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Title:	Development of capabilities to simulate the coupled thermal-hydrological-mechanical-chemical (THMC) processes during in situ oil shale production
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Development of capabilities to simulate the coupled thermal-hydrological-mechanical-chemical (THMC) processes during *in situ* oil shale production

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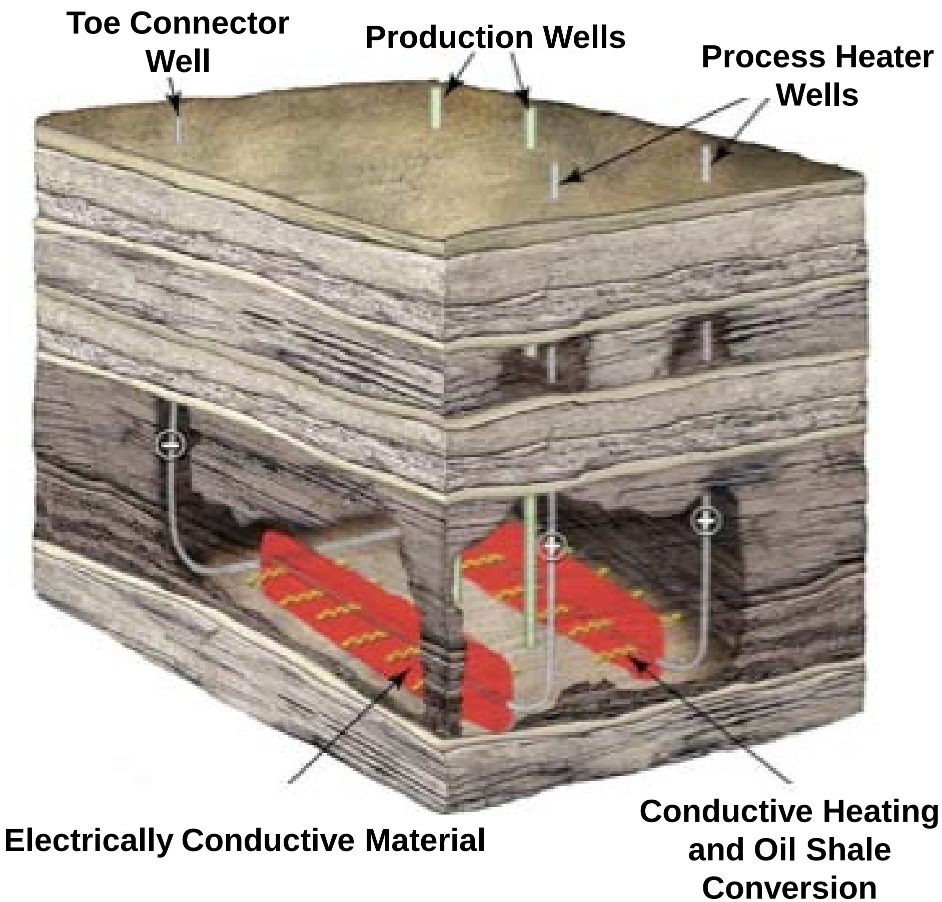
Motivation

Coupled thermal-fluid flow-mechanical-chemical processes are important in many subsurface energy and environment applications including

- Unconventional oil and gas production
- CO_2 sequestration
- Geothermal energy production
- Nuclear waste storage

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

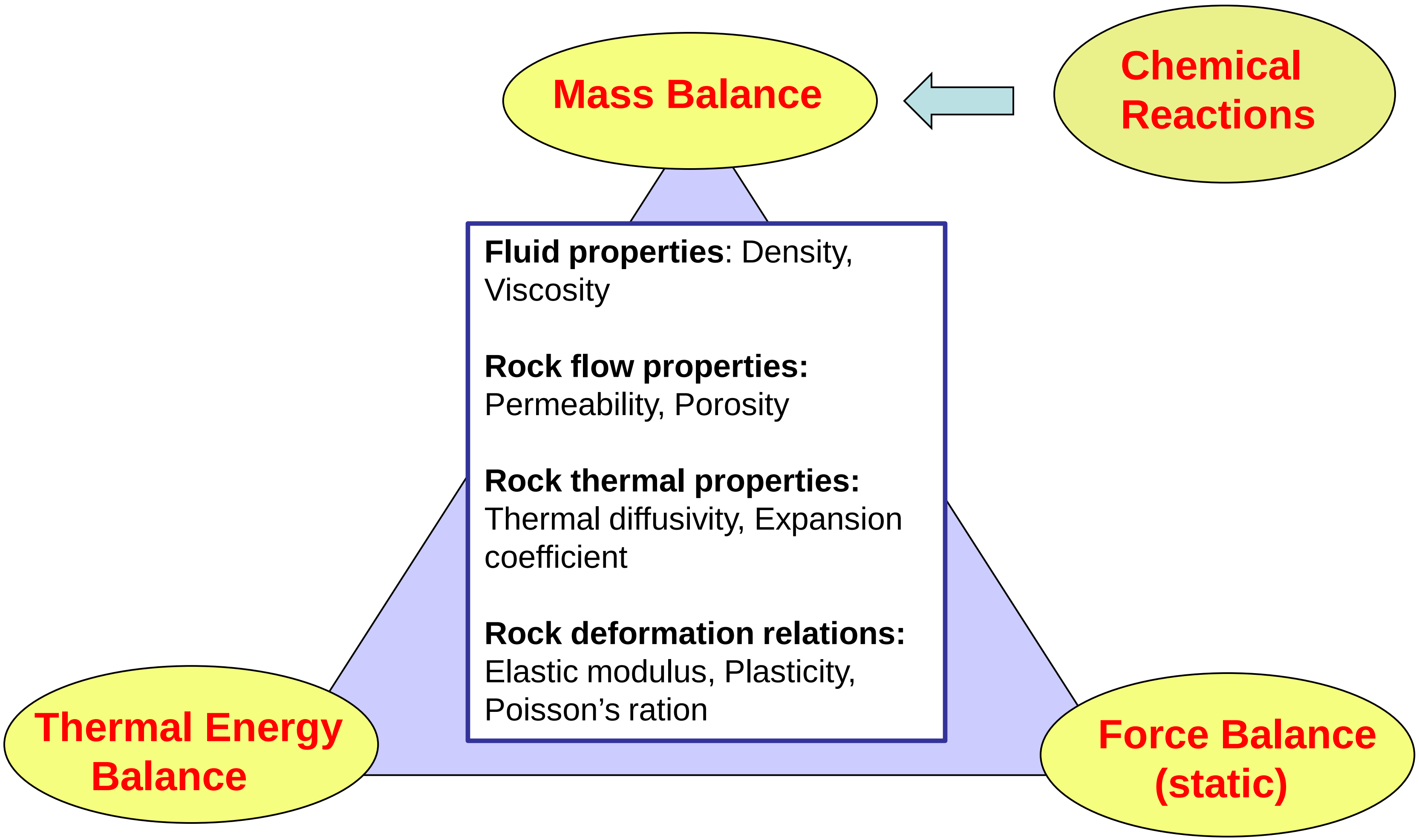
ExxonMobil's *in situ* oil-shale recovery process



