# Coupled THMC Modeling of $CO_2$ Injection by Finite Element Methods

Yin, S., Dusseault, M. B., & Rothenburg, L. (2011).
*Journal of Petroleum Science and Engineering*, *80*(1), 53-60.

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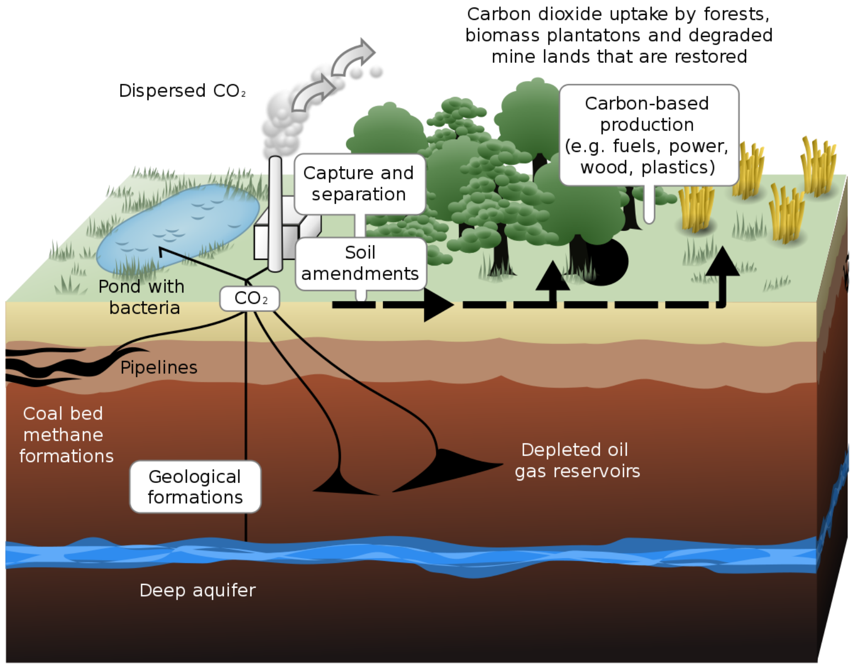
# Outline

- Introduction
- Methodology
- Results
- Conclusions

# Introduction

- Massive $CO_2$ sequestration is proposed to mitigate greenhouse gas emissions.
- It has been suggested that 7 Gt of $CO_2$ might be sequestered every year to maintain the balance of $CO_2$ emission.



- When adjusting $CO_2$ sequestration, reservoirs induce a range of strongly coupled thermal, hydraulic, mechanical and chemical processes (THMC).

- THMC includes:
  - Heat transfer
  - Multiphase fluid flow
  - Geomechanical response (strains and stresses)
  - Solute transport
  - Geochemical reactions between the fluids and formation minerals

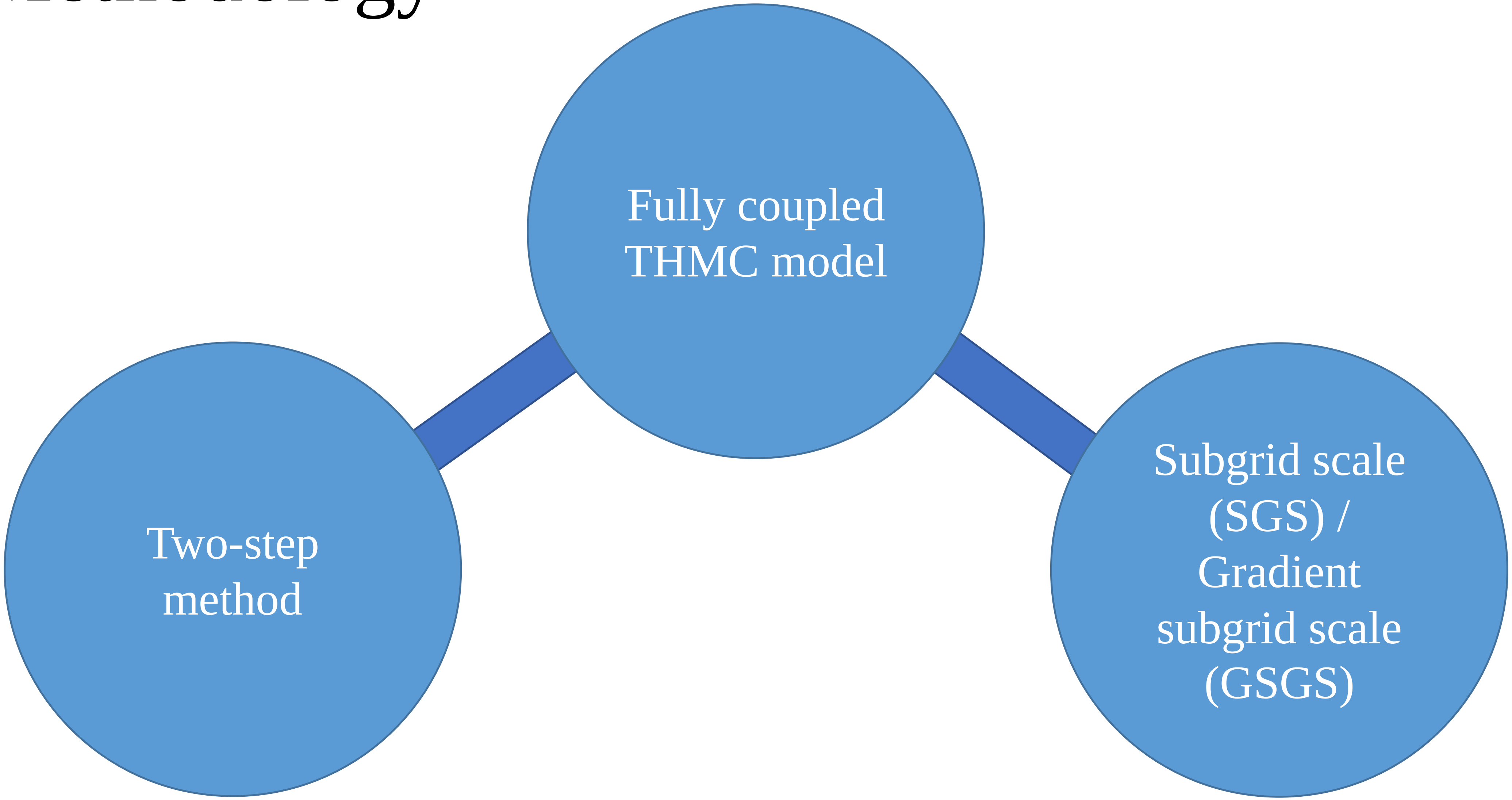
- Injecting such large amounts of $CO_2$ requires appropriate strata injection capabilities, well and caprock integrity.

