LA-UR-14-21986
Approved for public release; distribution is unlimited.

Title: Predictive Modeling of GTS Reservoirs

Author(s): Tucker, Matthew T.
Meyer, Brad A.
Bammann, Douglas J.

Intended for: GTS Structural Materials Working Group, 2014-03-04/2014-03-05
(Livermore, California, United States)

Issued: 2014-03-26

Predictive Modeling of GTS Reservoirs

Matthew Tucker, R&D Engineer
Douglas Bammann, LTVSM
Brad Meyer, Laboratory Fellow

W-7, Los Alamos National Laboratory

GTS Structural Material Working Group Meeting

March 4-5, 2014

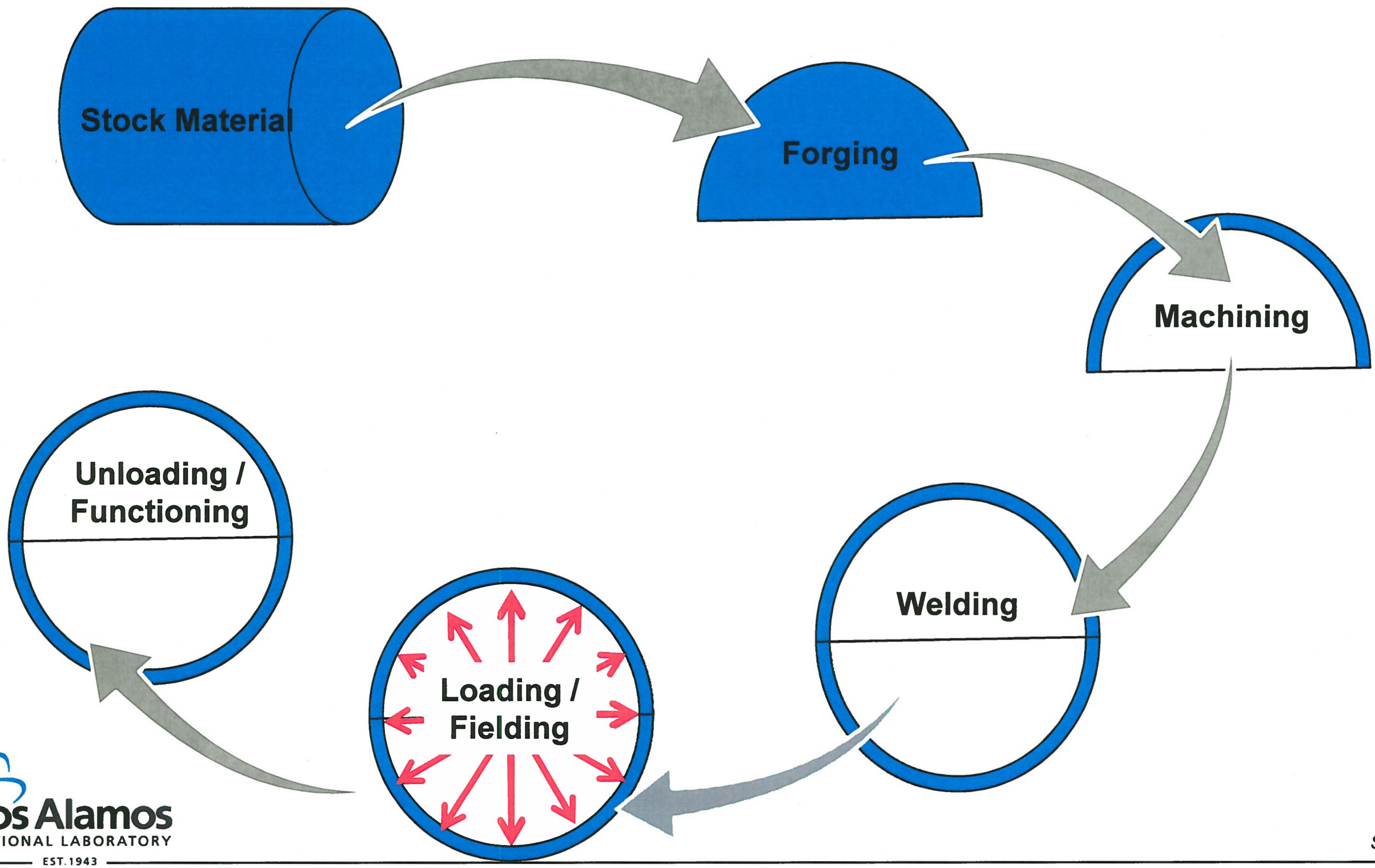
P.O. Box 1663
Los Alamos
NATIONAL LABORATORY
EST. 1943

