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A Review of Computer Models to Aid the Design and Assessment of IM Performance

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ABSTRACT

Nine permanent members of seven nations contributed to the progress of the group. In total eight meetings were arranged. During the meetings several visits to local facilities and test centres were organised; sometimes live IM tests could be witnessed. Each participating company presented its own methodology for IM scenario simulation. The product portfolios of the participating companies cover a broad field from igniters, shells, safety and arm units, warheads to missiles and also packaging. The IM threats for these various products are not all of equal significance and therefore most companies have put their own specific emphasis on different computer models. In this way the participants learned that for example thermal threats specifications can be met easier for warheads - existing mitigation devices can be integrated to guarantee moderate reactions. On the other hand, the propellant of missiles is very sensitive to elevated temperatures and can react very violently after decomposition started. Simulation of the Slow Cook Off aggression for energetic materials requires therefore good understanding of reaction kinetics.

According to the field of modelling (thermal, high speed mechanics), one of the problem which has been outlined is the lack of knowledge on the parameters which are needed as input for the different constitutive models, EOS or reactive models. Actually data are only available for few well known materials but for specific materials, the tests to retrieve such data or models require considerable effort and complex test facilities. It is also quite important to review the methodology how these material and behavior models and their parameters that are determined by particular laboratory tests are implemented in the analysis models.

Computer modelling covers the use of spread sheets, analytical models, in-house codes and very often the application of software tools that are based on Finite Element or Finite Volume theory - so called CAE tools. Usually these models are not truthfully predictive unless they have been adjusted to experimental results. There are many specialised applications. They are applied when simulating high speed events like bullet impact or shock transition but also when transient processes like heat transfer, burning or pyrolysis are studied.

Two quasi-open software tools, Fire Dynamics Simulation (NIST) and TEMPER (MSIAC), have been evaluated and checked for possible use within the participating companies. Pros and cons have been determined. A list of software tools as they are used by the participating companies for IM simulations has been prepared, their capabilities and fields of applications have been presented and assets and drawbacks were highlighted.

Several members of the Expert Working Group performed a gap analysis with respect to their capabilities in simulation of IM scenarios. After identifying the status quo a projection of future activities and necessary capabilities has been carried out. Most members predict a challenging increase of simulation in the fields of IM. All presentations held during the meetings are enclosed in this report.

This EWG proved that it is possible to exchange knowledge between collaborating companies even in fields where advances can be a decisive factor for business development. Though the topics are sensitive, the questions that have to be answered are very similar for many companies. This EWG served as a link between European companies which allowed some insight into the activities of IMEMG partners with respect to computer modelling in the fields of IM.

This review is only a first step for the IMEMG members to benefit from mutual exchange of experiences with respect to computer modelling. But there is a huge field where simulation experts are certainly looking for collaboration:

- Harmonisation of simulation procedures
- Definition of input data, material properties and test procedures to obtain these input data
- Coupling of codes
- Setup of live tests to obtain maximum input for simulation

All such activities could culminate in a study about ROI (return of investment) for computer modelling where we not only prove the gain of knowledge and a better understanding of the underlying physics of IM scenarios but also identify a significant opportunity to reduce expensive testing by smart simulation.

1. WHY TEMPER, WHY FDS?

Most companies of the EWG members rely on computer modeling of IM threats. This is an ideal supplement to necessary and required IM tests. Yet there is even more benefit when performing simulation. There is a good chance to gain more insight into the reaction process of products challenged by IM threats. Computer modelling enabled the companies to make good progress in understanding mechanisms and the sensitivity of parameters like material properties, tolerances, and test conditions but also for interpretation of test results and improvement of test setups. This will reduce the number of expensive tests and can optimize the design of munition with respect to IMness. The capabilities of computer modelling performed by experienced specialists will give a competitive edge. There is a huge bundle of software which is used by the companies. They are tailored for specific use, some are commercially available others are in-house codes which are restricted to the company. In any case details about this kind of simulation are hardly been communicated.

That is why open codes have been chosen for an evaluation by the EWG members. These tools are identical for all companies, yet individual experience matters again of course.

