# Numerical Simulation of Coupled Thermal-Hydrological-Mechanical-Chemical Processes During *In Situ* Conversion & Production of Oil Shale

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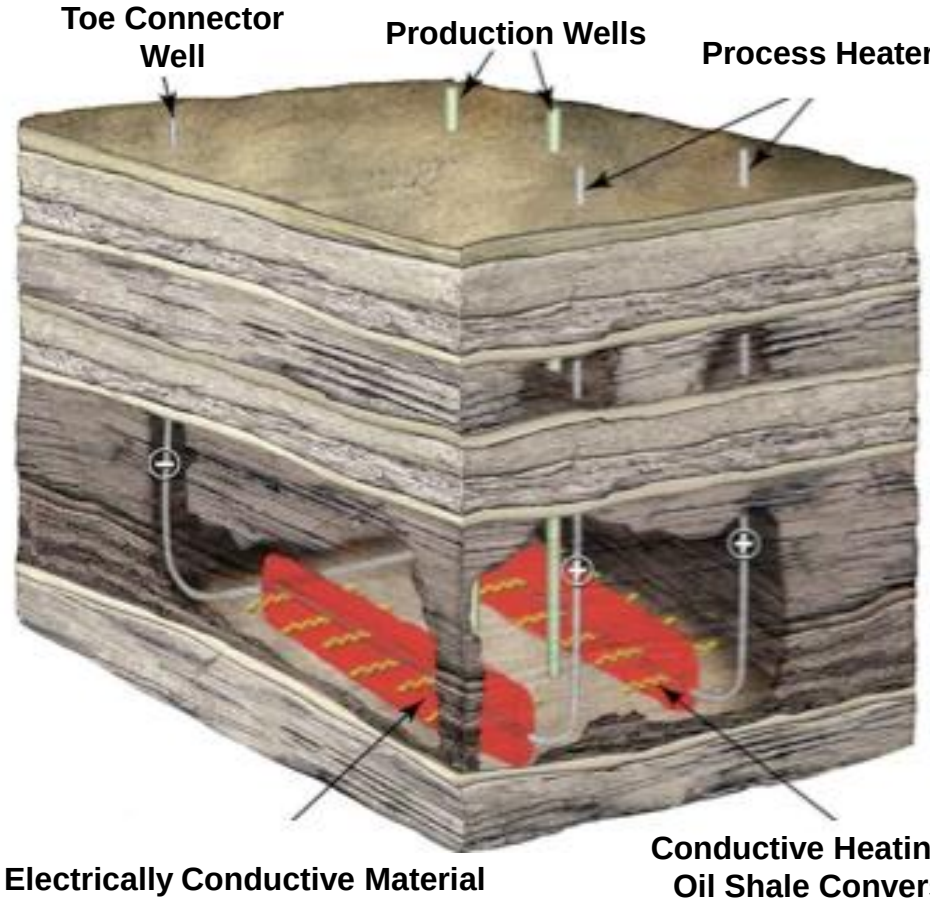
# Full physics modeling of *in situ* heating processes is challenging

**Mimicking *in situ heating* processes requires coupled thermal, mechanical, chemical, and multiphase flow modeling**




**Heating Element**

↓

**Heat transport**

↓

**Pyrolysis**

↓

**Creation of flow pathways by fluid generation**

↓

**Migration of generated fluids**

# Each aspect of oil shale simulation physics is complex in its own right

- **Thermal modeling**

$$\frac{\partial(\overline{C_p}T)}{\partial t} + \mathbf{U}.\nabla(\overline{C_p}T) = \nabla\cdot(\boldsymbol{\kappa}\nabla T) + Q$$

- **Chemical modeling**

$$r_i = f_i \prod_{j=1}^{N} c_i^{\gamma_{ij}}, \quad f_i = A_i \exp(-\frac{E_a^{\ i}}{RT})$$

- **Mechanical modeling**

$$\nabla\cdot\boldsymbol{\sigma} + \mathbf{F} = 0, \quad \boldsymbol{\varepsilon} = \mathbf{C}\cdot\sigma + \alpha\nabla T$$

