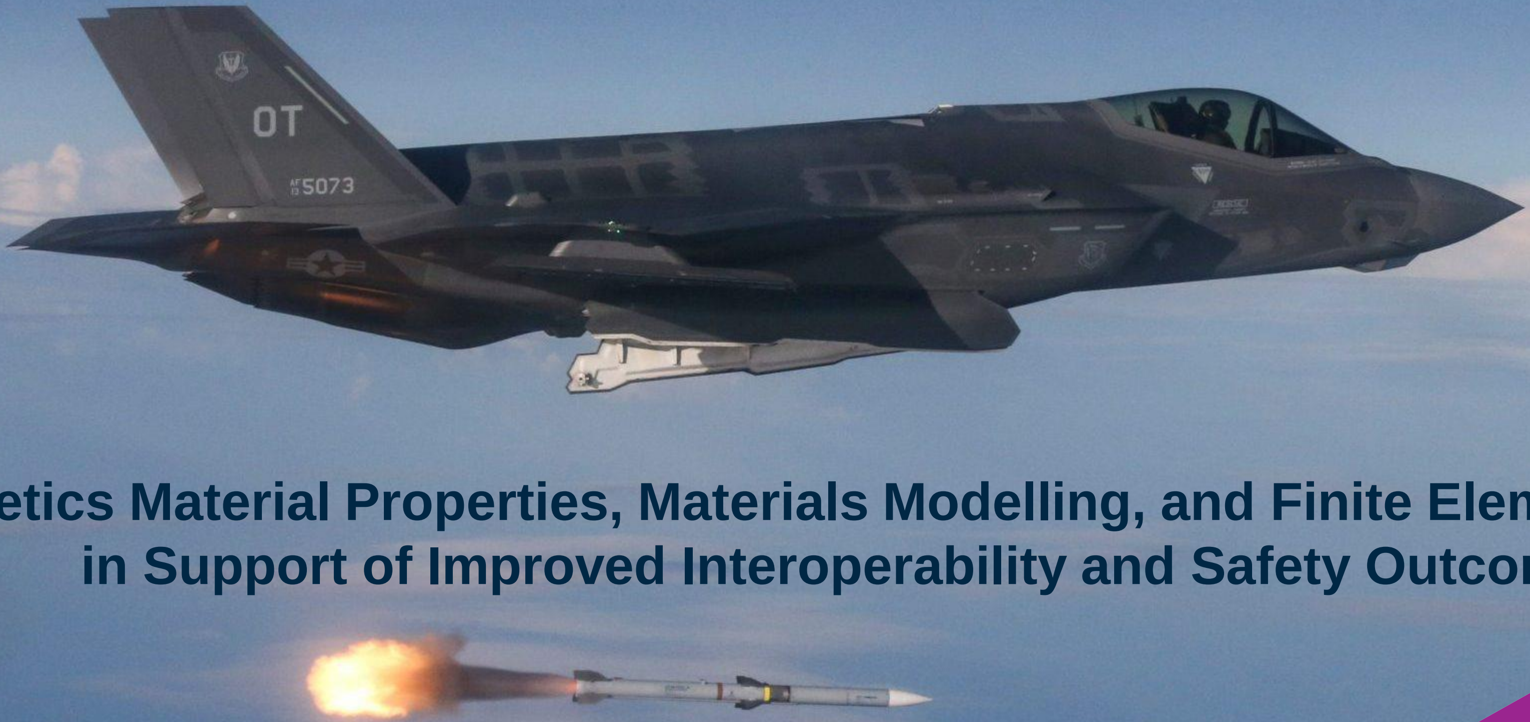
Numerical Modelling of Energetics for Air Domain GWEO



Energetics Material Properties, Materials Modelling, and Finite Element Analysis in Support of Improved Interoperability and Safety Outcomes

November 20th 2024

Photo courtesy of twz.com

Who We Are

Mr. Damion Hadcroft (Senior Principal Engineer)

- Over 20 years’ engineering experience.
  - 16 years Aerospace; 13 years Defence; 2 years Military Land Vehicles;
  - Multi-disciplinary expertise (structures; fatigue & fracture; dynamics; vibration; hardware integration; FEA).

Contact: dphadcroft@qinetiq.com.au

Mr. James Craigie (Team Lead)

- Lead for Weapons Integrity & Complex Analysis (WICA)
  - 10 years with QinetiQ Structural Integrity (SI) Programme.
  - Program leadership to specialist engineers from SI, Vibration & Aero elasticity disciplines.

Contact: jacraigie@qinetiq.com.au

The broader QinetiQ Australia Team:

- Tim Cooper, Joseph Tomazic, Cooper Watson

The QinetiQ UK Energetics Experts:

- Peter Gould, Andrew Rix, Mark Ashcroft

Context

- In FY23/24, QinetiQ was tasked by AEOSPO to perform an energetics modelling feasibility study.

- **Study across approximately 21 research papers, texts and standards, examining the feasibility of modelling energetic materials for a number of failure modes**.

- **Aims:**
  - To support a better understanding on weapon use & lifing
  - To improve the understanding of when weapon damage presents a safety risk

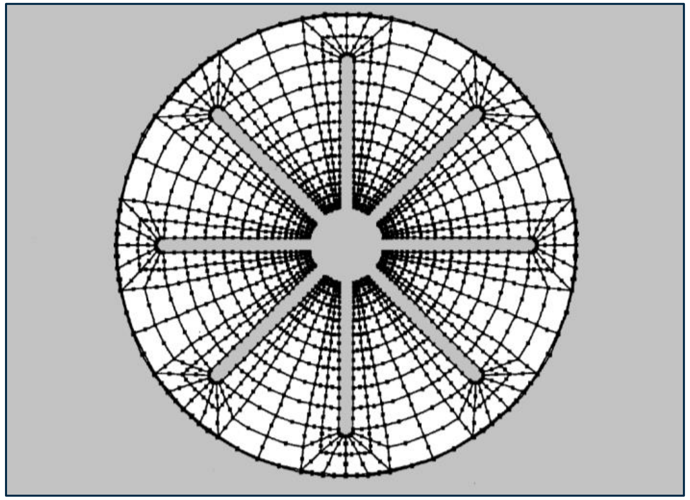
- **This presentation provides:**
  - A summary explanation of the science (material properties, failure modes, and modelling);
  - Discussion on the technical challenges;
  - Opportunities in-line with Safety and Interoperability objectives.

Our Goals for This Presentation

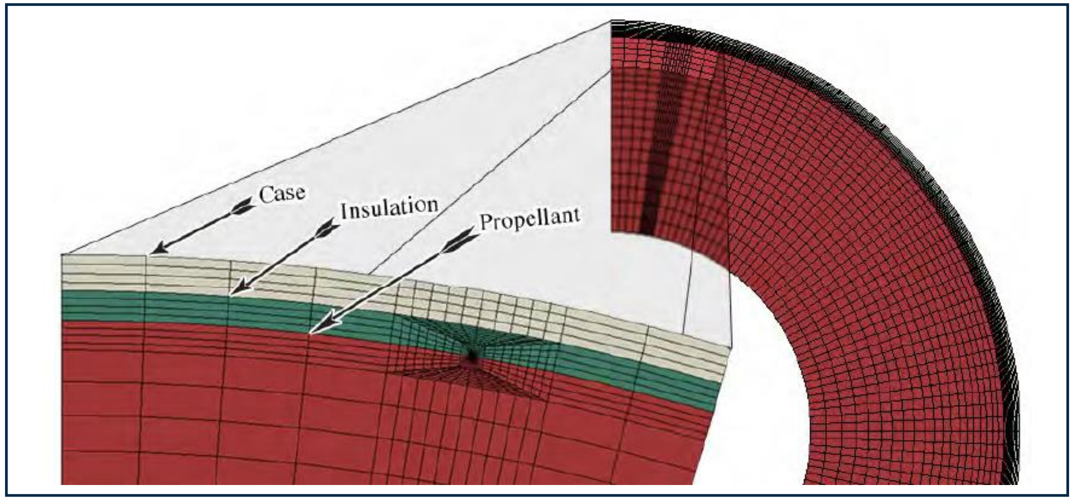
- Discuss previous examples of energetics modelling work.
- Outline energetics material mechanical behaviour.
  - In order to comprehend the technical complications associated with modelling energetics.
- Discuss important energetics material failure modes.
  - In order to grasp complexities and interactions.
- Provide examples of how numerical modelling can be applied to energetics.
  - Includes discussion on benefits and limitations.
- Explain how modelling can contribute to interoperability and safety goals.

