Mathematical Modelling of Energetic Materials, 3/4 December 2019

## Schedule

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| Tuesday | 13:15 | Introduction |
| | 13.30 | Ernest Baker<br>*High explosives: shear initiation, low velocity impact, slow heating rate effects and burn rate behavior* |
| | 14.35 | Robert Timms<br>*Asymptotic analysis of shear in energetic materials* |
| | 15.20 | coffee break |
| | 15.50 | Sally Said<br>*Modelling the combustion of explosives* |
| | 16.10 | David Torkington<br>*Mathematical models of shear band formation in high explosives* |
| | 16.30 | Kieran Quaine<br>*Finite element methods for the modelling of explosives* |
| | 18.30 | Workshop dinner<br>Blonde, 75 St. Leonard's Street, Edinburgh, EH8 9QR |
| Wednesday | 9.00 | Didier Picart<br>*Ignition of plastic bonded explosives submitted to low velocity impacts* |
| | 10.05 | Frank Smith<br>*On combustion of explosives: computations, analysis and comparisons* |
| | 10.50 | coffee break |
| | 11.20 | John Curtis<br>*Modelling HEVR at AWE* |

## Abstracts

**Ernest Baker** (Munitions Safety Information and Analysis Center, NATO HQ)
*High explosives: shear initiation, low velocity impact,*
*slow heating rate effects and burn rate behavior*

**Bio:** Dr. Baker (USA) joined the NATO Munitions Safety Information and Analysis Centre (MSIAC) in Brussels, Belgium on 1 June 2016 as the Technology Specialist Officer for Warheads Technology. Dr. Baker supports the MSIAC member nations with munitions science, technology and analysis supporting safety and insensitive munitions (IM) policy, standards, manufacturing, and development. Dr. Baker retired from the US Army Armament Research, Development and Engineering Center in May 2016 after over thirty years. He was the Senior Research Scientist (ST) for Insensitive Munitions (IM) and was strongly involved in the US DoD Joint IM Technology Program. Dr. Baker was also an adjunct professor of Mechanical Engineering at Stevens Institute of Technology.

**Abstract:** Dr. Baker's presentation includes a short narrative of his career and an overview of the NATO MSIAC. Dr. Baker will then provide technology overviews on high explosives experimentation and modeling for shear initiation and low velocity impact initiation. Dr. Baker will then provide overviews on the effect and standardization of slow heating rates on ignition and burn rate behavior of high explosives.

**Didier Picart** (CEA, DAM Le Ripault, Monts)
*Ignition of plastic bonded explosives submitted to low velocity impacts*

**Bio:** Mr Didier Picart received a PhD from the Université Paris 6 and from the Ecole Normale Supérieure de Cachan in 1994. He joins the Explosive Division of the CEA in 1994. In 2004, he has obtained the Habilitation Diriger des Recherches, the last degree required to reach academic research laboratories.

From 1995 until 2005, he managed a team in the field of the modelling of the mechanical behavior of High explosives, constitutive modelling and numerical simulations. He is now in charge of researches about the mechanical behavior of High Explosives and their safety (low velocity impacts, DDT). He has published more than 30 papers in international journals and has participated to 27 international conferences. He has been invited to the 2014 session of the Gordon Conference and chaired sessions during the 2014 Detonation Symposium, EUROPYRO 2015 and IMEMTS 2019. Lastly, he had co-organized the Workshop on Explosives (Tours FRANCE, 2015) and chaired a two-day session devoted to modelling during the MSIAC workshop on cook-off (Atlanta USA, 2016).

He managed a group of French manufacturers to provide national standards (AFNOR) for the characterization of the mechanical properties of energetic materials and to give requirements to improve the NATO STANAG. He is a member of the Insensitive Munition European Manufacturing Group (chairman of the Expert Working Group "Computer Modelling").

**Abstract:** The combustion to deflagration or detonation phenomenon in HMX-based pressed explosives is still poorly understood and as a result badly predicted today. Safety studies of pyrotechnic structures find benefit from a prediction of ignition conditions preliminary to any runaway of the reaction. We are interested here in the case of moderate mechanical impulses such as falls or impacts that do not directly lead to a shock-to-detonation transition.

Impact-induced pyrotechnic events are very complex phenomena, whose interpretation is hindered by difficulties coming from (1) the complexity of the dynamic loading, (2) the crucial role played by the non-linear behavior of the PBX, (3) the coupling of physical phenomena involving simultaneously deformation, self-heating, thermal conduction and chemical heat release and (4) the so-called but still unknown "hot-spot" process.

Therefore, any prediction of the full pyrotechnic event, including its violence, remains out of reach at present. We are only considering ignition rather than pyrotechnic reaction. This talk will present a numerical tool including our state of knowledge of the dynamic mechanical behaviour of our PBXs, the principles of the hot spot model development and a simplified heat equation. We evaluate the capabilities of the numerical tool for a large range of realistic impact scenario including drop-weight tests, Susan-tests, Steven-tests and a Taylor-test. The discussion highlights the relative good agreement between data and simulations as well as the future works that remain to be done.

