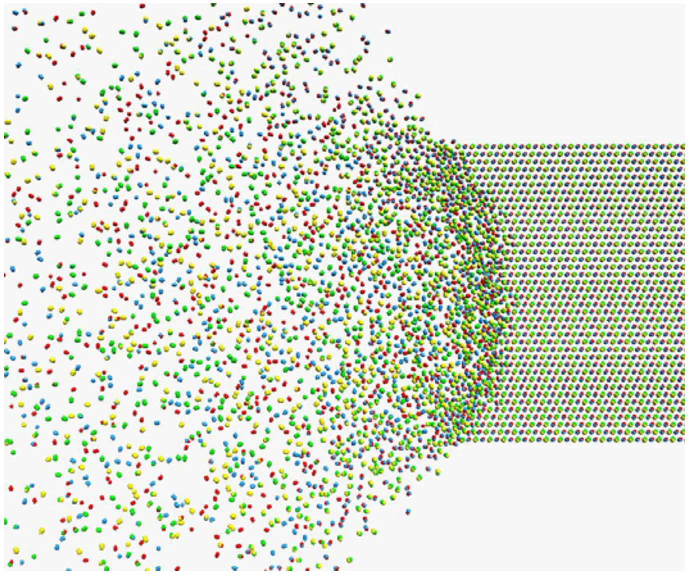
Challenges in the Modelling of Initiation, Growth and Propagation of Condensed Phase Detonation



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A presentation to: A joint meeting of:

The EPSRC Condensed Phase Reactive Flow Network
The UK Explosion Liaison Group
& The Smith Institute Industrial Mathematics KT Network

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1. Introduction

•Objectives of this talk are to:

- Outline the requirements for modelling in the field of military explosives.
- Describe the current capabilities and key deficiencies.
- Indicate the technical challenges and suggest the areas which require development.

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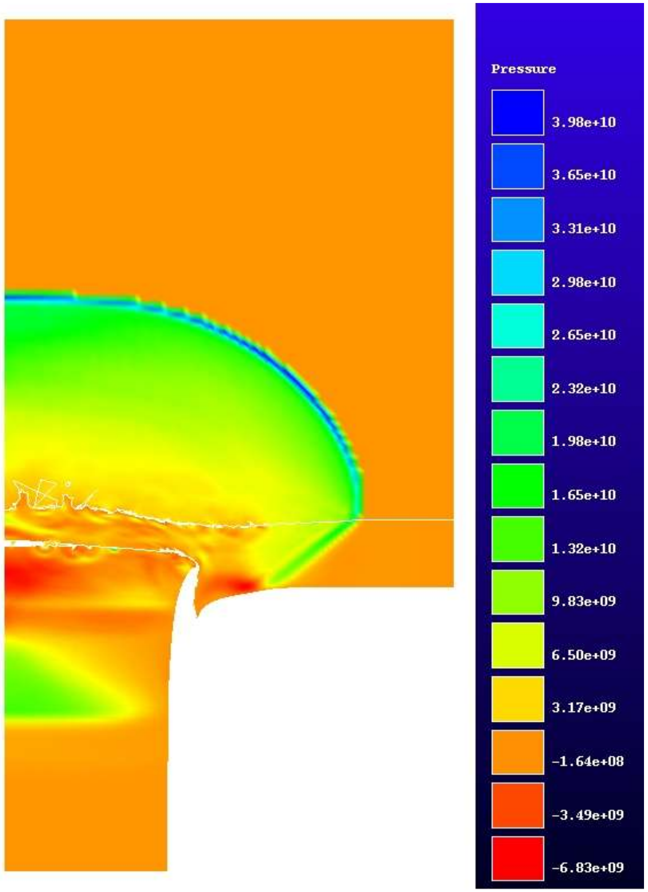
Requirements – Modelling Military Explosives



2. Requirements – Modelling Military Explosives

- The principal needs for modelling in the field of military explosives stem from the following requirements:
  - Performance prediction:
    - Optimisation of system designs.
    - At a more fundamental level, to guide the synthesis and formulation of potential new explosives.
  - Hazard prediction:
    - Safety (IM) assessment of existing systems (in conjunction with testing).
    - To help design mitigation for existing systems.
    - To guide the development of new materials for improved safety.
  - Compatibility / Stability / Life Assessment:
    - Understanding short term chemical compatibility issues.
    - Predicting service life (chemical and physical ageing).