Historical Examples of Energetics Modelling

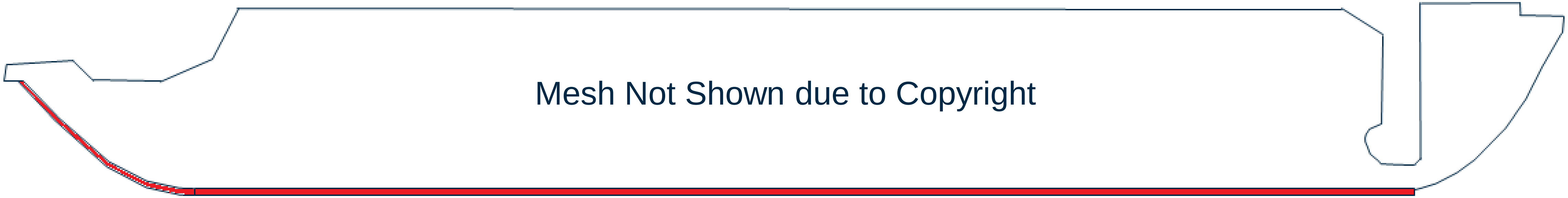
Of the 21 research papers investigated, some noteworthy examples:



Structural Assessment of Solid Propellant Grains
AGARD Advisory Report 350 (for NATO community)
ISBN 92-836-1063-6, Dec. 1997



Detectability of Delaminations in Solid Rocket Motors with Embedded Stress Sensors
Anhduong Q. Le, L.Z. Sun, and Timothy C. Miller (University of California, Irvine)
May 2012; sponsored by Edwards AFB, presented at JANNAF 2012



Mesh Not Shown due to Copyright

Sketch Depicting the Cross-Section Model of :
Structural assessment of a solid propellant rocket motor: Effects of aging and damage
H.C. Yıldırım, S. Özüpek
Journal of Aerospace Science and Technology, Jan. 2011

Energetic Material Properties

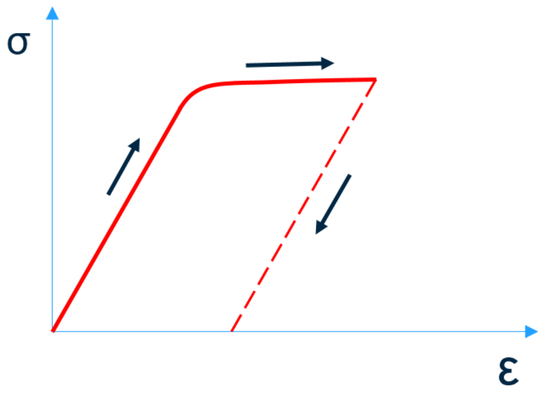
- Energetic materials are known to exhibit *‘**non-linear visco-elastic (NLVE) properties**[1]’.*
  - This will now be explained.

- NLVE properties will be explained in a *rheological* (mathematical) sense.
  - Based on a set of more commonly used material characteristics.

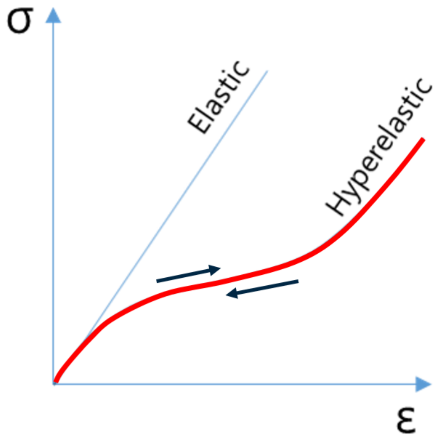
[1] *Ageing studies on AP/HTPB based composites solid propellants*
Published in the Journal of Energetic Materials Frontiers,
By Hamza Naseem et. al., 2021.

Types of Non-linear Materials

- **Non-linearity through plasticity**



- **Non-linearity through elasticity**



- **Combinations of these (to come)**

Hyper-elasticity

IMPORTANT CHARACTERISTICS

- **Full strain restoration upon load release**
- **No net work done over a stress cycle.**
- **No Time Delay for full elastic restoration.**

Some Rheological Models:

Mooney – Rivlin,
Ogden,
Arruda-Boyce
Yeoh,..

Arruda-Boyce 8 chain model:

Constant describing the initial shear modulus

Bulk modulus

$$\mathbf{T}_A = \frac{\mu_A}{J\overline{\lambda}^*}\,\frac{\mathcal{L}^{-1}\left(\overline{\lambda}^*/\lambda_A^{lock}\right)}{\mathcal{L}^{-1}\left(1/\lambda_A^{lock}\right)}\,\mathrm{dev}\left[\mathbf{B}^*\right] + \kappa[J-1]\mathbf{1},$$

Cauchy Stress

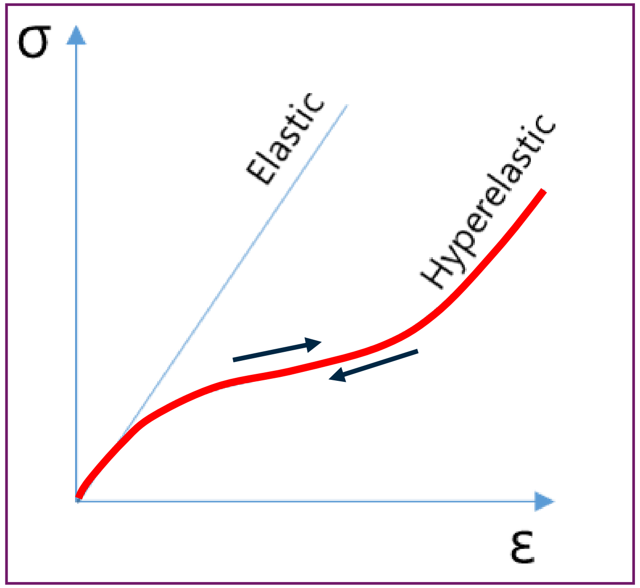
A limiting stretch constant

For further info. refer:
Journal of Mechanics of Materials, Vol. 33, pp. 523–530, 2001.