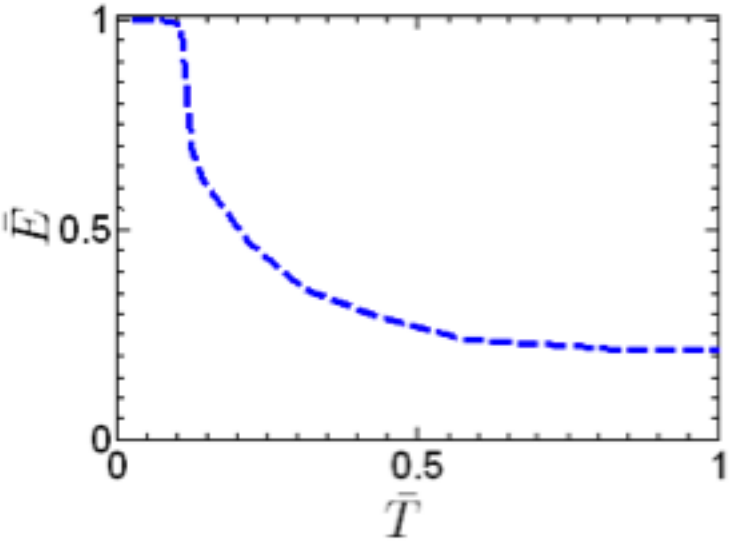
- **Multiphase flow**

$$\mathbf{q}_i = -\frac{k_{ri}}{\mu_i}\mathbf{K}\cdot(\nabla P - \rho\mathbf{g})$$

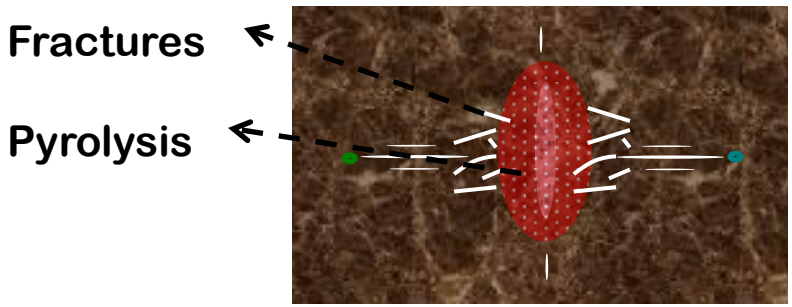
# Oil shale simulator's feature list is extensive owing to complex properties of oil shale


## Thermal and mechanical properties depend on temperature

Transversely isotropic thermal and mechanical properties




## Green River oil shale is non-porous and impermeable




Strong flow-mechanics coupling required to capture porosity/permeability creation during pyrolysis and by rock failure

# LANL's FEHM simulator is an ideal spring board for oil shale simulator development

- FEHM: Finite Element Heat and Mass
  - Had the coupled thermal-flow-mechanics simulation capability applicable to elastic response
  - Control volume-finite element (CVFE) approximation:
    - Control volume for mass/energy balance
    - Finite element for stress
- FEHM has been verified through extensive applications:
  - Groundwater modeling
  - Contaminant transport and reactions
  - Methane hydrate reservoir production
  - $CO_2$ sequestration
  - Geothermal

# Developing new thermal-hydrological-mechanical-chemical (THMC) modeling capabilities in FEHM

- Thermal:
  - Anisotropic, temperature-dependent thermal properties
- Hydrological (multiphase flow):
  - Black oil model: to be extended to compositional
  - EOS based properties
- Mechanical:
  - Anisotropic, temperature-dependent mechanical properties
  - Plastic/elastic deformation models
  - Stress-dependent changes in porosity and permeability
- Chemical:
  - Kerogen conversion into oil/gas/coke and subsequent reactions
  - User-specified stoichiometry and kinetics

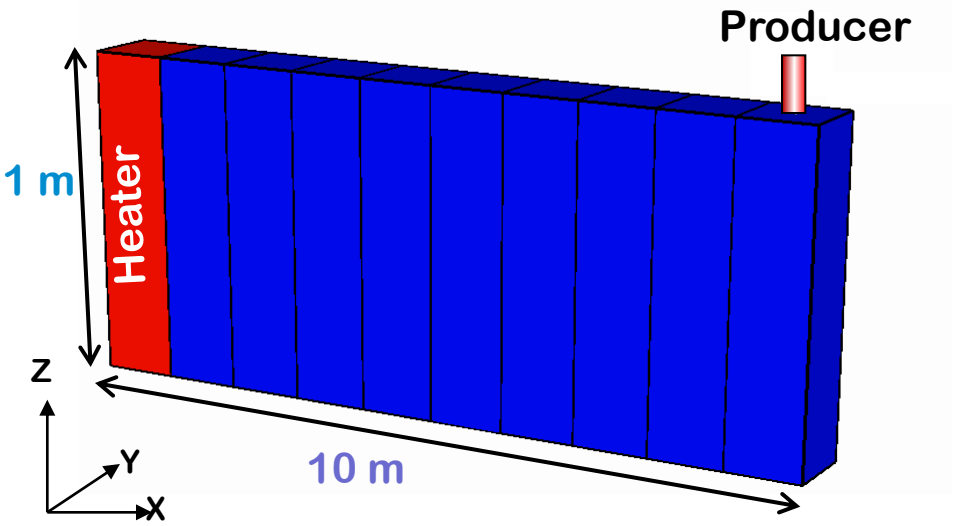
# Benchmarked some of FEHM's new THMC modeling capabilities against CMG's STARS

