INL/CON-22-69415-Revision-0

# Sensitivity Study of Multiscale and Phenomenological Elasto-Viscoplastic Grade 91 Material Models for Component-Scale Response

October 2022

Changing the World's Energy Future

Lynn Brendon Munday, Benjamin W Spencer, Aaron Tallman, M. Arul Kumar, Mark Messner, Aritra Chakraborty, Laurent Capolungo, Topher Matthews

Idaho National Laboratory

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**Idaho Falls, Idaho 83415**

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# Sensitivity Study of Multiscale and Phenomenological Elasto-Viscoplastic Grade 91 Material Models for Component-Scale Response

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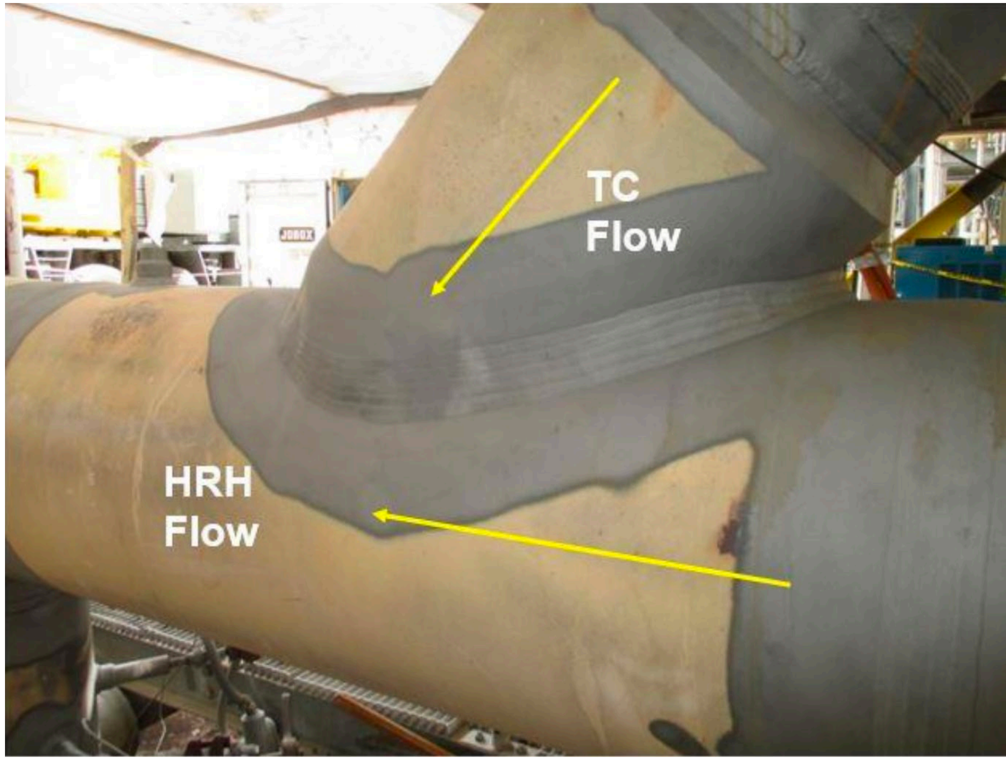
[c]Applied Materials Division, Argonne National Laboratory

Idaho National Laboratory

# Elasto-Viscoplastic Grade 91 Material Models

- Develop simulation capabilities for high temperature design and life-cycle prediction
- NEML - models for probabilistic design:
  - Phenomelogical
  - Fast running to provide large samples
  - Provide statistics of failure based on design criteria, e.g. ASME BVP code
- LAROMANCE - models for component life:
  - Incorporate microstructural data
  - Run at engineering length and time scales
  - Robust over range of stresses and temperatures

MOOSE



# NEML model overview

- Nuclear Engineering Material model Library (NEML)[1]
- Phenomelogical model fit to range of experimental data using Bayesian Markhov Chain Monte Carlo[2]
- Developed for monotonic loading

**Flow Rule**

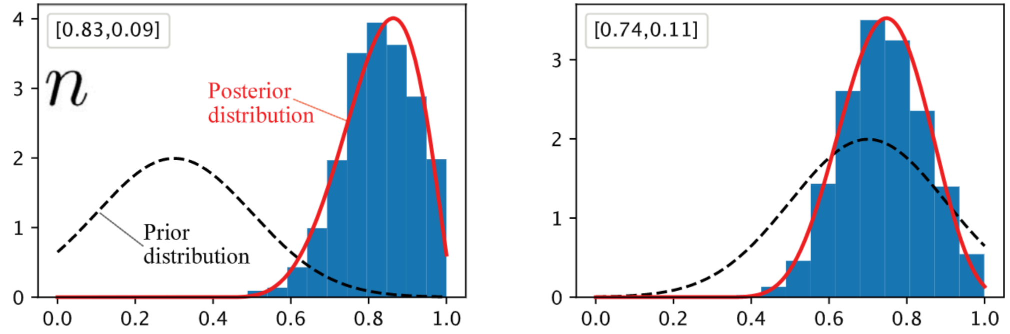
$$\dot{\epsilon}_{vp} = \left\langle \frac{\frac{\sigma}{1-\omega} - \sigma_0 - R}{\eta} \right\rangle^n$$

**Hardening Parameter**

$$R = Q\left[1 - \exp\left(-b|\epsilon_{vp}(t)|\right)\right]$$

**Damage Rate (fixed)**

$$\dot{\omega} = \left(\frac{\sigma}{A}\right)^{\zeta}(1-\omega)^{-\phi}$$




| parameter | 550 ° C | | 600 ° C | |
|---|---|---|---|---|
| | $(\mu, \sigma)$ | Bounds | $(\mu, \sigma)$ | Bounds |
| $n$ | $(11.09, 0.37)$ | $[9, 13]$ | $(8.455, 0.47)$ | $[7, 10]$ |
| $\eta$ | $(832.4, 23)$ | $[700, 950]$ | $(750.6, 41.9)$ | $[600, 900]$ |
| $\sigma_0$ | $(3.769, 0.83)$ | $[2, 10]$ | $(3.547, 0.66)$ | $[2, 5]$ |
| $Q$ | $(106.9, 8.7)$ | $[80, 130]$ | $(112.6, 8.19)$ | $[80, 130]$ |
| $b$ | $(47.99, 7.7)$ | $[30, 70]$ | $(44.00, 8.28)$ | $[20, 70]$ |
| $A$ | 517 | – | 650 | – |
| $\zeta$ | 12.5 | – | 10 | – |
| $\phi$ | 2.5 | – | 2.0 | – |
| $E$ | 174000 | – | 168000 | – |
| $\nu$ | 0.31 | – | 0.31 | – |

Elastic Constants

(a) Truncated normal distributions for NEML model parameters [4]. Units are MPa, mm, s.

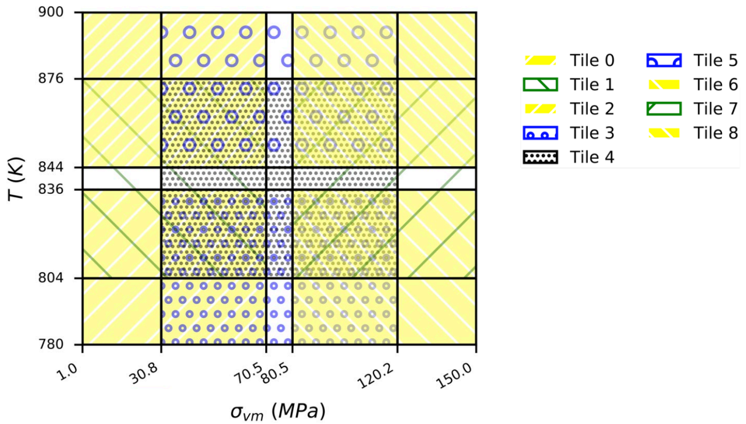
[1] https://neml.readthedocs.io/en/dev/#

[2] Chakraborty A, Messner MC. Bayesian analysis for estimating statistical parameter distributions of elasto-viscoplastic material models. Probabilistic Engineering Mechanics. 2021 Oct 1;66:103153.

