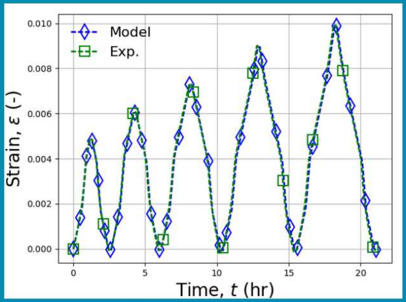
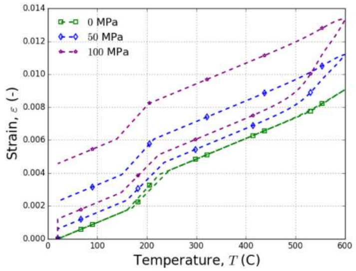
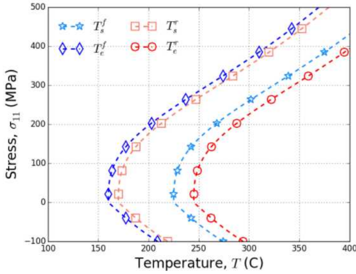
SAND2020-9575C

Glass-Ceramic Material Modeling: Theory, Implementation, and Application







Brian T. Lester
Kevin Long
Sandia National Laboratories

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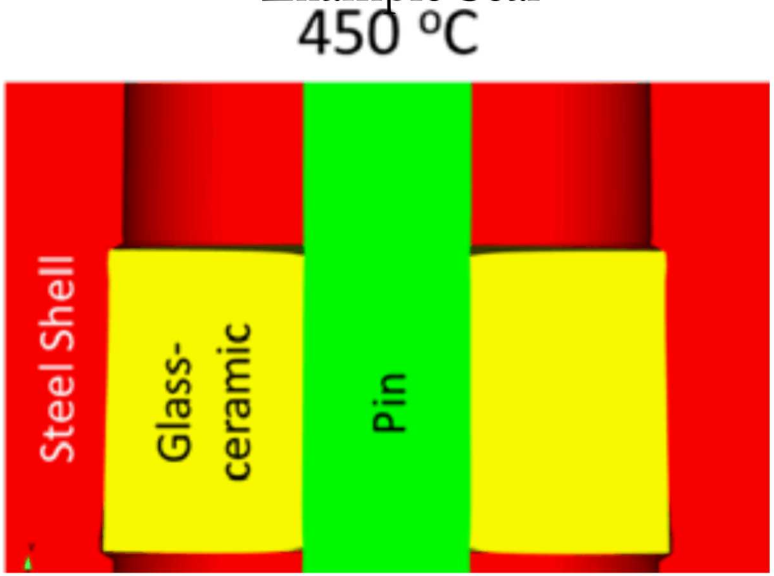
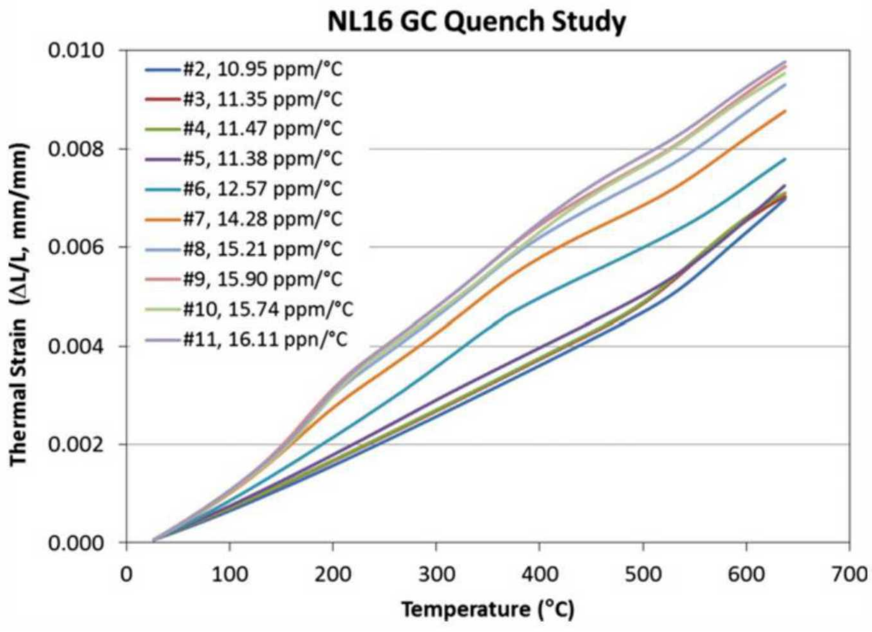
Glass-ceramic to Metal Seals (GcTMS)