- Very few fully-coupled THMC models have addressed the large-scale problem.

# Objective

- Analyze stress and pressure changes in rocks around a borehole during $CO_2$ injection.
- Understand heat transfer, fluid flow, geomechanics behavior, and reactive chemical transport by mathematical methods.

# Methodology



# Methodology

- Fully coupled THMC model
  - Based on FEM.
  - Combine theories of poroelasticity, thermoelasticity, and reactive solute transport.

# Equation of mechanics

General equilibrium equation in terms of effective stress

$$G\nabla^2 u + (G + \lambda)\nabla div u - \left(1 - \frac{K}{K_m}\right)\nabla p - K\beta_s \nabla T = 0$$

(Lewis and Schrefler, 1998; Yin et al., 2010)

*G*, $\lambda$: Lamé elastic constants
*u*: displacement
*p*: pore pressure
*T*: temperature
$\beta_s$ : volumetric thermal expansion coefficient
*K:* bulk moduli (bulk skeleton)
$K_m$ : bulk moduli (matrix mineral)

# Equation of hydraulics

General form of the continuity equation for fluid flow, incorporating Darcy's Law

$$\nabla^T\left(-\frac{k}{\mu}\nabla p\right)+\left(\frac{\alpha-\Phi}{K_m}+\frac{\Phi}{K_w}\right)\frac{\partial p}{\partial t}+\alpha\frac{\partial \varepsilon}{\partial t}-\left[(\alpha-\Phi)\beta_s+\Phi\beta_w\right]\frac{\partial T}{\partial t}=0$$

(Lewis and Schrefler, 1998; Yin et al., 2010)

$\alpha$: Biot's coefficient, equal to 1.0-$K/K_m$
$k$: permeability of the porous medium
$\Phi$: porosity
$\mu$: viscosity
$\beta_w$ : volumetric thermal expansion coefficient of the fluid

# Thermal equation

General form of the energy balance equation, including the thermal convection and thermal conduction terms

$$\nabla^T[-\lambda_T \nabla \boldsymbol{T}] + \rho_w c_w v \nabla \boldsymbol{T} + T\left[(1-\Phi)c_s \frac{\rho_s}{K_m} + \Phi c_w \frac{\rho_w}{K_w}\right]\frac{\partial \boldsymbol{p}}{\partial t}$$
$$+[-\Phi c_w \rho_w \beta_w T - (1-\Phi)\rho_s c_s \beta_s T + (1-\Phi)\rho_s c_s + \Phi \rho_w c_w]\frac{\partial \boldsymbol{T}}{\partial t} + Q_h = 0$$

(Lewis and Schrefler, 1998; Yin et al., 2010)

$\lambda_T$: porous medium thermal conductivity
$c$: specific heat capacity
$\rho$: density
$Q_h$: external sink or source
$v$: Darcy velocity

# Equation of chemical reactions

General form of the equation for solute transport of ith aqueous species, including both the solute diffusion and convection terms

$$\nabla^T(D_i \nabla C_i) + \Phi \frac{\partial C_i}{\partial t} + v_w \nabla C_i = R_i, i = 1, \dots, N$$

$C_i$: aqueous phase concentration of the ith species (moles of species/unit volume of solution)
$D_i$: dispersion coefficient
$R_i$: reaction rate
$v_w$: Darcy velocity

General form of the continuity equation for the jth species in the solid phase

$$\frac{\partial C_j}{\partial t} R_j, j = 1, \dots, M$$

$C_j$ : solid phase concentration of the jth mineral species (moles of species per bulk volume of rock)
$R_j$ : reaction rate

Rate law for the mineral dissolution and precipitation reaction

$$R_j = A_j k_j (1 - \frac{Q_j}{K_{eq,j}})$$

$A_j$: reactive surface area for mineral
$k_j$: rate constant of mineral j
$K_{eq,j}$: chemical equilibrium constant for mineral reaction j
$Q_j$: chemical affinity of mineral reaction j
$R_j$ : positive → precipitation, negative → dissolution

- Two-step method
  - Approach to solve the reactive transport equations.
  - Solve solute transport & chemical reactions separately.

- Subgrid scale (SGS) / Gradient subgrid scale (GSGS) method

  - Subgrid scale: A computational method used for stabilizing numerical solutions of advection-diffusion-reaction problems.