Rheological Model

$(\mu_A, \lambda^{lock}, \kappa)$

Hyperelastic element

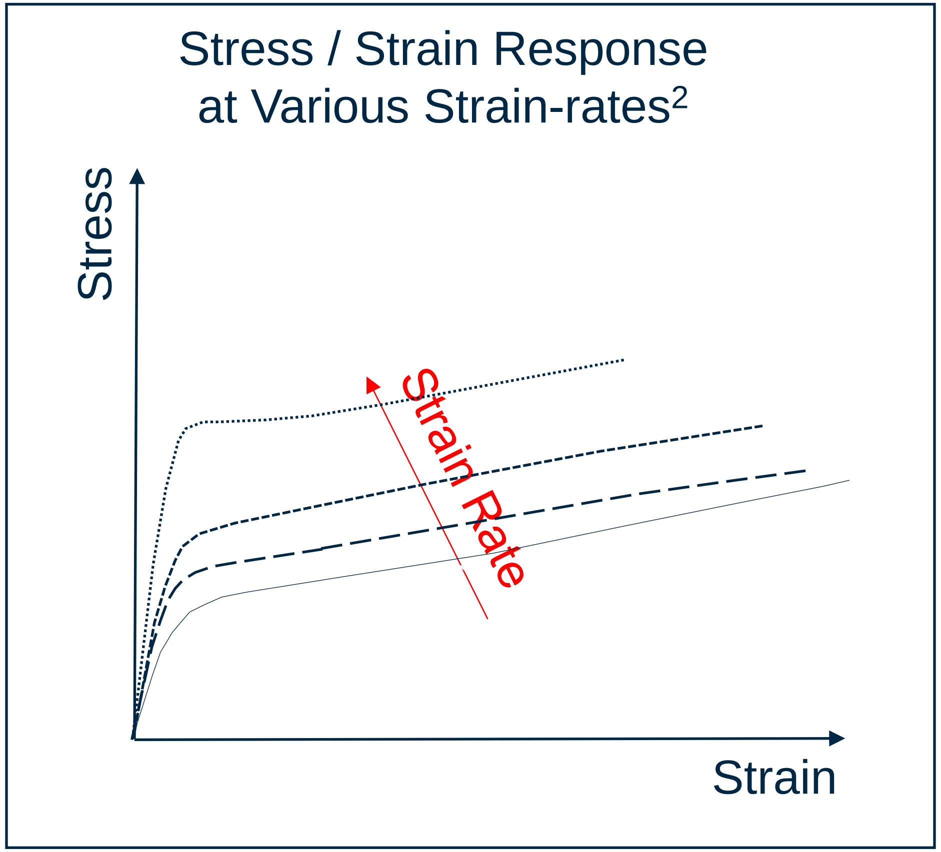


Hard rubber tends to behave like this under some conditions, but not always.

Visco-Plasticity

IMPORTANT CHARACTERISTICS

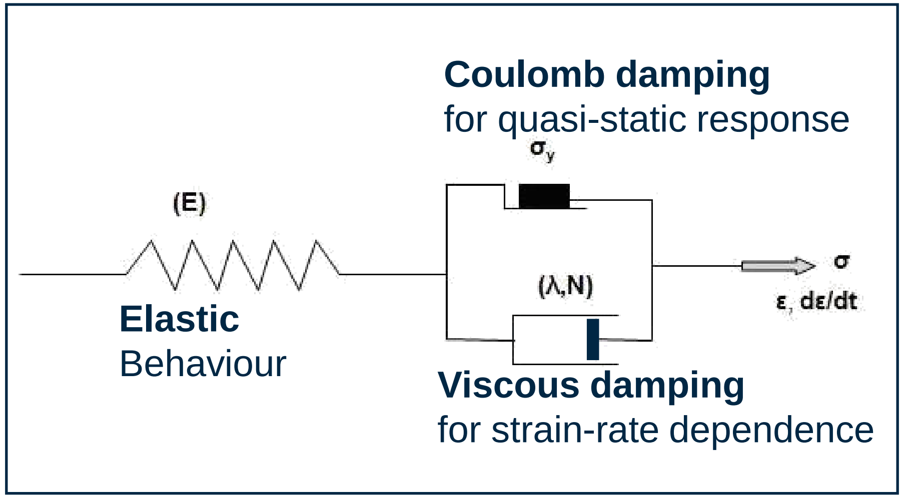
- **Incomplete strain restoration after load release (permanent set).**
- **Strain-rate dependence – time component.**



For further info. refer:
“Hyper-viscoelastic constitutive models for predicting the material behaviour of polyurethane under varying strain rates and uniaxial tensile loading”
By K. H. Badri et. al.
Published in:
Journal of Construction and Building Materials, 2020.

Visco-Plasticity Rheological Model:

Bingham Norton Model (there are others).



For further information refer:
“*Interactive Rheological Modeling in Elasto-visco-plastic Finite Element Analysis*”
By B. E. Melnikov et. al.
Published in:
15th International scientific conference - Underground Urbanisation as a Prerequisite for Sustainable Development, 2016

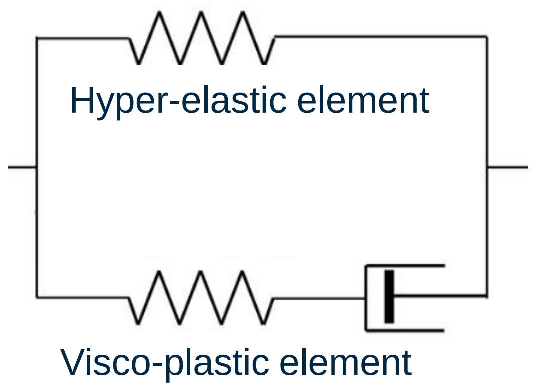
Visco-elasticity

IMPORTANT CHARACTERISTICS

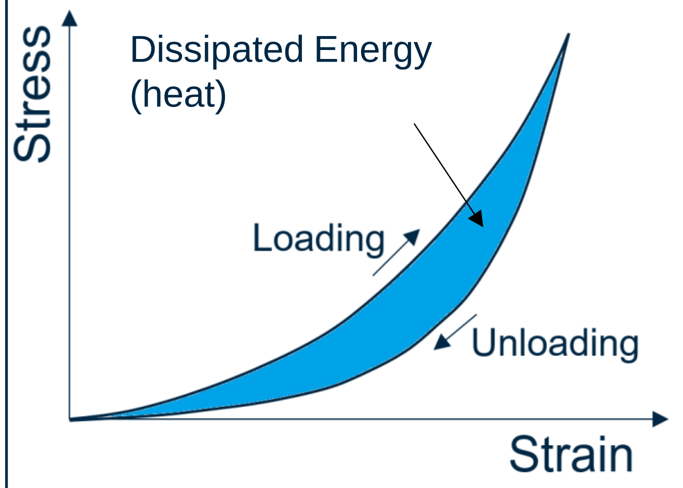
- **Full strain restoration following load release.**
- **Time Delay for full strain restoration.**
- **Unloading Path Differs from loading path.**
- **Dissipated energy (heat) with each loading cycle.**
  - Dissipated energy is a function of loading rate / frequency.
  - Elastic energy is a function of loading rate / frequency.
  - Stiffness is a function of loading rate / frequency.