# LAROMANCE model overview

- Surrogate model database generated from crystal plasticity model[1,2]
  - Viscoplastic self consistent CP framework
  - Inelastic strain from dislocation glide, climb and coble creep
  - For polynomial degree 2, α has 729 terms
  - Sigmoid function to interpolate between tiles

| parameter | Bounds |
|---|---|
| Cell Dislocation Density ($10^{12}\mathrm{m}^{-2}$) | [1, 3.5] |
| Wall Dislocation Density ($10^{12}\mathrm{m}^{-2}$) | [6, 18] |
| MX Phase Fraction ($\phi_{MX}$) | [0.008, 0.1] |
| von Mises Stress (MPa) | [1, 150] |
| Effective Strain (m/m) | [0.0, 0.08] |
| Temperature (°C) | [507, 627] |

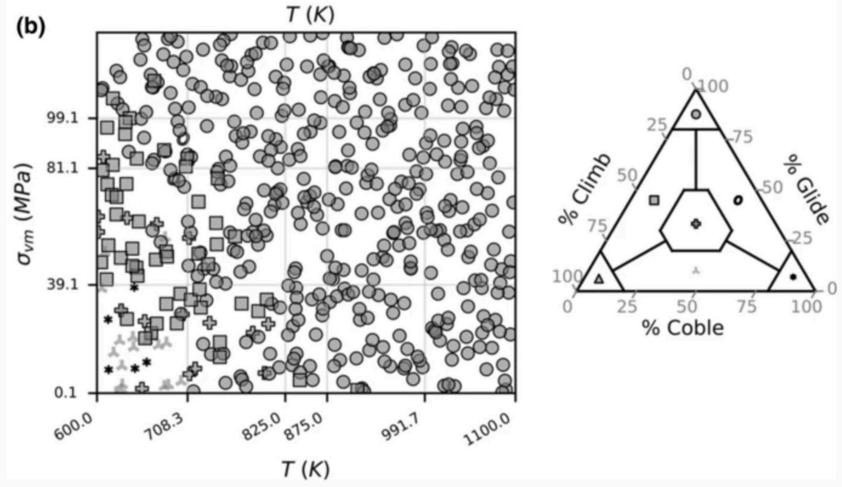



$$\dot{\varepsilon}_{ij} = \dot{\bar{\varepsilon}}_{\mathrm{vm}} \frac{3}{2} \frac{S_{ij}}{\bar{\sigma}_{\mathrm{vm}}}$$

$$\dot{\varepsilon}^{**}_{vm} \sim \sum_{0 \le i \ldots n \le N_{\mathrm{deg}}} \alpha^{ijklmn}_{\varepsilon} P^i\left(\bar{\rho}^*_{cell}\right) P^j\left(\bar{\rho}^*_{w}\right) P^k\left(T^*\right) P^l\left(\sigma^*_{vm}\right) P^m\left(\varepsilon^*_{vm}\right) P^n\left(\phi^*_{MX}\right)$$

$$\dot{\bar{\rho}}^{**}_{cell} \sim \sum_{0 \le i \ldots n \le N_{\mathrm{deg}}} \alpha^{ijklmn}_{\rho_{cell}} P^i\left(\bar{\rho}^*_{cell}\right) P^j\left(\bar{\rho}^*_{w}\right) P^k\left(T^*\right) P^l\left(\sigma^*_{vm}\right) P^m\left(\varepsilon^*_{vm}\right) P^n\left(\phi^*_{MX}\right)$$

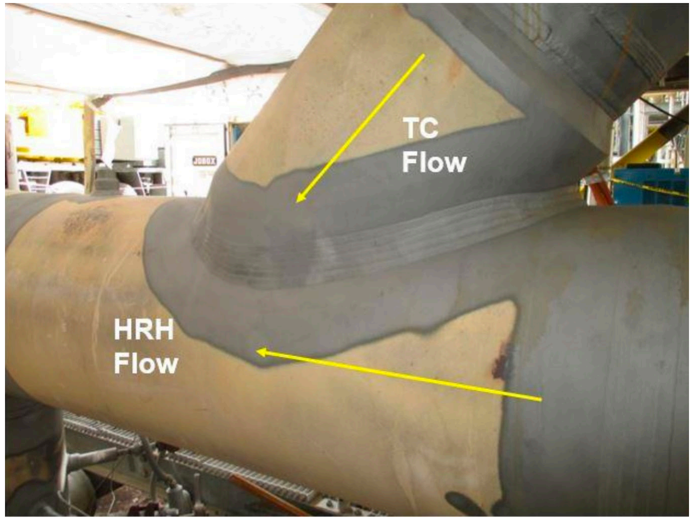
$$\dot{\bar{\rho}}^{**}_{w} \sim \sum_{0 \le i \ldots n \le N_{\mathrm{deg}}} \alpha^{ijklmn}_{\rho_{w}} P^i\left(\bar{\rho}^*_{cell}\right) P^j\left(\bar{\rho}^*_{w}\right) P^k\left(T^*\right) P^l\left(\sigma^*_{vm}\right) P^m\left(\varepsilon^*_{vm}\right) P^n\left(\phi^*_{MX}\right)$$

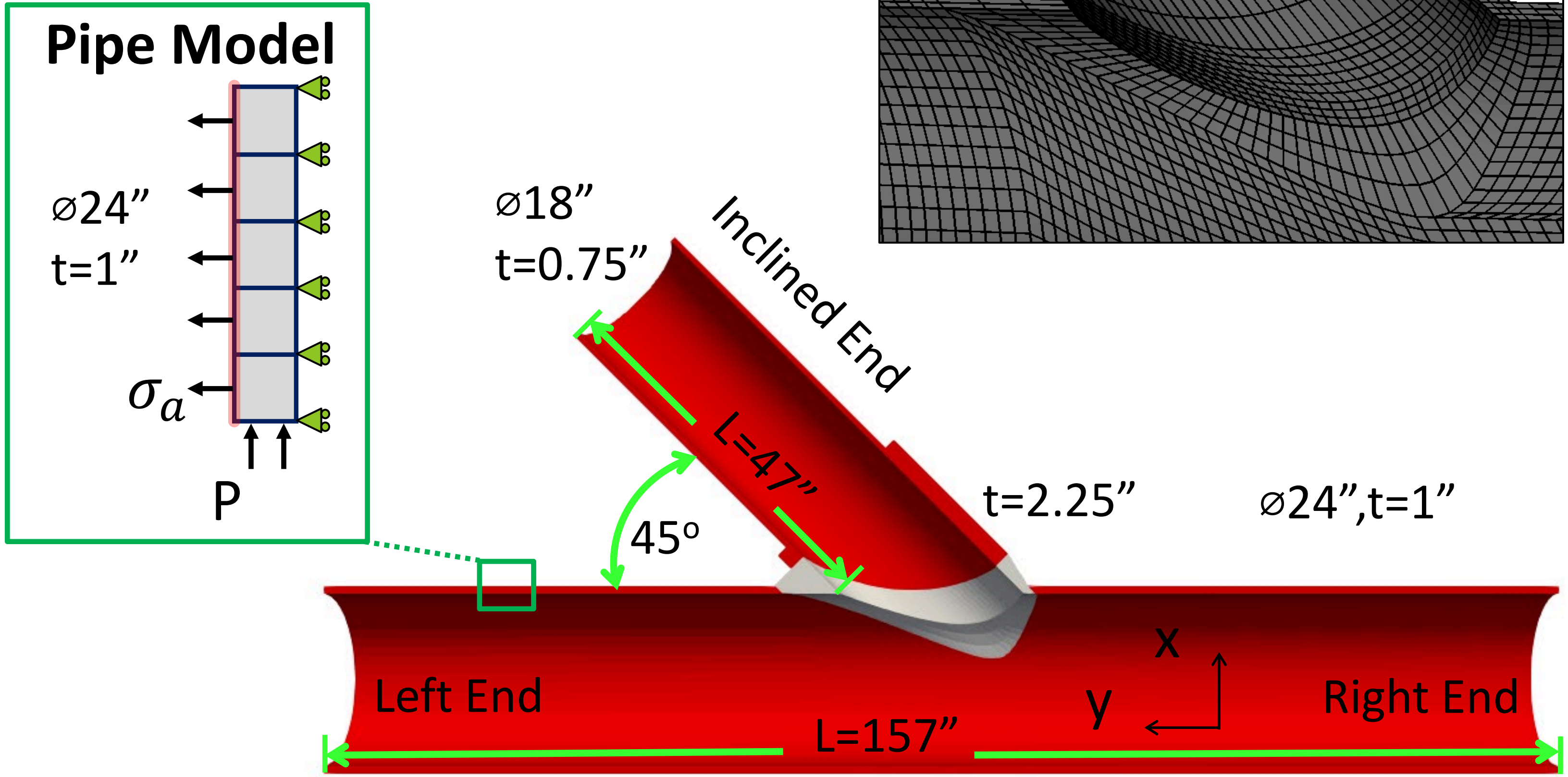


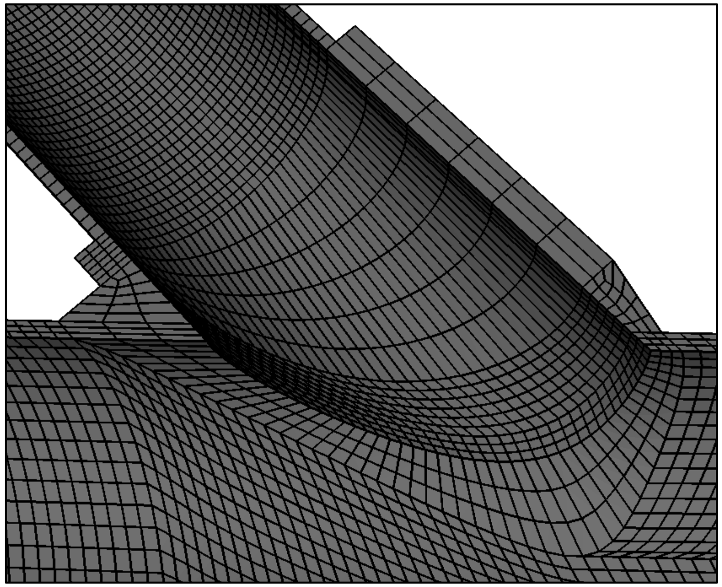

[1]Wen W, Kohnert A, Kumar MA, Capolungo L, Tomé CN. Mechanism-based modeling of thermal and irradiation cree behavior: An application to ferritic/martensitic HT9 steel. International Journal of Plasticity. 2020 ;126:102633.
[2]Tallman AE, Arul Kumar M, Matthews C, Capolungo L. Surrogate modeling of viscoplasticity in steels: Application to thermal, irradiation creep and transient loading in HT-9 cladding. JOM. 2021;73(1):126-37.