**John Curtis** (AWE & University College London)
*Modelling HEVR at AWE*

A very brief review of explosives is followed by the requirement to understand by modelling their response to mechanical and thermal stimuli. Some of the AWE experimental tests are described. The HERMES model for mechanical insults is introduced and it is shown how results using it have highlighted the potential importance of shear bands. Then some of the modelling of thermal stimuli is described. First the One Dimensional Time to Explosion Model (ODTX) is presented and then modelling of Deflagration to Detonation Transition with HERMES is shown, to highlight how burns can lead to detonation under the right conditions. The talk ends with discussion of modelling issues arising with shear and combustion.

**Kieran Quaine** (Heriot-Watt University)
*Finite element methods for the modelling of explosives*

This work is concerned with efficient and reliable numerical methods for challenges encountered in explosives, such as the modelling of runaway reactions and shear bands. Shear banding is a strain-localisation phenomenon expected to play a role in HMX plasticity. An applied stress is relieved by plastic flow in narrow regions (the shear bands), which leads to a localised energy release and may be associated with hot-spots and other regions of localised heating that can lead to ignition.

To more fully understand and quantitatively predict the key mechanisms of the onset of a reaction in a high explosive, caused by mechanical deformation, we require numerical methods to represent the extreme localised thermal and mechanical effects in shear bands. Current hydrocodes like LS-Dyna and ALE3D at AWE and LLNL struggle to represent these.

In this talk we will present two different finite element methods for the reliable computation of extreme physical problems. We discuss the challenges of traditional methods with blow up problems and localised features such as shear bands and how adaptive or enriched finite elements can be used to address these.

**Sally Said** (University College London)
*Modelling the combustion of explosives*

When an explosive burns, gaseous products are formed as a result. The interaction of the burning solid and gas is not well understood. More specifically, the process of the gaseous product heating the explosive is yet to be explored in detail. The present work sets out to fill some of that gap using mathematical modelling: this aims to track the temperature profile in the explosive and the gas response.

The work begins by modelling single step reactions using a simple Arrhenius model. The model is then extended to include three step reaction. An alternative asymptotic approach is also employed. There is close agreement between results from the full reaction-diffusion problem and the asymptotic problem.

Building on the above, a first gas model is a sequential scheme which accounts for gas created in the system. Here we track the temperature of the gas produced from the reaction. This model is to be extended to a continuous framework where we solve the equations numerically and possibly apply asymptotic analysis also.

**Frank Smith** (University College London)
*On combustion of explosives: computations, analysis and comparisons*

The interest here arises within a model of interaction evolving between thermal diffusion and one or more reactants, based on a simple Arrhenius representation. The single-step case is examined first for one spatial dimension and time. The typical values of certain parameters involved in the interaction are found to be extremely large or small, a feature which points towards the use and potential benefits of asymptotic analysis. The main extreme parameter is the effective diffusion coefficient and this leads early on to thin layers being produced near the ends of the spatial domain and a core in between. Core temperatures then can become very large. Later times see a gradual cooling down. The influences of other parameter values also turn out to be considerable. The three-step case is examined subsequently. Likewise the extension to incorporate substantial gas effects is under consideration. Overall comparisons of the analytical and computational results show quite close agreement over a wide range of the parameters.

**Robert Timms** (University of Oxford)
*Asymptotic analysis of shear in energetic materials*

Shear localization is often suggested as a potential accidental ignition mechanism in explosive materials, giving rise to so-called hot spots. In this talk, I will highlight a number of problems related to shear in explosive materials. As a more detailed example, a one-dimensional model for the initiation of shear bands in a reactive material will be discussed. The model accounts for thermal softening, strain hardening and strain-rate effects, and also considers heating due to chemical reaction via an Arrhenius source term. In the analysis, the thin zone of localization is identified as a boundary layer. It is found that the behaviour of the perturbations to the temperature, stress and strain hardening variable in the localization zone are governed by four dimensionless parameters which are known in terms of various material properties. The analysis highlights key physical quantities that control the reactive shear banding process and demonstrates how asymptotic techniques can give deeper insight into the mechanisms responsible for the accidental ignition of reactive materials.

**David Torkington** (Heriot-Watt University)
*Mathematical models of shear band formation in high explosives*
Shear bands are localised regions experiencing high strain rates. Shear banding is known to be an important mode of failure in granular materials and polymers, and many explosives consist of granules bound together by polymers. The high stresses in shear bands can produce hotspots through viscous dissipation, and so shear bands pose a significant threat to safety. We present a one-dimensional model of shear bands using a bi-viscous rheology, including precise asymptotic analysis describing the growth of a shear band. We also introduce a recent quasi-one-dimensional model of shear bands that accounts for the pressure drop across the material.