2. Requirements - Vision (5 Years)

- A robust ‘engineering’ modelling capability for hazard assessment. Ideally:
  - A common, agreed, UK approach/ set of tools
  - With clearly defined and reasonable (cost) requirements for input data
  - Able to handle SDT and all forms of BVR (even though empirically)
- A first-generation predictive tool-set for energetic materials properties (performance, hazard, and life assessment). Also a clearly defined route for the future development of the capability.
  - The predictive tools should, as a minimum, provide a qualitative, or preferably semi-quantitative, description of the main factors effecting performance and hazard (e.g. crystal size, molecular structure, porosity, etc.)

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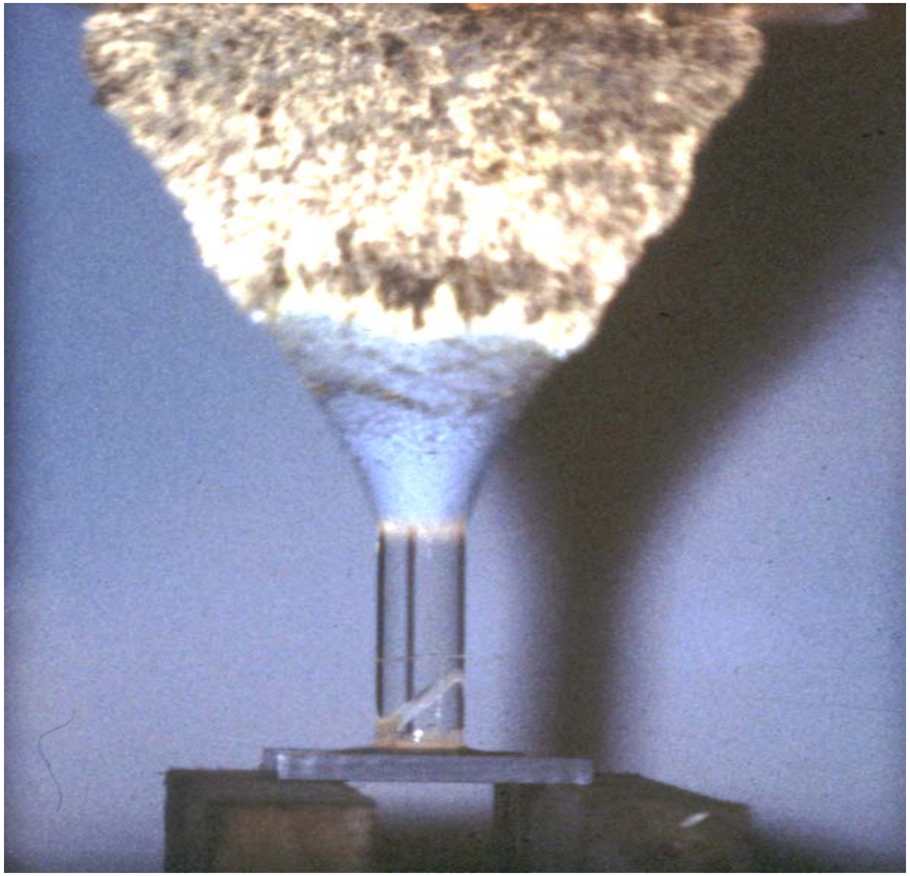
Current Capabilities



3. Current Capabilities - Where Are We Now (1)?

We currently have the following capabilities:

- Reasonable predictive capability for performance of ideal explosives and propellants.
- Very limited predictive capability for performance of non-ideal / enhanced blast explosives.
- Various semi-empirical models for SDT hazards, but no agreement on best approach or future development route.
- No modelling capability for BVR (in many ways the most important hazard).
- Promising, but stalled, capability for fundamental modelling based on MD.
- Reasonable experimental facilities to generate calibration/ validation data, but these will need some investment.

3. Current Capabilities - Where Are We Now (2)?

- First-principles performance prediction - Reasonable modelling capability (using quantum chemistry, crystal packing and ideal detonation codes), but no recent UK investment. Some opportunities for development, particularly with regard to improving crystal packing/polymorph prediction.
- Reactive flow modelling – Currently there are QQ (CHARM) and FGE (visco-plastic pore collapse) SDT models in different codes. Both approaches have merits and deficiencies. Models are semi-empirical at best and require significant experimental data to calibrate. Very significant development needed to establish a BVR modelling capability – currently some very limited work in this area mostly on material models.
- Molecular dynamics - Offers the potential to influence most areas of predictive modelling. No UK investment for ca. 6 years.
- Analytic (empirical) models – Some recent QQ development of these approaches. Opportunity for some further development and exploitation.