- Variety of industrial applications for glass-ceramics
  - Hermetic glass-ceramic to metal seals (GcTMS)
  - Subject to complex thermomechanical histories
- Need constitutive model for behavior
  - No real existing GC model

Example Seal



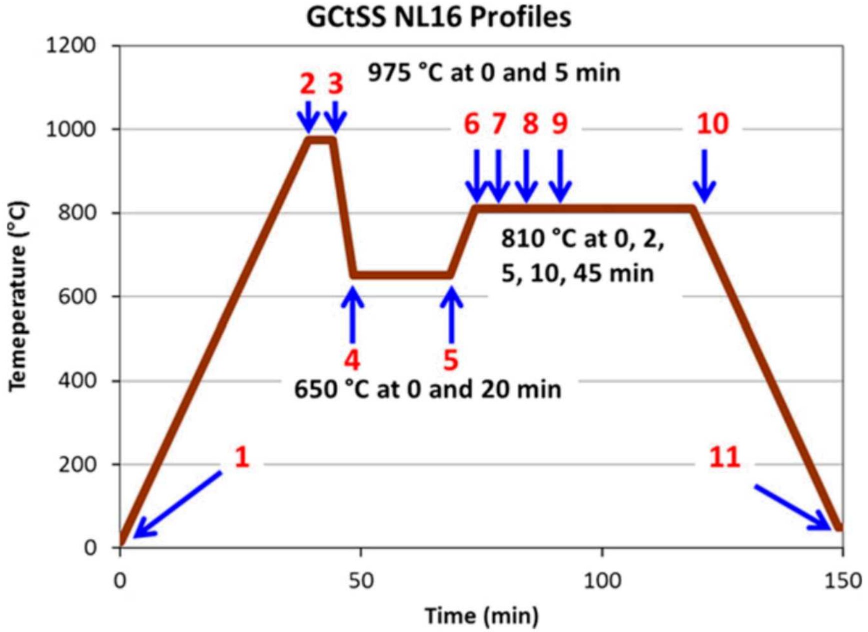
Dai *et al.*, 2017, *J Am Ceram Soc*, 100, pp.3652-3661



Dai *et al.*, 2016, *J Am Ceram Soc*, 99, pp.3719-3725

Glass-Ceramics – Microstructure

- Glass-ceramics are produced by inducing a ceramic phase(s) in an inorganic base glass
- Advantageous features arise from microstructure
  - Up to 5 constituents
  - Inelasticity from residual glass and silica polymorphs



