Modelling Cook-Off

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1. Introduction

European manufacturers involved in the design of munitions participate in the IMEMG association to promote insensitive munitions. The IMEMG Expert Working Group “computer modelling” builds up a map where computer models would be of assistance to design such munitions and to demonstrate their intrinsic insensitivity to STANAG stimuli. The group reviews the availability, the applicability and the capability of existing models, and then completes a gap analysis of the available computer models.

Models are used in the manufacturer community to design and develop new systems to, demonstrate their safety and for the assessment of insensitive munition labels, evaluate collateral damage, design ignition trains, improve processing and manufacturing technology, propose innovative packaging and study ageing of the systems. The group is focused on high explosives, propellants and pyrotechnics.

Previous works of the EWG have shown the lack of knowledge on the parameters which are needed as input for the different constitutive models, equation of state or reactive models. Data is available for few models and the testing to gain such data for models requires considerable effort and complex test facilities. The group has selected two open software tools to be share among the IM community: TEMPER (NATO MSIAC) and FDS (NIST) [1-2]. Group members also use other commercial software such as FLUENT, ABAQUS, COMSOL [3-5].

One of the recent works of the group have been focused on a gap analysis about modelling of the cook-off phenomenon based on the expertise of the members of the group and references available in the literature. The result of applying this expertise is detailed in the second part of this paper.

The third part of the paper is devoted to the numerical possibilities based on AOP-39 flowcharts [6]. This analysis clearly shows the regimes where modelling could be of interest and also domains of uncertainties and lack of models.

The last part of this paper gives some feedback from the IMEMG experts on the use of the open software tool FDS for the simulation of fires and thermal boundary conditions around munitions.

2. Gap analysis

Before ignition due to Cook-Off, a series of complicated events occurs [7]. In principle, each of the contributing processes is well understood. Scientists from various disciplines work on the modelling of phase transitions, such as melting, modelling the chemical reactions with full or reduced complexity, modelling material damage and material ageing. In each discipline, experiments are performed to advance the understanding of the processes and to obtain parameters of the models.

There are various approaches how all these models are combined in a computational simulation. The approaches range from high-complexity microscopic (quantum chemistry, molecular dynamics) to full scale engineering approaches. There are multi-scale approaches that couple different levels of detail within the same simulation. Even though it is agreed that the microscopic models offer the most fundamental description of reality, they are restricted to very small samples because the feasible computational effort is bounded by the available hardware.

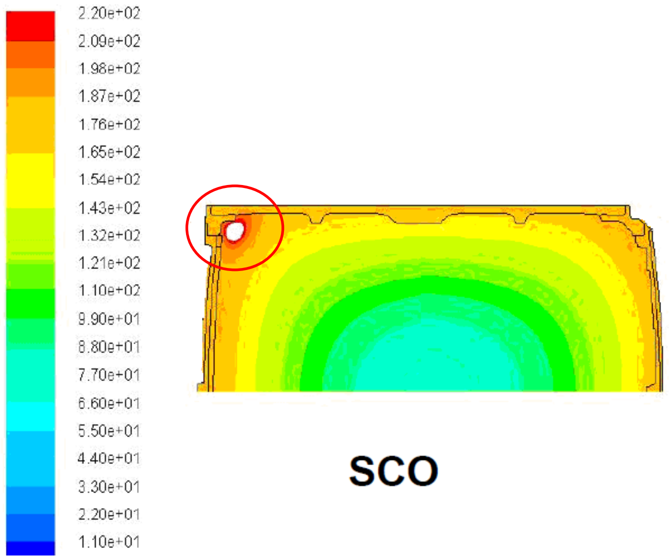

Figure 1: Determination of the location of ignition (white zone) into a munition submitted to a STANAG 4382 Slow cook test off using the FLUENT computer fluid dynamic code to optimize the design (thanks to Pablo Bernardez and Victor Benito from EXPAL). Colours refer to temperature in Celsius.

2.1. Gap: small scale vs. AUR

One of the knowledge gaps identified by the community is that the relation of small-scale testing to all up round (AUR) is not known very well. Such knowledge is important for both, experimental assessment and theoretical modelling. In both cases, testing and simulation, it is much easier and cheaper to avoid the complexity of the AUR and do small scale trials instead. Rigorous methods or formulae to estimate the reaction of the AUR from a small-scale test are not known. Neither is a database of small scale and related AUR test that would permit the derivation of empirical models on that topic.