3. Capabilities - Current

Models /Codes	SDT	BVR	Detonation Performance	Afterburn / Blast Performance	Combustion Performance	Life Assessment
CHARM (in DYNA, GRIM, EDEN)	Y (Semi-empirical)	N	Y (Semi-empirical)	N	N	N
FGE Model (in EDEN)	Y (Semi-empirical)	N	Y (Semi-empirical)	P (Partial, due to unknown particle combustion kinetics)	N	N
TOPAZ (Chemical)	N	P (Time & location of ignition, but not violence)	N	N	N	N
GAUSSIAN 03	N	N	Y (in association with MOLPAK & CHEETAH)	N	P (in association with MOLPAK & CHEETAH)	P (currently a research tool)
MD Codes (DYNAMITE & QUASIMODO)	P (currently a research tool)	P (currently a research tool)	P (currently a research tool)	N	P (currently a research tool)	P (currently a research tool)
MOLPAK	N	N	Y (in association with GAUSSIAN & CHEETAH)	N	P (in association with GAUSSIAN & CHEETAH)	N
CHEETAH (2 & 3)	N	N	Y	Minor capability	Y	N
Analytic Models (RECCONEX & Walker Wasley)	Y (Empirical)	N	N	N	N	N

QinetiQ

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Development Priorities

QinetiQ

4. Development Priorities (1)

Development priorities need to address the following key issues:

•Serious deficiencies in our ability to model hazards other than SDT. In general hazard modelling is not sufficiently mature / reliable to significantly reduce the high costs of safety / IM testing.

•Significant developments (e.g. higher power explosives) are unlikely to come from conventional chemistry, but will probably require new concepts (e.g. use of binaries, meta-stable or excited states) backed by fundamental theory / modelling.

4. Development Priorities (2)

Highest priorities:

- Develop BVR and improved SDT modelling capability. Reactive flow models will require:
  - Heat flow
  - 2-phase flow
  - Good material models to predict damage, surface area / hot spot evolution
  - Improved reactive flow model
- Start development of fundamental predictive modelling tool set. Requires:
  - A medium and long term strategy for the development of a multi-scale approach
  - MD studies of energetic materials likely to be a key component (feeds into material and reactive properties – e.g. hot spot mechanisms and coupling to chemistry)

These priorities imply that the major areas for investment / development are:

- Reactive flow modelling (and associated hydrocode developments)
- Multi-scale adaptive codes (molecular, meso, continuum)
- Material modelling