# Geometry engineering models

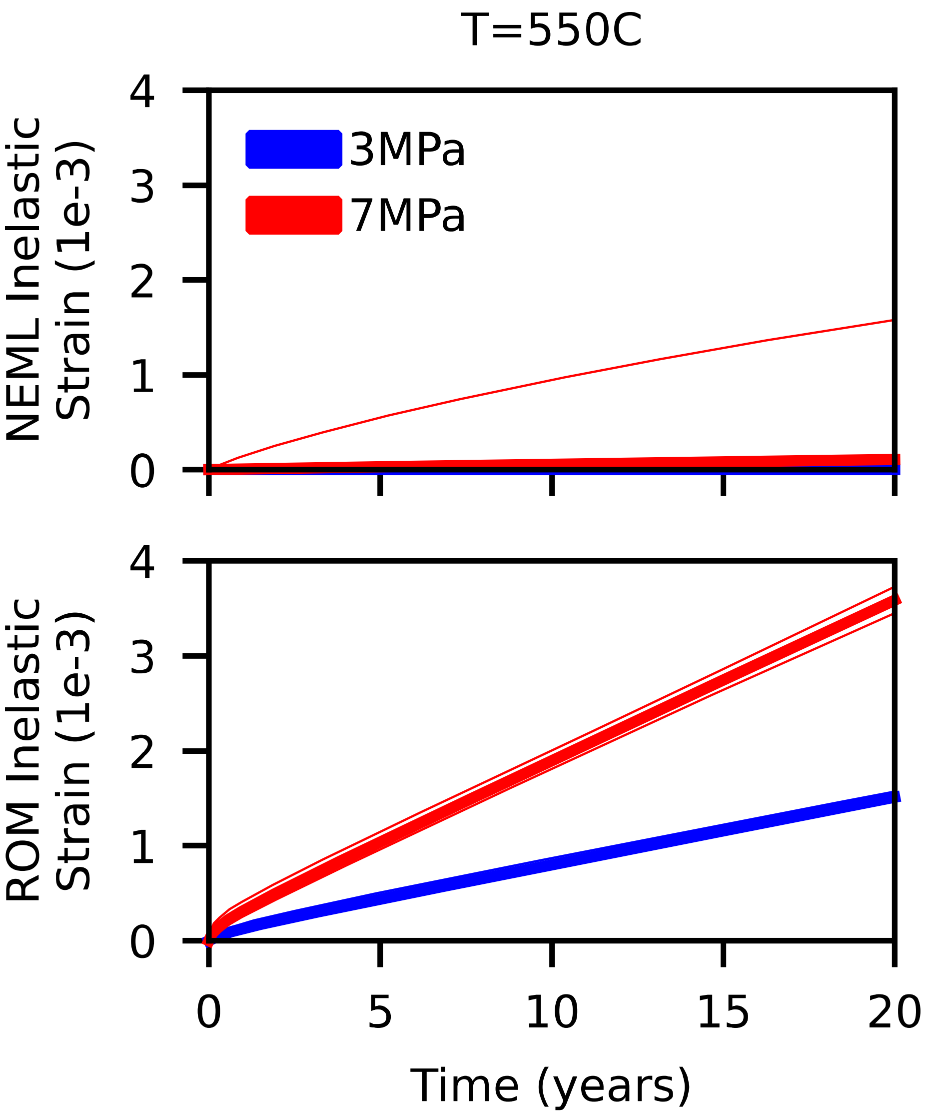
- Show stresses, etc.  Show pipe modle.
- Show



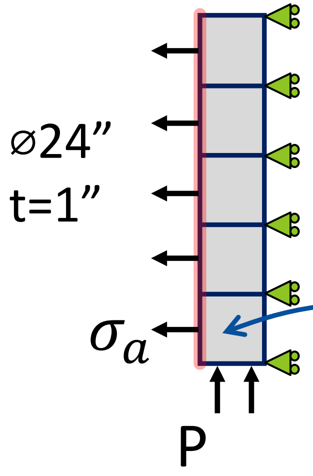



# Pipe Results: Stress-Strain History for T=550C

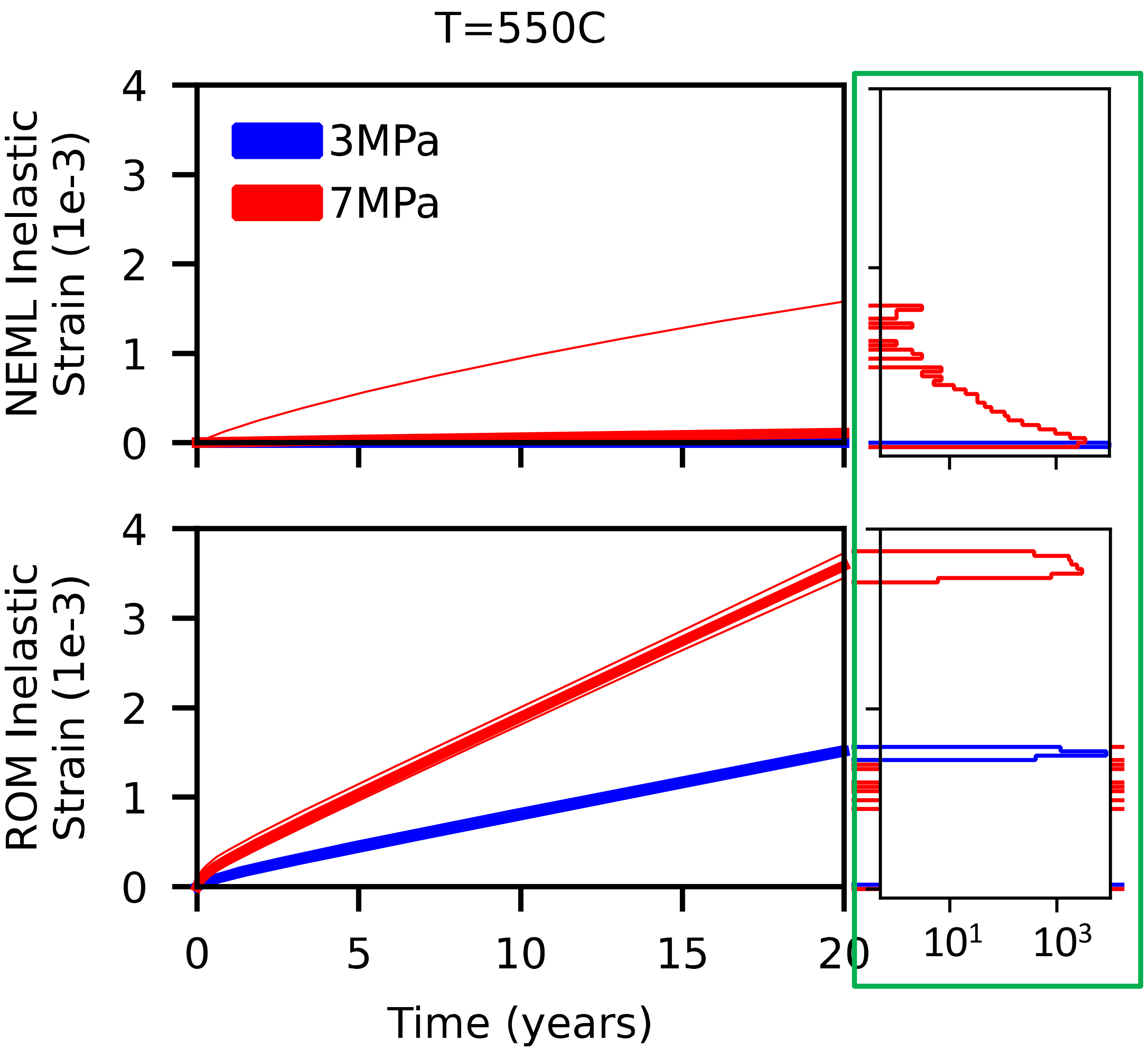



- 10,000 Parameters samples at each pressure
  - NEML sampled from truncated normal distributions
  - LAROMANCE sampled from uniform distributions over valid parameter range