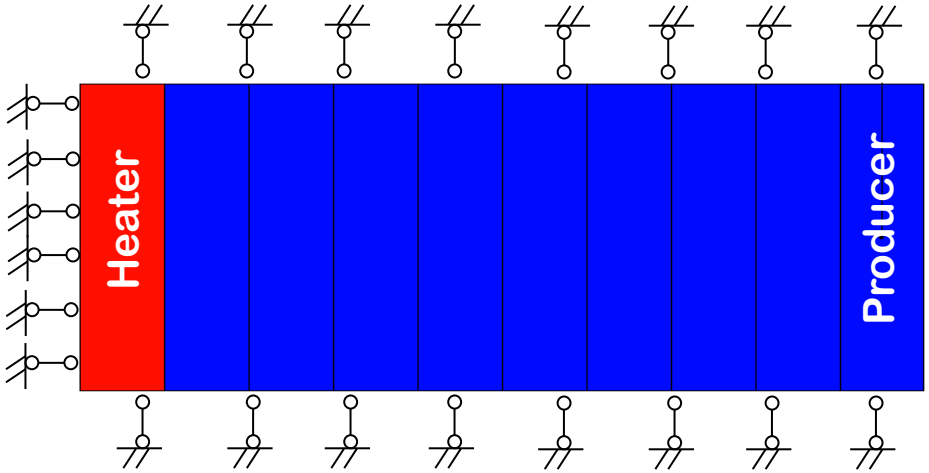
## Problem description:

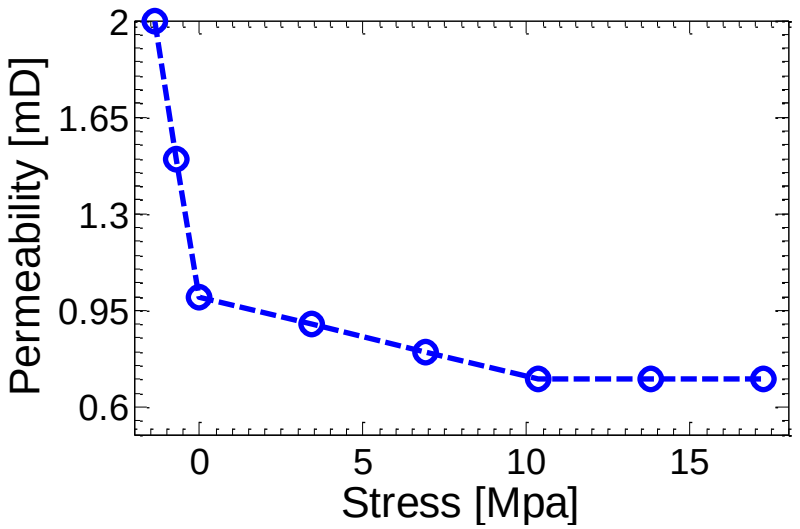
- Richness 35 gal/ton (GPT)
- $P_{Initial} = P_{well} = 5.54$ Mpa
- Stress-dependent permeability
- Q = 0.7 kW
- Reactions:

$$\text{Kerogen} \Rightarrow \text{Oil} + \text{Gas} + \text{Coke}$$

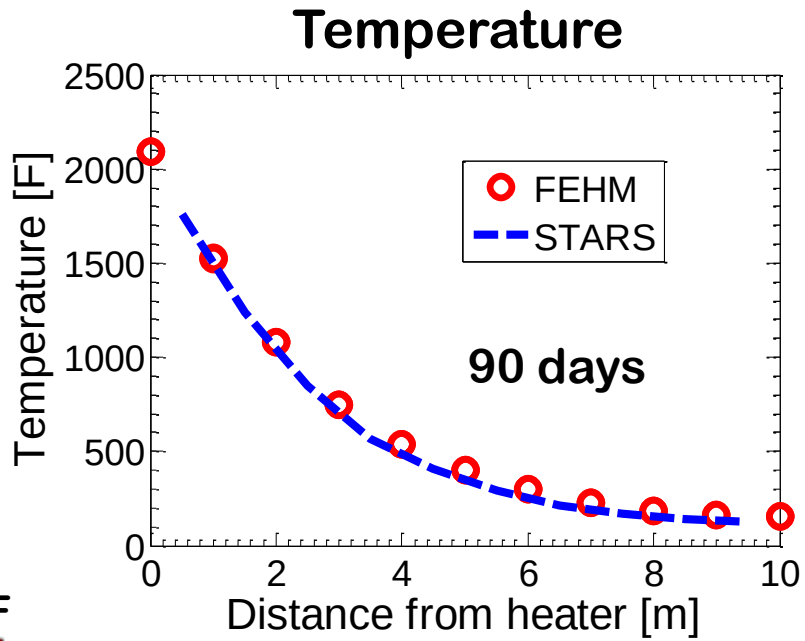
$$\text{Oil} \Rightarrow \text{Gas} + \text{Coke}$$