Heating Element
↓
Heat transport
↓
Pyrolysis
↓
Creation of flow pathways by fluid generation
↓
Migration of generated fluids

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

Numerical Model-Conservation Equations



Variables: pressure, temperature, saturation, composition, deformation

LANL's FEHM simulator is being modified 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:
  - Over 30 years of development and application
    - 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 (k-value based phase equilibrium)
  - 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

Component mass conservation

$$\frac{\partial A_n}{\partial t} + \overline{\nabla} \cdot \bar{f}_n + q_n + q_{nr} = 0$$

n– oil, water, gas

$$A_n = \phi\left(S_o \rho_o x_n + S_g \rho_g y_n + S_w \rho_w w_n\right)$$

Accumulation

$$\bar{f}_n = x_n \rho_o \bar{v}_o + y_n \rho_g \bar{v}_g + w_n \rho_w \bar{v}_w$$

Advection

$$q_n = \bar{q}_o x_n + \bar{q}_g y_n + \bar{q}_w w_n$$

Source/sink

$$q_{nr} = f\,(Kerogen\ Content)$$

Reaction

ϕ – Total porosity which includes solid with kerogen plus liquids and gas

$$\bar{v}_l = -\frac{k k_{rl}}{\mu_l}\left(\overline{\nabla} P_l - \rho_l \bar{g}\right) \quad k_{rl} = f\left(S_l' = \frac{S_l}{S_w + S_o + S_g}\right)$$

Total energy conservation

$$\frac{\partial A_e}{\partial t} + \overline{\nabla} \cdot f_e + q_e + q_{er} = 0$$

$$A_e = (1-\phi)\rho_r u_r + \phi\left(S_o\rho_o u_o + S_g\rho_g u_g + S_w\rho_w u_w + S_s\rho_s u_s\right)$$ Accumulation

$$\bar{f}_e = \rho_o h_o \bar{v}_o + \rho_g h_g \bar{v}_g + \rho_w h_w \bar{v}_w - K\overline{\nabla}T$$ Advection + conduction

$$q_e = \bar{q}_o h_o + \bar{q}_g h_g + \bar{q}_w h_w$$ Source/sink

$$q_{er} = \text{Heat of reaction}$$ Reaction

Static Stress Equilibrium Equations-Finite Element Formulation for infinitesimal elastic deformation, with pore pressure and thermal terms

$$\sum_i \left\{ \int \left[\frac{\partial N_j}{\partial x_l}(\lambda + 2G)\frac{\partial N_i}{\partial x_l} + \frac{\partial N_j}{\partial x_m} G \frac{\partial N_i}{\partial x_m} + \frac{\partial N_j}{\partial x_n} G \frac{\partial N_i}{\partial x_n} \right] \mathrm{dv} \right\} U_{l_i}$$

$$+\sum_i \left\{ \int \left[\frac{\partial N_j}{\partial x_l} \lambda \frac{\partial N_i}{\partial x_m} + \frac{\partial N_j}{\partial x_m} G \frac{\partial N_i}{\partial x_l} \right] \mathrm{dv} \right\} U_{m_i}$$

$$+\sum_i \left\{ \int \left[\frac{\partial N_j}{\partial x_l} \lambda \frac{\partial N_i}{\partial x_m} + \frac{\partial N_j}{\partial x_n} G \frac{\partial N_j}{\partial x_l} \right] \mathrm{dv} \right\} U_{n_i}$$

$$-\sum_i \left\{ \int \left[N_j \frac{\partial N_i}{\partial x_l} \frac{K}{H} \right] \mathrm{dv} \right\} \Delta P_i - \sum_i \left\{ \int \left[N_j \frac{\partial N_i}{\partial x_l} \frac{\alpha E}{(1-2\nu)} \mathrm{dv} \right] \right\} \Delta T_i$$

+ Body Force Terms + Surface Terms =0

$U_{l_i} =$ nodal displacements

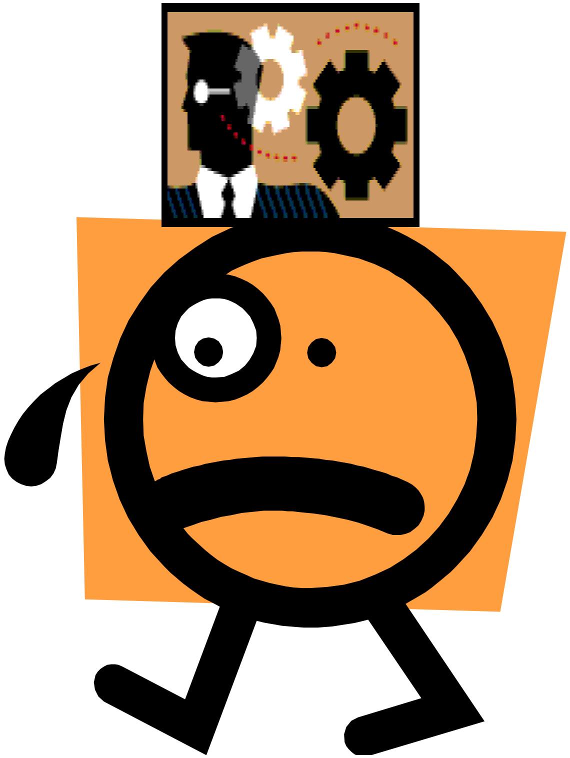
E	Young's modulus
υ	Poisson's ratio
u_i	Displacement
α	Coeff. of Thermal Expansion
$\frac{\alpha_B}{K}$	Biot coeff.

$$G = \frac{E}{2(1+\nu)}$$

$$\lambda = \frac{E_\nu}{(1+\nu)(1-2\nu)}$$

$$K = \frac{E}{3(1-2\nu)}$$

Modeling challenges



- Large changes in fluid pressure
- Large changes in temperature
- Large changes in stress
- Large problem size
- Highly nonlinear
- Many different space and time scales
- Matrix rock and fractures/faults are both important