  - Gradient subgrid scale: A technique that enriches the SGS method with an integral containing the gradients of the residual and the weighting space.

  - Mitigate numerical instabilities and spurious oscillations that may arise from unresolved small-scale features in the flow and transport processes.

  - Improve the accuracy and stability of the numerical simulations.

# Validation - reactive transport module

The chosen validation problem: Transport of three species with sorption and decay in a one-dimensional flow field.

$$R\frac{\partial C_1}{\partial t} = D\frac{\partial^2 C_1}{\partial z^2} - v\frac{\partial C_1}{\partial z} - k_1 C_1$$

$$\frac{\partial C_2}{\partial t} = D\frac{\partial^2 C_2}{\partial z^2} - v\frac{\partial C_2}{\partial z} - k_2 C_2 + k_1 C_1$$

$$\frac{\partial C_3}{\partial t} = D\frac{\partial^2 C_3}{\partial z^2} - v\frac{\partial C_3}{\partial z} - k_3 C_3 + k_2 C_2$$

Domain: one dimension (40cm)
Boundary condition:
Inlet: $C_{10} = 1.0, C_{20} = 0.0, C_{50} = 0.0$
Exit: no-flux

| Symbol | Meaning | Value |
|---|---|---|
| $C_1$ | *concentrations of species* | - |
| $C_2$ | | - |
| $C_3$ | | - |
| $D$ | *dispersion coefficient* | $0.018 cm^2/h$ |
| $v$ | *fluid velocity* | $0.1 cm/h$ |
| $k_1$ | *species reacion rate* | $0.05 h^{-1}$ |
| $k_2$ | | $0.03 h^{-1}$ |
| $k_3$ | | $0.02 h^{-1}$ |
| $R$ | *retardation coefficient* | 2.0 |