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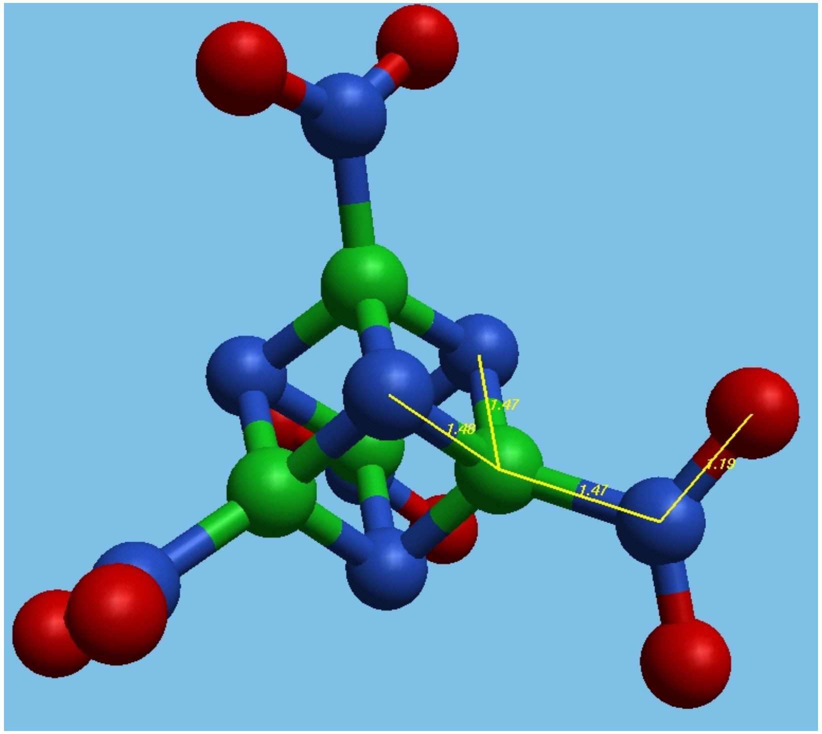
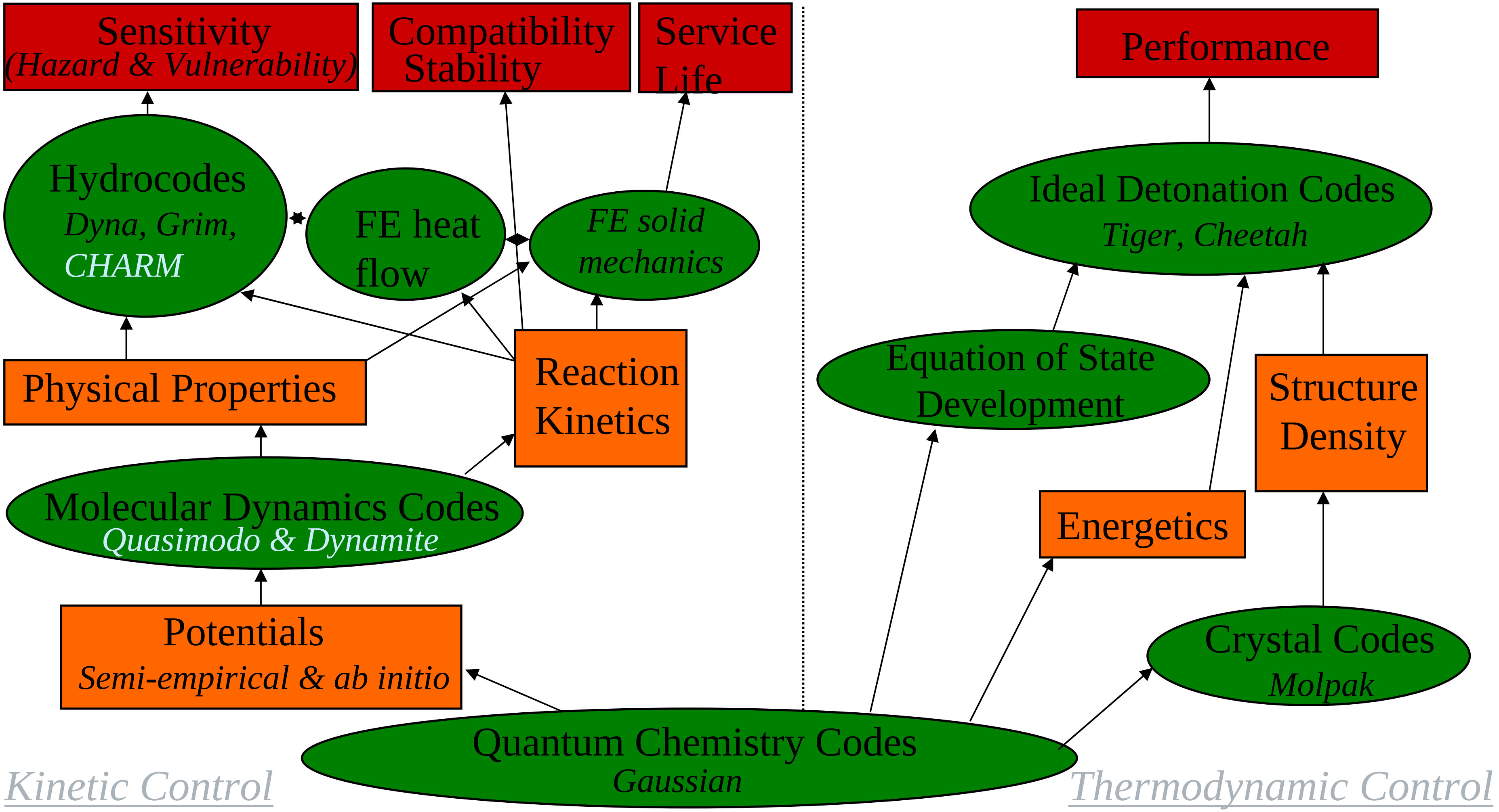
Strategy & Technical Challenges