- **Strain rate / time / frequency dependent material properties.**
  - Described by *Dynamic Modulus.*

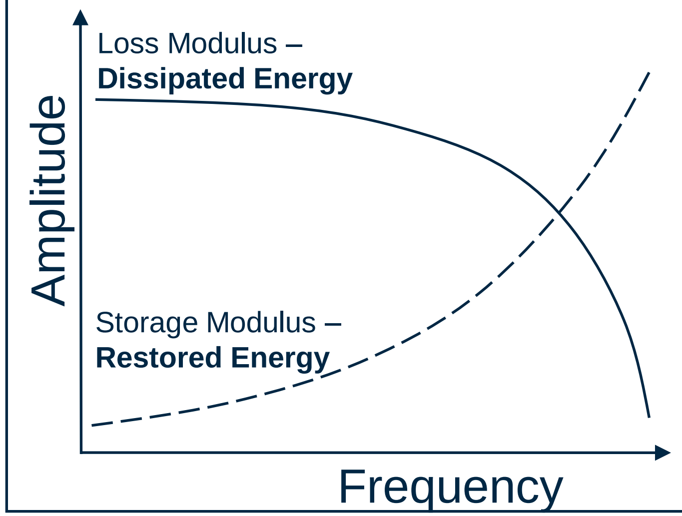
Rheological Model



Strain Response Features



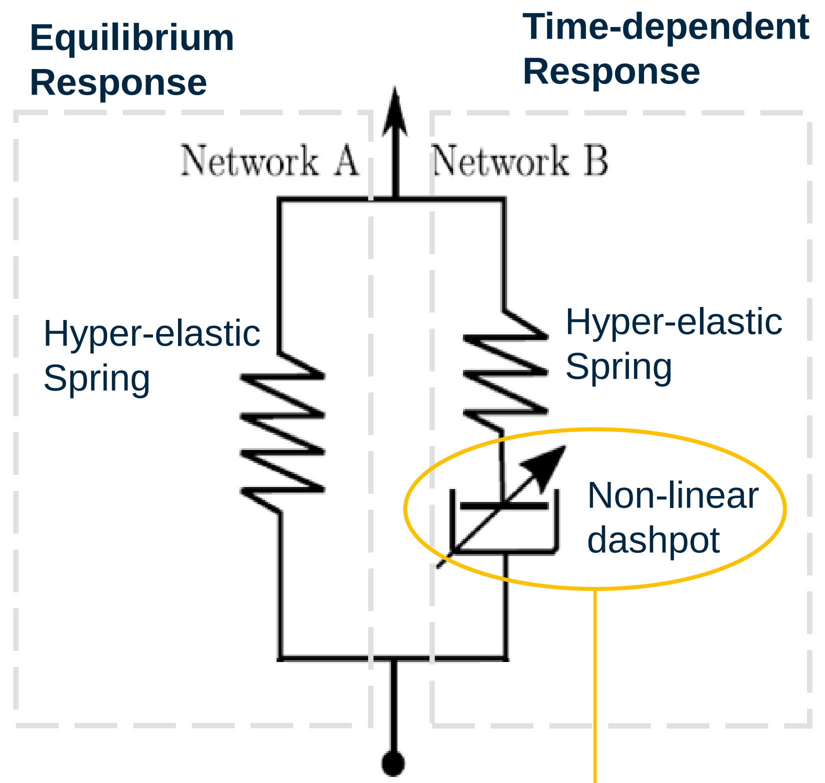
Dynamic Modulus Behaviour

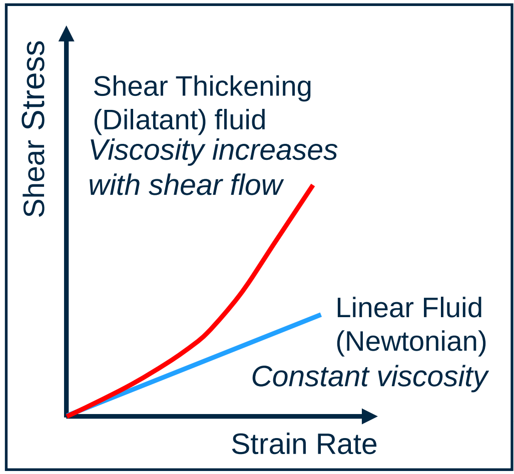


Non-linear Visco-elasticity

- Similar to visco-elastic, but with a non-linear dashpot (damping).
- **Bergström Boyce** material model is underpinned by polymer science and empirical behaviour data.
- **The material model can be used to create new finite element definitions.**
- Careful work required to determine the **9 constitutive material model parameters.**

1-dimensional Rheological Representation of the Bergström-Boyce Constitutive Model

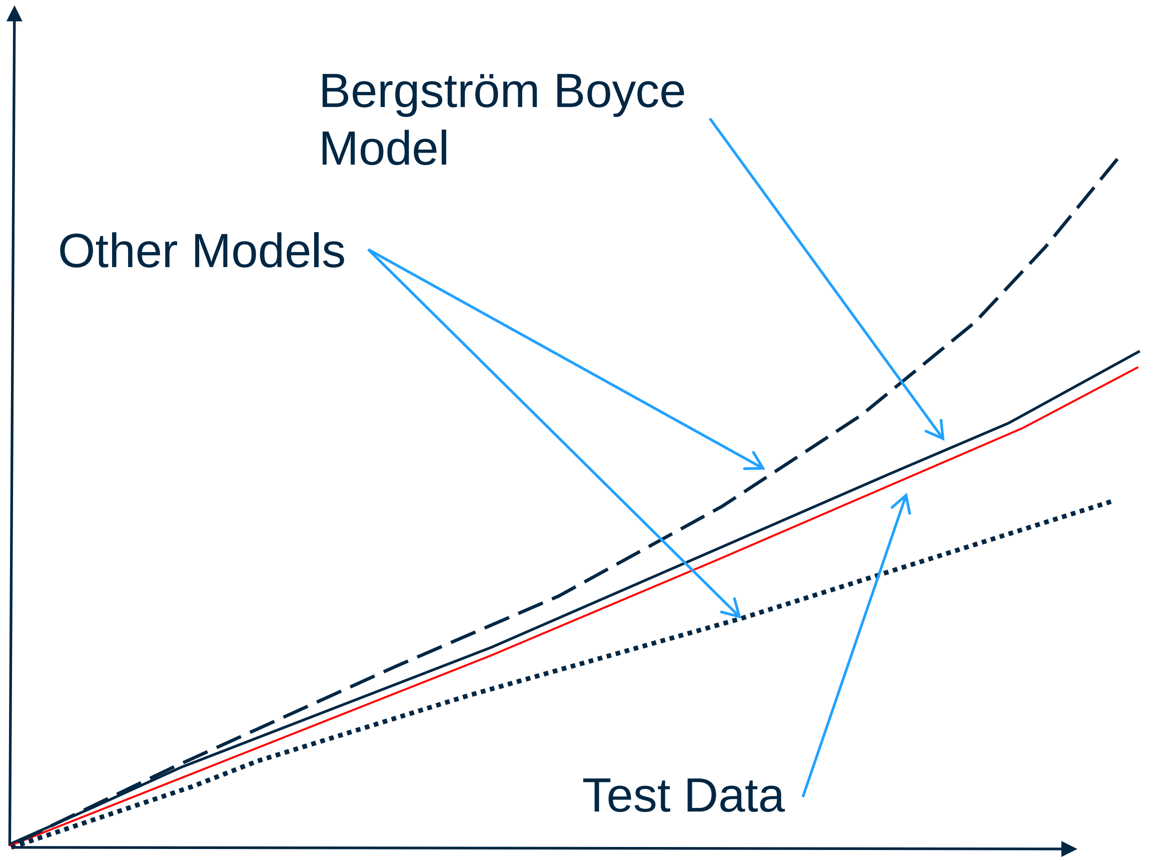




Constitutive Model Performance

- Bergström **thesis shows good correlation** between test and model under various configurations[2].
- Explored **range of different materials** (no energetics data uncovered at this point).
- Test Coverage:
  - *Time dependent material behaviour.*
  - *Numerous materials / filler content.*

Typical Model Correlation to Test – Bergström Boyce



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2. **For further information refer:**
Large Strain Time Dependent Behavior of Elastomeric Materials
For the doctoral thesis of Jörgen S. Bergström
Massachusetts Institute of Technology, June 1999.

Determining Constitutive Model Parameters

- **Smarter Test Strategies.**
  - Re-thinking the nature of testing to suit polymer material technology.