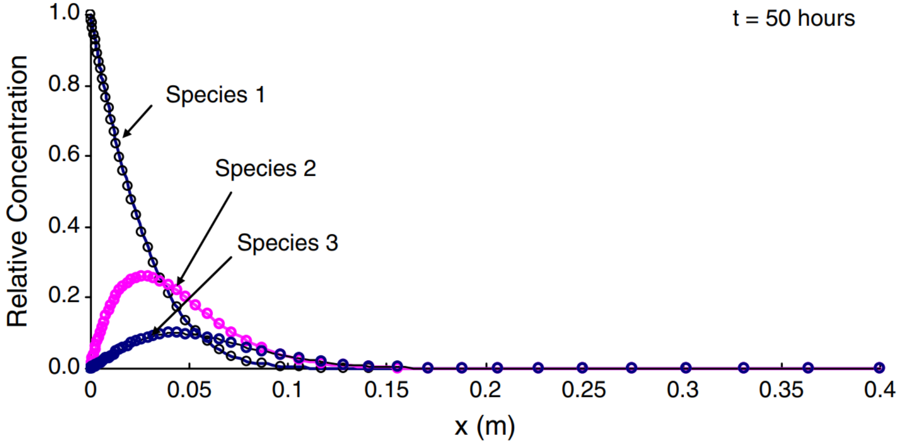



**Fig. 1.** Relative concentration of species at t = 50 h.

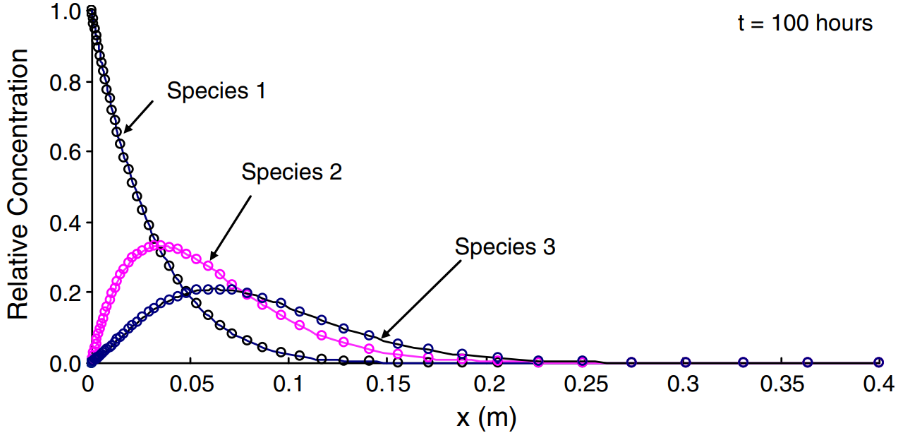



**Fig. 2.** Relative concentration of species at t = 100 h.

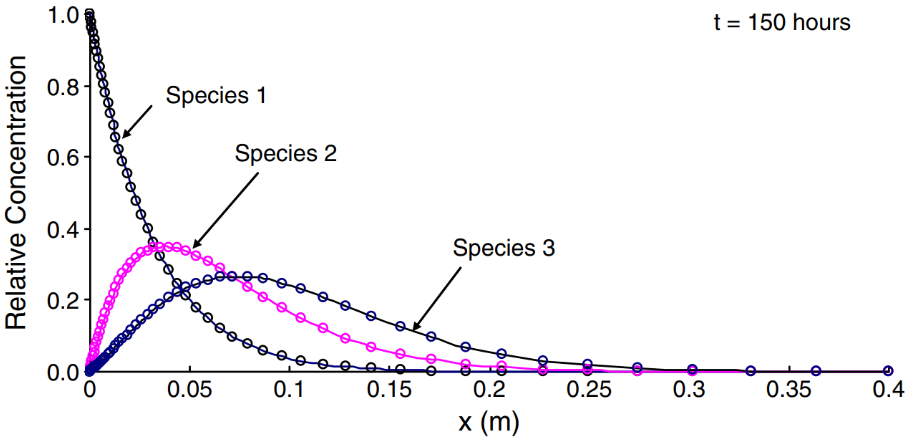



**Fig. 3.** Relative concentration of species at t = 150 h.

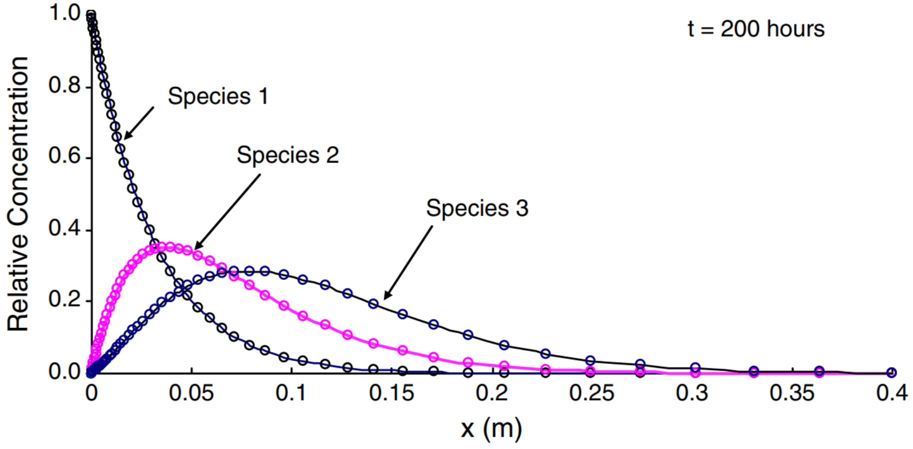



**Fig. 4.** Relative concentration of species at t = 200 h.

- Circles: Numerical results
- Solid line: Analytical results

# Pure Hypothetic Simulation

Suppose injection of $CO_2$ saturated water into a carbonate aquifer.

| Information of aquifer and well | |
|---|---|
| formation | pure calcite ($CaCO_3$) |
| porosity | 0.25 |
| depth | 1500m |
| horizontal far-field stress | $\sigma_{hx} = \sigma_{hy} = 3.2*10^4$kPa |
| vertical stress | $\sigma_v = 2.2*10^4$kPa |
| initial pore pressure | $p_0 = 1.4*10^4$kPa |
| radius of open hole well | $r_w = 0.127$m |
| injection pressure | $p_i = 2.0*10^4$kPa |
| Initial temperature of aquifer | $70^{\circ}$c |
| temperature of water | t =$10^{\circ}$c |

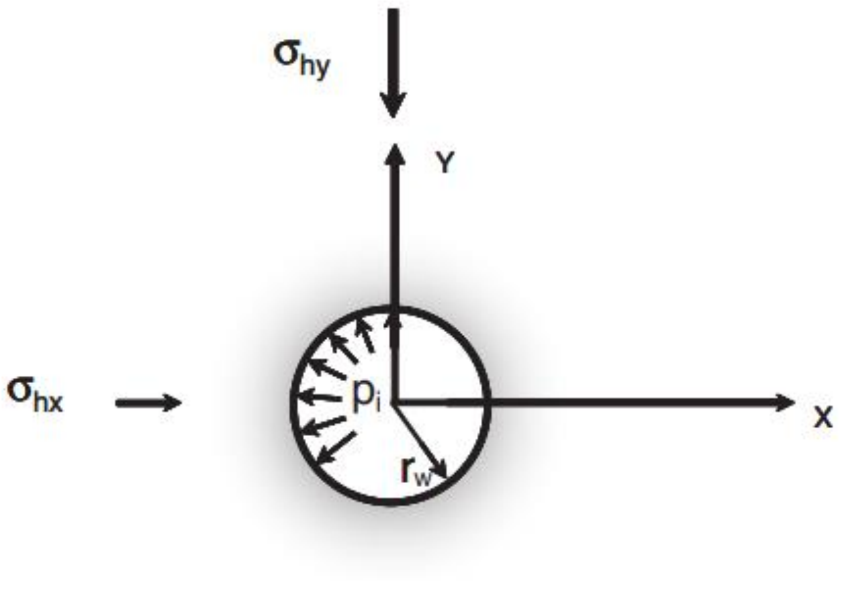



**Fig. 5.** Geometry of the wellbore and far-field stresses.

*Model is restricted to single phase flow and elastic porous media due to the complexity of the problem.

# Chemical reactions

Chemical reactions happen during injection:

$$CO_2 + H_2O \Rightarrow HCO_3^-$$

$$H_2CO_3 \Leftrightarrow H^+ + HCO_3^-$$

Reaction between the acidic solution and the rock mineral during injection:

$$CaCO_3 + H^+ \Leftrightarrow Ca^{2+} + HCO_3^-$$

| Symbol | Meaning | Value |
|---|---|---|
| Initial concentration of $H^+$ | - | $1.0*10^{-4} mol/m^3$ |
| Initial concentration of $Ca^{2+}$ | - | $4.0 mol/m^3$ |
| Initial concentration of $HCO_3^-$ | - | $4.0 mol/m^3$ |
| Chemical equilibrium constant of reaction | - | $1.6*10^5$ |
| Initial temperature of aquifer | - | 70°c |
| $E$ | - | $1.5 * 10^6 kPa$ |
| $v$ | Darcy velocity | *0.30* |
| $K_m$ | bulk moduli (matrix mineral) | $1.4 * 10^6 kPa$ |
| $K_w$ | bulk moduli (water) | $1.0 * 10^6 kPa$ |
| $k$ | permeability of the porous medium | $0.987 * 10^{-16} m^2$ |
| $\mu$ | viscosity | *1 cP* |
| $\rho_s$ | density (solid) | $2.5 * 10^3\ kg/m^3$ |
| $\rho_w$ | density (liquid) | $1.0 * 10^3\ kg/m^3$ |
| $\beta_s$ | volumetric thermal expansion coefficient of the skeleton | $2.0 * 10^{-5} K^{-1}$ |
| $\beta_w$ | volumetric thermal expansion coefficient of the fluid | $2.0 * 10^{-4} K^{-1}$ |
| $c_s$ | specific heat capacity of solid | $0.4 kJ/kg - K$ |
| $c_w$ | specific heat capacity of water | $4.2 kJ/kg - K$ |
| $\lambda_T$ | porous medium thermal conductivity | $\frac{2.65J}{m - s - K}$ |
| $D$ | dispersion coefficient | $1.5 * 10^{-7} m^2/s$ |

# Fully coupled THMC solution - stress

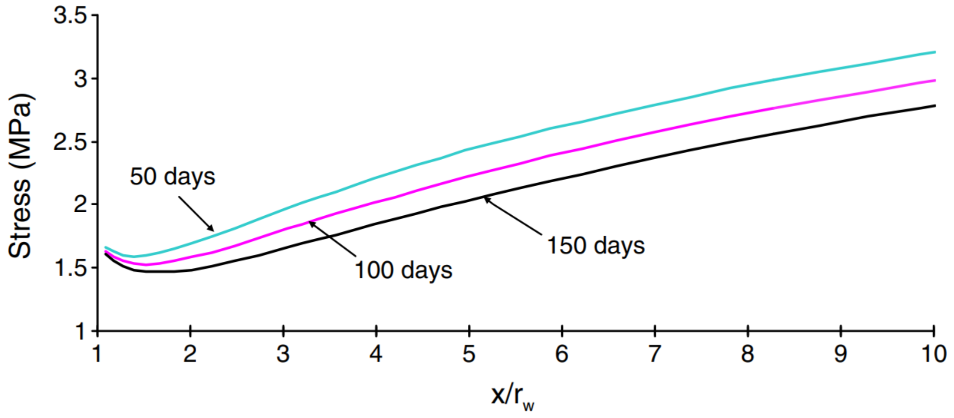



**Fig. 6.** Effective tangential stress profiles at different times.

Effective tangential stress around the wellbore declines over the time under the combined impact of cooling and chemical reaction effects.

Induced hydraulic fracture more likely to take place.