5. QinetiQ Energetic Material Modelling Strategy



Sensitivity
(Hazard & Vulnerability)

Compatibility
Stability

Service
Life

Performance

Hydrocodes
Dyna, Grim,
CHARM

FE heat
flow

FE solid
mechanics

Ideal Detonation Codes
Tiger, Cheetah

Physical Properties

Reaction
Kinetics

Equation of State
Development

Structure
Density

Energetics

Molecular Dynamics Codes
Quasimodo & Dynamite

Potentials
Semi-empirical & ab initio

Crystal Codes
Molpak

Quantum Chemistry Codes
Gaussian

Kinetic Control

Thermodynamic Control

5. Strategy – Key Technical Challenges

Principal technical challenges:

- Wide range of length and time scales control the important processes:
  - Molecular, crystal, meso, continuum length scales cover nanometres to metres (difference ~ 10^9).
  - Time scales for MD as short as femtoseconds, detonation propagation takes microseconds (difference ~ 10^9), other processes (e.g. BVR) can take milliseconds to seconds (difference ~ 10^{12} – 10^{15}).
- Uncertainties about the critical physical and chemical processes, e.g.
  - Mechanisms leading to, and temperatures of, hot spots.
  - Complexity and inadequate knowledge of chemical decomposition pathways.
  - Conditions at shock front – e.g. is translational temperature overshoot significant.

5. Strategy - BVR

BVR is the highest priority as it poses the most common threat and we have no modelling capability.

There is currently a small MoD funded R&D programme in this area but a much larger and more comprehensive effort is required.

We generally assume that BVR behaviour is controlled by all, or some, of the following processes:

- Deformation
- Ignition
- Combustion
- Detonation

Whilst we can divide the problem into these stages it is clearly necessary for the models dealing with each to be coupled.

We now briefly consider each of the basic processes in turn.

5. Deformation

- Deformation can result from both the initial stimulus and the subsequent response / reaction of the energetic material. Hence, although inert material response models are usually generated separately from reactive ones, they will need to be closely coupled when implemented.
- We can hypothesise that damage, and in particular crack formation, plays a key part in BVR. Consequently, a major requirement of the material models will be the prediction of the size and number of cracks and thus available surface area created as a function of insult stimuli and containment.
- Clearly improved material models capable of predicting bulk and localised temperatures and surface area are required.

5. Ignition

A number of hot-spot ignition models exist as part of the current SDT modelling capability. These include, pore collapse mechanisms (adiabatic collapse and viscoplastic), and friction/shear models. These are still potentially of relevance to BVR, particularly if detonation is the end result.

However, the initial ignition for a BVR scenario may involve other mechanisms such as:

- Cook-off resulting from general thermal insults
- Localised ignition from hot fragments
- Ignition resulting from large macroscopic damage (e.g. setback forces)

Ignition is clearly relevant to the overall hazard modelling capability (SDT and BVR) and future advances will probably be dependant on new fundamental experimental research to further clarify the relevant hot-spot mechanisms in different loading regimes.

5. Combustion

Combustion poses a new challenge for the modelling of explosives.

Following ignition our assumption is that BVR occurs when pressurisation by the product gases causes flame penetration of cracks and voids. The switch from largely conductive heat transfer to a convective process can then lead to a rapidly increasing burn rate and potentially violent event.

The combustion phase poses the greatest modelling challenge and could be addressed at a number of levels:

- Detailed flame models – not likely to be tractable in the near term given time and cost constraints and the complexity of systems of interest
- Semi-empirical models of convective burning with multi-phase flow
- Approximate analytical models along the lines of the WSB approach
- ‘Engineering’ models based on simple pressure dependant burn rates.

5. Detonation

When detonation occurs as the end result of a BVR process it is generally known as DDT, or in some specialised cases XDT.