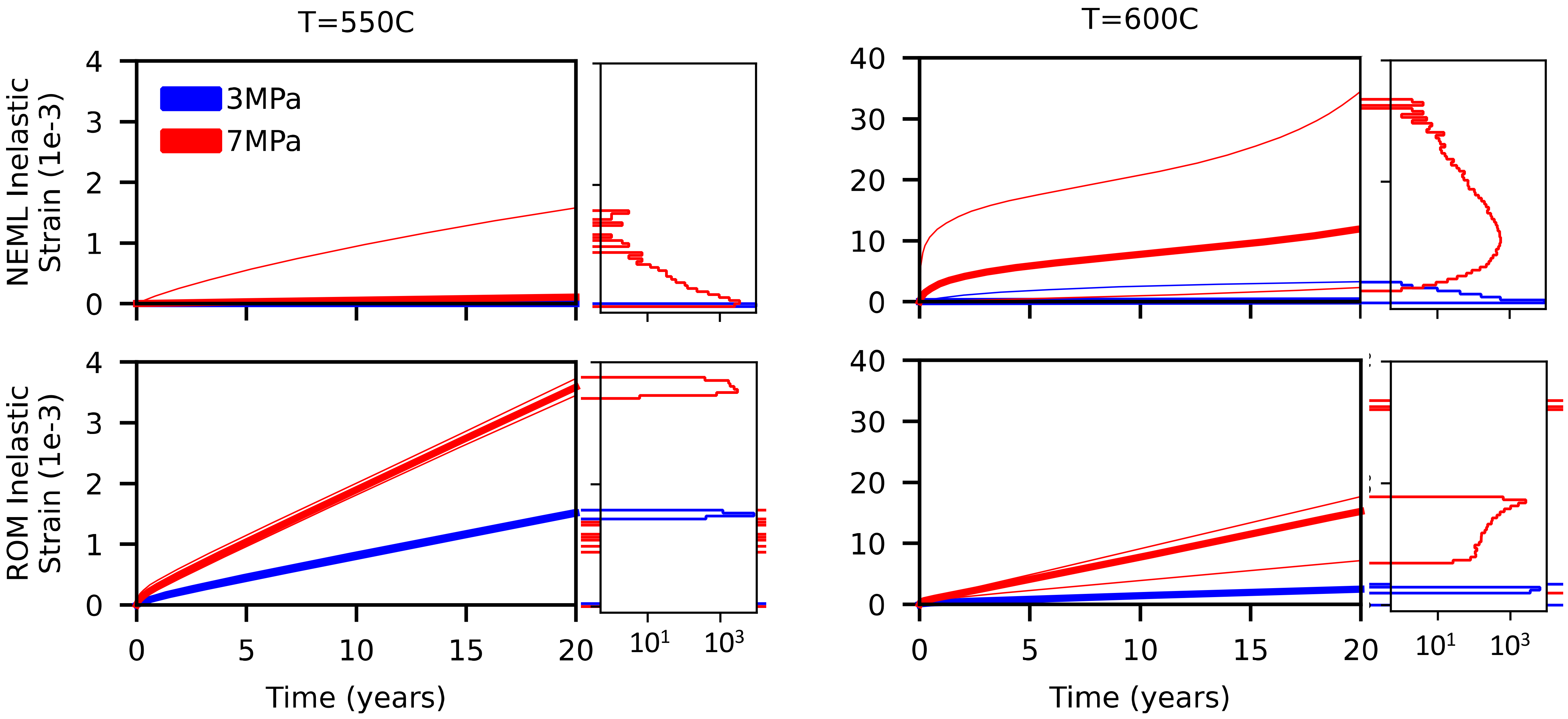



$$\max \sigma_{vm} = \left( \frac{\sqrt{3} r_o^2}{r_o^2 - r_i^2} \right) P \approx 11P$$

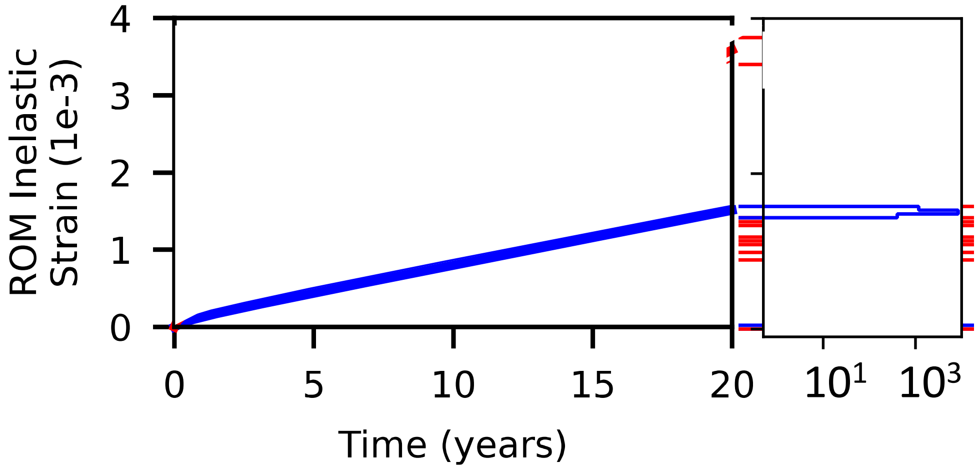
# Pipe Results: Inelastic Strain Histogram at 20 yrs



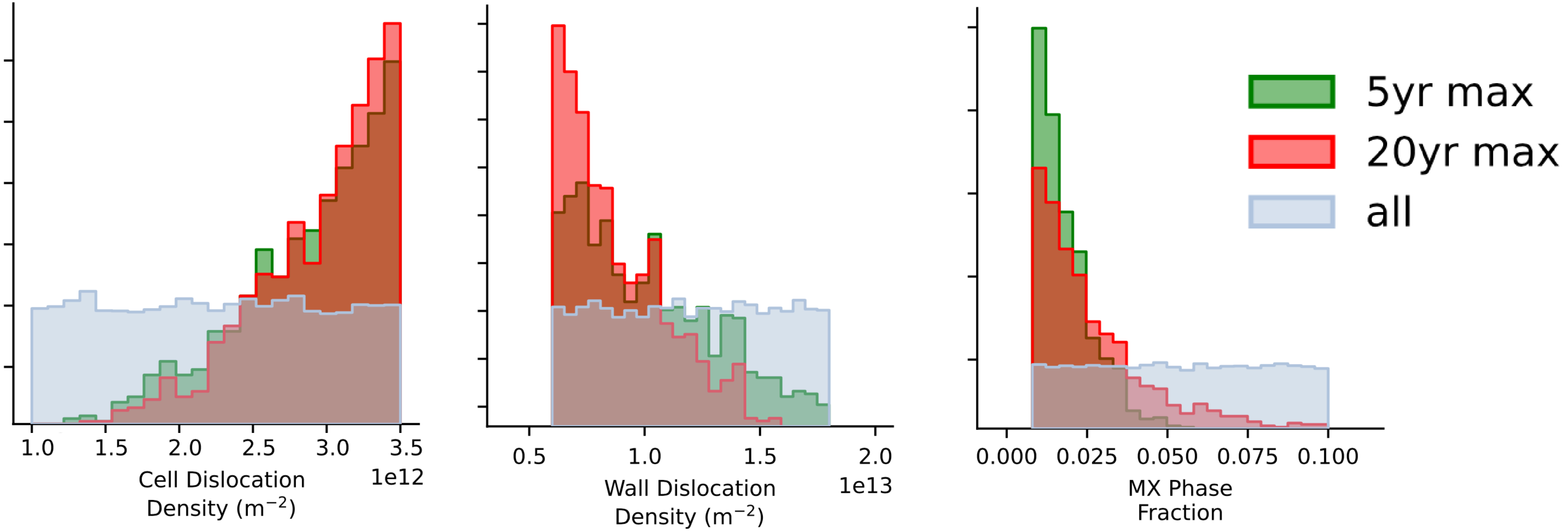
# Pipe Results:  Stress-Strain for T=550C and T=600C



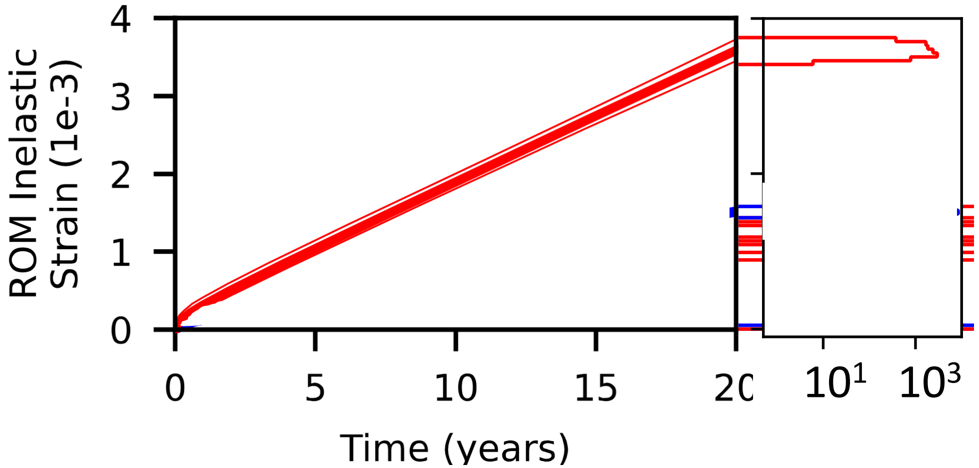
# **LAROMANCE MODEL:** T=550C, P=3MPa ($\sigma_{max}$=33MPa)