Drivers

- **Ability to confidently reduce structural safety factors would allow for more flexibility for future stockpile systems**
  - Require a predictive capability
    - Better implementation of what we know
    - Interaction of experimentation and modeling to determine knowledge gaps and develop techniques to probe them
    - Implementation of predictive capabilities with validation and verification from cradle to grave

The use of highly optimized reservoir designs from cradle to grave would have a significant positive impact on the stockpile, but requires a higher level of our understanding of materials and manufacturing processes.

Reservoir Cradle to Grave Process



Predictive Capability Development

Stock Material

- **Goal:**
  - Predict effects of chemistry and process changes

Forging

- **Goal:**
  - Predict resulting mechanical properties including recrystallization and texture
  - Modify process to meet requirements

Machining

- **Goal:**
  - Predict resulting mechanical properties
  - Modify process to meet requirements

Welding

- **Goal:**
  - Determine best process parameters for desired properties
  - Predict formation of cracks

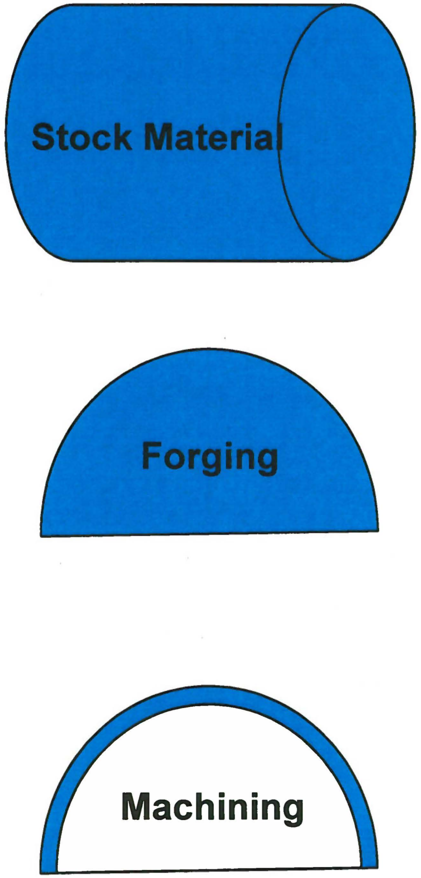
Loading / Fielding

- **Goal:**
  - Understand hydrogen/material interactions

Unloading

- **Goal:**
  - Predict test results measured through surveillance
  - Use surveillance data to inform modeling

Predictive Capability Development



Stock Material

- **Tools available:**
  - Documentation

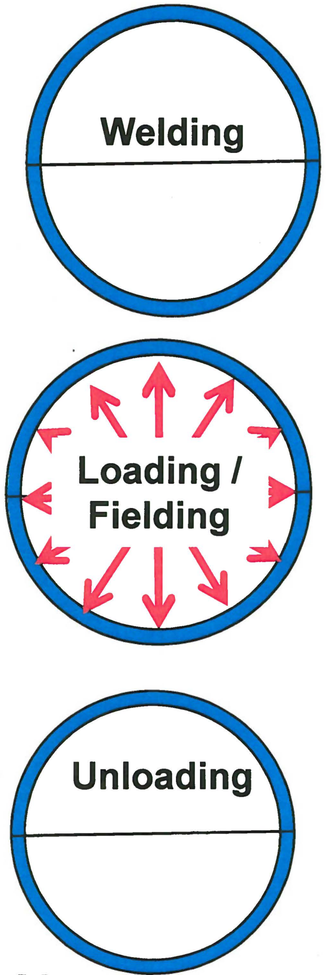
Forging

- **Tools available:**
  - Predictive modeling
  - Mechanical test data
- **Tools needed:**
  - Spatial map of final properties for next manufacturing step