TEMPER is a unique and powerful tool that utilizes a library of empirical or semi-empirical models dedicated to IM assessment. It is an “open source”, Object-Oriented Programming project, allowing full flexibility to add custom models or to enhance existing ones. Temper provides a library of stimuli, mitigation devices (anything in the real world able to convert an initial stimulus into a "residual" stimulus), explosive-containing structures and models. TEMPER has the ability to perform parametric or stochastic simulations by varying one or two parameters of the problem

Details and a procedure how to obtain TEMPER can be found at:

→ http://www.dod-msiac.org/

Fire Dynamics Simulator (FDS), is a 3-D computational fluid dynamics (CFD) model of fire-driven fluid flow. It is developed and validated by the National Institute of Standards and Technology (USA). FDS is a tool to simulate fundamental fire dynamics and combustion.

Appropriate for low-speed thermally driven flow (buoyancy forces) putting its focus on formation of smoke and heat transfer by fire. Interesting analysis features are heat transfer by convection and radiation between gas and surfaces of solids, pyrolysis, spreading of flames and formation of fire.

FDS solves numerically the Reynolds-averaged form of the Navier-Stokes equations (RANS)

Thermal radiation is calculated by means of Finite-Volume-Method (FVM) using the identical discretisation as for CFD.

Details of features, comprehensive literature, background information, demos and implementations can be found at:

→http://fire.nist.gov/fds

2. SIMULATION TOOLS AND AREAS

The attached list is an excerpt of applied software packages as they are used by the companies of this working group for simulation of IM scenarios and threats. Most of them are offered commercially and are occasionally fitted to the actual use by writing subroutines or by coupling with other codes. Many of them offer multi-physics features or allow coupled analysis, i.e. thermo-structural coupling. Some of the codes were developed by the companies themselves or by government agencies and there use is restricted or limited. Nowadays codes can be run in a HPC environment on clusters or multi-core workstations. This is essential as these codes are getting more and more sophisticated and can handle quite complex problems and huge model sizes. Simulation is done for events like impact where bullets or fragments hit a target, deform and penetrate the housing, transfer shocks and initiate a violent reaction. But also simulation for a full-scale FCO or SCO condition have been performed where conditions like wind, reaction kinetics, pyrolysis or consumption of intumescent paint has been taken into account

IM Simulation Tools Used by the Companies of the EWG Members

Tool	Characteristics	Used for	Degree of Use	Capabilities	Pros/Cons
ANSYS workbench	major general purpose FEA code	Prepare geometry, mesh, bondaries and conditions. In addition and many pyhsical phenomena	often	Heat transfer, static analysis, acoustic, electromagnetism, multiphysics , …	commercially available, user interface, suite of modules
Autodyn	FEA code, explicit, Lagrange/Euler solver short time dynamics	Slow Burn (deflagration/ convective burning) ,impact, penetration, structural strength of design, interior and terminal ballistics, fragmentation, ignition, ignition train	often	high strain rate (impact, energetic computation), ignition and growth, JWL	commercially available, de facto standard
LS/HI-DYNA	FEA code, explicit, Lagrang solver short time dynamics	Impact, penetration, structural strength of design, interior and terminal ballistics, fragmentation, ignition, ignition train; *Detonics :* - HX reactive models characterization - warhead design *Dynamics :* - Behavior models characterization - warhead design *Vulnerability :* - Behavior and reactive models characterization - warhead and motors response	often	high strain rate (impact, energetic computation), ignition and growth, JWL	commercially available, de facto standard
Ekvicalc					
Split-X	Gurney based analytical fragmentation code	fragmentation of shells, warheads, parametric study	often	3d Gurney, multiple initiations, arena tests	commercially available, easy GUI
MSC/Marc	FEA code,implicit,explicit, nonlinearities	impact, penetration, structural strength of design, SCO (reaction kinetics), FCO, drop shock	often	heat transfer, static, nonlinear analysis (material, geometric, contact), dynamic, reaction kinetics	commercially available, user interface; parallel computing
MSC/Dytran	FEA code, explicit	impact,penetration, FSI, SD, drop shock	limited	high strain rate (impact, energetic computation), ignition and growth, JWL	commercially available; parallel computing
Thafem	Heat transfer (2d)				
Comsol	FEA code, multi physics, PDE solver	heat transfer, electromagnetism	potential increased use	coupled multiphysics simulation, pre-processing , post-processing	commercially available, suite of modules
TEMPER (*)	analytical code to predict explosive reactions	BI, FI, SR, shape charge	limited	suite of stimuli, mitigation, targets, suite of empiracal models for initiation of explosives, parametric study, optimization	free of cost, source code avaiable, simple GUI, postprocessing actually only by outdated version of Excel
FDS (*)	CFD, Fire Dynamics Simulation 3d, burning, pyrolysis, reaction kinetics	dedicated to fire problems, fire structures, sprinklers cooling study, FCO,	limited	flows, turbulence, combustion, soot, conjugate heat transfer, pyrolysis,	free of cost, powerful for global phenomenology, limited geometry representation
Abaqus	FEA code, implicit,explicit, Lagrange/Euler solver, nonlinearities	impact, penetration, structural strength of design, FCO, drop shock *Mechanical analysis :* - Energetic materials behavior law characterization - Warhead and motor design (grain and bonding) *Thermal analysis and vulnerability :* - Energetic materials reactive model characterization - Warhead and motor response to heating	often	heat transfer ,nonlinear analysis, high strain rate (impact, energetic computation), static and dynamic	commercially available