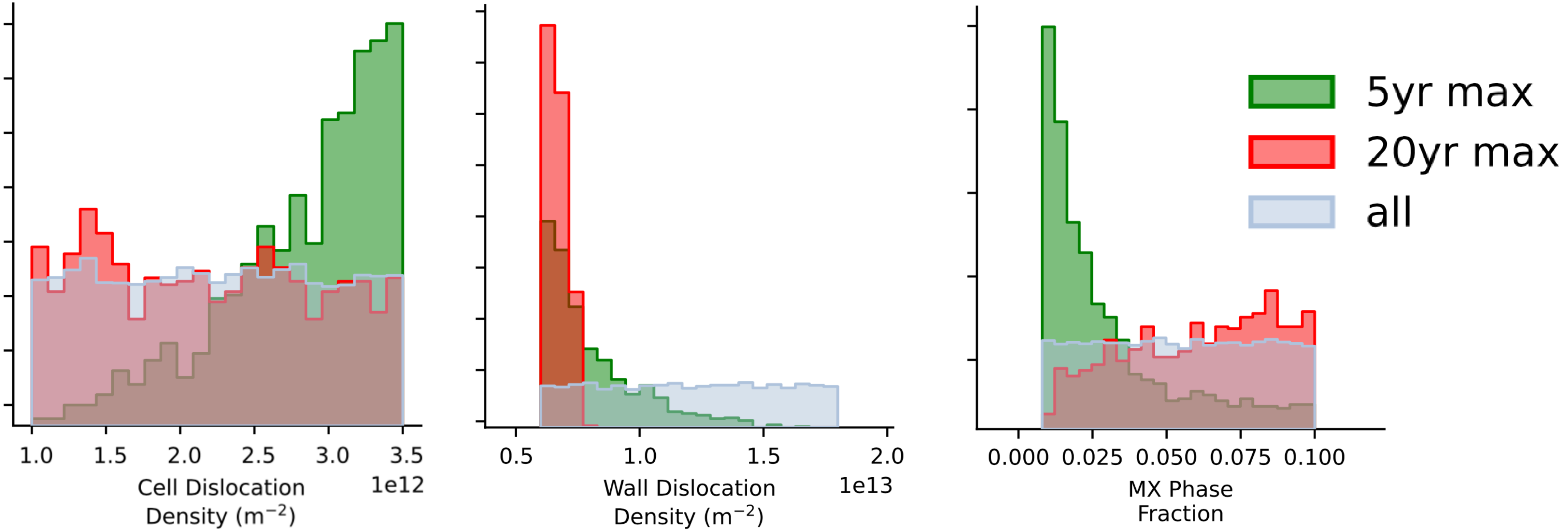

Parameters leading to top 10% of maximum inelastic strain after 20 years for T=550C, P=3MPa



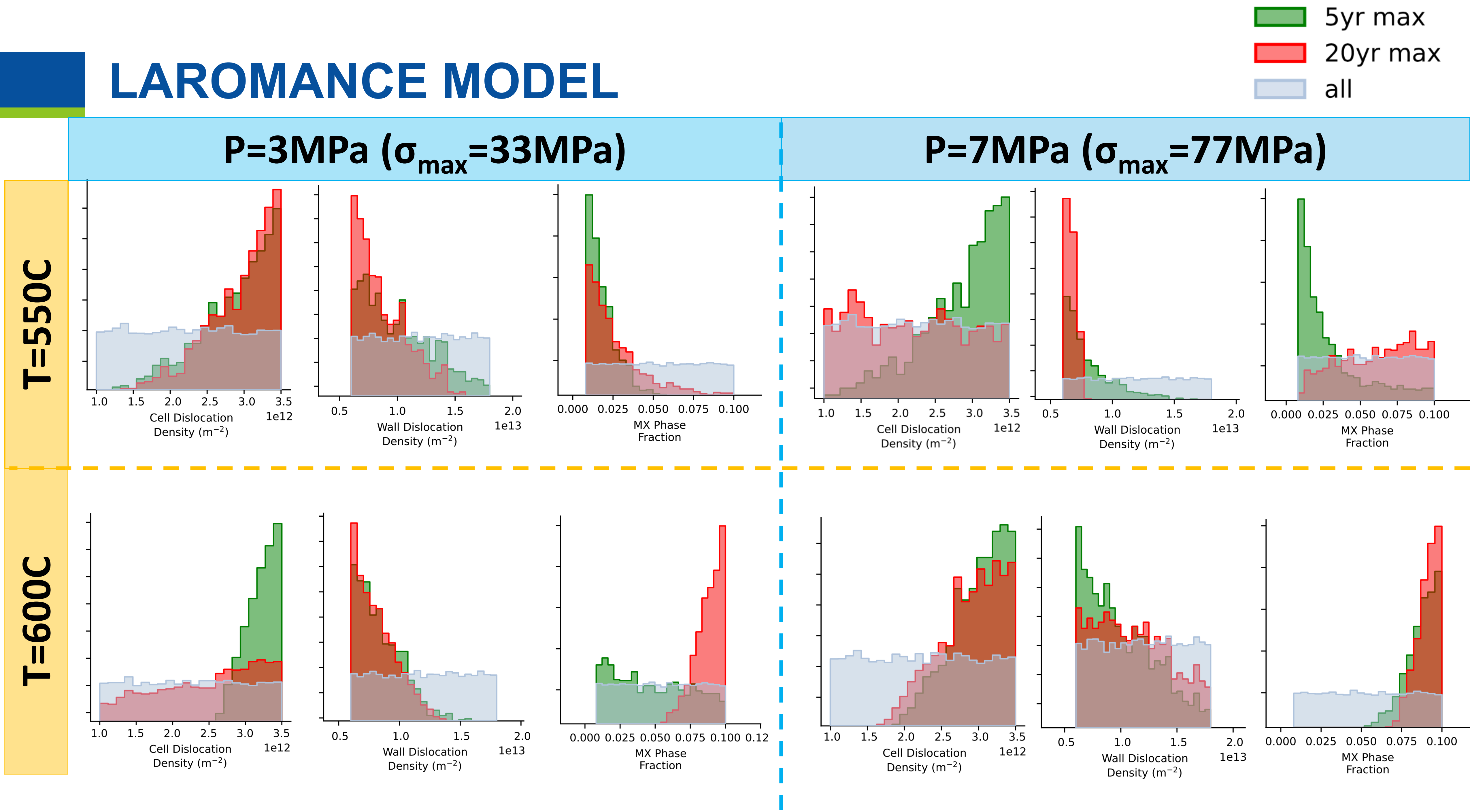
# **LAROMANCE MODEL:** T=550C, P=7MPa ($\sigma_{max}$=77MPa)



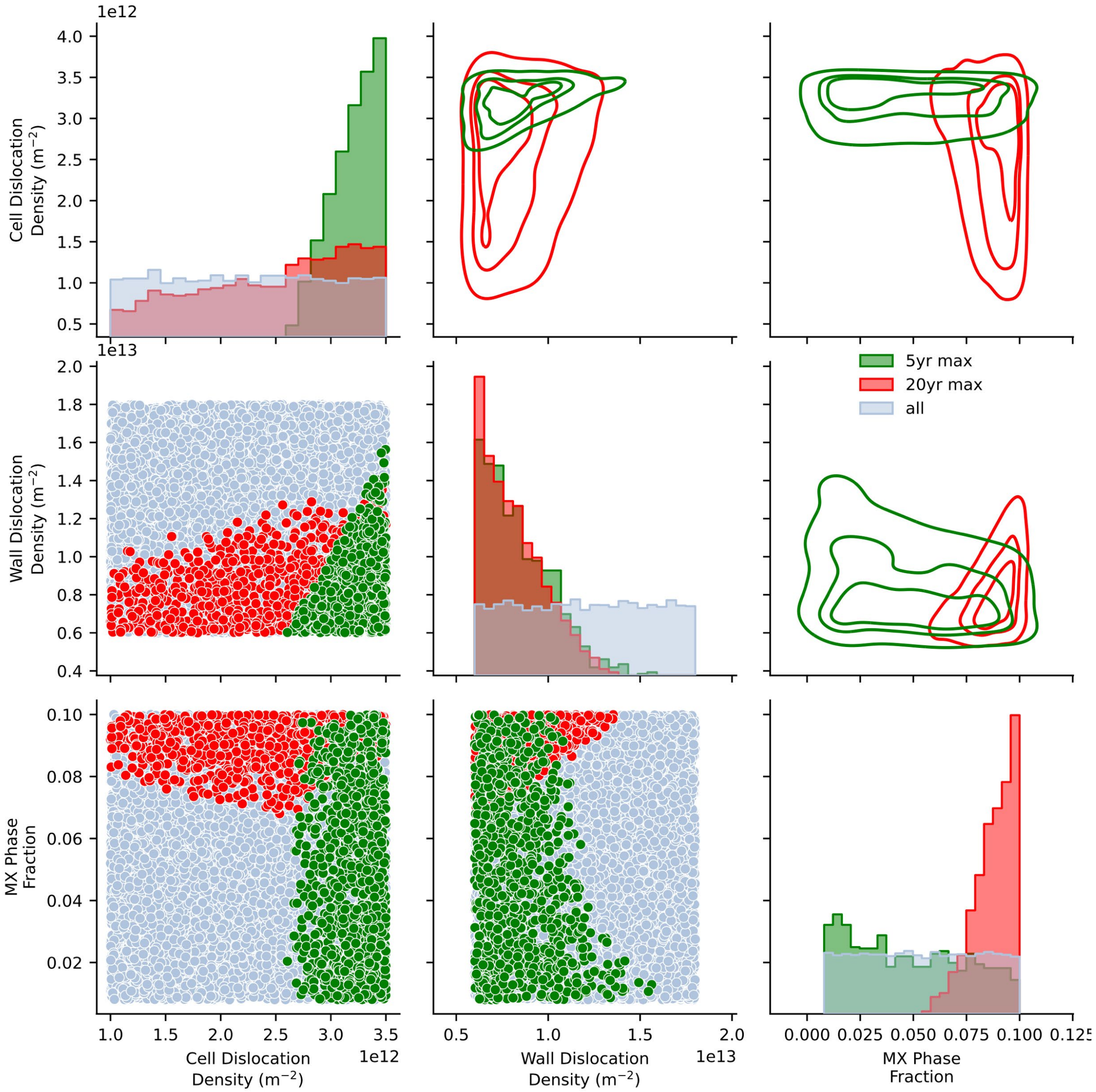

Parameters leading to top 10% of maximum inelastic strain after 20 years for T=550C, P=7MPa



