temperature profiles of the casing and within the high explosive charge as well as the reaction progress. A significant reaction progress is observed after 200 s through a significant increase in reactive heat in the outer layer of the high explosive charge. This results in a rapid temperatures rise at approx. 215 s with high explosive temperatures exceeding casing temperatures. This marks the event of an ignition of the HE charge leading to a reactive warhead output.

Figures 9 and 10 provide spatial temperature contour plots of a such a MK-82 warhead in 2D and 3D, respectively, at three different instances in time. They show well that heat is absorbed at the long cylindrical casing section and transferred to high explosive layers directly underneath. The major volume of the high explosive charge, however, remains unaffected at temperatures below 30 degrees C through fast cook-off time regimes of a few minutes.

4.2 Assessing mitigation potentials through coatings

Mitigation potential by intumescent coatings was assessed with thermo-kinetic COMSOL simulations. Thermal exposition results in a swelling of such coatings creating an effective barrier against the heat flux through a small heat transfer coefficient. The objective is to provide an additional time delay between 200 and 300 s until the reaction threshold is reached [9]. Two different coating materials of carbonizing foams were assessed considering a thickness of one millimeter of effective insulation layer. Material properties of this effective intumescent layer are given in Tab. 2.

Figure 11 provides thermo-kinetic simulations results of these coating materials. A reaction delay of less than one minute is obtained in case of coating material A. Coating material B, however, features better insulation properties resulting in delay times of approx. two minutes. Although these low-price materials provides an effective mitigation method, their application process is time-consuming and requirements for environmental temperature ranges and life times may be critical.

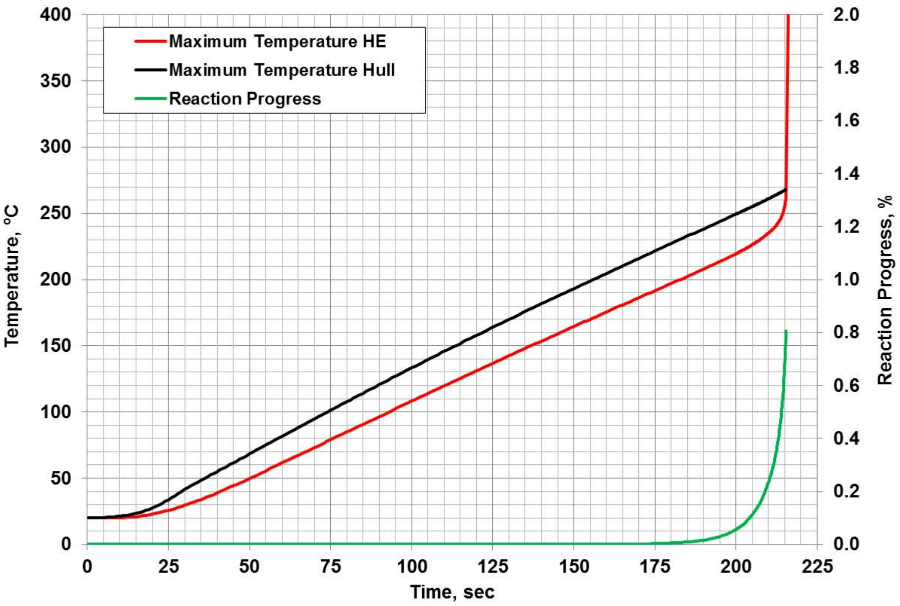


Figure 8. Temperature-time profiles showing formation of hot spots and resulting steep temperature increase in the HE charge.

