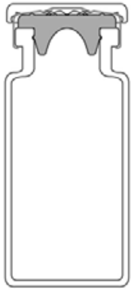
Evaluation of Cryogenic CCS Seal Integrity using an Incremental Computational Approach

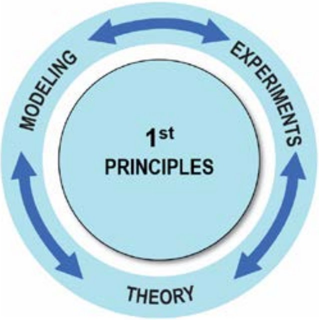
Objectives



1. 1st Principles insight into Cryogenic Container Closure

Underlying Objectives

2. 1st Principles can guide risk assessment and design plans
3. Computational Modeling > checking
4. A successful tool matures through the product life cycle



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Introduction

- A 1st Principles focus = ↑ efficiencies and ↓ risks
- Computational model(s) in parallel with development, not an *after-thought*.
- Appropriate to current objectives
  - Feasibility → Can it work? *(Subsystems level)*
  - Early Design → Identify sensitivities
  - Detailed design → Establish design margin *(System level)*
  - Sustaining → 'Curve balls' & process support
- Analysis and Experiments should ***complement***, not supplement.
- ASME V&V 40

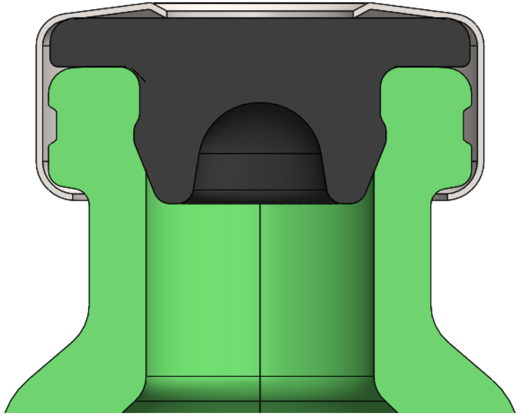
Typical Incremental Computational Approach

1. Identify theory of operation
2. Develop a Minimum Viable Computational Model
   - Define Objective
   - Explore physics-based 1st Principles understanding for functionality
   - Scale and execute computational model
   - Verify results
   - Iterate and/or expand conditions
3. Expand computation model and test plan for next development phase
4. Maintain model through transfer to manufacturing
   - Digital Twin, IIOT, Design Changes, root cause analyses…

Case Study

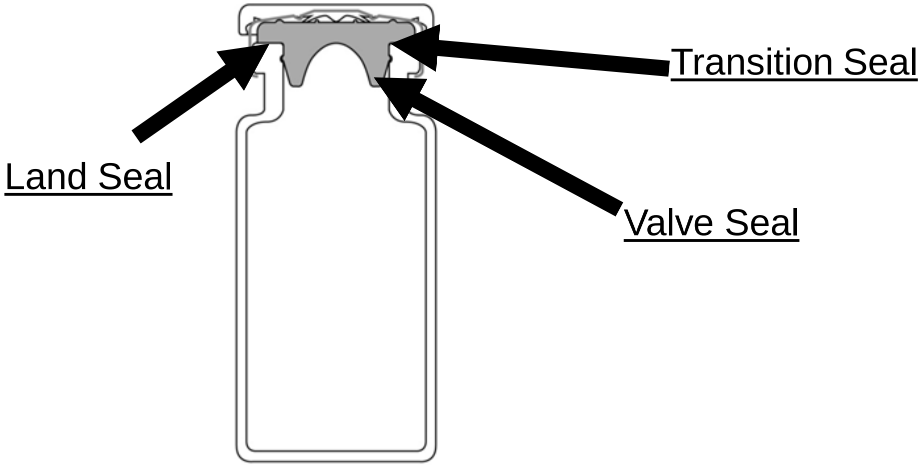
Can Seal Integrity be maintained at cryogenic storage for a ‘typical’ plastic 2ml Vial and standard assembly lines?