How coupling occurs in the equations

- **Explicit terms in equations**

  effective stress and thermal stress in the Force Balance

- **Dependence of coefficients**

  ϕ (ε,σ ,p,T) K (ε,σ ,p,T)

  In fractured media, permeability has power (cubic or higher) dependence on aperture . Growing body of literature, a number of permeability-deformation models

- **Dependence of rock properties and reaction kinetic parameters**

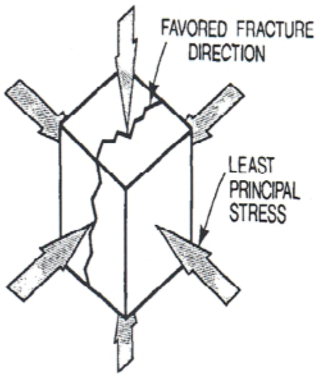


Figure 1. Stress element and preferred plane of fracture (after Hubbert and Willis, 1957).

Flow and stress coupling

Permeability – Aperture – Deformation – Strain - Stress

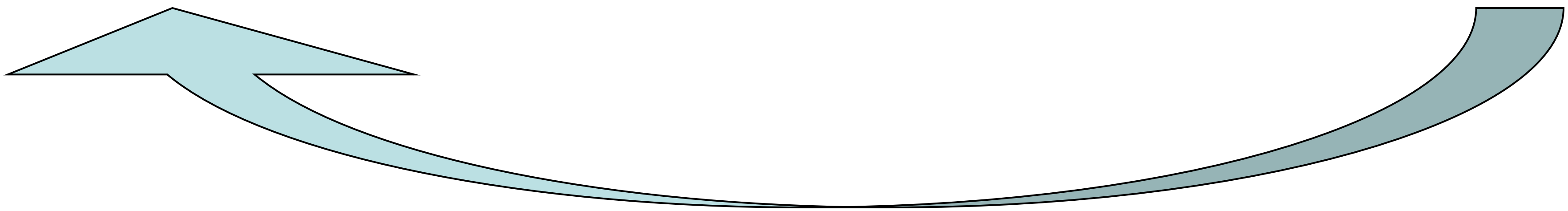
- Power Law

- Mechanical
- Hydraulic

- Tensile
- Shear

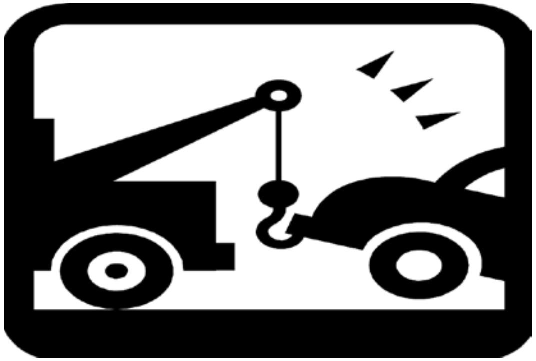
- Elastic
- Plastic

- Tectonic
- Gravity
- Thermal
- Pore Pressure



Growing body of literature, a number of permeability-deformation models

Levels of coupling



Desirable to be able to choose between fully implicit coupling and explicit coupling, depending upon the domain of interest

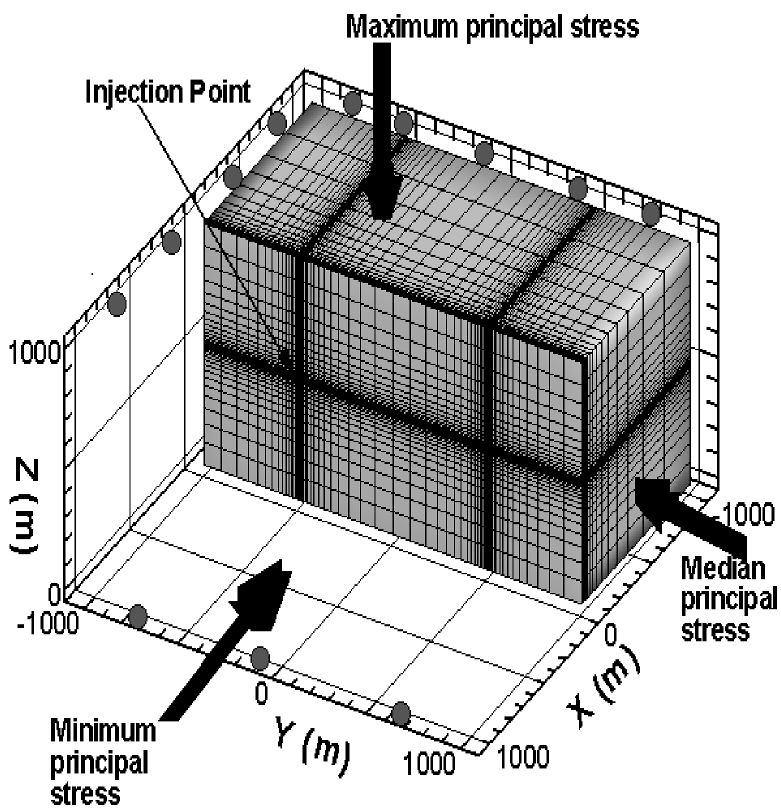
For example, near-field (~10’s m) strong gradients might be expected requiring full coupling (microseismicity, surface deformation, fracture generation due to pore pressure) where as in the mid-field (~km) (microseismicity, surface deformation) explicit coupling may be sufficient, and far-field (10’s km) may be adequately treated by uncoupled models.