As an example, DSC (differential scanning calorimetry) characterization techniques can be used to obtain accurate and complete chemical kinetic models for energetic materials. However, the size of the sample (few mm^3) can yield erroneous data or many discrepancies depending on the percentage of the binder/crystal that was in the sample and which differs from the macroscopic and homogeneous part. These differences yielded an incorrect prediction of the time to initiation of a rocket motor and then an accidental event.

2.2. Gap: Properties at/near ignition

Owing to the short timescale of the processes just prior to ignition, there are knowledge gaps on the material properties at this stage. All experimental efforts need very sophisticated techniques to allow reliable measurements to capture high speed phenomena.

Work is in progress to investigate the chemical reaction kinetics in more detail and to compare phenomenological kinetics (few stages) to extremely complete ones (few hundred stages). The physical (thermal, mechanical) properties just prior to ignition are topics of recent experiments. Also, the shape of the energetic component can change for unconfined material such as propellant due to pyrolysis and foaming. It was also observed in experiments that damage evolution (e.g., micro- and macroscopic crack growth) plays an important role in ignition.

However, these effects are not included in current computer models. In general, the modelling of the properties at ignition is at an early stage (at best).

2.3. Gap: What happens after ignition?

In general, the modelling community is quite confident about the prediction of the circumstances of ignition (when, where and under which boundary conditions). Of course, the knowledge of the exact thermal flux contours around a munition submitted to a fire (for example during the STANAG 4240 test) is still studied to improve the description of the thermal boundary conditions. To help such determination, the software tool FDS could be of interest.

In contrast, it is very hard to predict what happens after ignition (thermally damaged material, phase change, coupling between the gas released by the combustion and the fragmentation of the case). Particularly, one would like to know, whether there is slow burning, a deflagration or even a detonation. Obviously, such predictions are very valuable for the IM engineer. Currently there are no generally accepted models for such predictions. There are experiments in progress to systematically study DDT (deflagration to detonation transition). Such experimental data may result in empirical models in the near future.

It is pointed out, that the problems for modelling are related to the (often neglected) mass transport in the materials due to the intrinsic permeability of energetic materials. Additional complications arise from the fact that ullage, voids and cracks, the latter being yielded by the heat and the differential dilation of materials, seem to play an important role in the process. Voids and cracks emerge right at the time of reaction in a stochastic way and are notoriously hard to model.

2.4. Gap: Violence / What happens after reaction?

Even if our modelling correctly predicts the type of reaction, it is still challenging to quantify the violence of the event. It is generally agreed that violence is a monotonic function of pressure. Since pressure is force over area, it is understood that violence can be diminished by lowering the force of the event or by enlarging the area the force acts on.

In live testing, it proves to be very hard to measure the pressure inside and outside of the sample. Consequently, it is hard to calibrate or verify our computer model with such experiments even though pressure is easily available everywhere in the computational domain.

While fragments often pose the biggest threat, modelling natural fragmentation is very challenging and not generally trusted. While fragment tracking is easy in principle, it is rarely included in computer models. Prediction of the fragment mass and velocity is possible in case of detonation (for example using SPLIT-X [8], confirmed and compared using finite element codes as ABAQUS or LS-Dyna [9]). EDEN [10] enables simulating the whole event from the propagation of detonation to the prediction of the mass and velocity of the fragments. Temperature of the fragment is also determined.

The violence of reaction of rocket motors is quite different from all other devices, such that the usual violence metrics do not fit very well. A cause comes from the unknown geometry of the energetic component at ignition due to the initial bore collapsing and material foaming.

2.5. Gap: Benchmarks / What to compare with an experiment?

The confidence in the results of computer models could be improved by far if there was a collection of benchmarks agreed to by the community. Such benchmarks should come in the form of experiments and results ranging from small to full-scale tests.
Candidate quantities are temperature, time to initiation, location of initiation, pressure, expansion of the casing, fragment velocity, size and mass; these quantities being either difficult to calculate and/or measure.
However, there is no consensus in the community on which quantities from the computer-models should be compared to which experimental quantity.