# Fully coupled THMC solution

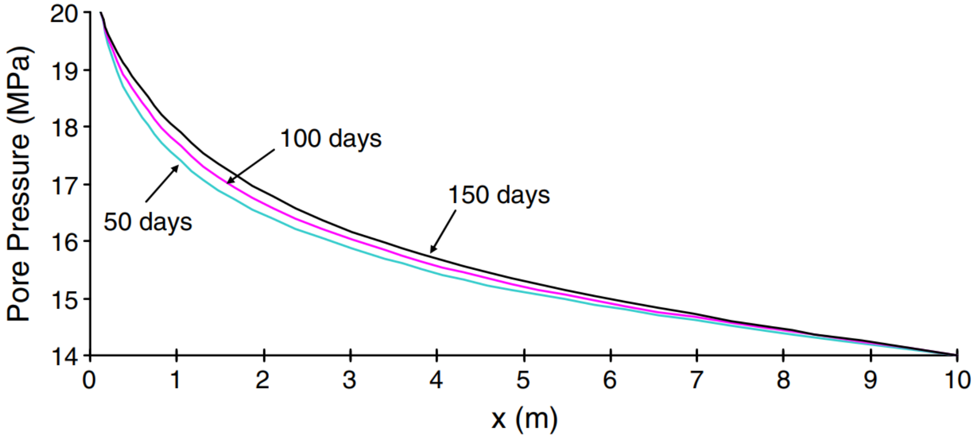



**Fig. 7.** Pore pressure profiles at different times.

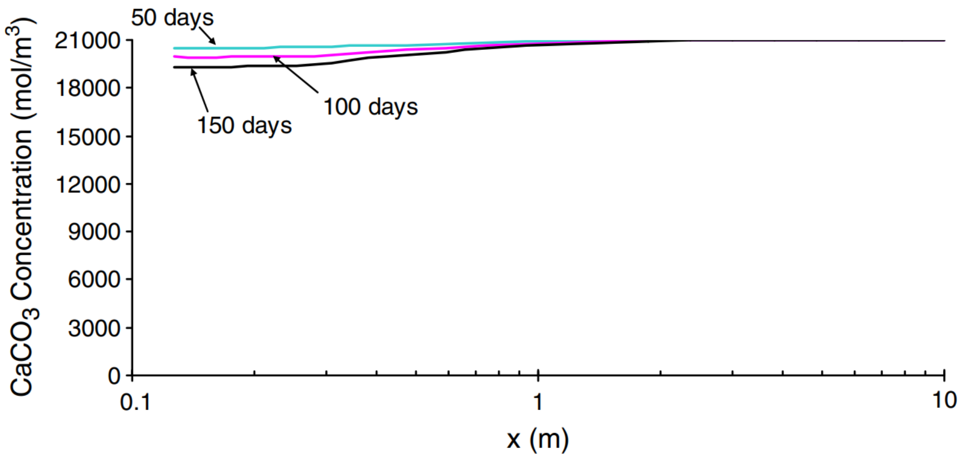



**Fig. 9.** Calcite concentration profiles at different times.

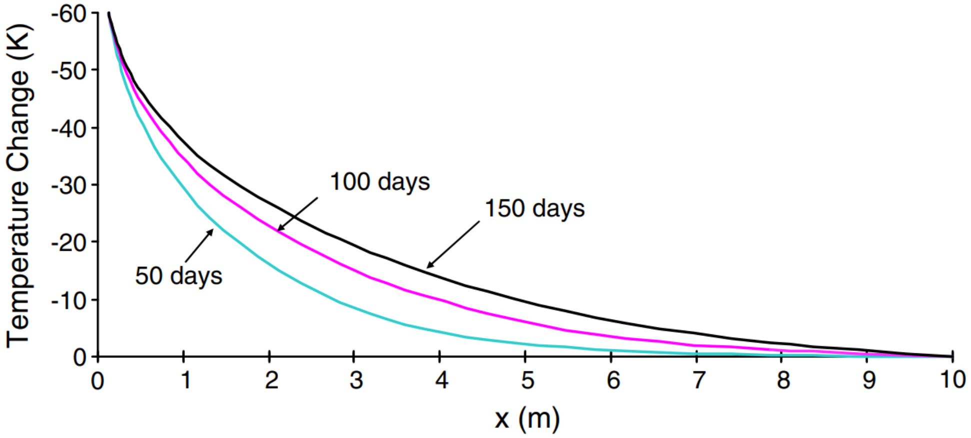



**Fig. 8.** Temperature profiles at different times.

- Both pore pressure and temperature increase with time.
- The concentration of $CaCO_3$ around the wellbore is declining with time

# Fully coupled THMC solution - relationship of porosity and permeability

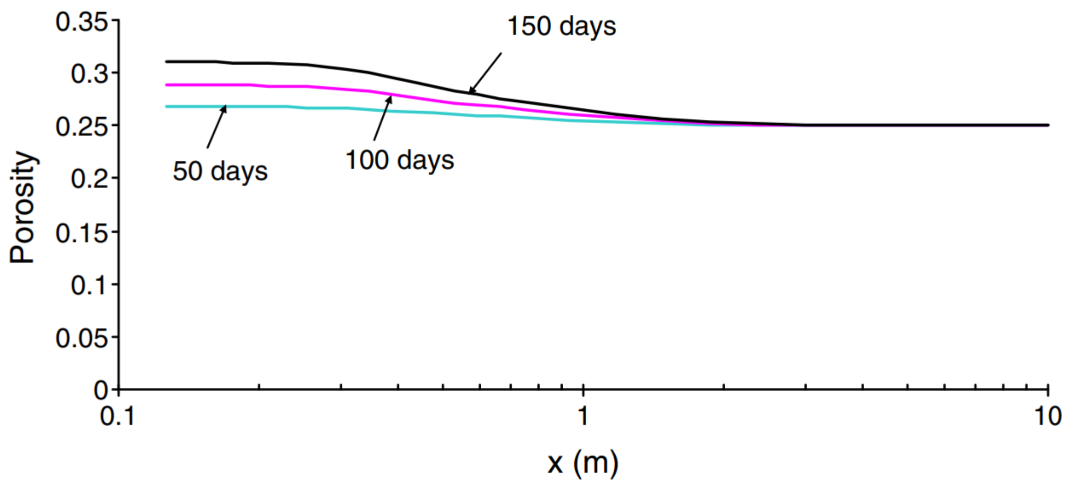



**Fig. 10.** Porosity profiles at different times.

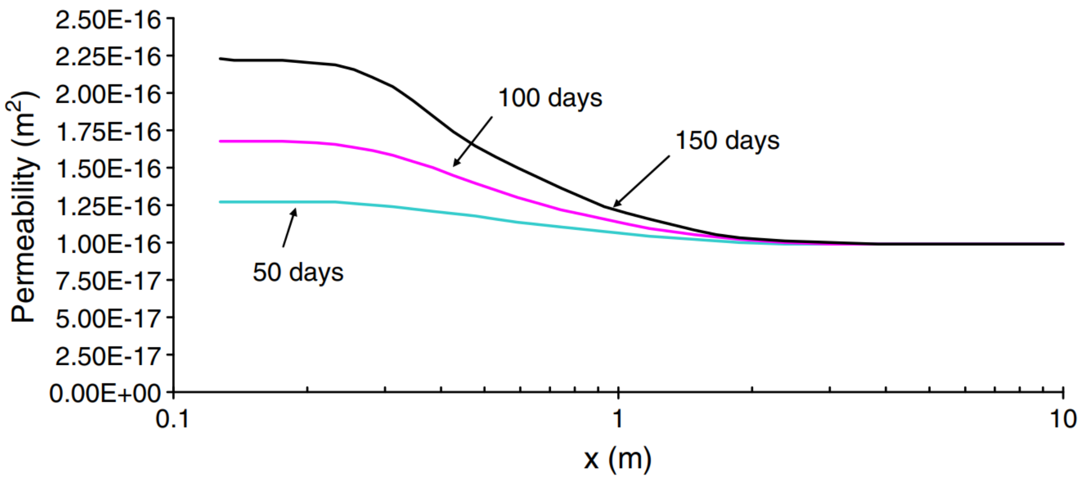



**Fig. 11.** Permeability profiles at different times.

A relatively small increase in porosity can lead to substantial increase of permeability of the formation rock.