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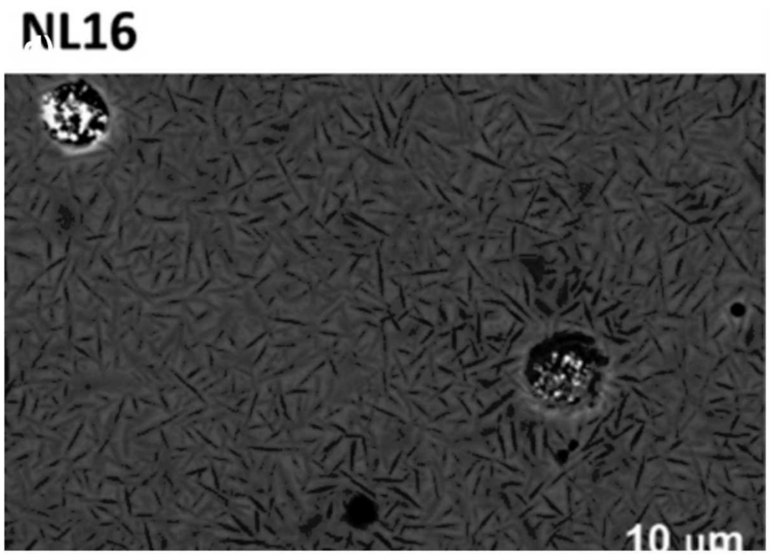


Rodriguez *et al.*, 2016, *J Am Ceram Soc*, 99 (11), pp.3726-3733

Glass-Ceramic Model

- Seek macroscale representation of glass-ceramics via use of internal state variable/continuum thermodynamics theory
  - Thermoviscoelastic theory for response of residual matrix (inorganic base glass)
  - Utilize shape memory alloy (SMA) theory as basis (Lagoudas model) for phase transformations

$$G\left(\sigma_{ij}, T, t, \xi, \varepsilon^{t}_{ij}; \delta^{i}\right) = G^{\mathrm{te}}\left(\sigma_{ij}, T, \xi; \delta^{i}\right) + G^{\mathrm{in}}\left(\sigma_{ij}, T, t, \xi, \varepsilon^{\mathrm{t}}_{ij}; \delta^{i}\right)$$

σ_{ij}, T, t	External State Variables
$\xi, \varepsilon^{\mathrm{t}}_{ij}$	Internal State Variables
δ^{i}	Constituent Volume Fractions

- Rate-independent transformation
  - Utilize $J_2 - I_1$ transformation function and associated flow rule
  - Combines parts of Qidwai & Lagoudas (IJP, 2000) and Lagoudas *et al.* (IJP, 2012)

$$\phi\left(X_{ij}\right) = \gamma_1\left(J_2\right)\sqrt{3J_2} - \gamma_2 I_1$$

Viscoelasticity

- Hereditary integral based formulation
  - Creep – not relaxation – spectra needed for use of Gibbs free energy
  - Shift-factor relates "material" and "laboratory" time

$$t^* = \int_0^t \frac{\mathrm{d}s}{a(s)}$$

- Investigate impact of two shift factors
  - WLF – equilibrated shift factor

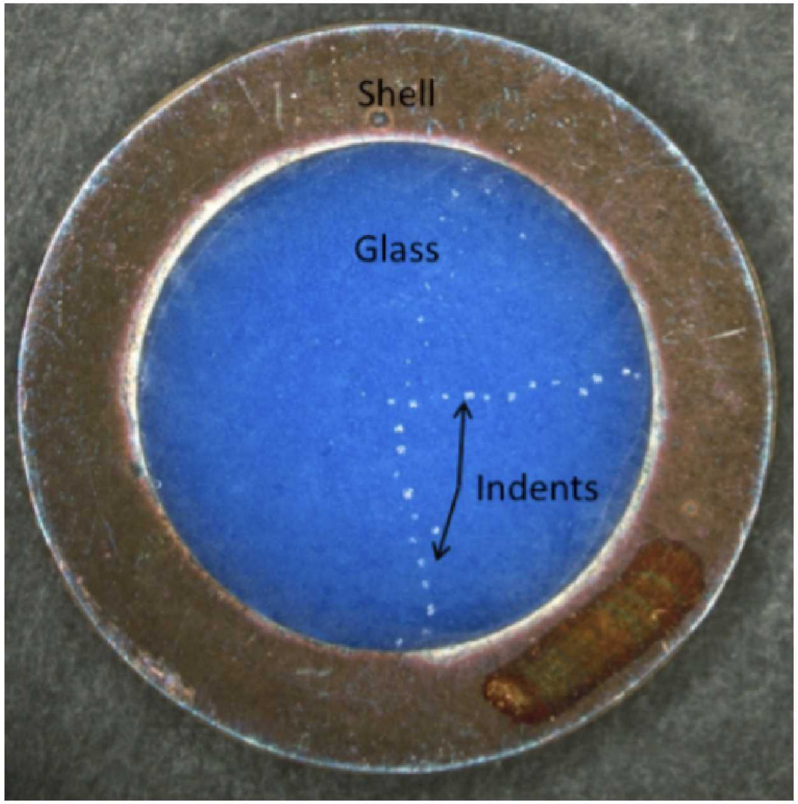
$$\log_{10} a = \frac{-C_1 (T - T_{\mathrm{ref}})}{C_2 + (T - T_{\mathrm{ref}})},$$