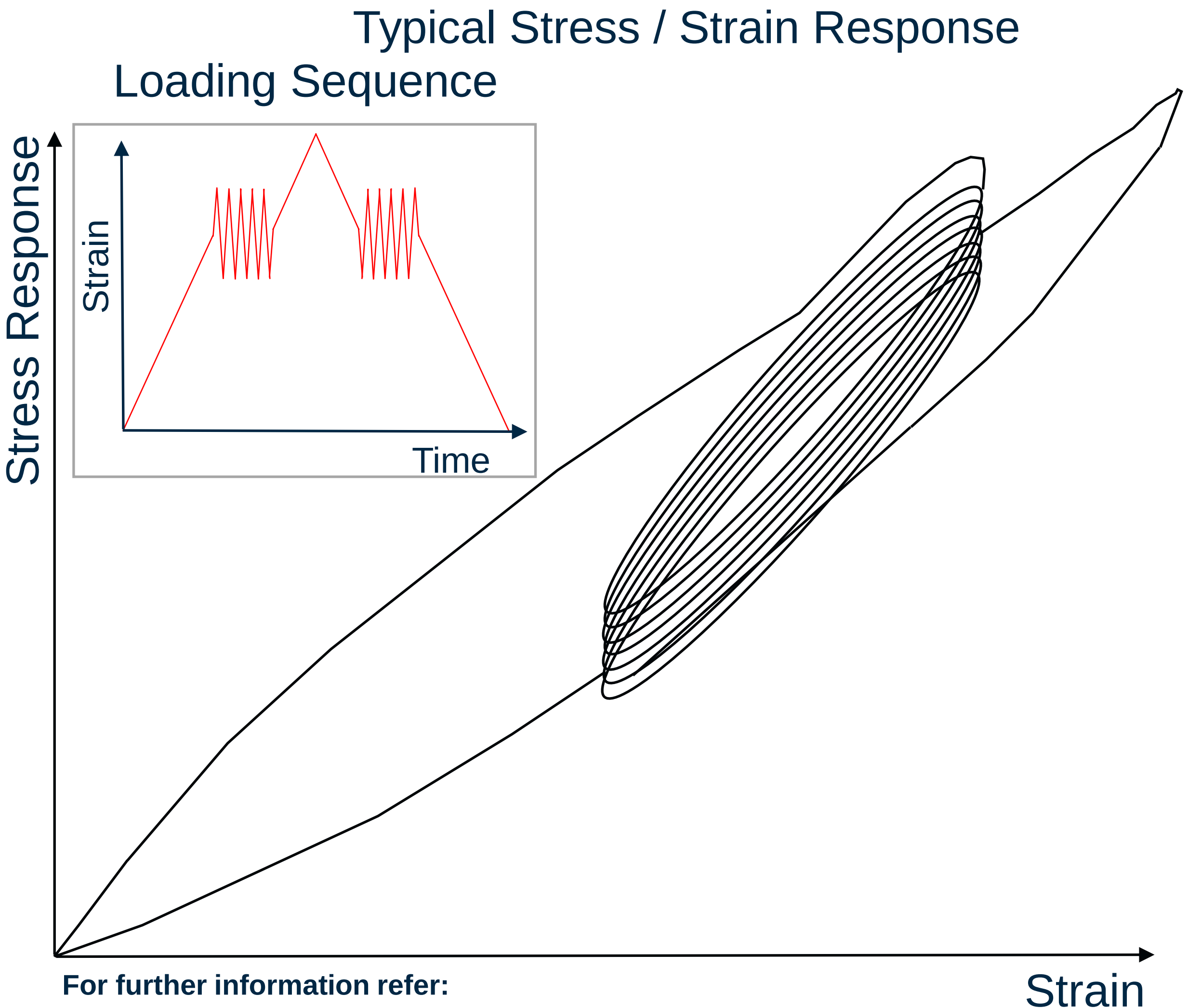
- **Clever Software / math.**
  - New tools that can extract material model parameters from test data.

Determining Constitutive Model Parameters

- Why test to failure?
- Why test with single strain-rates?

→ **Testing a single coupon with multiple loading cycles and/or multiple strain-rates offers a pathway to reduced test efforts for material characterisation.**

→ **As few as two or three laboratory tests to characterise a material for the Bergström-Boyce material model[3].**

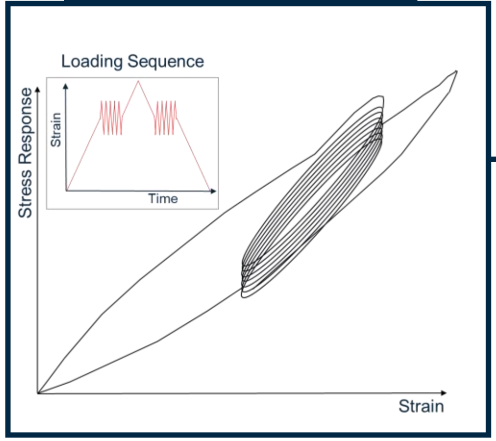


For further information refer:
Large Strain Time Dependent Behaviour of Elastomeric Materials
For the doctoral thesis of Jörgen S. Bergström
Massachusetts Institute of Technology, June 1999.

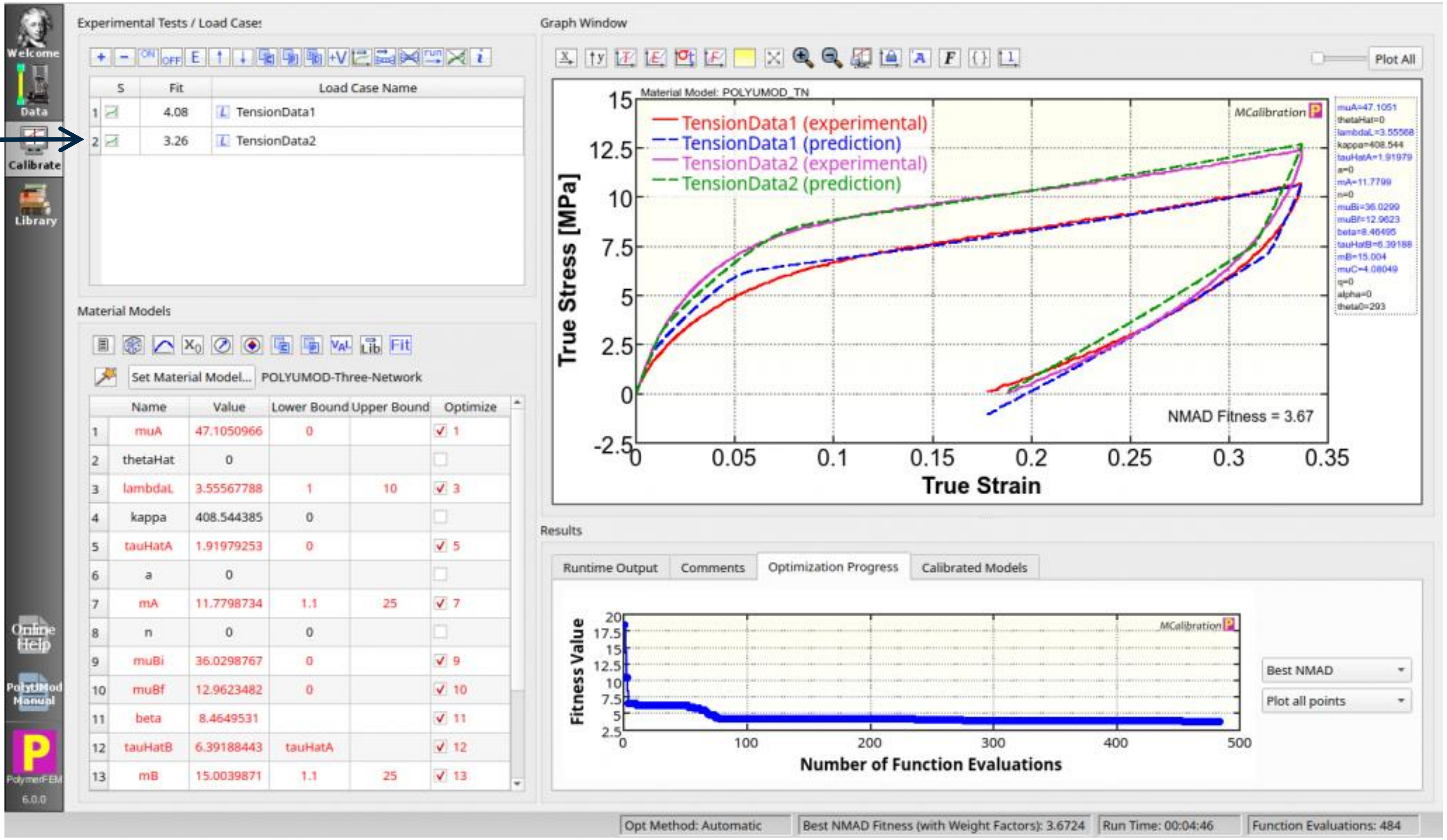
[3] Additional tests may be necessary to cover ageing, temperature, and other causes for property variations.