3. A map of model possibilities using AOP-39

Allied Ordnance Publication AOP-39 [6] provides guidance on the assessment and development of insensitive munitions (IM). The process for determining the response level of a munition to each IM threat is based on the hazard assessment protocols. These protocols are ordered procedures described, in Annexes C-F, by a flowchart through which modelling can be applied.
In the Annex C dedicated to fast and slow heating, the simplified protocol given in Figure 2 helps to determine the response level of a munition based on an overall review of physical mechanisms that may occur during cook off.
According to STANAG 4439, no response more severe than Type V (burning) is required for the slow and fast heating threats. Therefore, under this assumption, a simplified modelling approach could be applied in considering that simulations are expected to mainly determine the time to initiation, the location of the initiation and the conditions of deconfinement. From a numerical point of view, these data can be easily obtained by using common computer models. Moreover, the question about the normal surface regression can be answered by using experiments (closed-bomb, combustion in a heavily confined tube…), data on similar munitions or expert analysis.
The location of ignition gives an indication of the possibility of an abnormal regression. Ignition into the bulk can yield a violent reaction, while ignition at the boundary, with the help of deconfinement of the casing, typically results in normal regression.
Propulsion can also be predicted using suitable calculation codes. Consequently, designing munitions in order to ensure deconfinement (deconfining device, self-deconfinement, fusible material before reaction can be achieved by using this simplified approach.
In contrast, the use of computer models to study and predict Type I to Type IV responses is most challenging. Indeed, the modelling approach is confronted with two main difficulties. The first one concerns the ability of burning models to adequately describe the evolution of

the explosive material in the case of a volumetric reaction compared to a normal surface regression. The second difficulty is related to the deflagration-to-detonation Transition (DDT) mechanism. This open topic has been widely studied experimentally and numerically. However, to our knowledge, quantitative criteria have not yet been established to predict DDT. Moreover, several DDT models are proposed in the literature, but none of them is implemented in a commercial code. Yet these issues are essential to the determination of thermal and mechanical loadings which will drive the deformation of munition inert materials. From there, modelling methods are able to estimate the failure of munition inert components and consequently the resulting fragment characteristics (size, mass, velocity) needed to define the response level.

Lastly, all computer models need input parameters to conduct simulations. These parameters are usually identified from experimental data. Annex C of AOP-39 [6] provides two tables (C-1 and C-2) which give examples of data required to analyze fast/slow heating and tests that can be used to generate the required data for each mechanism. These tables can be applied to define the characterization of model parameters for inert and energetic materials

In conclusion, the simplified protocols proposed in AOP-39 can help to establish a map of model possibilities for each of the IM threats.