# Impact of Chemical Effect

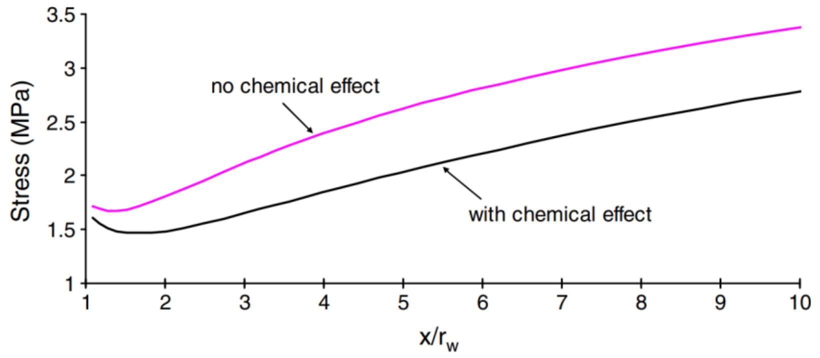



**Fig. 12.** Effective tangential stress profiles with and without chemical effect at 150 days.

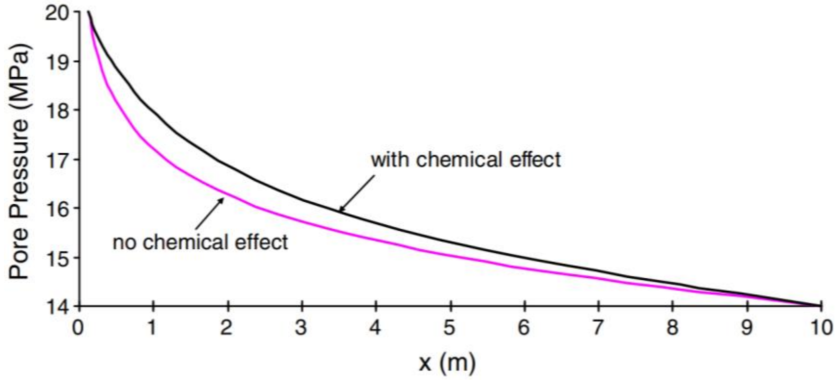



**Fig. 13.** Pore pressure profiles with and without chemical effect at 150 days.

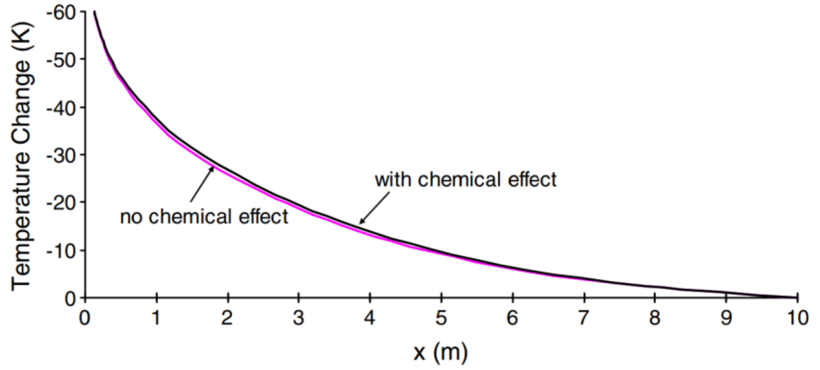



**Fig. 14.** Temperature profiles with and without chemical effect at 150 days.

Mineral dissolution near the wellbore contributes to the reduction of effective shear stress.

No increase in porosity and corresponding increase in permeability caused by mineral dissolution.

→ Pressure permeability process become slower.

→ Darcy velocity is lower. → Temperature changes are smaller.