Machining

- **Tools available:**
  - Mechanical test data
- **Tools needed:**
  - Implementation of predictive modeling
  - Spatial map of final properties for next manufacturing step

Predictive Capability Development



Welding

- **Tools available:**
  - Fairly reliable residual stress
- **Tools needed:**
  - Implementation of predictive modeling
  - Validation of predictive modeling

Loading / Fielding

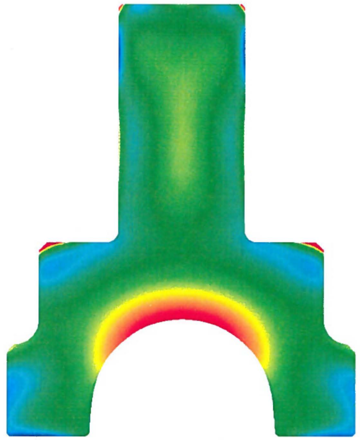
- **Tools available:**
  - Mechanical test data on H effects
- **Tools needed:**
  - Development of predictive model including physics based failure mechanisms for H
  - Validation of predictive model

Unloading

- **Tools available:**
  - Surveillance data
- **Tools needed:**
  - Development of predictive model including physics based failure mechanisms for H
  - Validation of predictive model

Current State – Forging

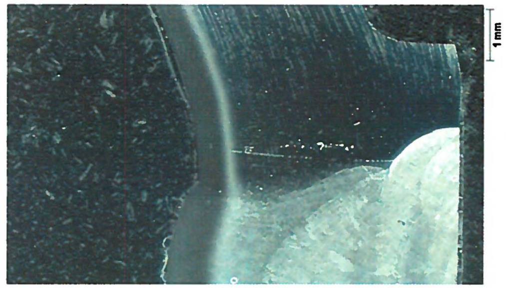
- **Development of mechanical and microstructural properties for majority of reservoir**
  - KCP works with vendors on forging development and has implemented FEA
  - Techniques available for measuring residual stresses with same techniques as for welding
    - Drawbacks are that a free surface must be exposed modifying the stress state or a very shallow area can be measured given an "unstressed" baseline measurement can be made
  - We need to be able to carry history effects forward from forging including accurate spatial information

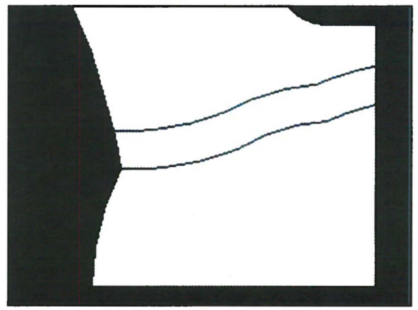


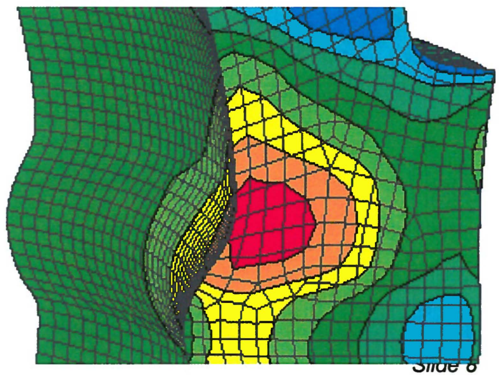
Extremely important process that determines majority of final reservoir structural performance

Current State – Welding

- **Most critical area for unexpected failure**
  - Welding induces property evolution to the developed forged properties
  - Current methodology is to model welding process and match measured residual stress measurements for coupling back to FEA for structural analysis
    - Not suited to predictive capability necessary for weld development
  - Modeling approach relies on marginally compatible commercial packages for stress state mapping
  - Measurement requires either exposing a stressed free surface therefore modifying the stress state or measuring a very shallow area given that an "unstressed" baseline measurement can be made