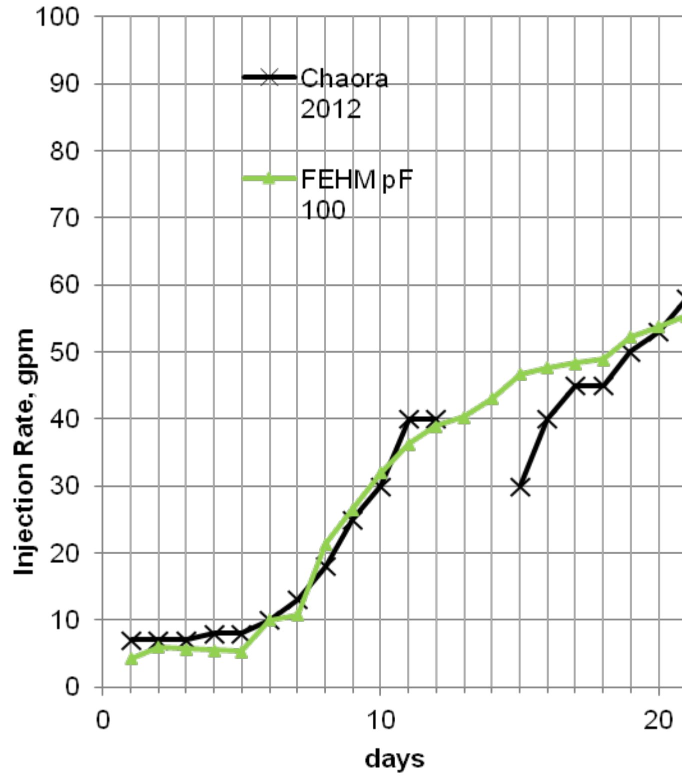
Example: coupled flow-stress modeling (permeability change)

Comparison with field data

Injection of cold water into a geothermal reservoir at pressure below fracture opening.
2km x 2km x 1km grid with specified far-field stresses.
Shear failure using Mohr-Coulomb criteria (Permeability function of shear stress)

Key Conclusion:
Good match of field observations with model, permeability enhancement due to thermal stresses is important.





Cross-validation of FEHM's oil-shale simulation capability with CMG's STARS

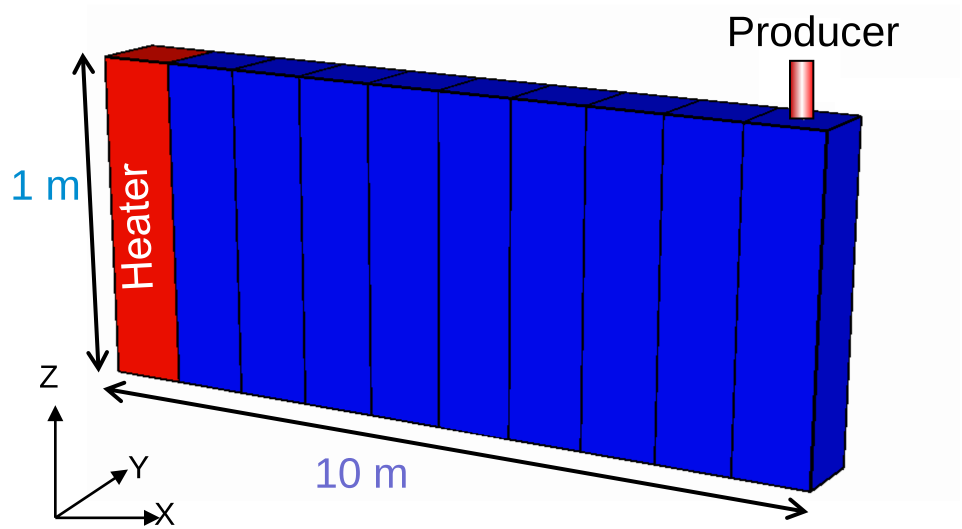
Benchmarked some of FEHM's new THMC modeling capabilities against CMG's STARS

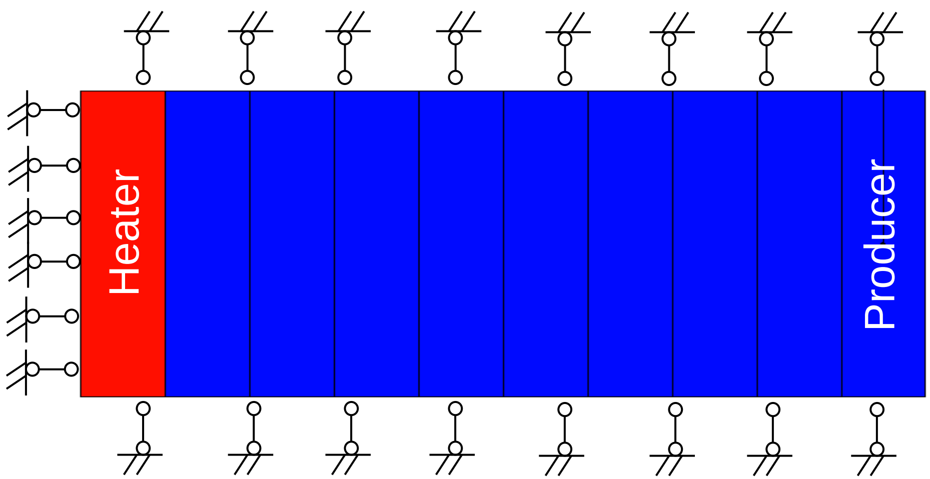
Problem description:

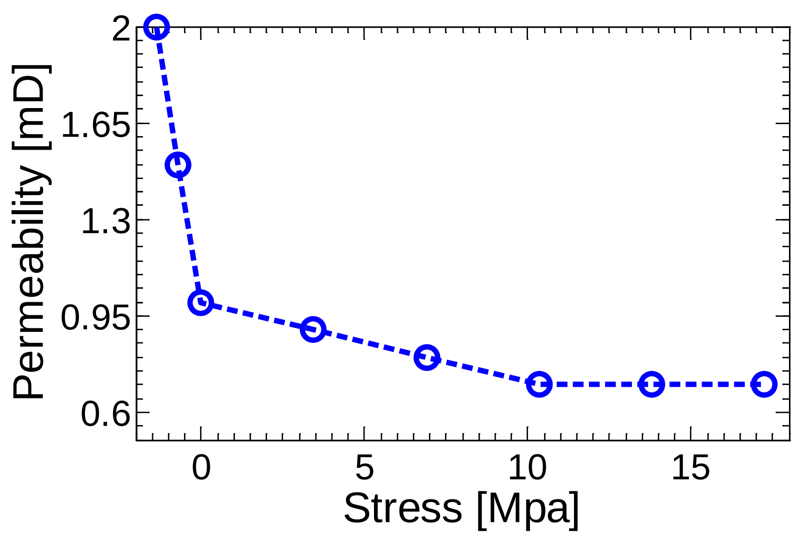
- Richness 35 gal/ton (GPT)
- $P_{Initial} = P_{well} = 5.54$ Mpa
- Stress-dependent permeability (empirical)
- Q = 0.7 kW
- Reactions:

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

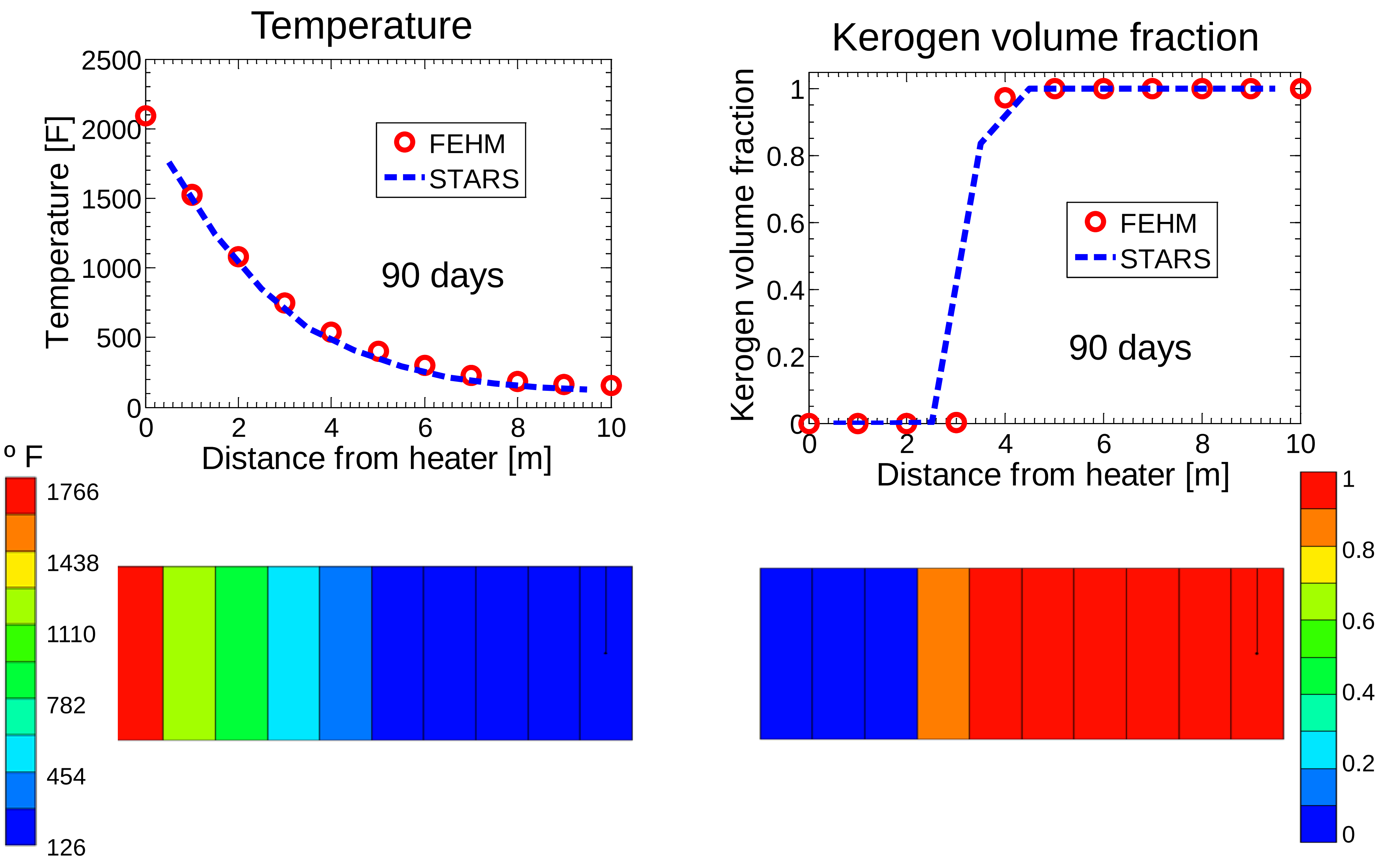
$$\text{Oil} \Rightarrow \text{Gas + Coke}$$