- Feasibility is hypothesized based on:
  - D.H. Weitzel’s 1962 success of highly compressed o-rings
  - Exploratory CTE calculation resulting in residual compression at -180^{o}C.
  - Prior literature nominal success with low statistical confidence



Identify Theory of Operation

- Traditionally, the face seal (Land Seal) is considered to be primary seal.



Minimum Viable Computational Model Objective

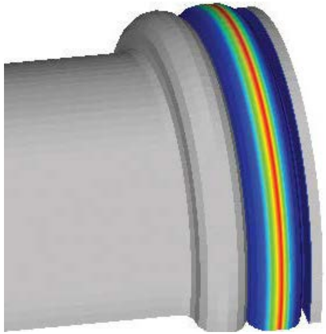
- Numerous factors through the product life cycle can affect the seal integrity.
- For initial feasibility, factors are down-selected to explore success

Component Manufacturing	Product Assembly	Cryogenic Storage	Use
• Tolerances • Surface quality • Material variations • Washing • Coatings • Sterilization • Post Processing • Storage • Local defects • Etc.	• Compression force • Crimp height • Timing • Temperature • Alignment • Etc.	• Temperature • Time • Rate • Transit • Environmental • Etc.	• Environment • Use cases • Etc.

Understanding the Physics of Sealing

- Elastomeric sealing = Contact Stresses + Contact Width.
  - Product usage, material stiffness, surface properties, assembly deformations, etc
  - Typically - experimentally derived.
- For feasibility, an analysis of an o-ring with similar hardness used to set specifications.
  - *(2ml hand calcs - RSF value ~ 27 N (6lbf))*
- Sealing stresses of rigid plastics are typically over an order of magnitude higher. Should be developed for temperatures below Tg.