An overview where the companies utilize the benefits of simulation in the fields of IM is given in Figure **1.** Simulation is now applied to a widespread area of IM proof. This covers activities like design, development, IM testing and even manufacturing of munition. Actually there are even simulations how evacuations should be performed in an optimized way when fire has been caught on a vessel and smoke is propagating. Another application couples the effects of a blast with the follow up of spreading fire and smoke which can lurk a propagating threat. High Performance Computing and the possibility to cover multiphasic features in the simulation will dramatically improve the way IM scenarios can be examined by means of computer models. Coupling of codes which can combine their specific benefits is emerging. An example is a procedure where the output of a blast event will serve as initial condition for a simulation of fire propagation. This will allow simulating events with very different time domains.

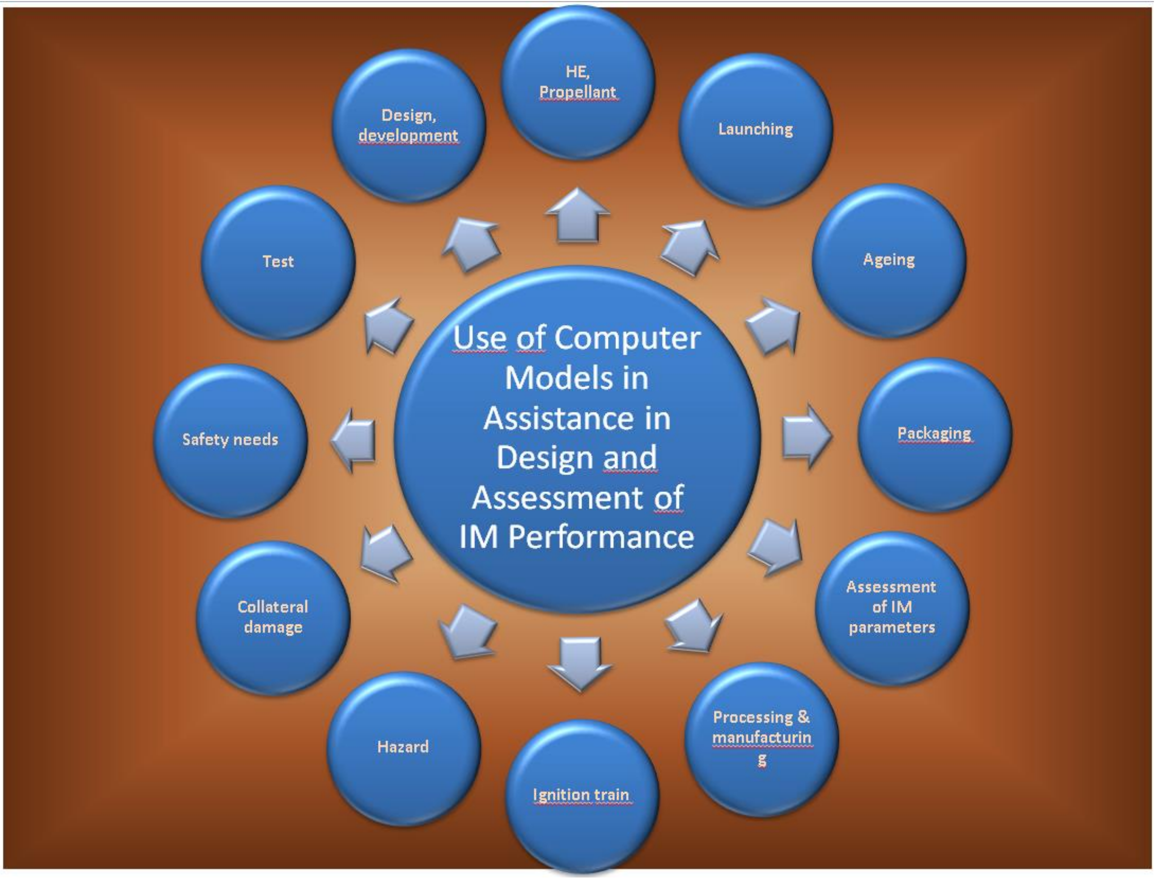


Figure 1

3. COOPERATION, SUPPORT

Often the companies do not have adequate equipment or man power to provide necessary input data for simulations. For sophisticated simulations many specific material properties are needed which require quite intricate testing of the energetic and also inert materials. Also when it comes to testing, on full or small scale, there are often regulations that force the companies to look for support by test centres or they have even to go abroad.

- Nammo cooperates a lot with the Norwegian Defence Research Establishment (FFI) and China Lake
- MBDA BC uses resources and capabilities of Fraunhofer ICT, TNO (*Nederlandse Organisatie voor toegepast-natuurwetenschappelijk onderzoek*), several Bundeswehr facilities (WTD92, WTD52)
- BAES Munitions utilises its internal company linkages between other parts of BAE Systems e.g. Bofors and the Advanced Technology Centres (ATC).

  BAES gets support by:

- Defence Ordnance Safety Group (DOSG),
- Health and Safety Executive (HSE),
- Defence Science & Technology Laboratory (Dstl),
- Defence Equipment & Support Agency (DE&S)

Academia:

- Aberdeen University
- Cambridge University (Cavendish Laboratory)
- Imperial College (Institute of Shock Physics)
- Cranfield University (DCMT Shrivenham)

4. FINDINGS, CONCLUSION AND RECOMMENDATIONS

Evaluation TEMPER

TEMPER utilizes a library of empirical or semi-empirical models dedicated to IM assessment. Companies use this product often in the beginning of a development to get first idea of the IMness of their products and to perform parameter studies, which are easy to handle by using TEMPER.