Clever Software – Mcalibration

Experimental Data



Finite Element Definitions



	S	Fit	Load Case Name
1		4.08	TensionData1
2		3.26	TensionData2

Set Material Model... POLYUMOD-Three-Network

	Name	Value	Lower Bound	Upper Bound	Optimize
1	muA	47.1050966	0		☑ 1
2	thetaHat	0			☐
3	lambdaL	3.55567788	1	10	☑ 3
4	kappa	408.544385	0		☐
5	tauHatA	1.91979253	0		☑ 5
6	a	0			☐
7	mA	11.7798734	1.1	25	☑ 7
8	n	0	0		☐
9	muBi	36.0298767	0		☑ 9
10	muBf	12.9623482	0		☑ 10
11	beta	8.4649531			☑ 11
12	tauHatB	6.39188443	tauHatA		☑ 12
13	mB	15.0039871	1.1	25	☑ 13

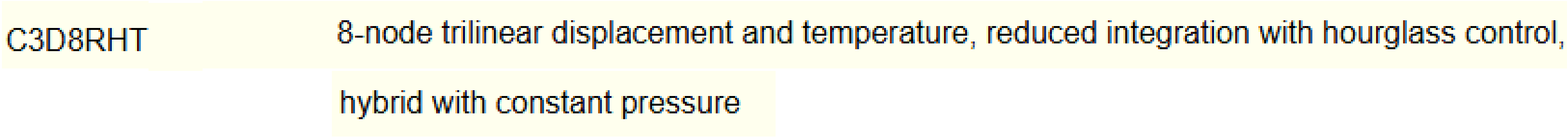
Opt Method: Automatic | Best NMAD Fitness (with Weight Factors): 3.6724 | Run Time: 00:04:46 | Function Evaluations: 484

Graphic courtesy of polymerFEM.com

Some Finite Element Considerations

✓Relevant finite element types exist.

- Element definitions that support NLVE materials.



C3D8RHT	8-node trilinear displacement and temperature, reduced integration with hourglass control, hybrid with constant pressure

✓Material model stability important, but solutions available.

- For numerical model convergence.
- Can be addressed by in-built stability tools as part of material model development (e.g. Drucker Stability).

✓Abaqus FEA software meets the requirements of this problem-space.

- has non-linear visco-elastic capabilities.
- Used by QinetiQ for energetics modelling in the past.

Additional Complexities for Energetic Materials

- **Mullins effect**
  - Material softening over the first few cycles (history dependence).
  - Can be modelled e.g.
    Ogden and Roxburgh method, 1999
- **Temperature dependence**
  - Mechanical property changes with temperature.
  - Can be modelled e.g.
    WLF method.
- **Humidity vulnerabilities**
  - Material shown to soften with humidity exposure.
- **Build / Batch variations**
  - Statistical variability between batches or fabrication methods.
- **Changes with age**
  - Material shown to harden with age.

Summary of Material Property Discussion

- Energetic materials are known to behave in a **non-linear visco-elastic** fashion.

- **Material properties are sensitive to ageing, environmental exposure, loading history and statistical variability[4].** Results must accordingly be treated with care.

- **Material mechanical properties can be modelled** through the application of rheological models to describe the constitutive behaviour.

- While material mechanical **properties are numerous and complex, they can be determined through smart testing and commercial software**.

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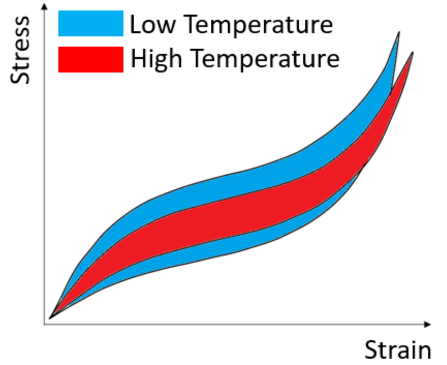
[4] Refer additionally Chapter 2.2.4 of *“Solid Propellant Grain Structural Integrity Analysis, Space Vehicle Design Criteria (Chemical Propulsion)”* NASA SP-8073, June 1973.

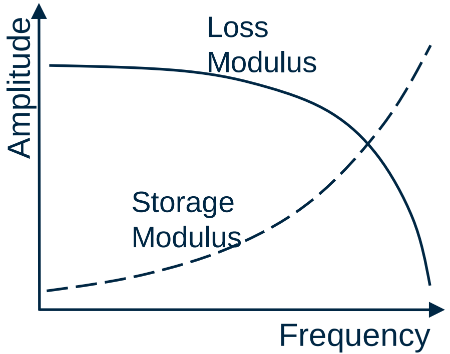
Energetic Material Failure Modes

Hysteresis and Hysteretic Heating

Recall: Material Properties are Temperature Dependent

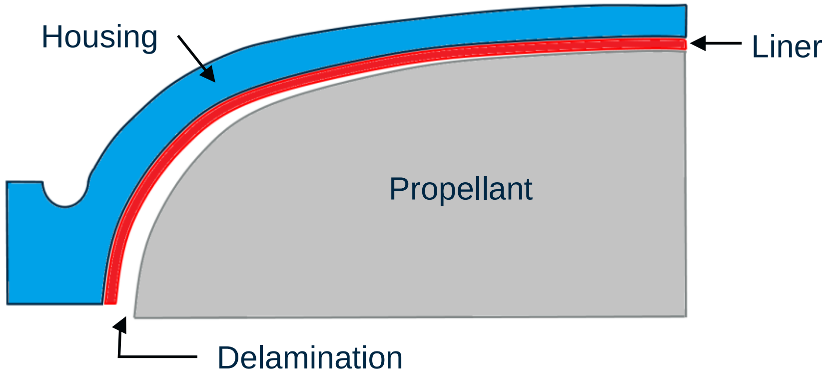


Recall: Dynamic Properties are Frequency Dependent



- Material deformations cause heating, which causes material temperature increases.
- Materials undergo temperature-induced softening, which changes the hysteresis behaviour.
- The dispersal of hysteretic heating depends on the specific heat of adjacent material; and thermal conductivity properties.