Generic O-Ring

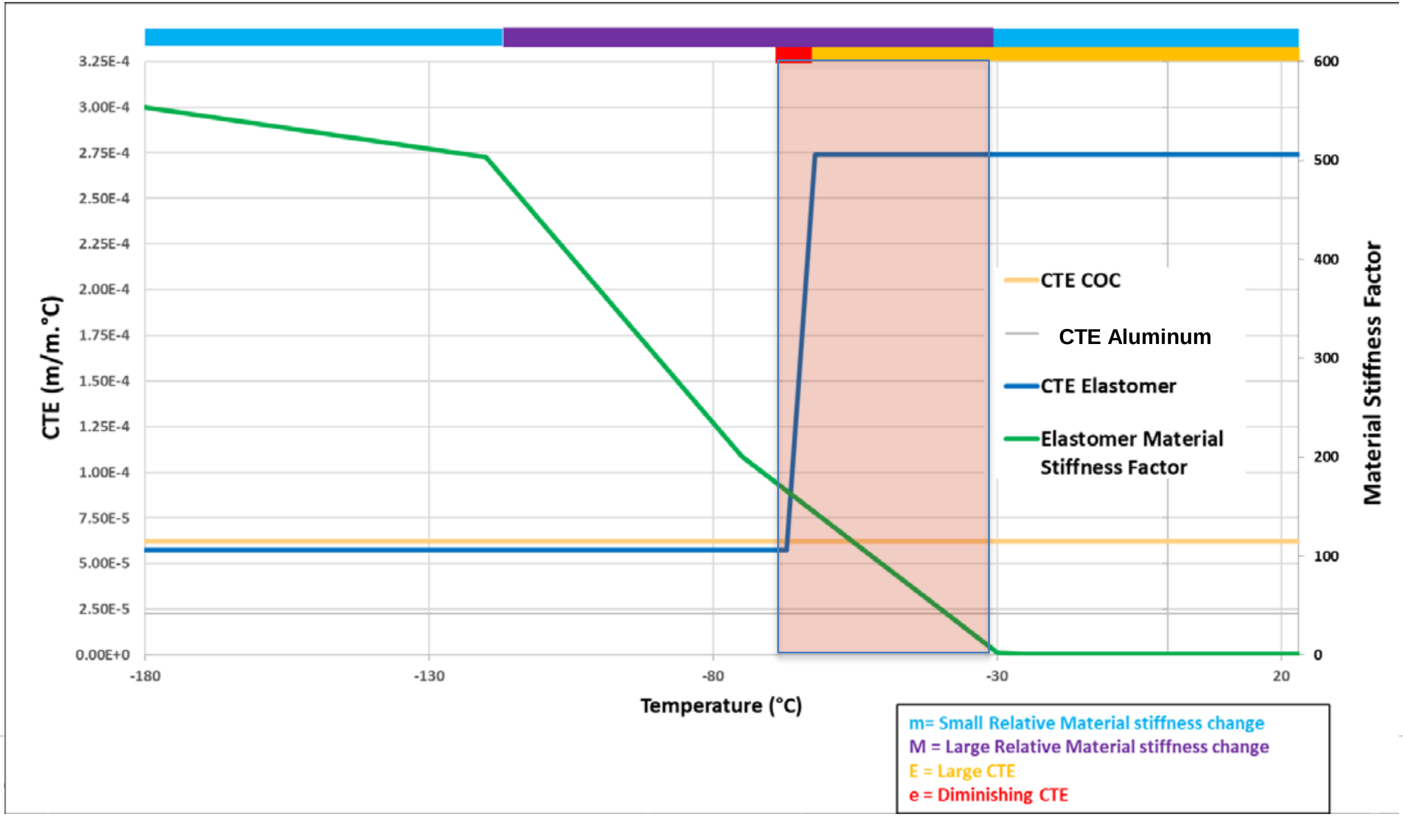


Red > 0.3MPa
>0.3mm

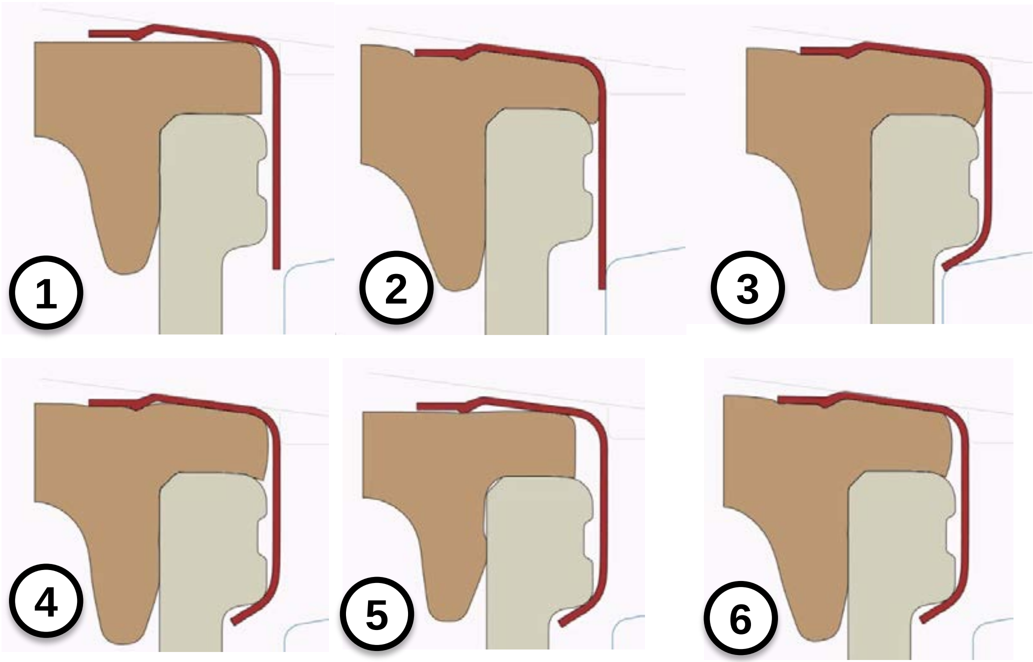
1st Principle Material

- Elastomeric seals known to be hyperelastic & viscoelastic
- Cryogenic storage typically not recommended by elastomer suppliers
- Preliminary material testing performed to develop a basic understanding of:
  - ***How do part dimensions change with temperature?***
  - ***How does material stiffness change with temperature?***
- Assumed to be the minimum input necessary for a feasibility model.
  - If feasibility is confirmed, extensive testing would be recommended to explore resin variations, transient properties, failure mechanisms, etc.