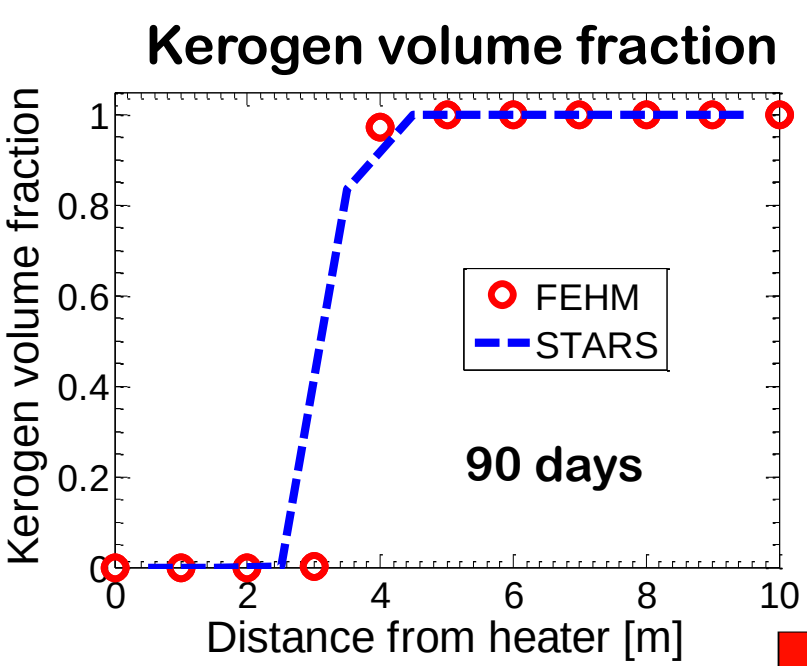


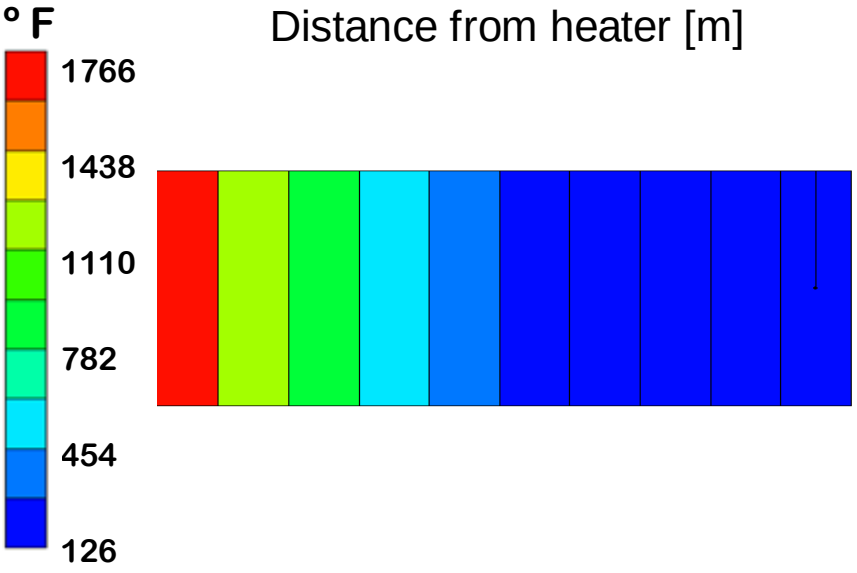



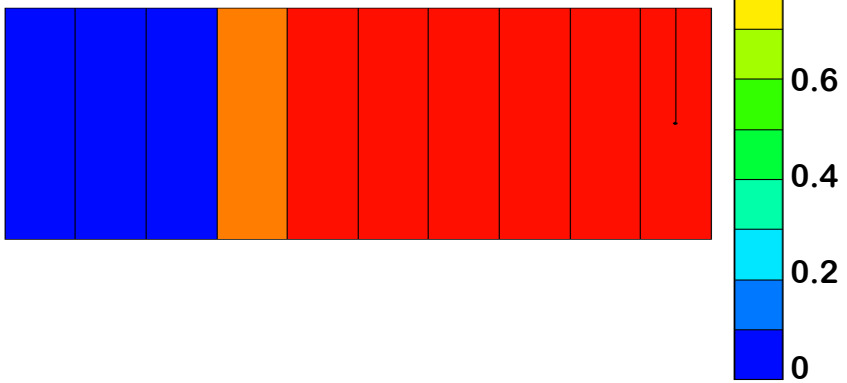



# FEHM's new THMC modeling predictions compare well with CMG's STARS