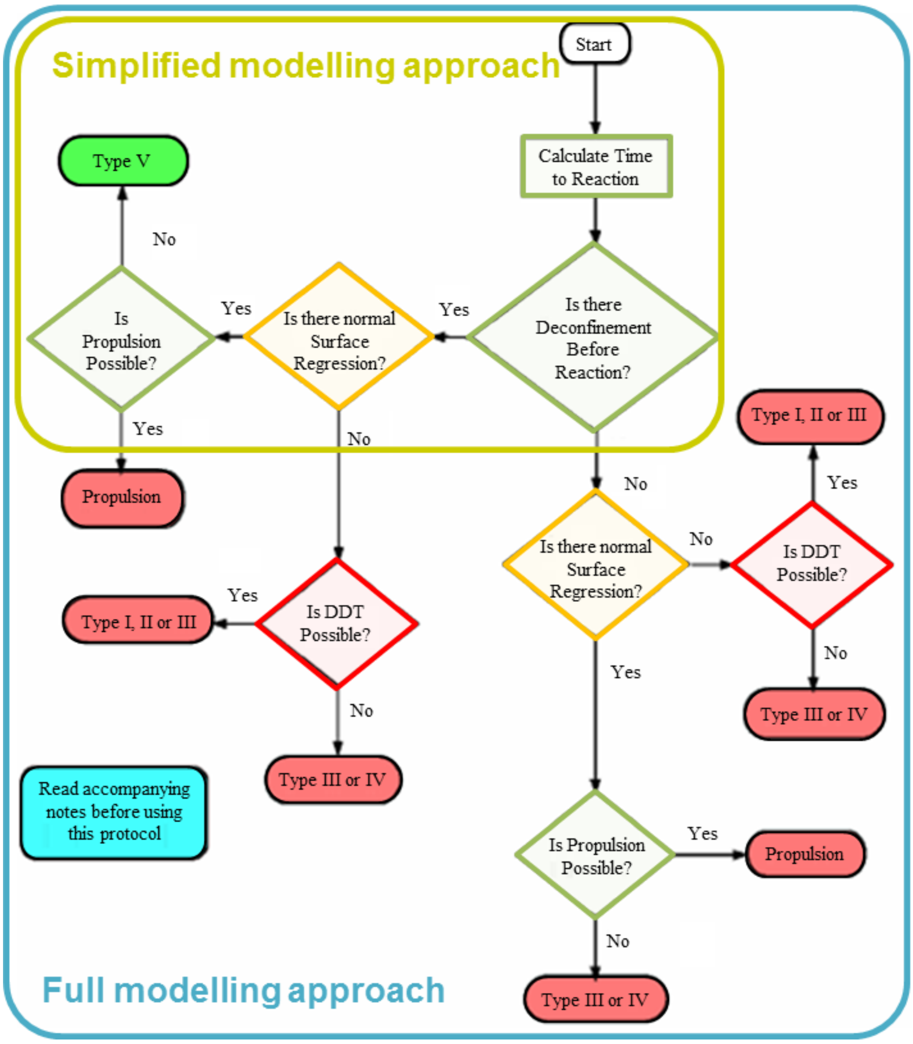

Figure 2: Simplified hazard protocol according to AOP-39 Annex C Fig C-1. Green squares, rhomboids or lozenges indicates that common computer models are available, orange ones indicate case-by-case analysis supported by experiments and red ones refer to scientific domains with few available models.

4. FDS: evaluation for cook off prediction

The FDS (Fire Dynamic Simulation) software tool can be downloaded from the internet [2]. The software has been used in the IM community to evaluate the boundary thermal conditions of munitions submitted to different fires. FDS was evaluated as a candidate to determine thermal gradients between the top, bottom and also axially across the munition. The aim was to determine convective and radiative fluxes. The main feedbacks of the users (including the conclusions from the IMEMG EWG on Fast Cook-Off) were:

- Curved structures are not well meshed except very fine mesh (which is increasing the cost of the simulation and requires large scale computation).
- The results on heat fluxes are currently unconvincing and are still under study.
- Many turbulence models are provided in FDS making the choice difficult for an engineer.
- A mesh-dependence of the temperature was highlighted.
- The influence of the combustion model was also discussed.

It does mean that FDS can only be used to qualitatively determine the boundary conditions except making large scale simulations. Some of the companies of the IMEMG association are turning their attention to STARCCM+ [11], FLUENT (CFD codes) or to OPENFOAM [12].

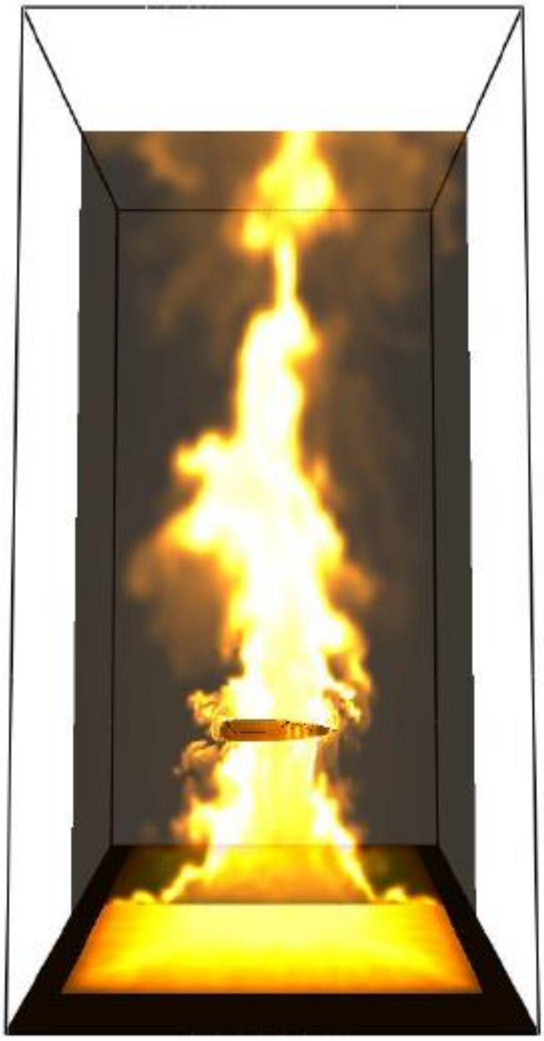

Figure 2: Simulation of a 155mm munition submitted to a fuel fire (thanks to Paul Locking from BAE Systems Land UK) using FDS.

5. Conclusion

European manufacturers take advantage of the IMEMG Expert Working Group to share data and information about up-to date models and computer solutions to help the design of their pyrotechnic systems and for the assessment of safety objectives (Insensitive Munition Signature). This paper has been devoted to cook-off scenarios.
The prediction of the development of violent reaction (burning, deflagration and/or detonation) remains hardly tractable. The logic sequence provided in the fourth part of this paper has re-emphasized that the deflagration-to-detonation transition is still an open question.
The gap analysis provided in the second part of the paper shows that many topics remain on the table for the engineer who tries to model a system in a fire.
However, today computer modelling as part of the IM design process predicts ignition time and location with a good level of confidence. These results and the expertise of the teams help to determine the level of reaction.

6. References

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