1st Principles Material



Initial Computational Model

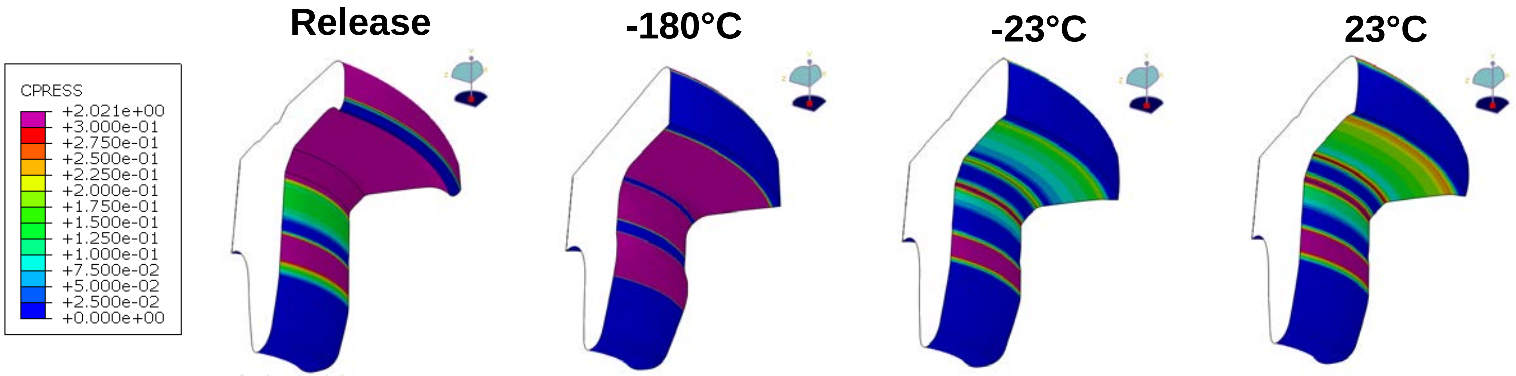


- Assume:
  - Hyperelastic, temperature dependence
  - No time dependence

1. Resolve Stopper Interference
2. Compress to 140N (32lbf)
3. Crimp
4. Release Crimp and Load
5. Temperature sweep to -180°C
6. Temperature sweep to +23°C

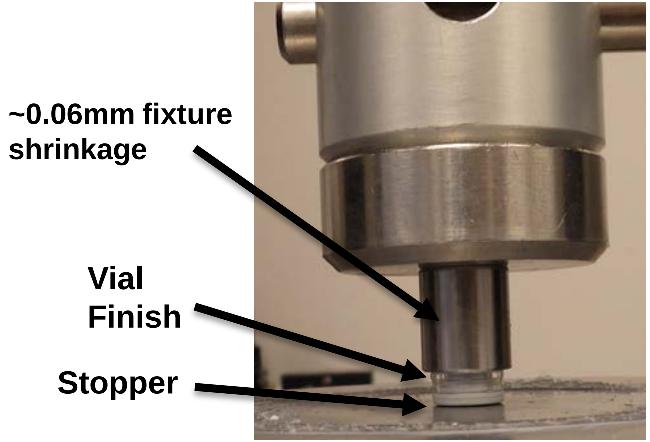
Initial Computational Results

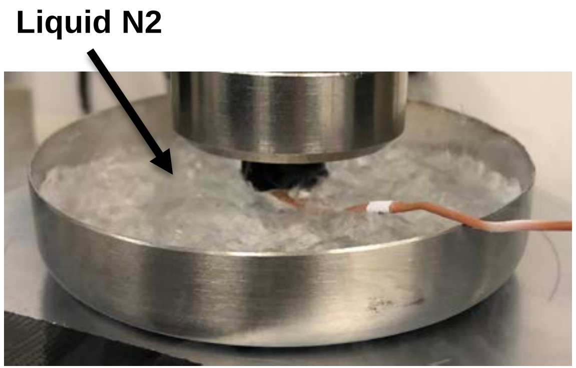
- Pink surfaces = Contact stress > assumed specification
- Primary seal maintains contact but fails to meet target contact stress during the warm up cycle. (Transition Zone)
- Although counterintuitive, the results seems to correlate to prior literature that sealing can be achieved however does not meet the robust requirements.