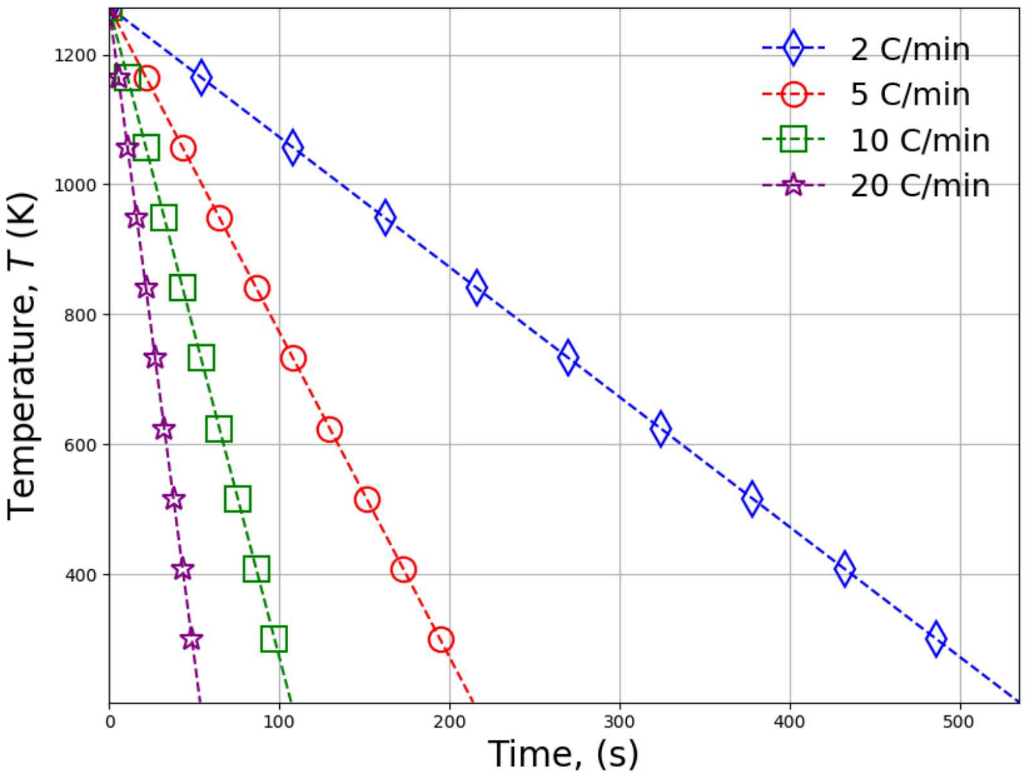
  - WLF-Lag
    - Incorporate some history dependence
    - Sealing problem exhibits large temperature ranges of interest (RT << T_g)

$$\log_{10} a^{\mathrm{WLF\_Lag}} = \frac{-C_1 \left(T - T_{\mathrm{ref}} - \int_0^t (1 - j_v(t^* - s^*, 0)) \frac{\partial T}{\partial s} \mathrm{d}s\right)}{C_2 + \left(T - T_{\mathrm{ref}} - \int_0^t (1 - j_v(t^* - s^*, 0)) \frac{\partial T}{\partial s} \mathrm{d}s\right)}$$