Four companies evaluated TEMPER. Some of them were already experienced others introduced this tool recently. All members of the EWG had the chance to participate a life tutorial by Dr. François Peron, at that time member of MSIAC. He gave an overview about the basic idea, the capabilities and applications of TEMPER and highlighted some of the empirical models for initiation of explosives like Jacobs-Roslund, Peugeot, Held and other.

The EWG members appreciated the clearly arranged GUI of TEMPER. The analytical approach requires only very moderate CPU time and hardware requirements but of course has trade-offs with respect to the geometrical complexity of a real component. The GUI is intuitive. The output is a go or no-go label. The software allows performing parametric studies and stochastics in a quite effective way. There is a possibility to implement own materials, models, mitigations and stimuli. Evaluators also like the access to MSIAC databases and that it is free of cost.

All of the participating users blamed the outdated version of Excel that is used for results evaluation. Most companies do not support usage of this expired version. MSIAC has been contacted yet no solution has been provided right now.

NAMMO performed an intensive study on impact and sympathetic reaction with 155mm shells utilizing the features of TEMPER.

BAE Systems also values the assets of TEMPER in the beginning of a development but also argues that the databases are outdated and that the documentation should be improved. They see a chance to use TEMPER to back-fit model parameters.

Evaluation FDS

FDS is a very powerful tool to simulate fundamental fire dynamics and combustion. It enables users to simulate FCO and SCO threats. It is a big advantage to be able to introduce well defined boundary conditions like wind speed which in a real test is quite difficult to arrange. But wind speed is a major driver for the results. By doing FCO simulation the effect of an inadequate wind condition can be eliminated.

FDS is a 3-D computational fluid dynamics (CFD) model of fire-driven fluid flow. Therefore it is necessary that a user has a fundamental background on fluid dynamics. Although it has a simple GUI and a post processing module (Smokeview) that can evaluate results in a much preconfigured way it is a full-fledged CFD code and the expertise of an experienced user is recommended.

4 companies contributed to the evaluation of FDS, see attached listing. Others did not yet install FDS either due to lack of time or because they are actually missing experienced people.