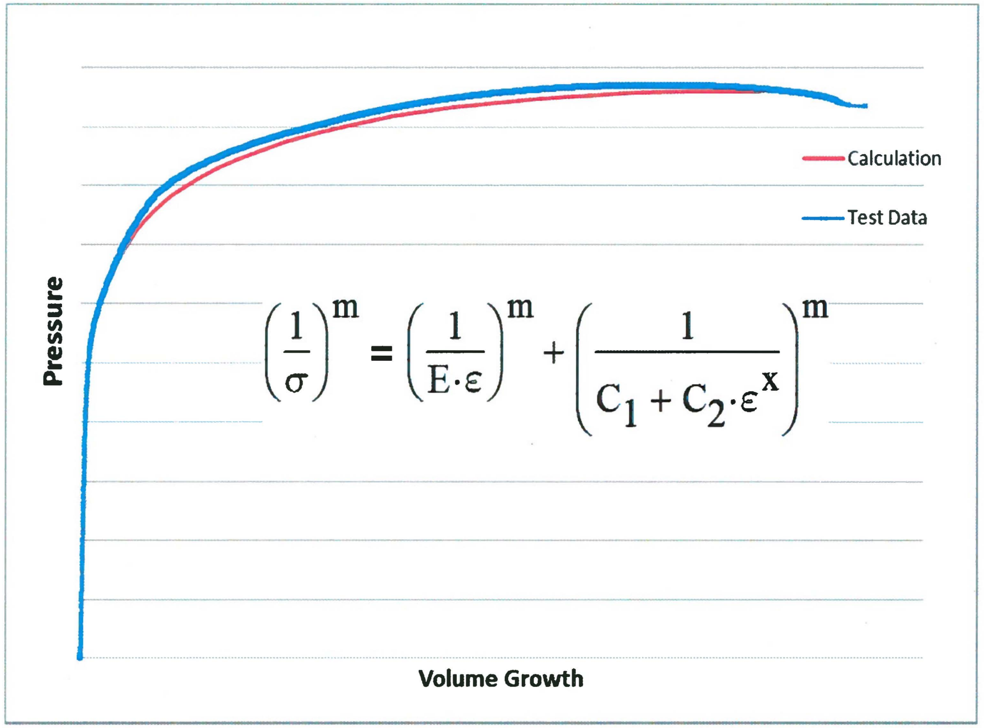




Current State – Fielding

- **Required agreement between model and test data for man-safe certification**
- **Very accurate prediction of reservoir yield and burst pressure using model fit to forge test data**

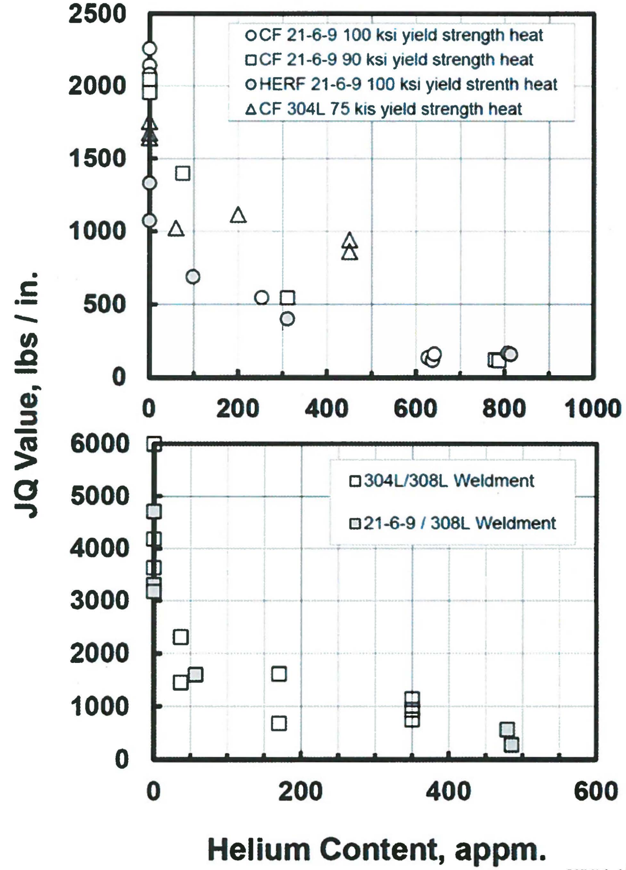
Excellent structural verification model and accurate **predictions** provide evidence of process understanding