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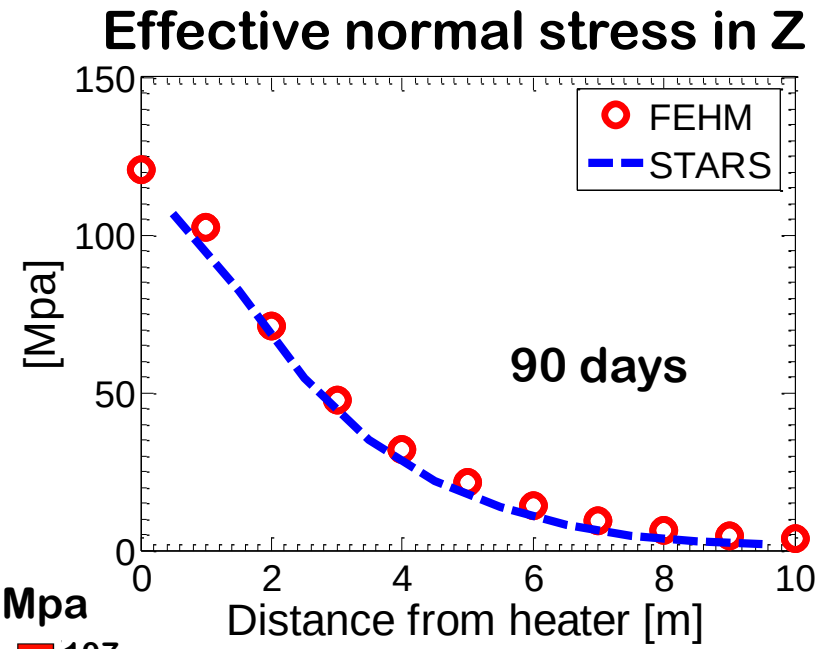
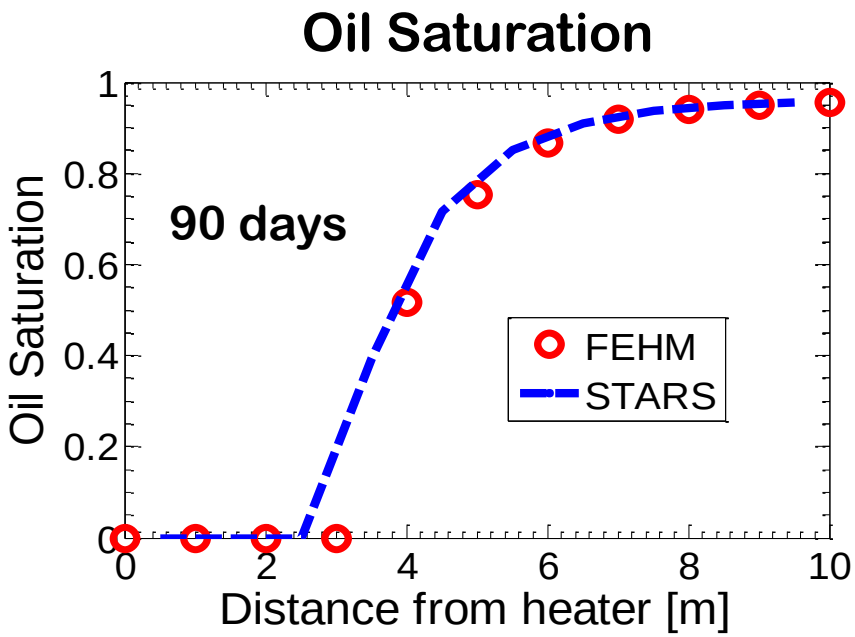
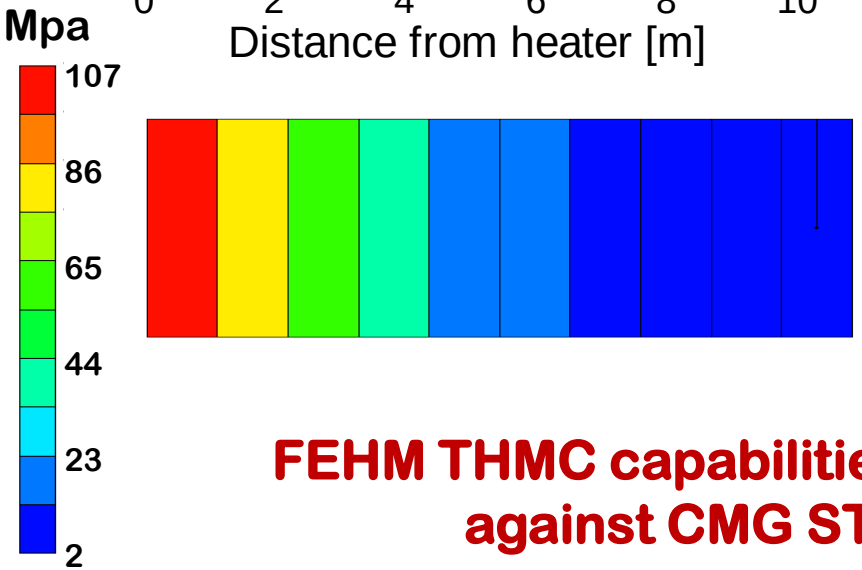
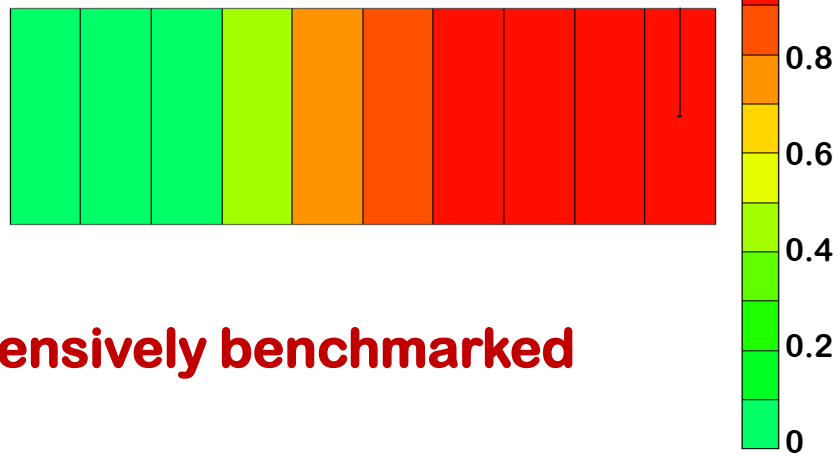