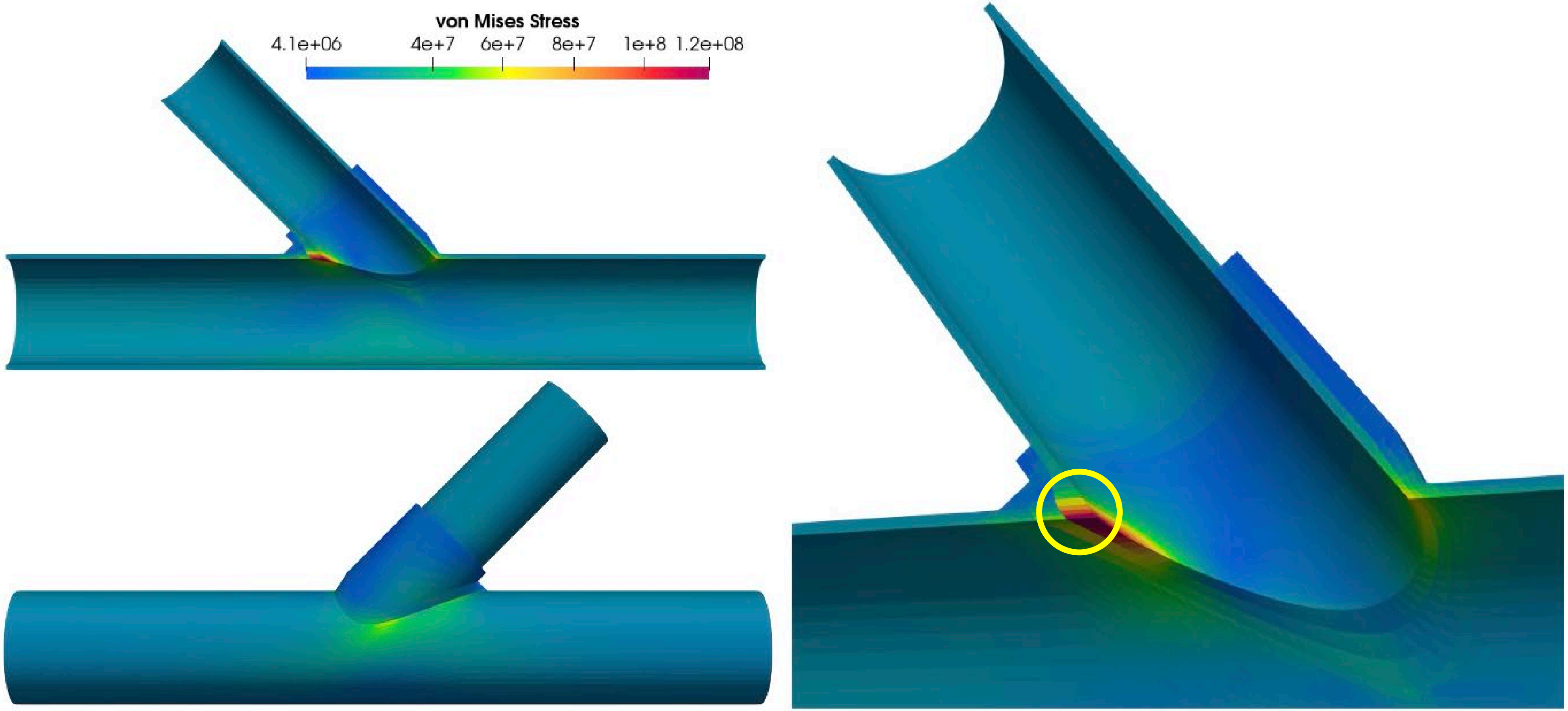
# LAROMANCE MODEL



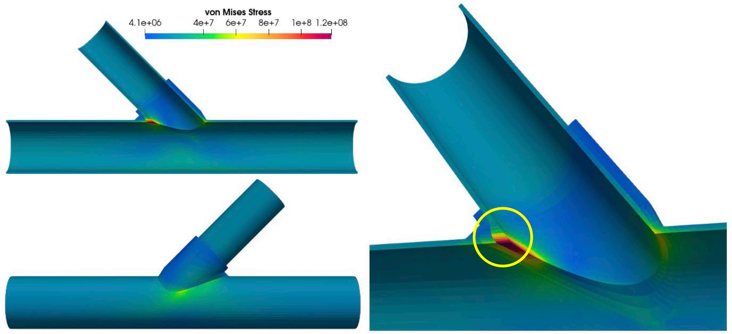
# Pipe Results: Cross Correlation - T=600C, P=3MPa