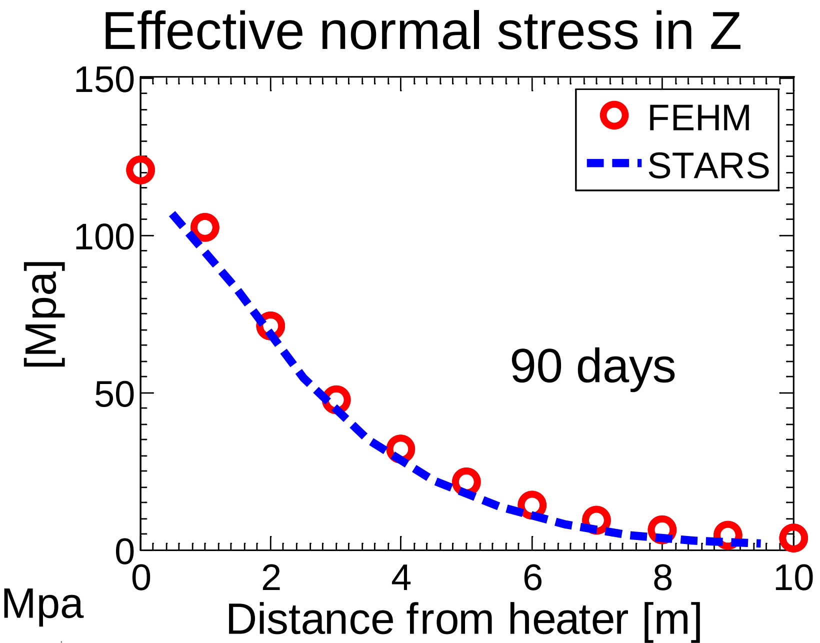


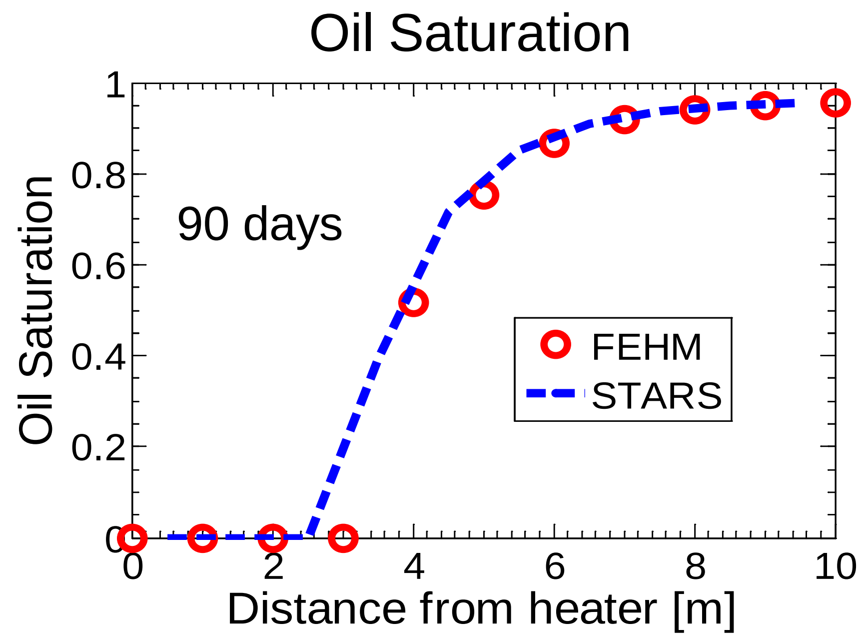


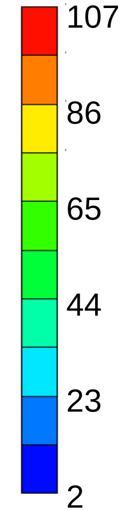
FEHM's new THMC modeling predictions compare well with CMG's STARS

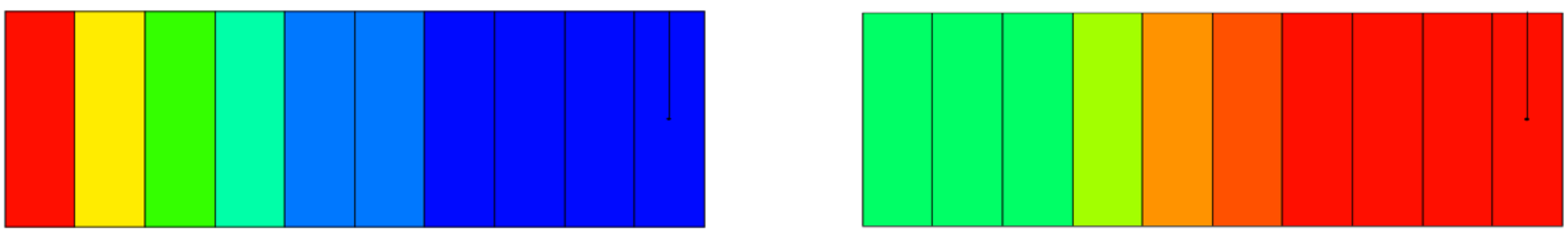


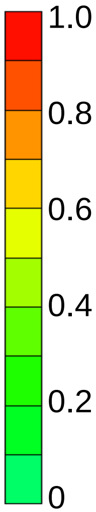
FEHM's new THMC modeling predictions compare well with CMG's STARS







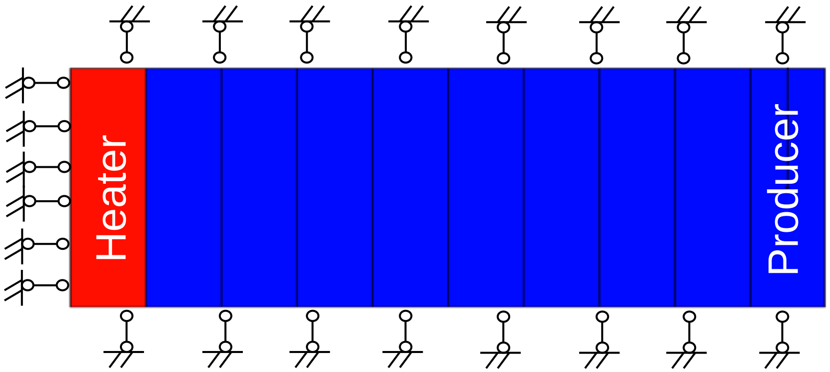




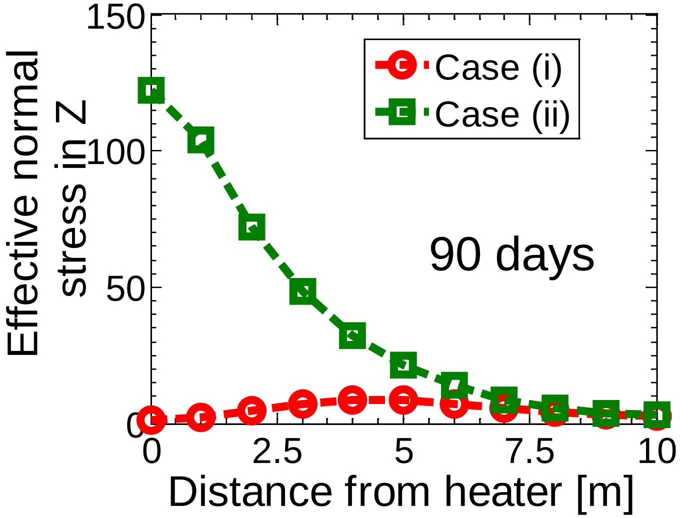
FEHM THMC capabilities extensively benchmarked against CMG STARS

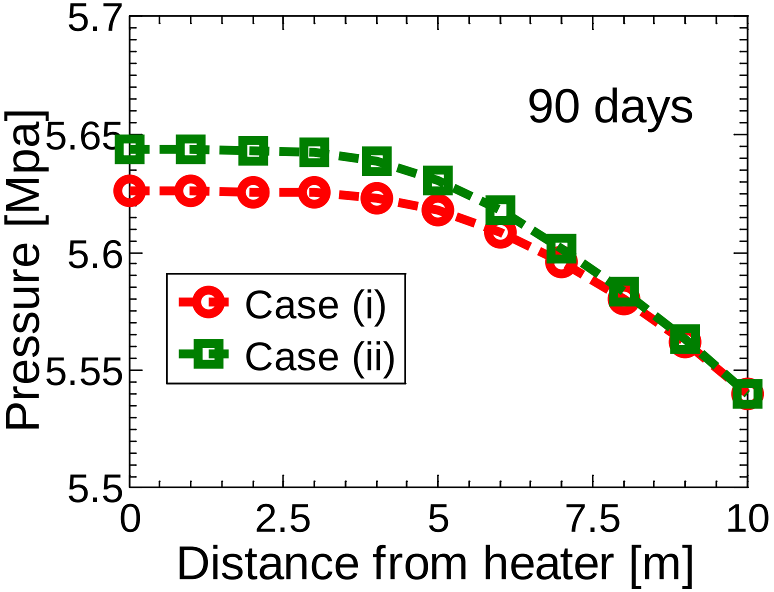
FEHM's new THMC modeling capabilities go beyond contemporary commercial simulators