MBDA Bayern-Chemie uses FDS for some preliminary work on FCO testing when they started a comparison between gas and fuel fire.

MBDA F relied on FDS when they performed a study about cooling effects on time to reaction for a rocket motor during a FCO test. They also performed phenomenology studies on mixing flow zone during a liquid fuel fire in an under-ventilated compartment and the effects of wind on JP5 fuel fires.

BAES has worked for many years developing a fire modelling capability. The model has been used extensively in designing both ships and submarines. This modelling normally takes the form of an energetic event producing heat/temperature and smoke. As part of these models an assessment is made of the likely crew human reactions and also covering fire detection and suppression (water sprays, venting etc.) which could be activated. Crew modelling also covers visibility of the possibly crowded escape routes. Normally many varied simulations are run to assess the implications of proposed design alterations such as controlled ventilation scenarios.

Expanding this work under direct UK Government funding (DOSG), BAES has together with Fluid Gravity Engineering (FGE) been developing a coupled model which links the short timescale energetics modelling of FGEs Eden model and then coupled its outputs with the longer duration FDS model. Significant work was carried out on the required complex mesh resolution and was successfully concluded. The result was such that a secondary material fire following on from a detonation of various TNT charges could be predicted both with and without external air entrainment from series different vents. The work is considered important for detailed analysis of secondary detonation and fires. This work is ongoing.

SAFRAN Herakles gained extensive experiences in using FDS through versions 4 & 5, and today version 6, for modeling of current fuel fires for increasing temperature calculations in closed magazines and various configurations. Also they developed a specific methodology to model fires of energetic materials taking into account of packaging, quantity, arrangement and sprinklers effects.

FDS is for free! Companies who evaluated FDS praised the ample capabilities and features. Beginners are pleased by a sound documentation and the tutorial, included databases and open user interfaces. The speed is impressive, supported by the possibility to perform parallel computing. In FDS the geometry is represented by cubicles only. This is speeding up the analysis but on the other side only poor representation of curved surfaces is reached.

Users would welcome an improvement of post processing features in a way which is better tailored to their specific needs.

All companies agreed in good marking for FDS. They will further explore this software and intend to utilize its capabilities even more in the future.

5. GAP ANALYSIS (STATUS 2014)

Following diagram reflect the author's idea about the development and application of software tools in their company with respect to simulating/ modelling of IM scenarios according STANAGs. Each company will put a different focus and emphasis depending on their products and technology. 'Necessary 'in this context means that the author states there is a lack in competence or capability or a change in philosophy with respect to demonstration of IM-ness . Putting more effort on modelling and simulation will improve the design. 100 % does not mean that the scenario can be simulated from the very start of the threat to the very end but i.e. it is satisfying if reaction kinetics during SCO can be described quite accurate to determine an ideal condition for a mitigation device.

The gap analysis results in a graph reflecting the status quo and a plan how companies will increase the field of IM simulation during coming years to support the product design and evaluation. An "ideal" plan reflects the schedule at the time when this planning has been done for the first time. Most companies forecast a permanent rise in number and importance of simulation of IM scenarios within their companies.

MBDA Bayern-Chemie puts a lot of effort in the simulation of thermal threats because this is actually the most challenging threat for their products. They will continue to improve their simulation capabilities in coming years with similar intensity. Starting in 2013 they intend to expand their simulation capabilities with respect to high speed events like bullet impact, fragment impact or at a limited level to shape charge jet.