Current State – Fielding

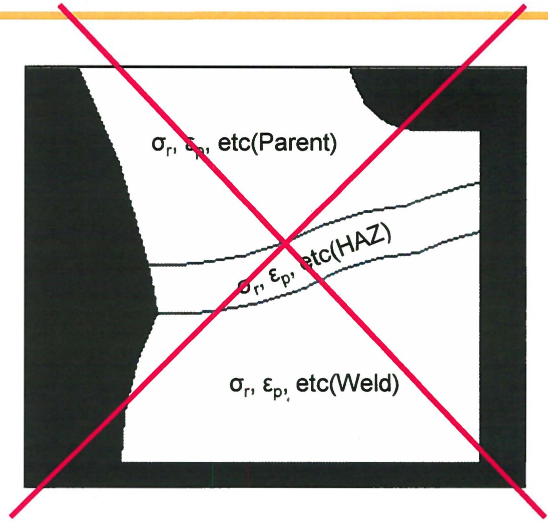
- **Tritium/Helium effects have been studied for decades and consistent data provides confidence for design**
  - Most difficult data to obtain due to hazards and time constraints
  - Most critical data for avoidance of unexpected failure
  - Only available data is from within the complex

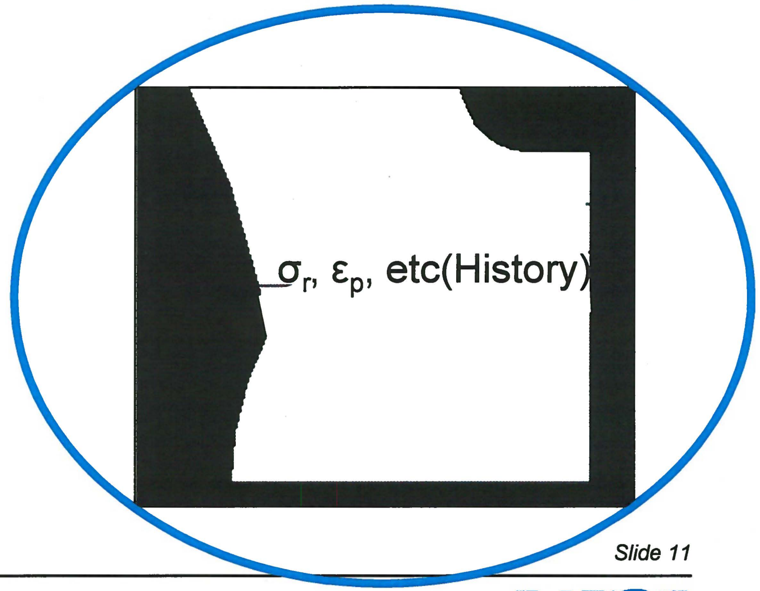
Unique problem for our industry so we are responsible for making sure we understand what is important



Approach Going Forward

- **Development and implementation of a unified multistage physics-based modeling capable of capturing known process and environmental effects as well as predicting unforeseen issues**
  - Single modeling flow capable of handling
    - Complex solid modeling input
    - Forging process input and output
    - Welding process input and output
    - Loading and fielding input and output
    - Failure prediction due to:
      - Ductile failure
      - Known hydrogen-material interactions
      - Competing theories on hydrogen-material interactions





Physics-Based Modeling of Hydrogen Effects – Embrittlement Theories

- **Stress-induced hydride formation and cleavage**
  - Metals with stable hydrides (Group Vb metals, Ti, Mg, Zr, and their alloys)
  - Supported by experimental observations
- **Hydrogen enhanced localized plasticity**
  - Increased dislocation mobility
  - Localization of slip in front of crack tip
  - Failure by plastic deformation mechanisms (localizations) enhance crack growth or grain boundary initiated failures
  - Supported by experimental observations
- **Hydrogen-induced decohesion**
  - Decrease in the strength of the atomic bonding by the hydrogen solutes