Thermal softening



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





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

Its critical to model change in permeability with stress

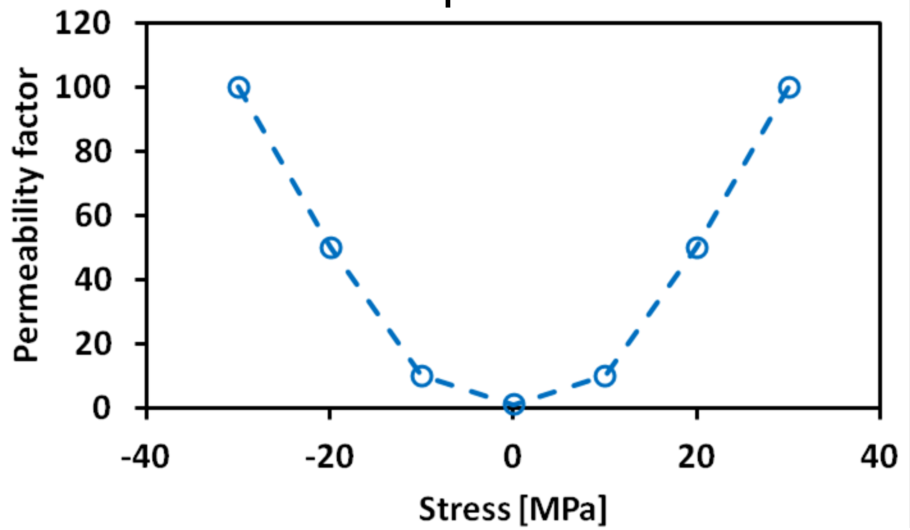
- Creation of permeable pathways due to change in stresses is critical for success of *in situ* process
- Permeability creation due to pore pressure change
  - Local effect
  - Need models that accurately capture change in permeability at continuum scale
- Our stress-perm model is limited in its ability to capture these sub-continuum scale pore-pressure effects
  - We used another hypothetical model in order to demonstrate how sub-continuum scale effects can be captured in continuum models

Model to demonstrate effect of pore-pressure change on permeability

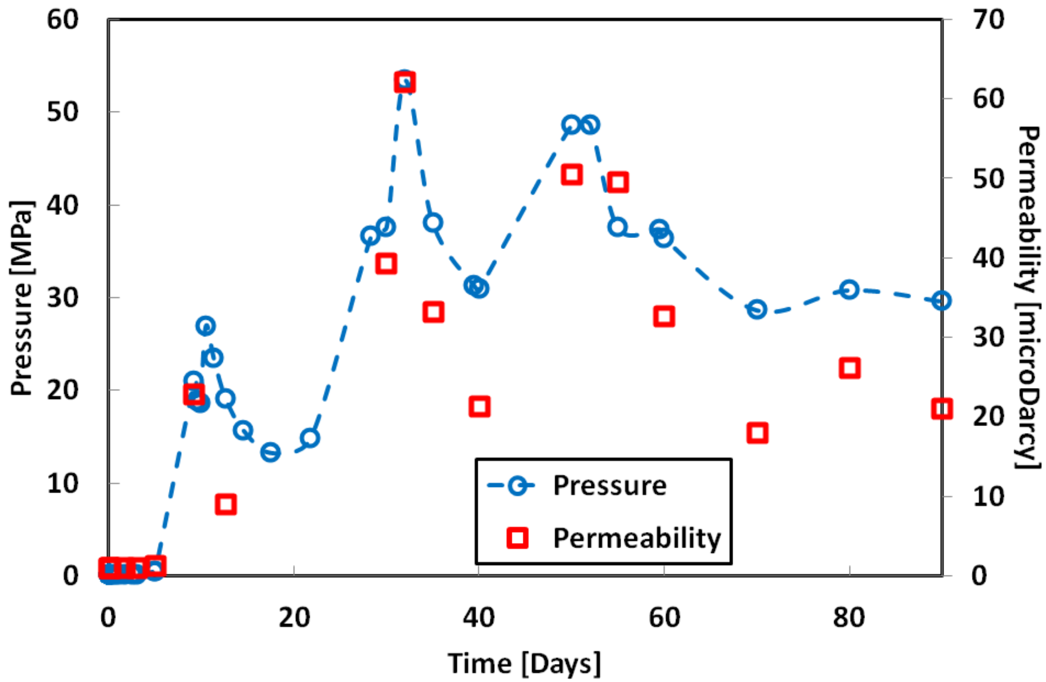
Problem description:

- Same as before except:
- Initial permeability 1 μ–Darcy
- Different stress-dependent permeability (hypothetical)
- No thermal stress effect (thermal expansion coefficient 0.0)