Delamination / Disbond



For further information refer:
"Ageing studies on AP/HTPB based composites solid propellants"
By *Hamza Naseem et. al.*

- Temperature induced expansion and contraction can create interface stresses that cause bond failures.
- Separation about constituent laminates or layers described as delamination or 'de-bonding'.
- Bond strength properties not clear at this point - could be determined from test and likely to vary with age.

Finite Element Analysis Capabilities

What FEA Can Do

- **Modelling material response as a result of thermal shock.**
- **Modelling interface response between dissimilar materials** (e.g. rocket propellant and liner) when exposed to temperature changes**.**
- **Modelling material response under a range of load configurations.**
- ***Qualitative* information through back-to-back comparisons is seen as especially suitable**.

What FEA Cannot Do

- **Reporting precise stress or strain values when inputs are highly variable.**
  - Not reasonable.
- **Some multi-physics problems may contain too many unknowns.**
  - Excessive uncertainty for meaningful results.
- **Certain types of problem require linear solvers.**
  - Some numerical methods cannot be performed in non-linear FEA.

Most challenges to energetics modelling involve the complexity and stability of model inputs (esp. materials), and not the numerical modelling process.

Useful Strategies for Numerical Modelling – Comparative Studies

Sensitivity Studies

- Great value can be found in comparison runs, where ***one variable is incrementally changed, and results sensitivity is studied.***
- This is an example of applying *the scientific method* with finite element models.
- It is frequently the case that most modelling effort lies in building a model, and that running the model repetitiously is not costly, and very informative*.*

Back-to-back Comparisons

- **Back-to back comparisons of materials, load cases, and boundary conditions** are all examples.
- **Focus on comparison runs** i.e. changing parameters, re-running models, comparing results, and learning.

→ **Repetitious work is well-suited to computers and the same applies to numerical modelling.**

→ **Repeating model runs under different configurations, or with incremental variations, can generate useful data efficiently.**

→ **Relevant for comparisons of differing Configurations, Roles and Environments (CRE) which aligns with Interoperability objectives.**

Example Previous Work of This Nature – Further Reading

- An Example of back-to-back comparative FEA is presented below.

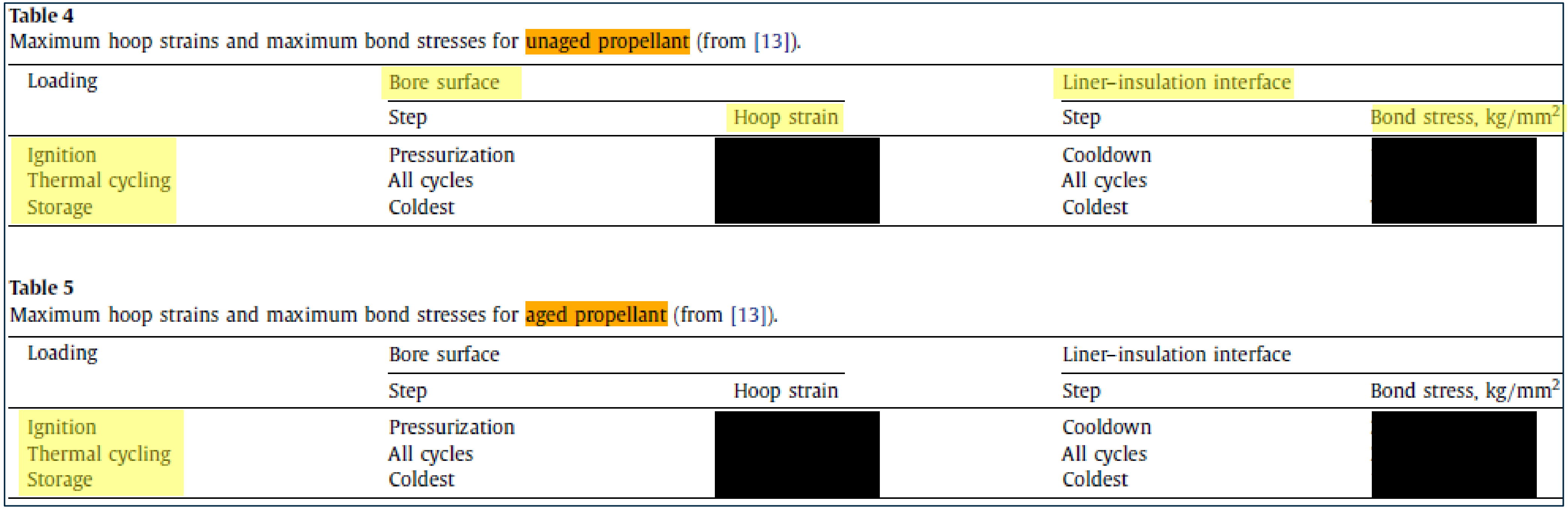


Table 4

Maximum hoop strains and maximum bond stresses for unaged propellant (from [13]).

Loading	Bore surface		Liner–insulation interface	
	Step	Hoop strain	Step	Bond stress, kg/mm^2
Ignition	Pressurization	[redacted]	Cooldown	[redacted]
Thermal cycling	All cycles	[redacted]	All cycles	[redacted]
Storage	Coldest	[redacted]	Coldest	[redacted]

Table 5

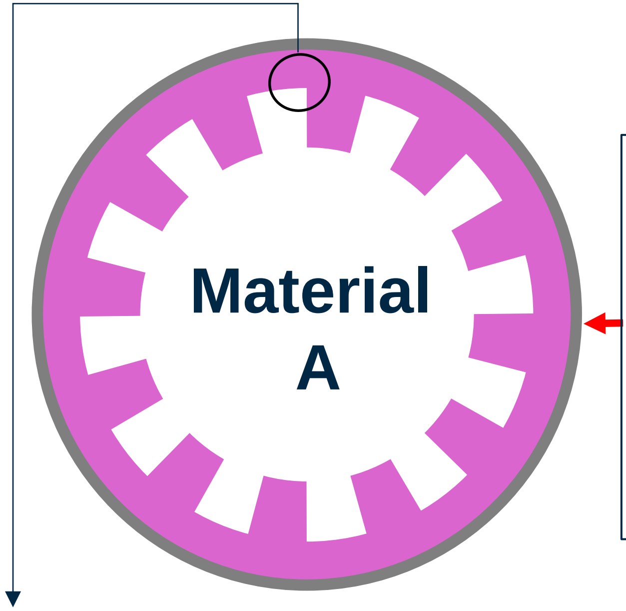
Maximum hoop strains and maximum bond stresses for aged propellant (from [13]).