Two types of DDT have been recognised:

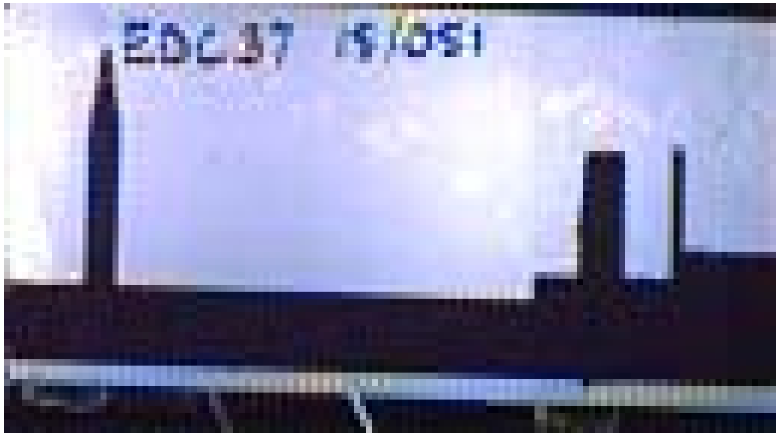
- Type 1 – This involves plug formation and is relevant to granular beds or highly damaged energetic materials. Simple models exist for this mechanism.
- Type 2 – Convective, with no plug formation. No validated models.

The term XDT is often used to describe detonations which occur when energetic material is extensively damaged (e.g. spalled material) and then re-shocked or re-compressed. The exact mechanism leading to detonation is still uncertain and further experiments are needed to assist model development. XDT is a very serious threat for some rocket motors.

An example of XDT in EDC37 under fragment impact is shown in the next 2 slides

5. EDC37 Charge / Void / Steel plate

5. XDT – EDC37
Projectile - 150° conical tip, Velocity = 688m/s



5. BVR - Summary

We see BVR as the key area requiring model development to assist in the assessment of IM compliance.

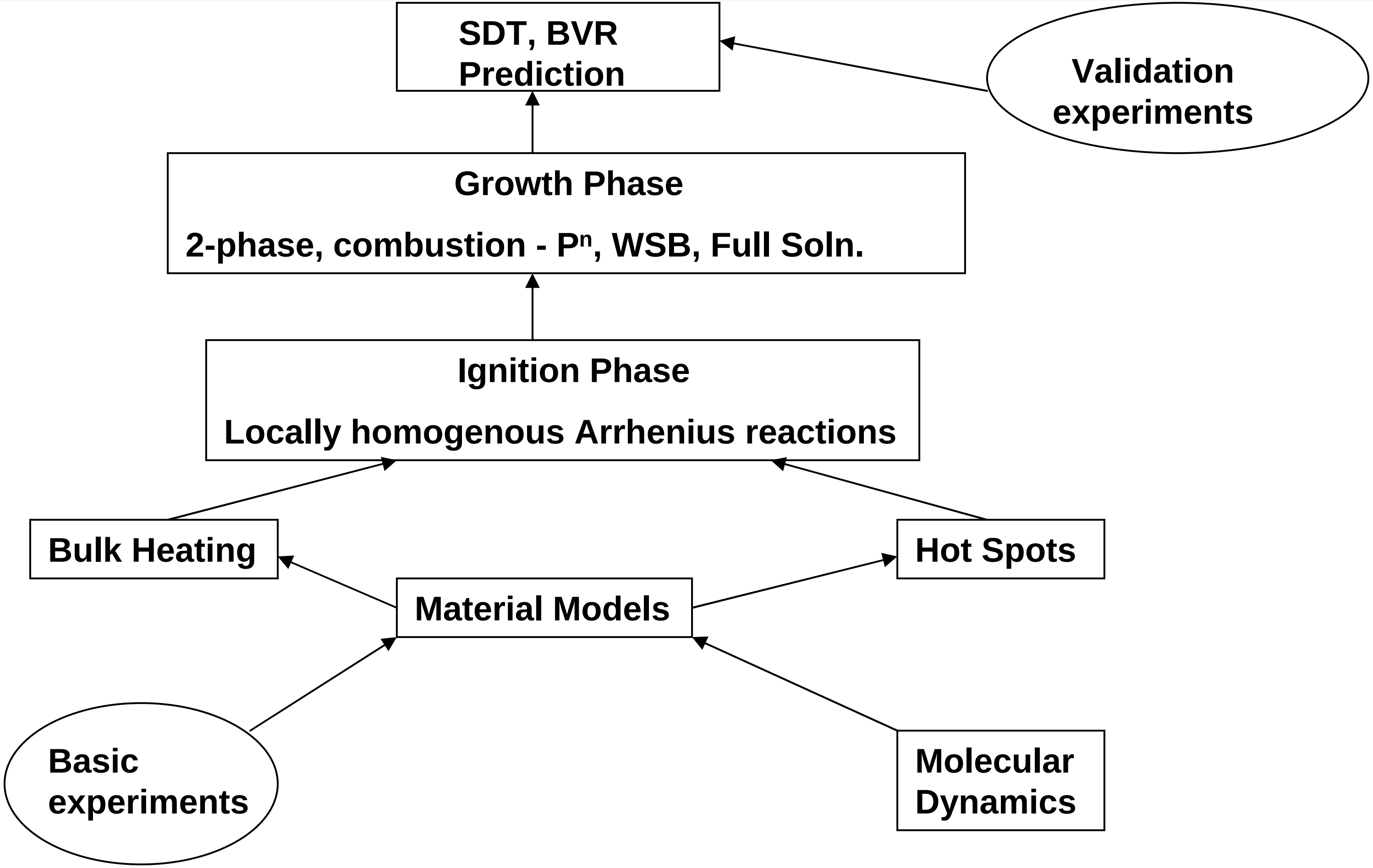
Little or no validated modelling capability exists for BVR, most assessments being based on the results of integral tests (e.g. tube tests, friability tests).