Example Problem – Simple Seal

- Simple seal used as representative example problem
  - Common test for prediction and measurement of residual stress
  - GC Seal enclosed in concentric metal (stainless steel) shell
  - Cooled from above T_g to RT; Representative of sealing process
  - Consider different shift factor forms

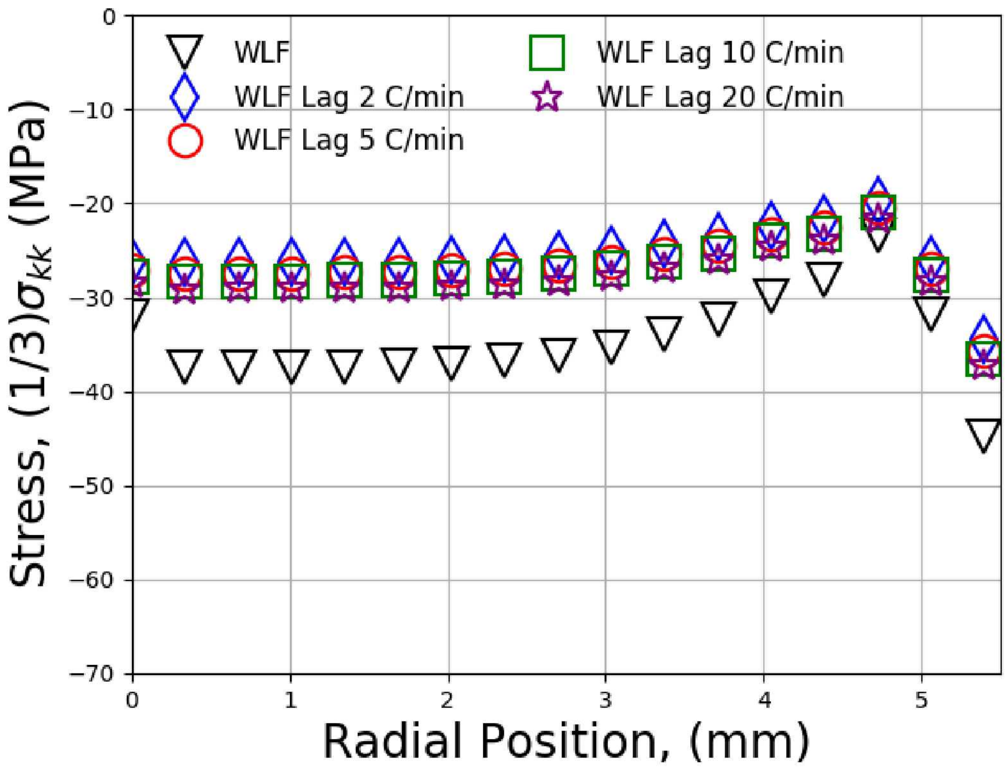




Jamison et al., SAND2017-10894

Simple Seal – Pressure

- Look at prediction of residual (hydrostatic) stress through radius
  - Common metric for model validation (tests forthcoming)
  - Residual stresses important for aging and (potentially) fracture
  - See strong impact of model form on final predicted form