# Impact of Thermal Effect

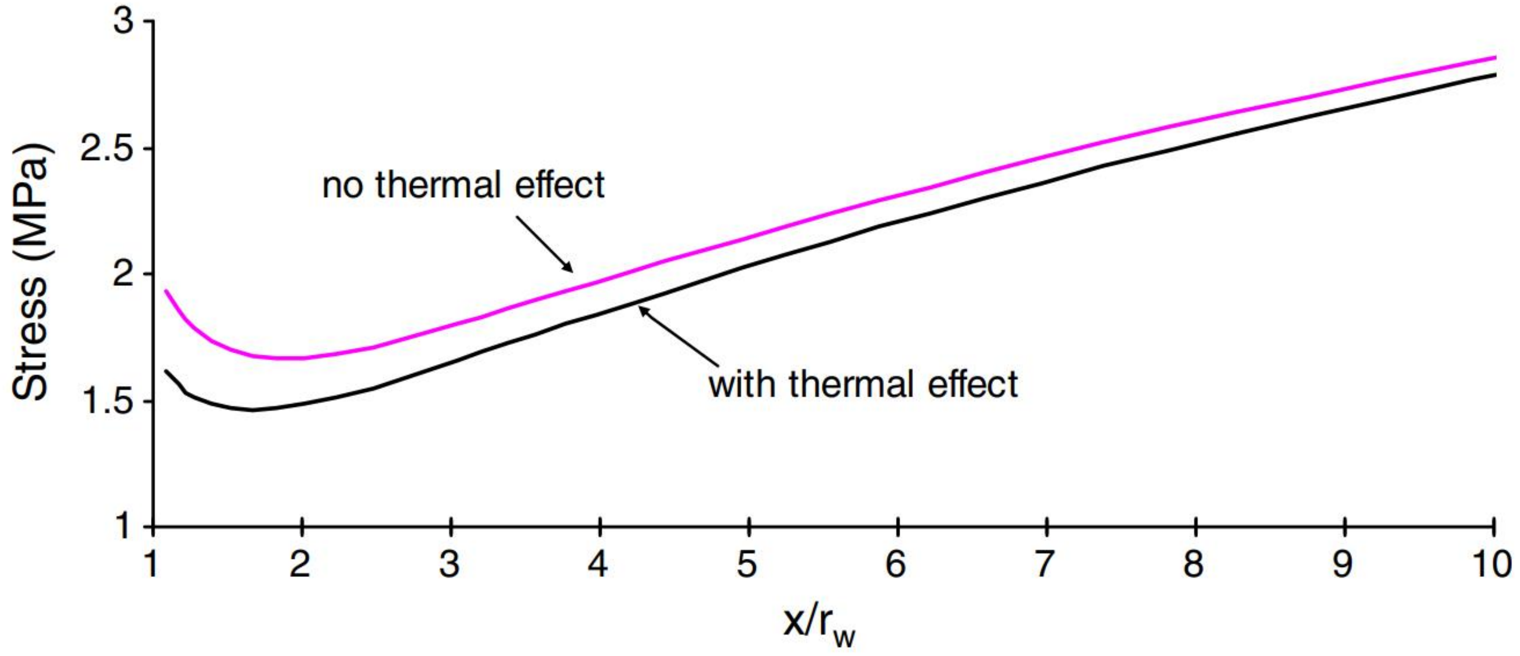



**Fig. 15.** Effective tangential stress profiles with and without thermal effect at 150 days.

Cooling effects (shrinkage) render the stress state around the wellbore more favorable for hydraulic fracturing, which will enhance well injectivity.

# Impact of the Stabilized FEM Scheme

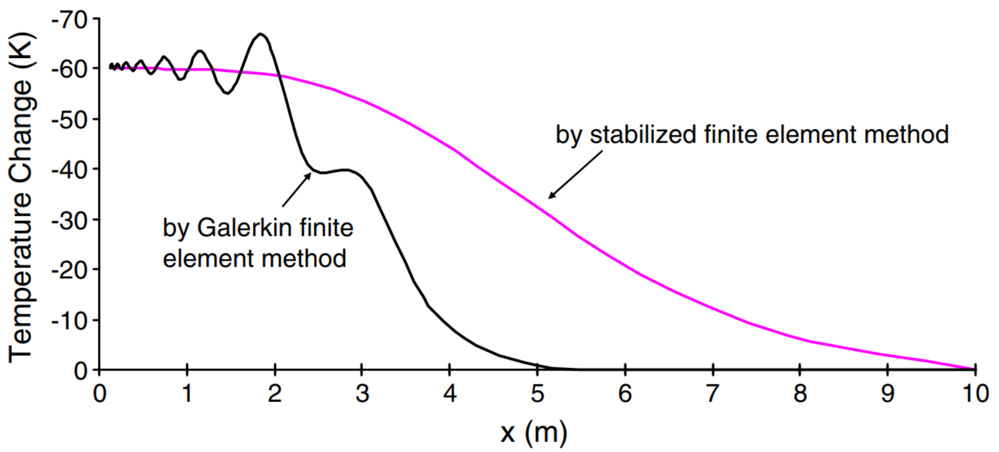



**Fig. 16.** Temperature change profiles generated by Galerkin FEM and stabilized FEM.

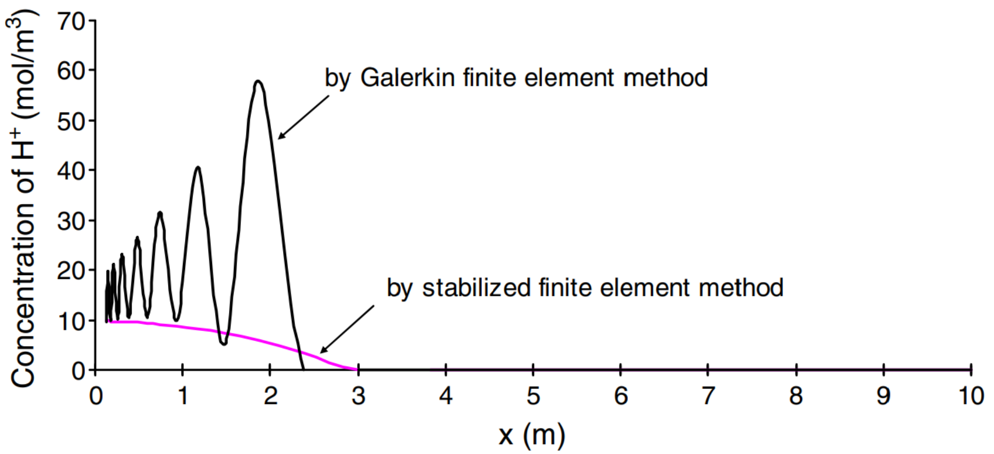



**Fig. 17.** $H^+$ concentration profiles generated by Galerkin FEM and stabilized FEM.

The stabilized finite element model reduces the numerical oscillations in transient advection-diffusion problems.

# Conclusions

- Thermal and chemical effects have a significant impact on stress and pressure change around the injection area.

Thank you for your attention.