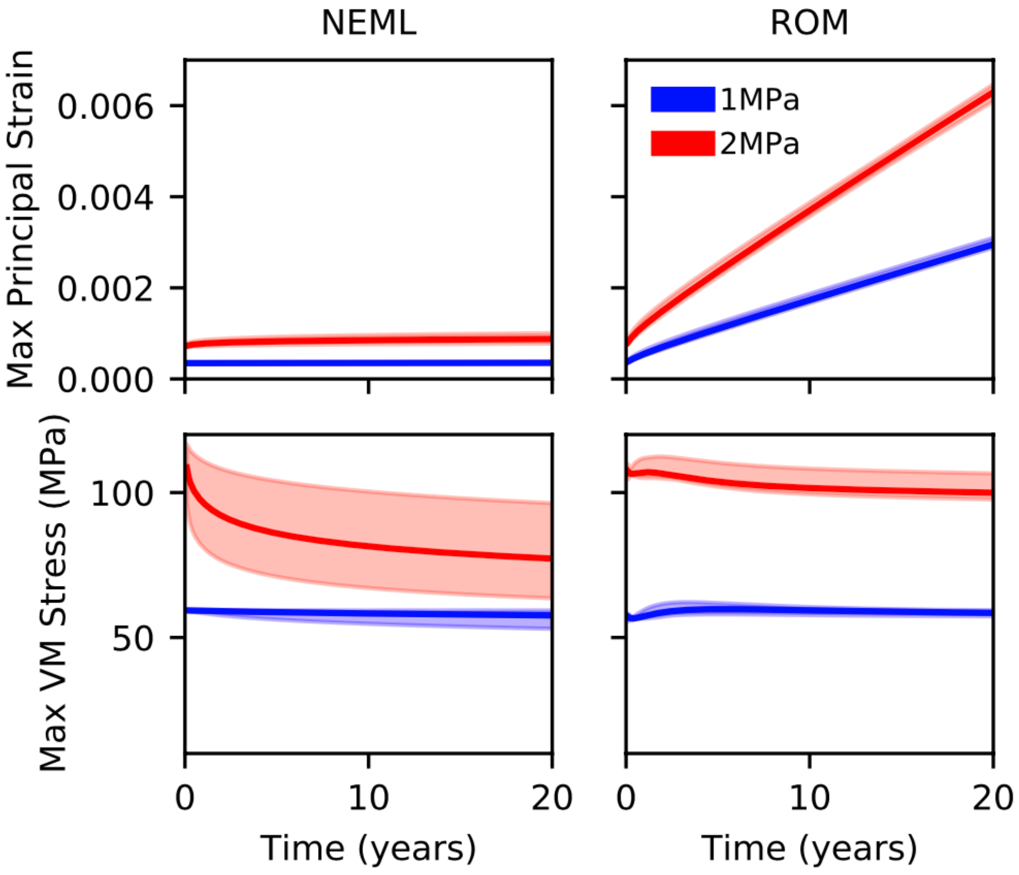


# Pipe Lateral Simulations: T=550C, P=2MPa

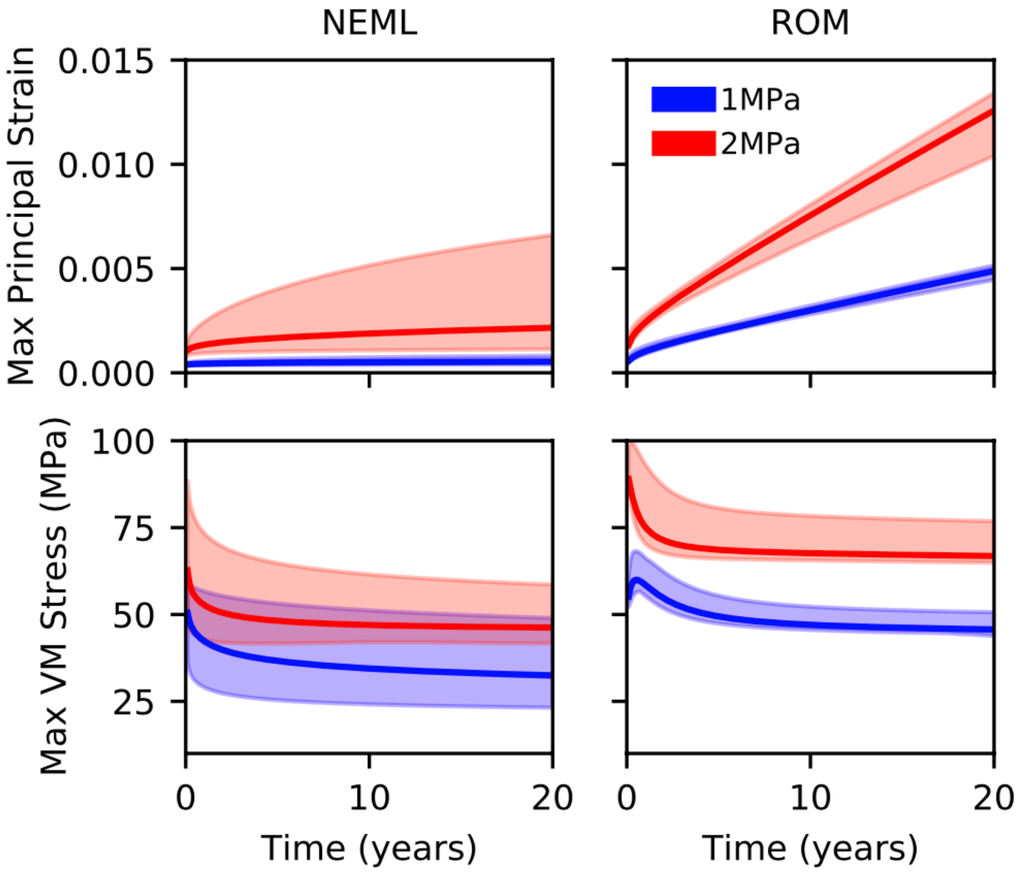


# Pipe Lateral Simulations



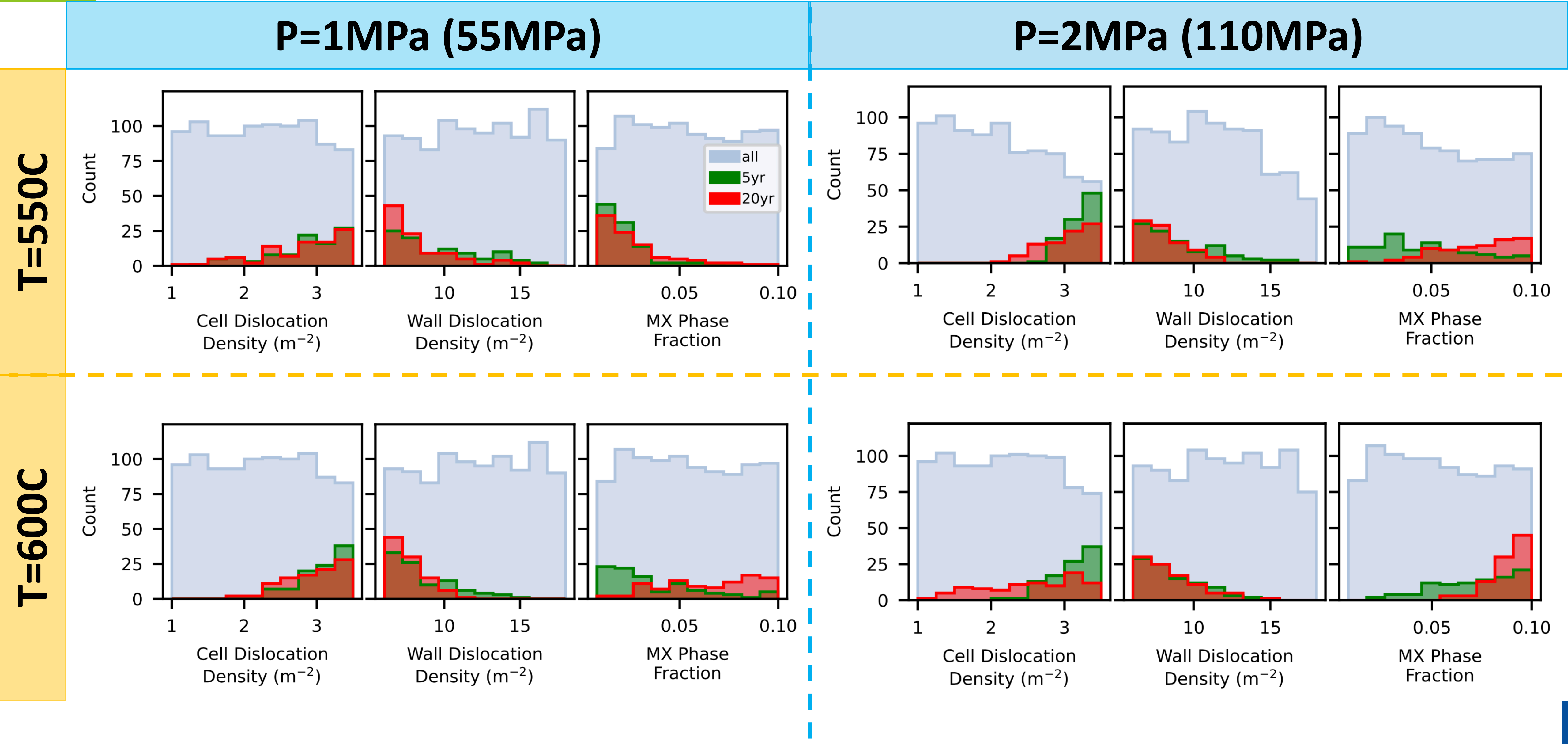




(a) Temperature = 550°C



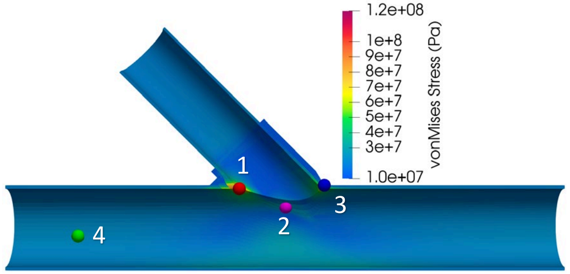

(b) Temperature = 600°C

# NEML, laromance stress strain.



# Future Work

- Get better sampling of LAROMANCE model for pipe lateral.
- Run Simulations at a single pressure, collect results at different locations.
- Check LAROMANCE parameter ranges for MX phase fraction - 10% seems high

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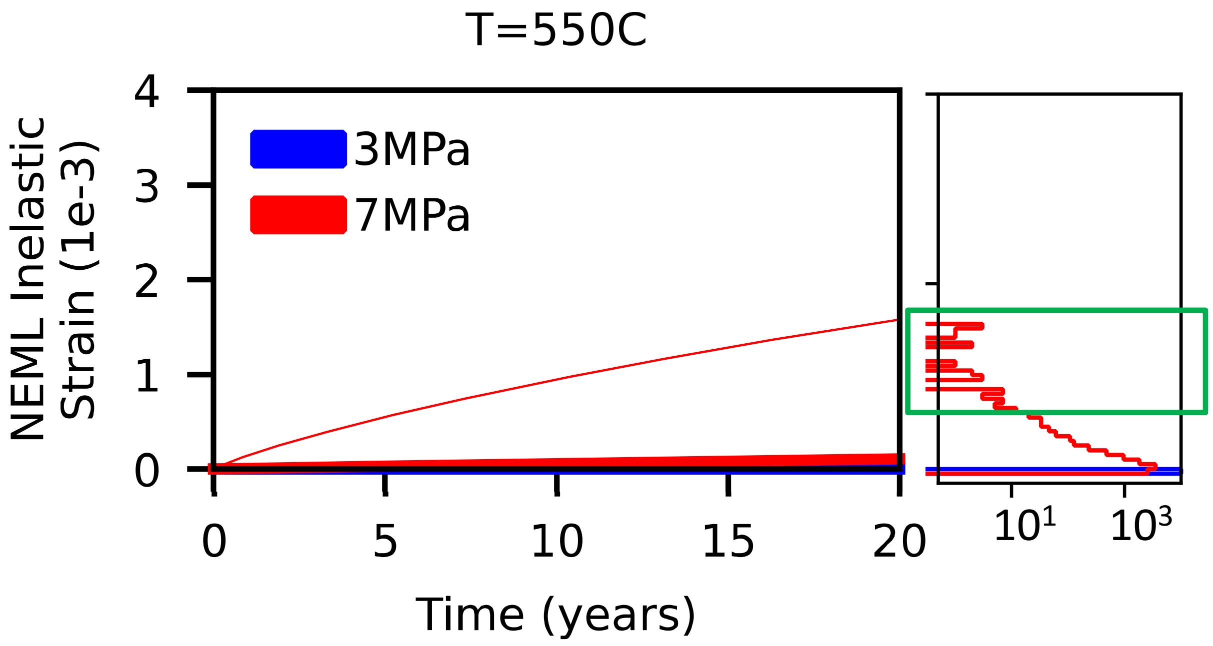
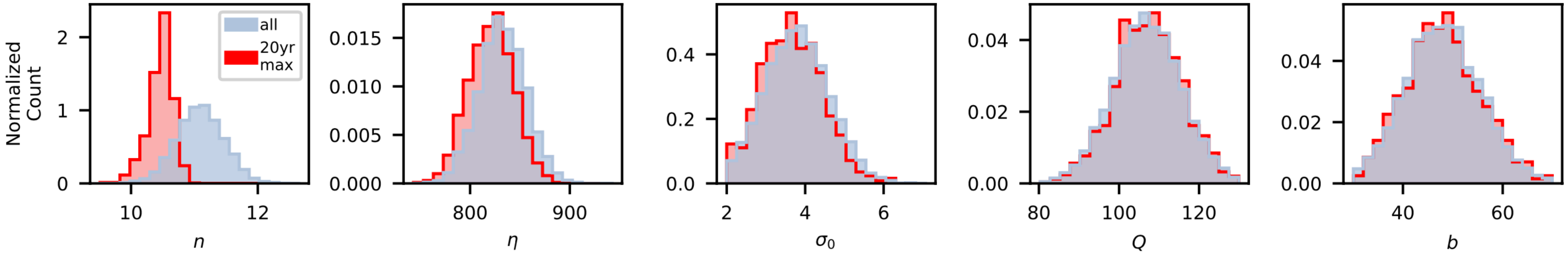
# Extra Slides
# NEML Parameter Sensitivity T=550C, P=7MPa