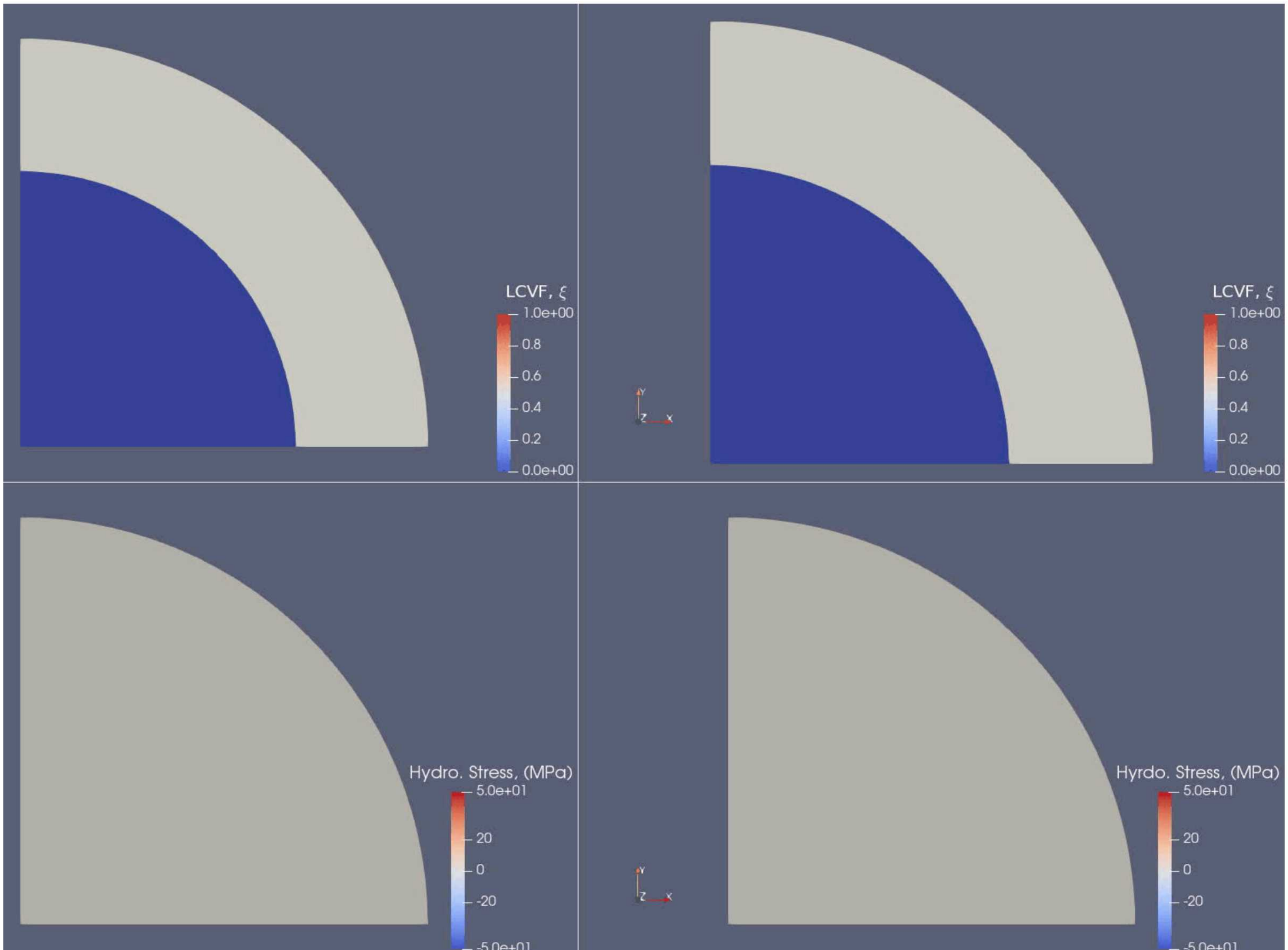


Simple Seal Results

WLF | **WLF Lag – 2ºC/min**

Low Cristo. Vol. Fraction, ξ (Vol. Frac. of Cristo. Only)

Hydrostatic Stress



Conclusion and Summary

- Developed new phenomenological constitutive model for glass-ceramic materials
  - Coupled viscoelasticity and phase transformation
  - 3D numerical implementation

- Results show promise for use in modeling seal applications
  - Validation against simple, existing experiments
  - 3D form considered for simple seal case

- Future work
  - Expanded validation exercises
  - Study impact of different flow-rules/shift factors

Acknowledgements

- Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This paper describes objective technical results and analysis. Any subjective views or opinions do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

Questions?