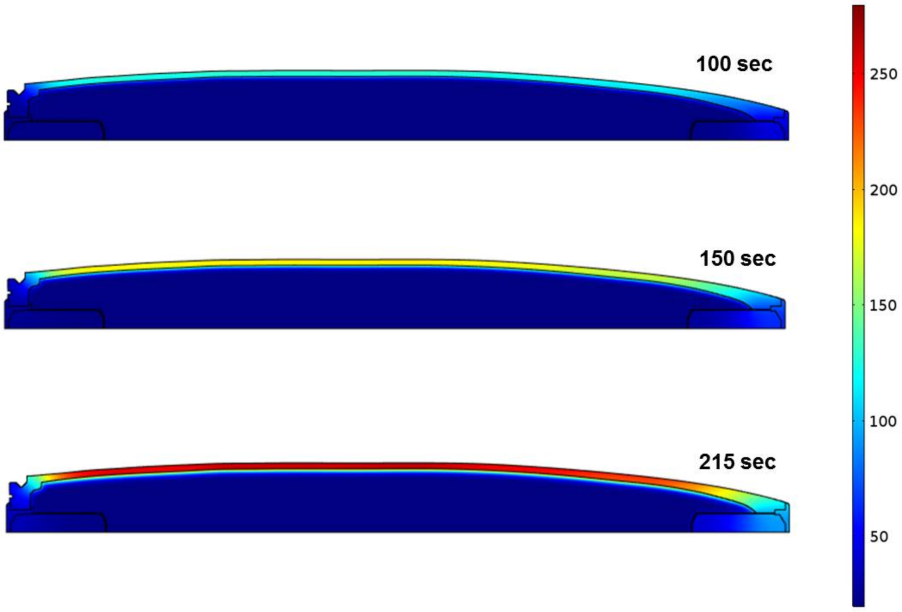


Figure 9. 2D contour plots of spatial temperature distributions (in degrees C) of a MK-82 bomb at different instances in time.

5 Conclusions

A fast-cook off modeling and simulation study was performed using at first a simplified thermal model without reaction kinetics that was implemented into ANSYS Mechanical and allowed an initial assessment of critical parts and components of warheads. A new modeling approach including reaction kinetics using COMSOL Multiphysics provides an accurate prediction of spatial temperature profiles and hot spot forming of full-scale warheads. This allows prediction of reaction times and temperatures and allows, in addition, an assessment of potential mitigation technologies such as intumescent coatings. These thermal models can be easily applied to other full-scale warhead systems allowing a prediction of their IM conformance.

In future, applying temperature sensors inside or underneath the casing and inside the high explosive charge of small-scale or full-scale test vessels will allow further verification and optimization of thermal simulation models. Resulting effects such as burning or deflagration reactions may be predicted by including conservation equations and considering gas pressures and the mechanical behavior of inert warhead components in simulations.