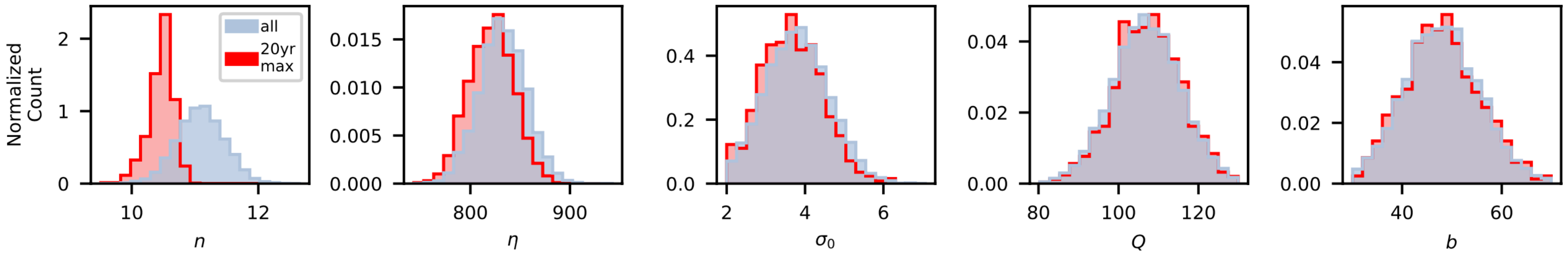

Parameters leading to top 10% of maximum inelastic strain after 20 years for T=550C, P=7MPa

**Flow Rule**

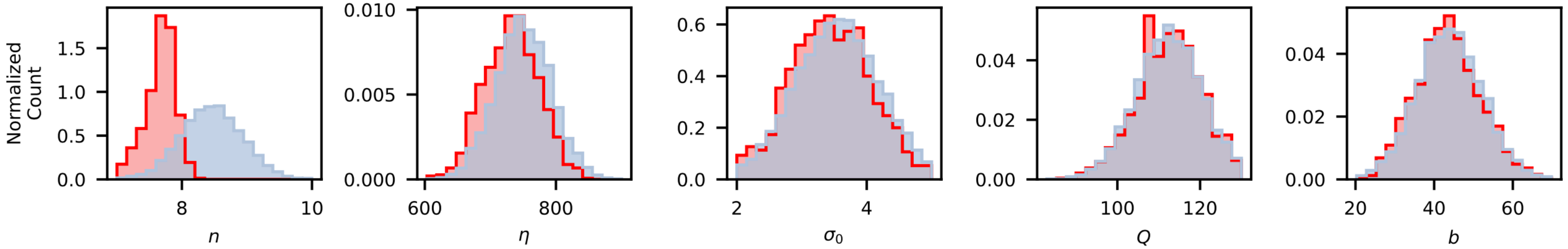
$$\dot{\epsilon}_{vp} = \left\langle \frac{\frac{\sigma}{1-\omega} - \sigma_0 - R}{\eta} \right\rangle^{n}$$



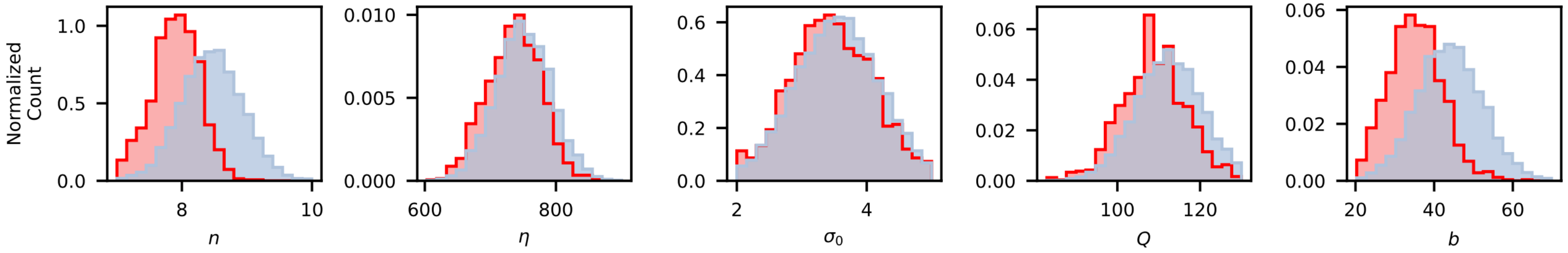
# Pipe Results: Parameter Sensitivity NEML




(a) Temperature = 550°C, Pressure = 7 MPa




(b) Temperature = 600°C, Pressure = 3 MPa




(c) Temperature = 600°C, Pressure = 7 MPa

Rate sensitivity exponent, n
Hardening parameter, b

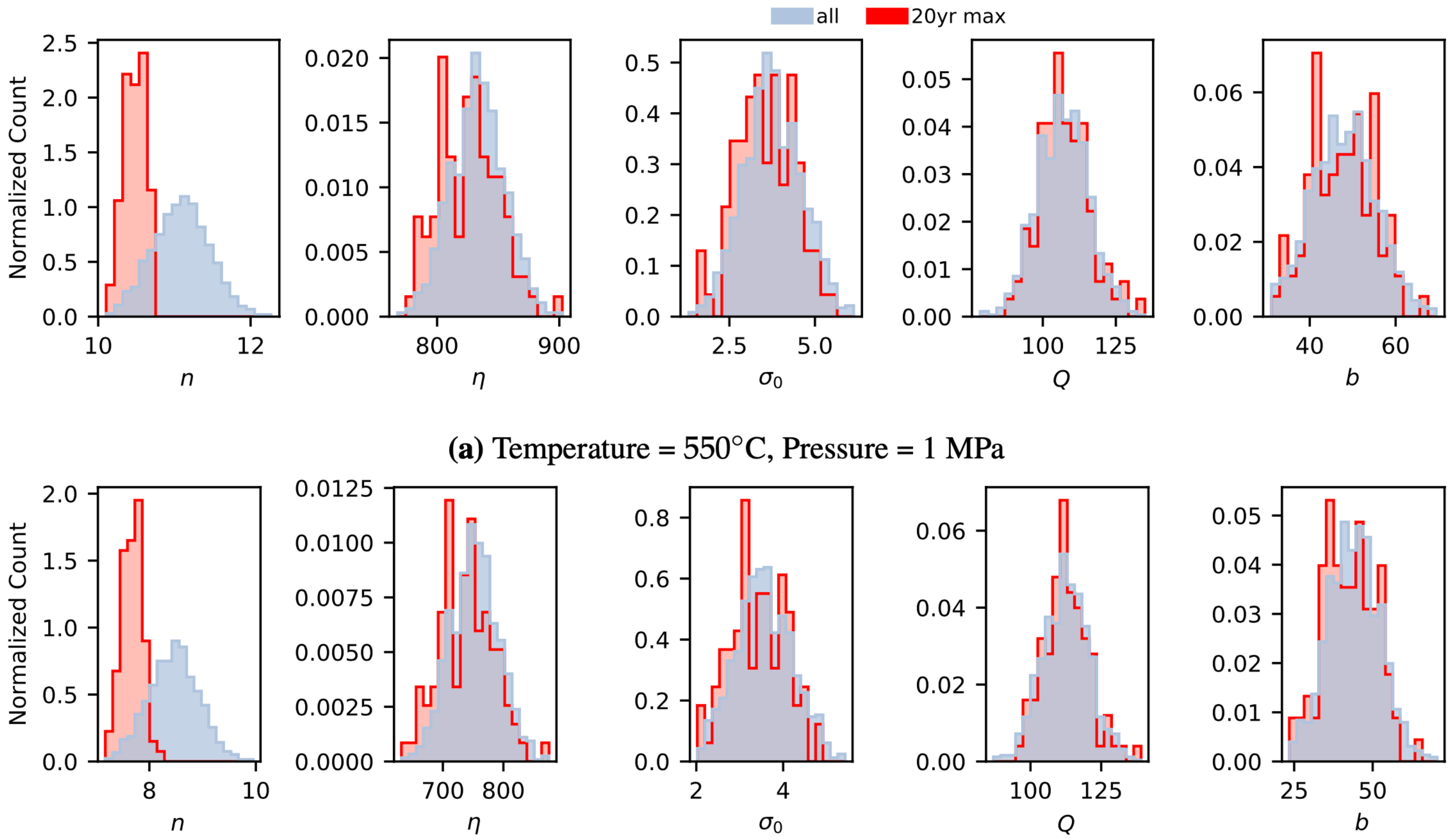
Flow Rule

$$\dot{\epsilon}_{vp} = \left\langle \frac{\frac{\sigma}{1-\omega} - \sigma_0 - R}{\eta} \right\rangle^{n}$$

Hardening Parameter

$$R = Q\left[1 - \exp\left(-b|\epsilon_{vp}(t)|\right)\right]$$

# Pipe lateral:  Parameter Sensitivity NEML




**(a)** Temperature = 550°C, Pressure = 1 MPa

**(b)** Temperature = 600°C, Pressure = 2 MPa

Rate sensitivity exponent, n
Hardening parameter, b

Flow Rule

$$\dot{\epsilon}_{vp} = \left\langle \frac{\frac{\sigma}{1-\omega} - \sigma_0 - R}{\eta} \right\rangle^{\boxed{n}}$$

Hardening Parameter

$$R = Q\left[1 - \exp\left(-\boxed{b}\left|\epsilon_{vp}(t)\right|\right)\right]$$