New material (inert) and reactive models are required and these will need associated experimental programmes.

With regards to reactive modelling the main effort will probably be required in the combustion / growth phase, with ignition, at least initially, being treated using existing models.

The next slide shows a simple schematic of how the components of an integrated model development programme might interact.

5. Strategy - Predictive Hazard Model



SDT, BVR Prediction

Validation experiments

Growth Phase

2-phase, combustion - P^n, WSB, Full Soln.

Ignition Phase

Locally homogenous Arrhenius reactions

Bulk Heating

Hot Spots

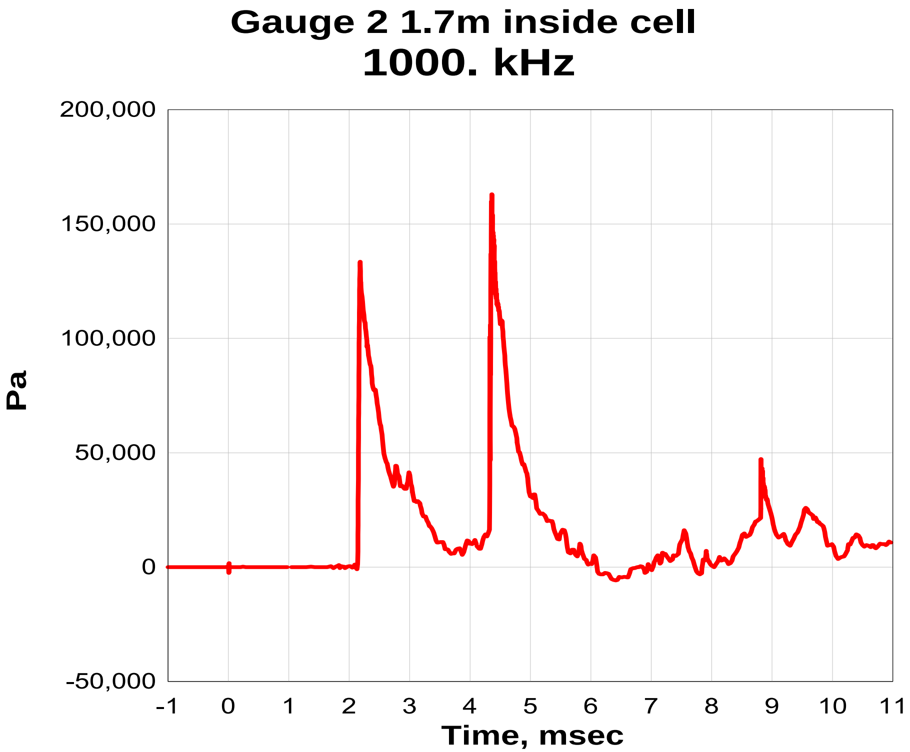
Material Models

Basic experiments

Molecular Dynamics

6

Conclusions



6. Conclusions

- There is a need for improved modelling of condensed phase explosives for a wide range of reasons. For military explosives the two key requirements are:
  - Improved hazard modelling of weapon systems.
  - Longer term fundamental studies to support the development of new materials and concepts.
- Issues:
  - Lack of long term R&D funding from MoD.
  - Co-ordination of research – e.g. Common codes, or duplication of effort?
- Possible ways forward:
  - Co-ordinate through a regular forum (academia and industry). Can we find a way to continue the Network in some form?
  - Make greater use of joint MoD/EPSRC grants.