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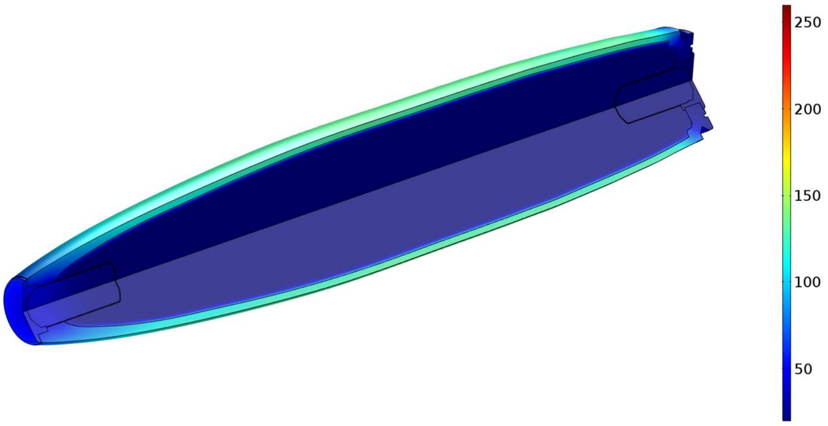
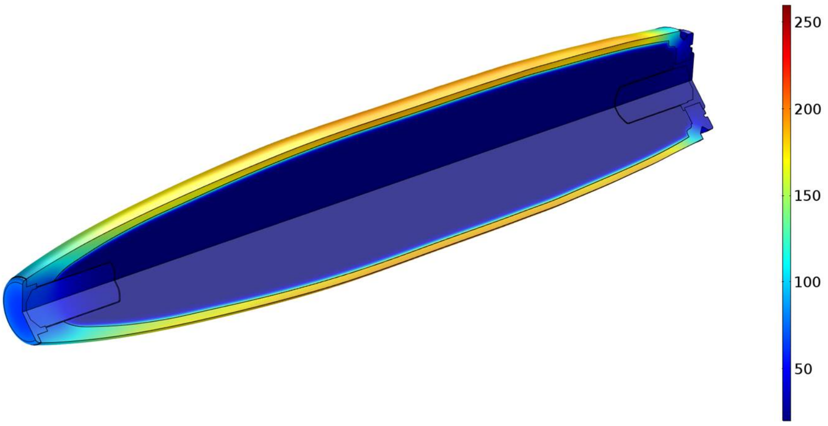
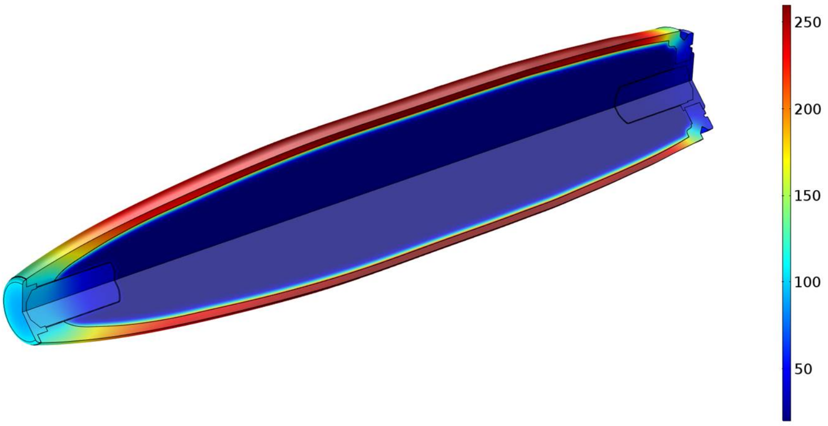


(a) After 100 seconds.



(b) After 150 seconds.



(c) After 215 seconds.

Figure 10. 3D temperature plots (in degrees C) of a MK-82 warhead simulated with COMSOL.

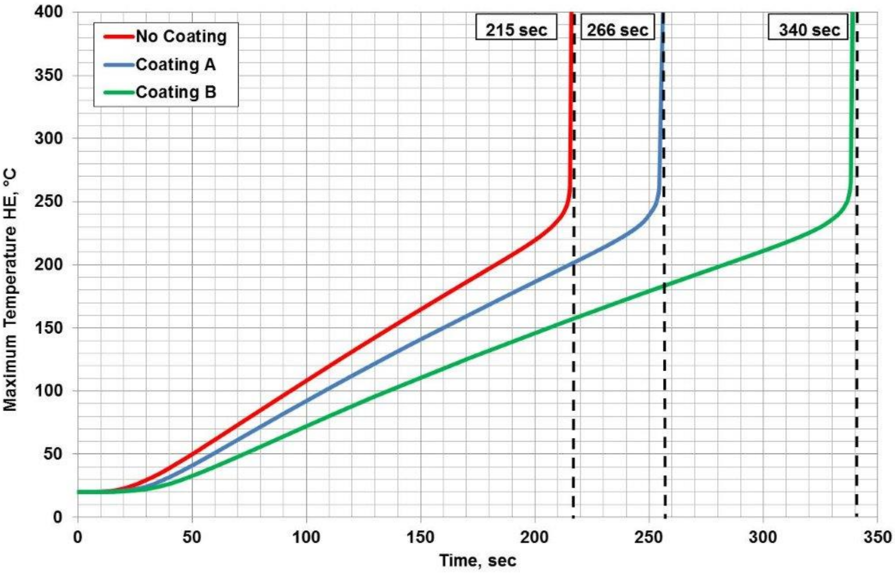


Figure 11. Temperature-time profiles showing effects of coatings applied on MK-82 bomb casings.

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