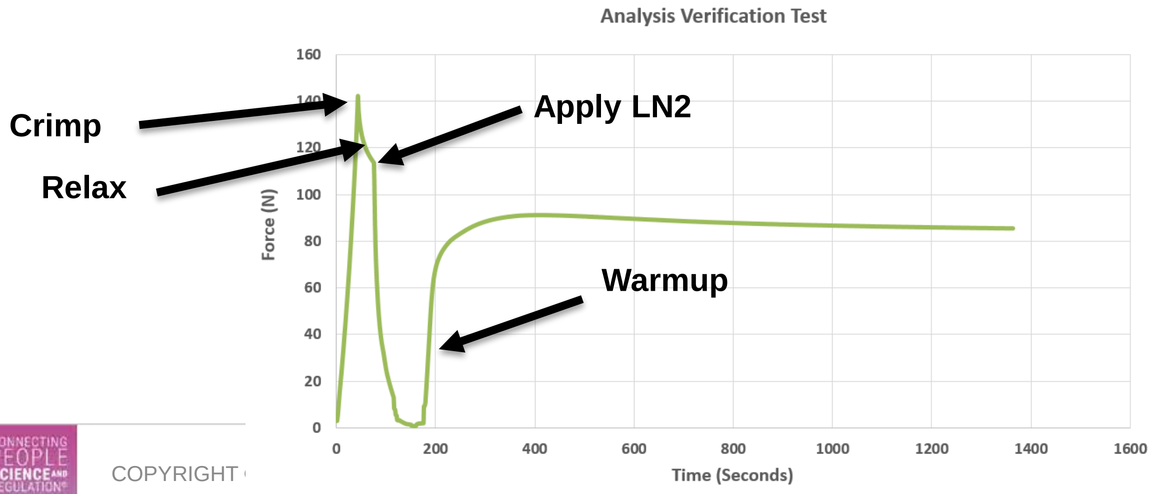


Verify Results

- At -180C, the load is greatly reduced (~140N to 4N)
- Analysis indicates a significantly higher force
- Initial analysis definitions are <u>insufficient</u> to evaluate <u>cryogenic</u> conditions. Must be further developed.



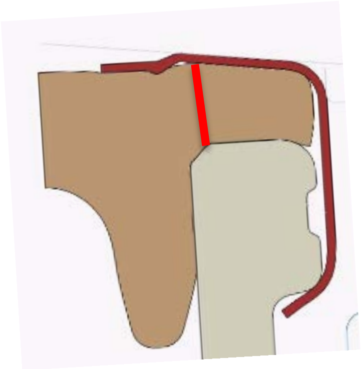




Verify & Interpret Results

- However, verified at room conditions (~2% Error)
- The model utilized to explore the sensitivity of the system.
- The below table summarizes the typical contact pressure at the face seal as **GREEN** if >0.3MPa, **YELLOW** if <0.3MPa, and **RED** if no contact.