Stress-perm model



Pressure and permeability at heater node

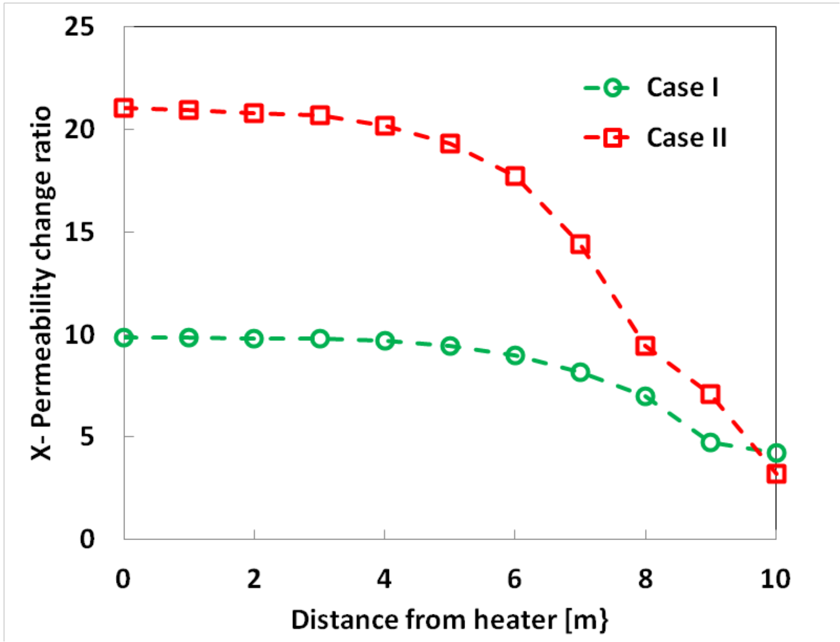


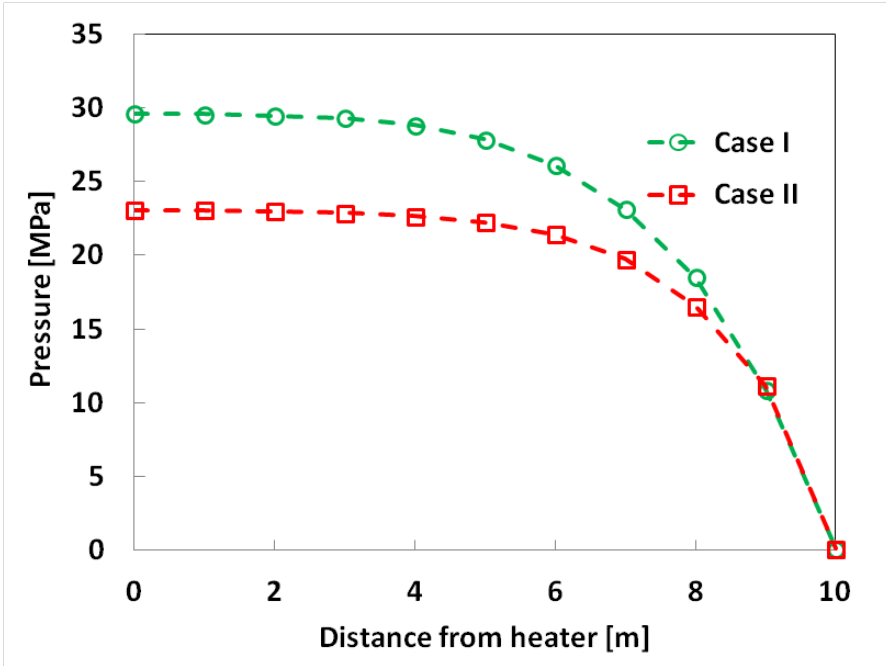
FEHM's new THMC modeling capabilities go beyond contemporary commercial simulators

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

Implicit coupling of permeability change

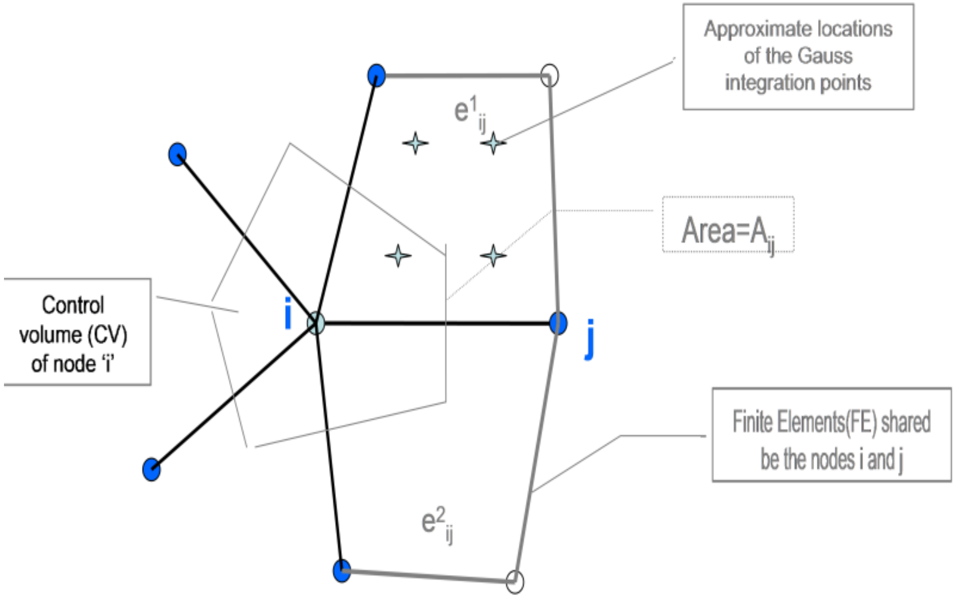
Derivative of the mass flux between two connected nodes I and j wrt a node k connected to one of them:

$$\frac{\partial q^{ij}}{\partial \overline{u}_k} = K^{ij} \cdot \frac{\rho}{\mu} \cdot (A_{ij} / l_{ij}) \cdot (P_j - P_i) * \frac{\partial pF^{ij}}{\partial \overline{u}_k}$$

$$\frac{\partial pF^{ij}}{\partial \overline{u}_k} = \frac{1}{N_{ij-e}} \sum_{elements-ij} \frac{\partial pF^{ij-e}}{\partial \overline{\sigma}_e} \cdot \frac{\partial \overline{\sigma}_e}{\partial \overline{u}_k}$$

$$\frac{\partial \overline{\sigma}_e}{\partial \overline{u}_k} = \frac{1}{Ve} \sum_{gp} | J | \overline{\overline{D}} \cdot \overline{\overline{B}} \cdot \overline{\overline{I}}$$

pF^{ij-e} **is an effective permeability factor representing stress/deformation effects**



NOTE: In FEHM, properties are input at nodes and assigned to the CV. properties on FE are obtained by using appropriate averages/interpolations

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 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 the *in situ* conversion processes
- Models to effectively capture change in permeability due to stress change are needed in continuum-scale formulations
- We are currently developing capabilities to implicitly simulate change in permeability due to stress change
  - Multi-phase formulation
  - Plastic deformation

Acknowledgements

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- The capabilities for simulation of geomechanical processes have been developed through the Zero Emission Research & Technology (ZERT-II) project under DOE's Carbon Sequestration Program.
- The application to geothermal field test was funded through US DOE's Geothermal Technologies Program

Background Slides

Parameter values

PARAMETER	**VALUE**
Formation temperature	190^0 C
Initial pore pressure	9 MPa
Bottom hole injection pressure	13.1 MPa
Injection temperature	170^0 C
Principal in situ stresses	
Maximum	22.6 MPa (vertical)
Intermediate	18.1 MPa
Minimum	13.8 MPa
Thermal conductivity	3 W/m/K
Heat capacity	820 J/kg/K
Porosity	10%
Initial permeability*thickness	9 md.m
Shear failure-permeability model parameters	
Friction Coefficient	0.8
Cohesion	2 MPa
Permeability multiplier (all directions)	100
Young's modulus	30 GPa
Poisson' ratio	0.15
Coeffficient of Thermal Expansion	10^{-4} $/^0$C
Biot poroelastic parameter	0.5

Example of application to non-Orthogonal grid: Inclined, weak fault