Degradation often a result of synergistic action

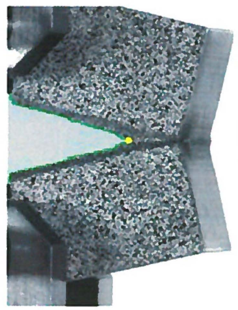
Physics-Based Modeling of Hydrogen Effects

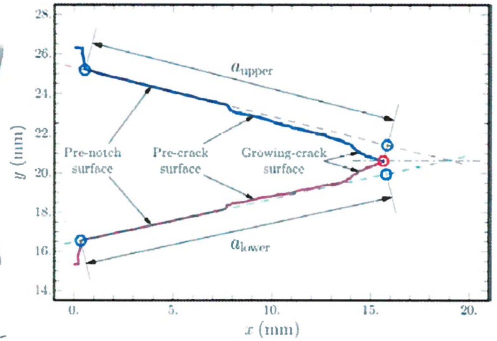
- **Internal State Variable Model (ISV)**
  - Strain rate and temperature dependent
  - Allows history tracking from one process to the next
    - Necessary improvements in averaging ISV during remeshing
  - ISV must be physically based to track properties from one process to the next (dislocations, microcracks, etc)
  - Kinematics / Thermodynamics result in fully coupled thermal-mechanical theory (diffusion of heat, hydrogen, etc)
  - Micro / meso based bounds on parameter space provides a multi-scale coupling
- **Hydrogen (ISV) coupled with dislocation model**
  - Effect of hydrogen on dislocation (changes in mechanical properties – yield, hardening, etc)
  - Dislocation trapping as another method of hydrogen transport
  - Hydrogen / dislocation / microcrack interaction
    - HELP, blocking of dislocation emission results in cleavage

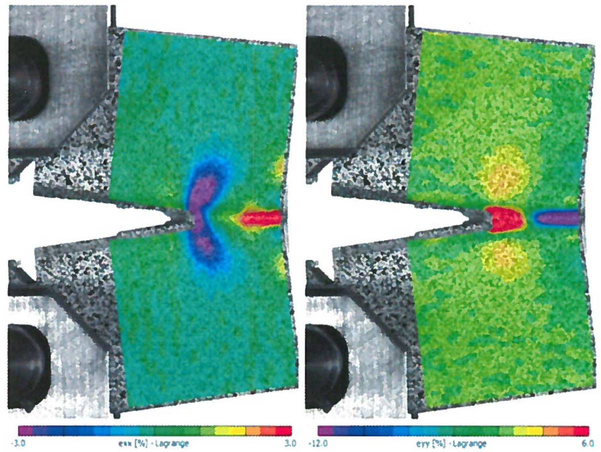
Model each probable mechanism and let loading conditions determine appropriate contributions

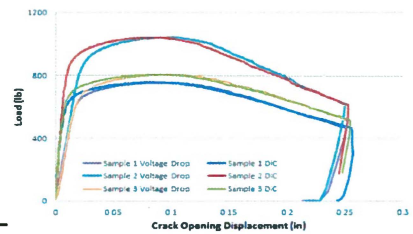
Physics-Based Modeling of Failure and Fracture

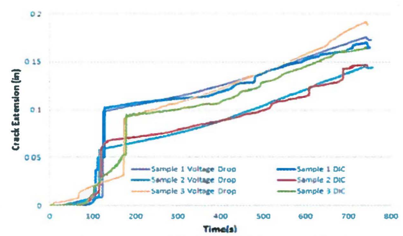
- **Fracture toughness specimen coupled with digital image correlation provides excellent test bed for model validation to 3D stress state and fracture evolution**
  - Simple to compare load vs crack opening displacement
  - The goal is to extract as much information as possible from each test for model validation
  - Additional mechanisms can be probed during traditional test
    - Crack initiation
    - Small scale visualization of crack propagation











Conclusion

- To improve knowledge and predictive capabilities to the degree needed for more structurally efficient reservoirs, significant work must be done experimentally and theoretically
- Fortunately, many tools are in place but need to be validated and implemented
- We need to stay up to date with industry where applicable
- We have to go on our own where no outside interest exists