	Baseline RSF=140N	Reduced Crimp load, RSF=90N	0.25mm Tighter Crimp	0.25mm Less Crimp	Baseline, LMC
Initial Room Temperature					

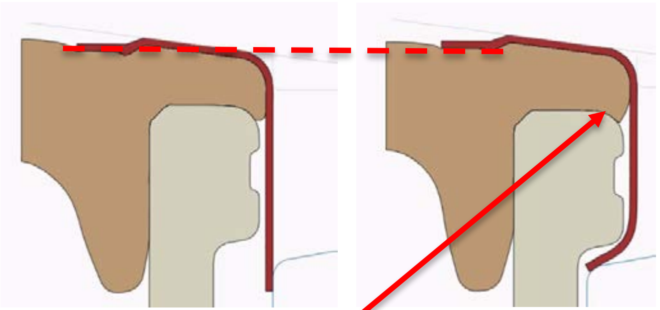


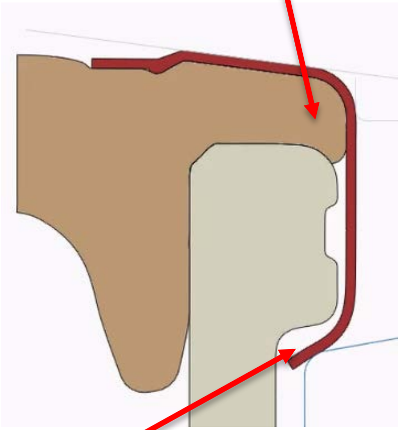
Observations

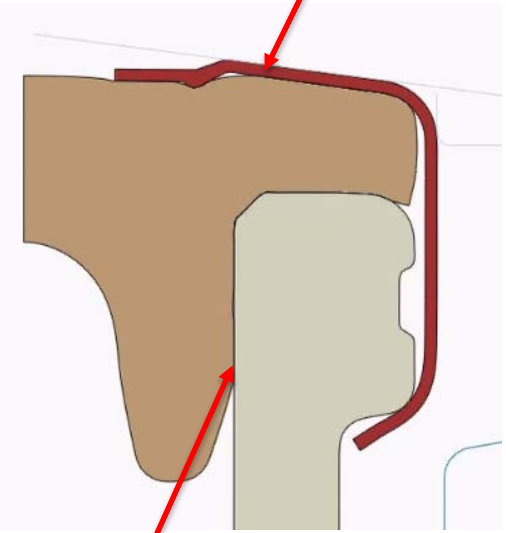
Fixture geometry affects compression

Confined compression

Crimping affects preload







Preload and Crimp Geometry affects overhang

Crimp affects compression

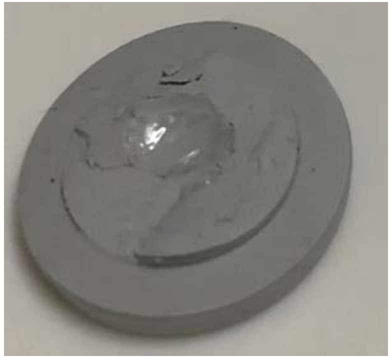
High friction reduces the compression

Explore Material Model Limits

- Quick ‘binder clip’ experiment at -40^{o}C and 23C to investigate counterintuitive analysis results.
- Current model would predict that the -40C stopper would straighten
- The room temperature stopper quickly recovered its shape,
- The -40C stopper maintained its shape and slowly recovered as it warmed.