Loading	Bore surface		Liner–insulation interface	
	Step	Hoop strain	Step	Bond stress, kg/mm^2
Ignition	Pressurization	[redacted]	Cooldown	[redacted]
Thermal cycling	All cycles	[redacted]	All cycles	[redacted]
Storage	Coldest	[redacted]	Coldest	[redacted]

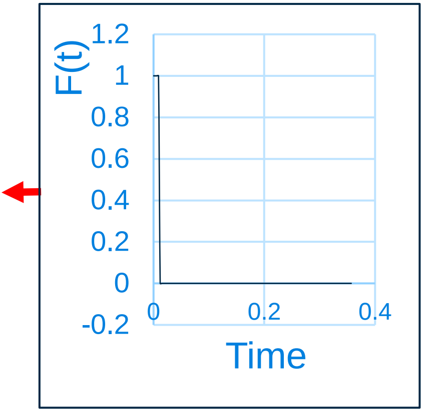
Refer: "Structural assessment of a solid propellant rocket motor: Effects of aging and damage"
H.C. Yıldırım, Ş. Özüpek
Published in the Journal of Aerospace Science and Technology, 2011

Data Values Redacted due to Copyright

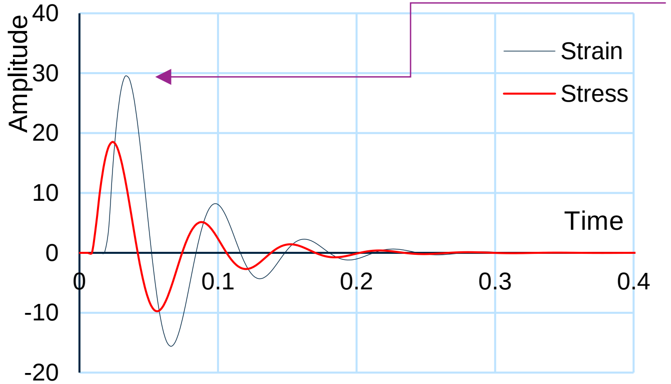
Back-to-back Comparison Example - Mechanical Shock Response



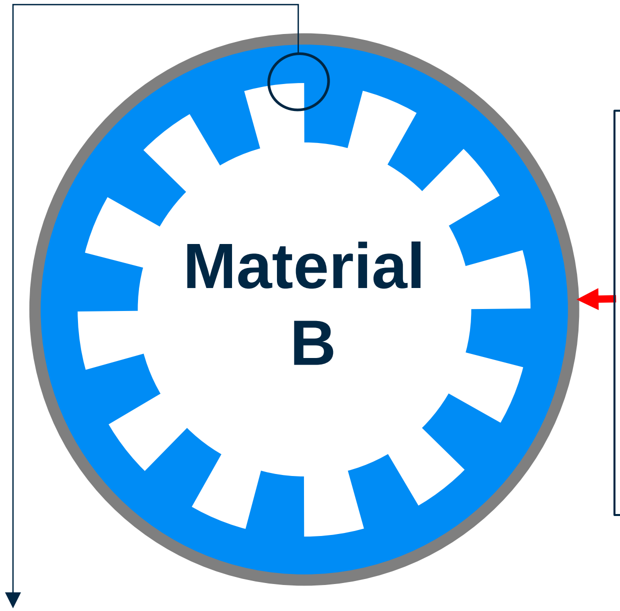
Impulse Load



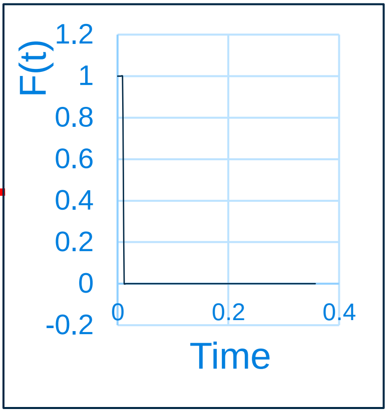
Stress and Strain Response



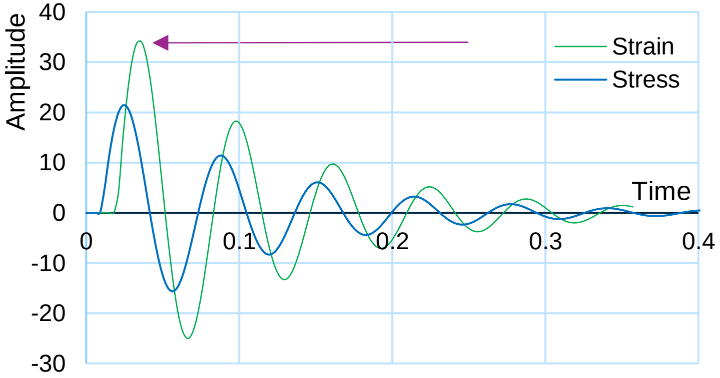
Compare peak strains



Impulse Load

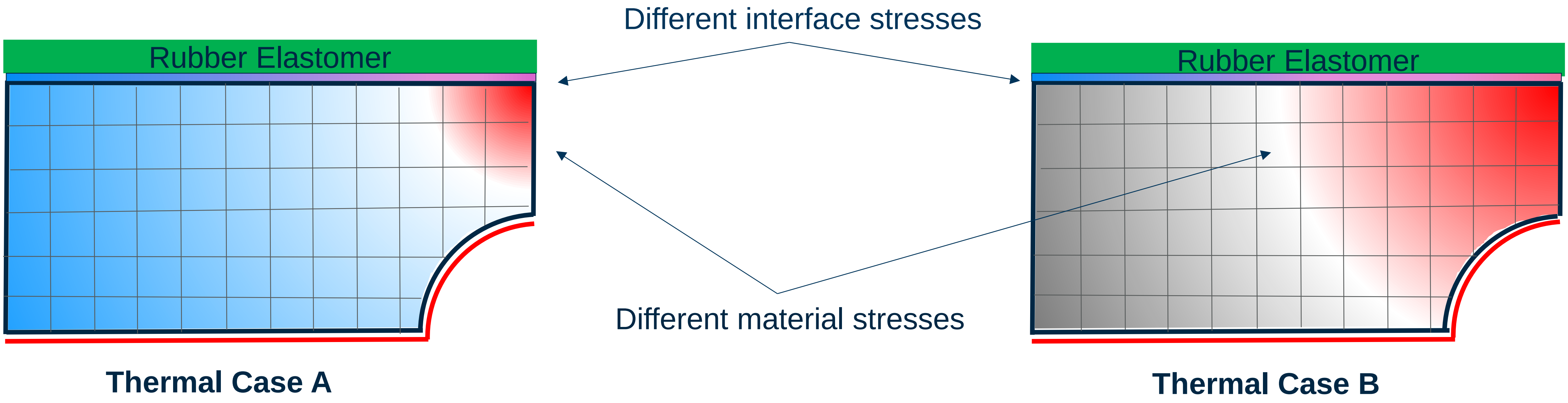


Stress and Strain Response



Comparative change in material strain levels due to changed material condition can be studied.
→ Support to safety case for ageing energetic materials.

Back-to-back Comparison Example -Thermal Cases



Back-to-back thermal cases may help to understand the effects of differing CRE.
→ Support to interoperability analysis and associated safety cases.

Potential Challenges

- Challenges to **constitutive model development** (rheological model parameters).
- **Material property variability** can affect confidence in results (batch / lot variability).
- **Material property sensitivities** influence confidence in results (environmental, etc.).
- **Unforeseen numerical modelling challenges** – new territory in non-linear visco-elastic modelling.

A model is only as good as the information that it is founded upon.

Conclusion

- **QinetiQ work shows numerous examples where finite element models of energetics have allowed meaningful and relevant results**.
- **Numerical modelling of energetic materials is thus considered feasible and of potential utility to Safety and Interoperability aims**.
- **Mechanical material property complexities; their variability; and their sensitivity to change present challenges to the modelling of energetic materials.**
- Materials and failure mode complexities are seen as limitations that can prohibit models from delivering quantitative results; however, research shows that qualitative / comparative modelling strategies can be useful in-line safety and interoperability objectives, especially if used alongside other methods, such as physical testing.

Our Vision

- Test-validated numerical models, working in concert with test and surveillance data, to:
  - **Improve the understanding of energetic material behaviour**.
    → improved failure predictors and failure management.
  - **Provide insight and guidance for targeted surveillance** strategies.
  - **Improved interoperability and safety outcomes**.
    → improved understanding on material behaviour under differing CRE.

If this direction is successful, it will improve the understanding of energetic material behaviour under differing CRE; beneficially impact safety outcomes, and reduce sustainment costs.

Thank You for Your Attention

Questions

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