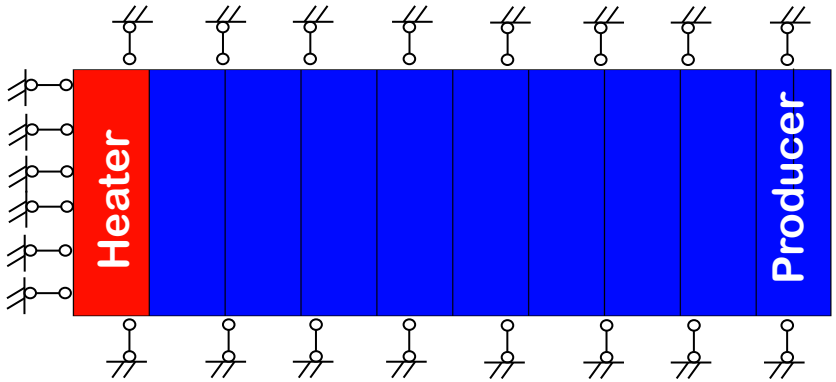



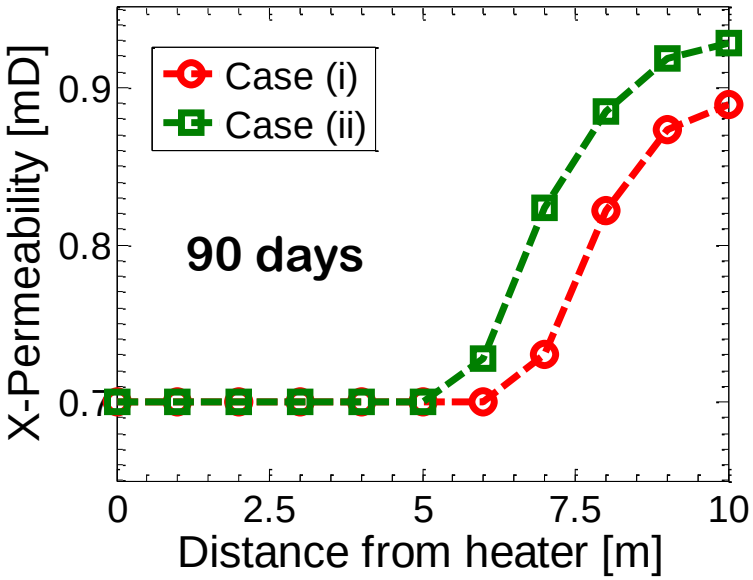




**FEHM THMC capabilities extensively benchmarked against CMG STARS**

# FEHM's new THMC modeling capabilities go beyond contemporary commercial simulators

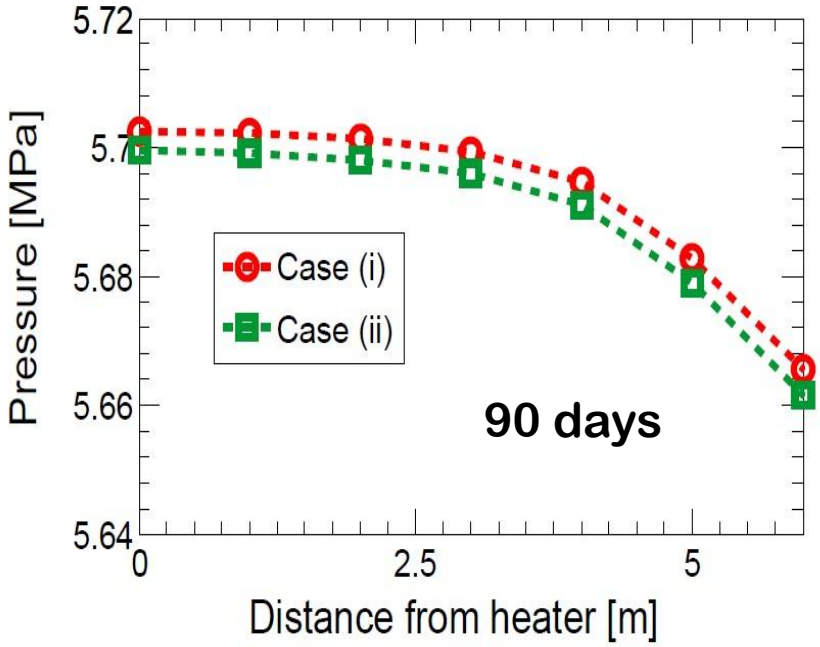
## Directional permeability-stress dependence