Folded Stopper

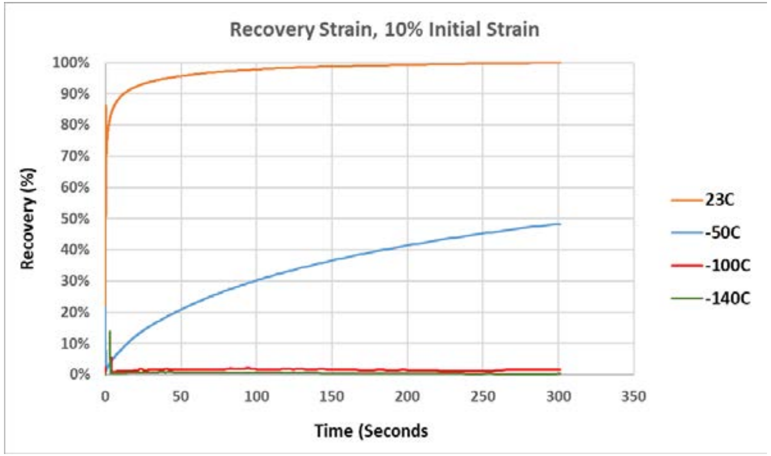
23C

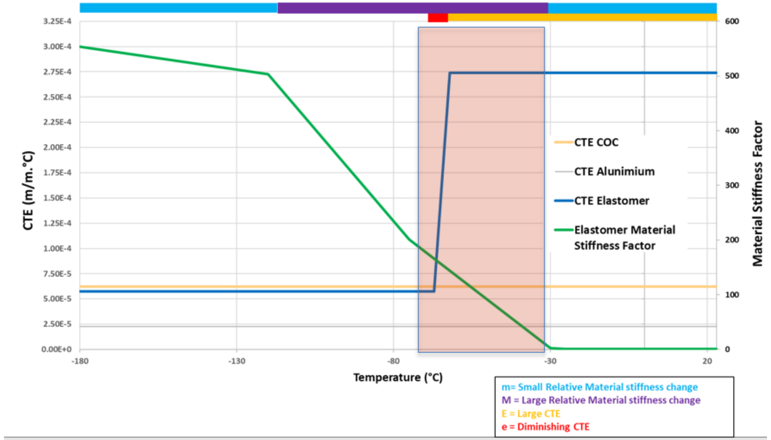


-40C

Material Investigation - Recovery

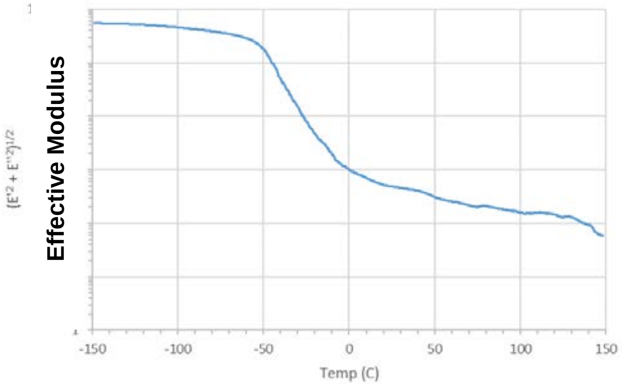
- DMA used to verify the binder clip experiment
- Material's recovery is <u>time and temperature</u> dependent.
- The previous material model must be revised to account for 'freezing'
- This phenomenon further complicates the transition region