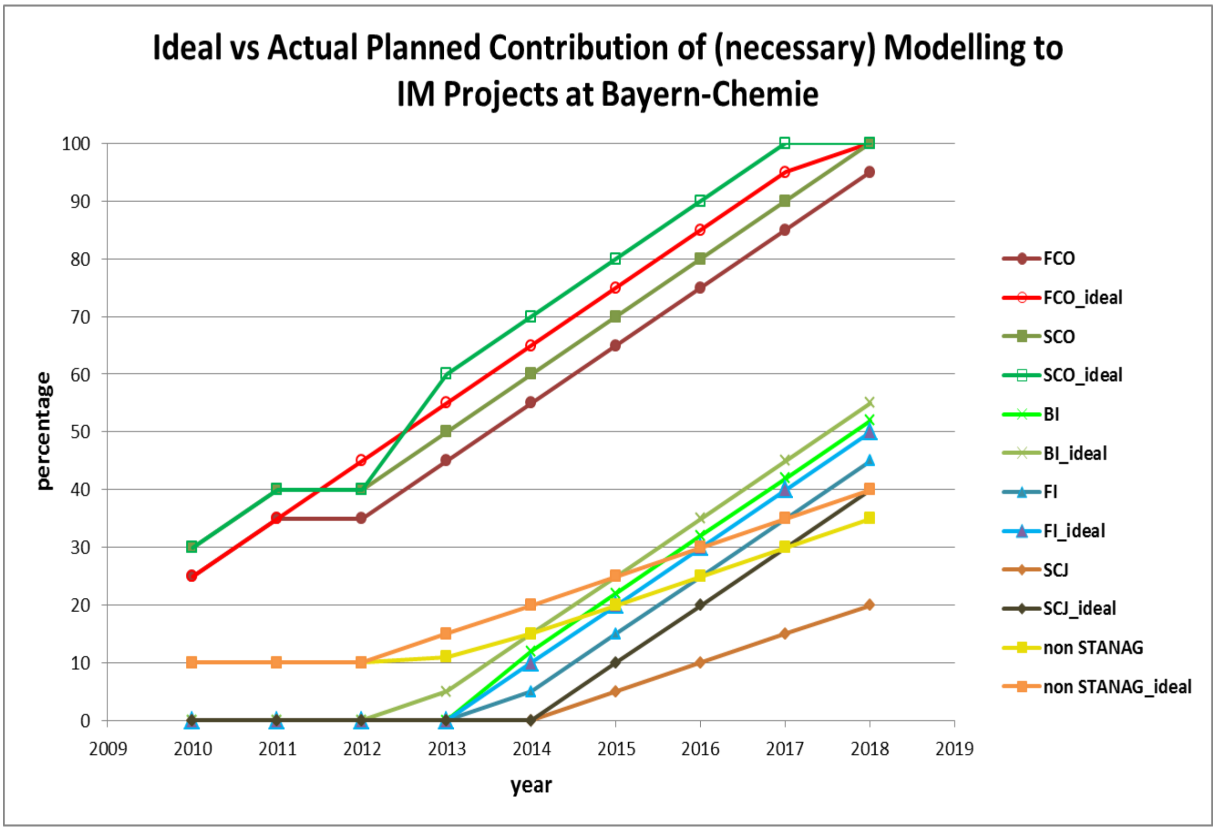
Since a couple of years Nammo relies on simulation primarily supporting the design. From 2013 they also perform simulation of STANAG events and they feel that it is even necessary to boost these capabilities. Their focus is on simulation of impact and shape charge aggression.

RWM Italia started quite early to simulate bullet impact and fragment impact. These are the threats their products are exposed to in the field. There are plans to expand simulation to examine Slow Cook Off conditions.

BAE System has a lot of experience in simulating detonics and impact events. With respect to simulation of IM scenarios according STANAG they also see a need to enhance these activities during coming years. Their priority will remain bullet impact simulation, but an upswing tendency for the coming years can be recognized for the simulation of thermal scenarios and the shape charge jet hazard.

Some of the companies made an initial planning in the years between 2010 and 2012. This is marked by the index "ideal". When the actual evaluation has been made (in most cases at the end of 2014) an obvious delay could be observed often. This tool can be used when updated regularly to detect the reasons for a laggard mechanism and where there is a need to catch up.

Example:



6. FUTURE ACTIVITIES

The actual review represents a kaleidoscope of applications that are in use at companies who deal with IMness of products. In most cases industry relies on CAE tools which are tailored to specific use. The tools are powerful and rely on implemented models that have been developed over decades. Parameters are available for some materials where institutes or research departments spent a lot of time and money to determine these data. It is a permanent challenge for the modelling community to find reliable data for their computations and how different approaches can be compared. Especially for new HE and many propellants there is a lack of these data.

Therefore follow on activities for the EWG were proposed:

- Gathering material data relevant for simulations (i.e. ignition and growth, EOS for propellants)
- Recommendations for use of analysis tools
- Workshop on FDS , including coupling to other codes
- Round Robin simulations FDS, TEMPER
- Workshop on FSI
- Collaboration with MSIAC's working group on simulation
- Improving collaboration of EWGs (FCO, Computer Models)
- Design of trials and experiments only for use in establishing data specific for modelling purposes. (As current routine testing fails to determine modelling specific parameters.)