**Case (i):** $K_i = f(\max_{j \neq i}(\sigma_{jj}))$

**Case (ii):** $K = f(\sigma_{mean})$

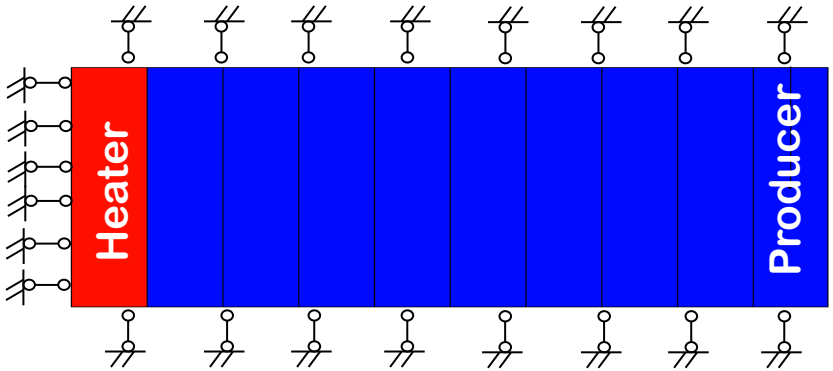


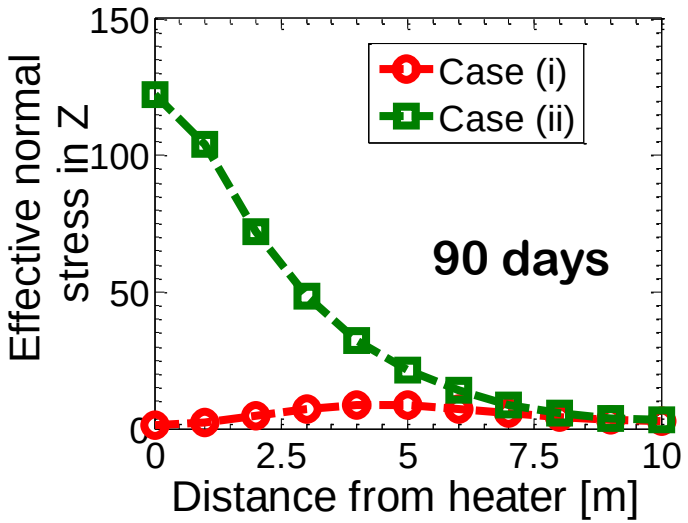

**Impacts pressure and hence recovery**

**Critical to correctly model permeability evolution**

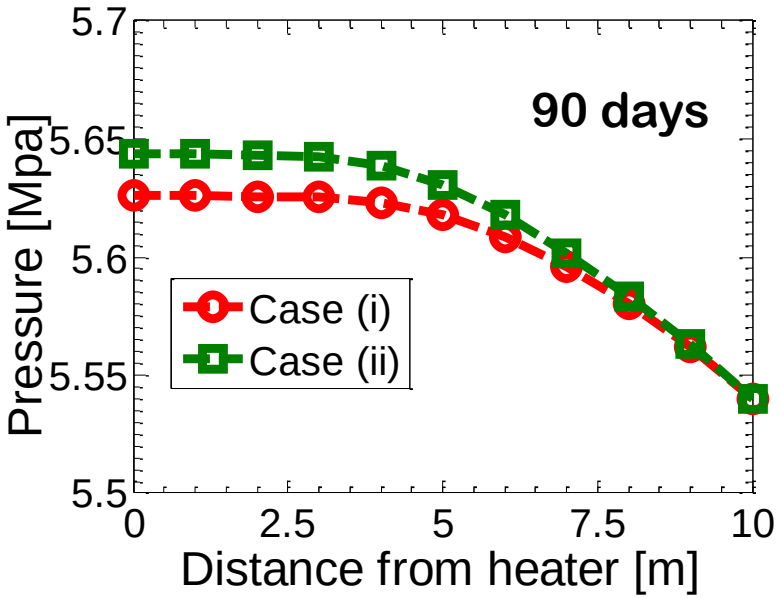
# FEHM's new THMC modeling capabilities go beyond contemporary commercial simulators

## Thermal softening




**Case (i): thermal softening**
**Case (ii): no temp. dependence**




**Changes in rock properties with temperature will impact fluid recovery and formation stability**

# New THMC modeling capabilities in FEHM enable comprehensive modeling of *in situ* conversion processes

- New thermal-hydrological-mechanical-chemical (THMC) capabilities have been developed in FEHM to numerically simulate *in situ* conversion processes.
- Some THMC modeling capabilities have been extensively benchmarked against CMG's STARS and Abaqus.
- FEHM's new THMC modeling capabilities go beyond commercial simulators. These capabilities are critical for effectively modeling *in situ* conversion processes.
- Future developments include:
  - switching to implicit formulation
  - compositional fluid description

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