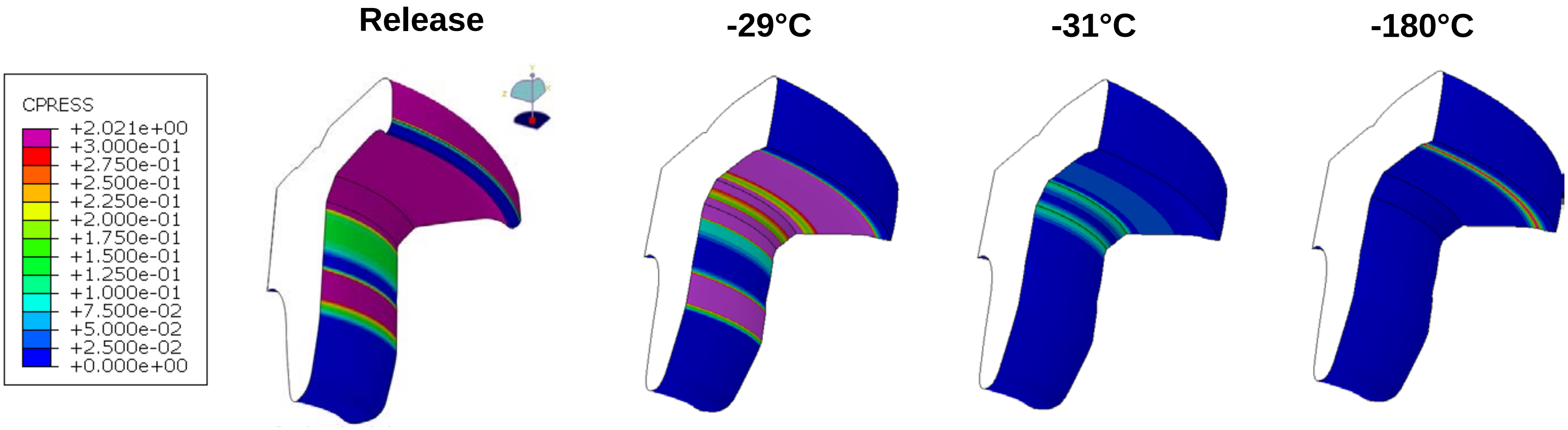
Revised Computational Model

- An abbreviated ‘binary’ recovery material model rather than fully developing all time dependencies.
- Assume full recovery at temperatures greater than -30C and zero recovery at less than -30C.
- -30C selected because it reflects the temperature where the rate change in effective modulus occurs.
- This method is assumed to be conservative for temperatures lower than -30C.

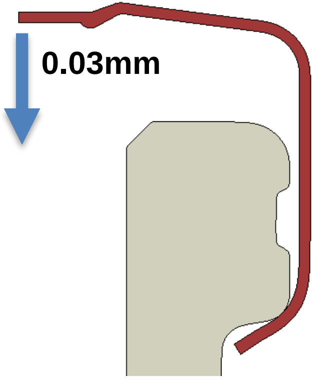


Revised Computational Model

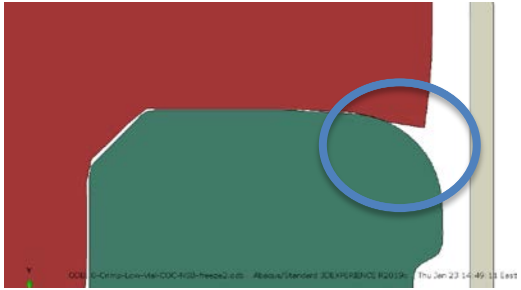
- Primary seal maintained until the ‘freeze point’.
- Contact Maintained, design margin is small
- Contact transitions from the ID to the OD



Key Learnings



1. Below the 'freeze zone', less dependent on initial crimp force and more dependent on:
   - Relative CTE differences
   - Internal stresses of the Crimp and Vial
2. Shape and temperature of Stopper 'freeze' is critical to sealing
   - If it 'freezes' early – the CTE of the Stopper is greater than the Vial and the overhang on the Vial OD creates sealing surface.
   - If it 'freezes' later – the CTE differential is less and contact stresses are driven by the ability of internal stresses of the Crimp and Vial to compensate for continual thermal shrinkage.
3. Sealing appears feasible, however is expected to be sensitive



Discussions

<u>Why different from CTE hand calculations</u>

- Did not include material property effects due to temperature/time

<u>Why different from Weitzel's findings?</u>

- Different materials, geometry, or compression
- Gough-Joule effect?

<u>Is this different from previous test results?</u>

- Feasibility is shown in both but with low design margins
- Rate of cooling
- May indicate more exotic properties resulting in sealing
  - Polymer entanglement, diffusion of processing material, etc.

Case Study Conclusions

- Primary sealing mechanisms transitions from
  - Large elastomeric compression, to
  - CTE driven ‘rigid’ contact
- Understanding the material transition zone and timing is critical
- Low design margins → Higher fidelity model and test fixture recommended
  1. Test method should better compensate fixture shrinkage
  2. Material model should include the temperature, time, and rate dependence for recovery
  3. More complex material behavior should be investigated, (Gough-Joule, CTE vs. initial strains, polymer entanglement, diffusion, etc.)

Incremental Approach Comments

We demonstrated an approach to building a minimum viable computation model which can:

- – Develop a physics-based understanding of a system and key elements.
- – Provide a road map for appropriate explorations
- – Predict future challenges
- – Improve program efficiencies
- – *Stimulate novel solutions*

Standards and References

1. D. H. Weitzel, R. F. Robbins, P. R. Ludtke, and Y. Ohori, "Elastomeric Seals and Materials at Cryogenic Temperatures," ASD-TDR 62–31, Part II (1962).

Acknowledgements

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Q&A's

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