Physical Processes and Modeling Studies of CO_2 Storage in Subsurface Formations

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MINES | Carbon Capture, Utilization and Storage

Outline

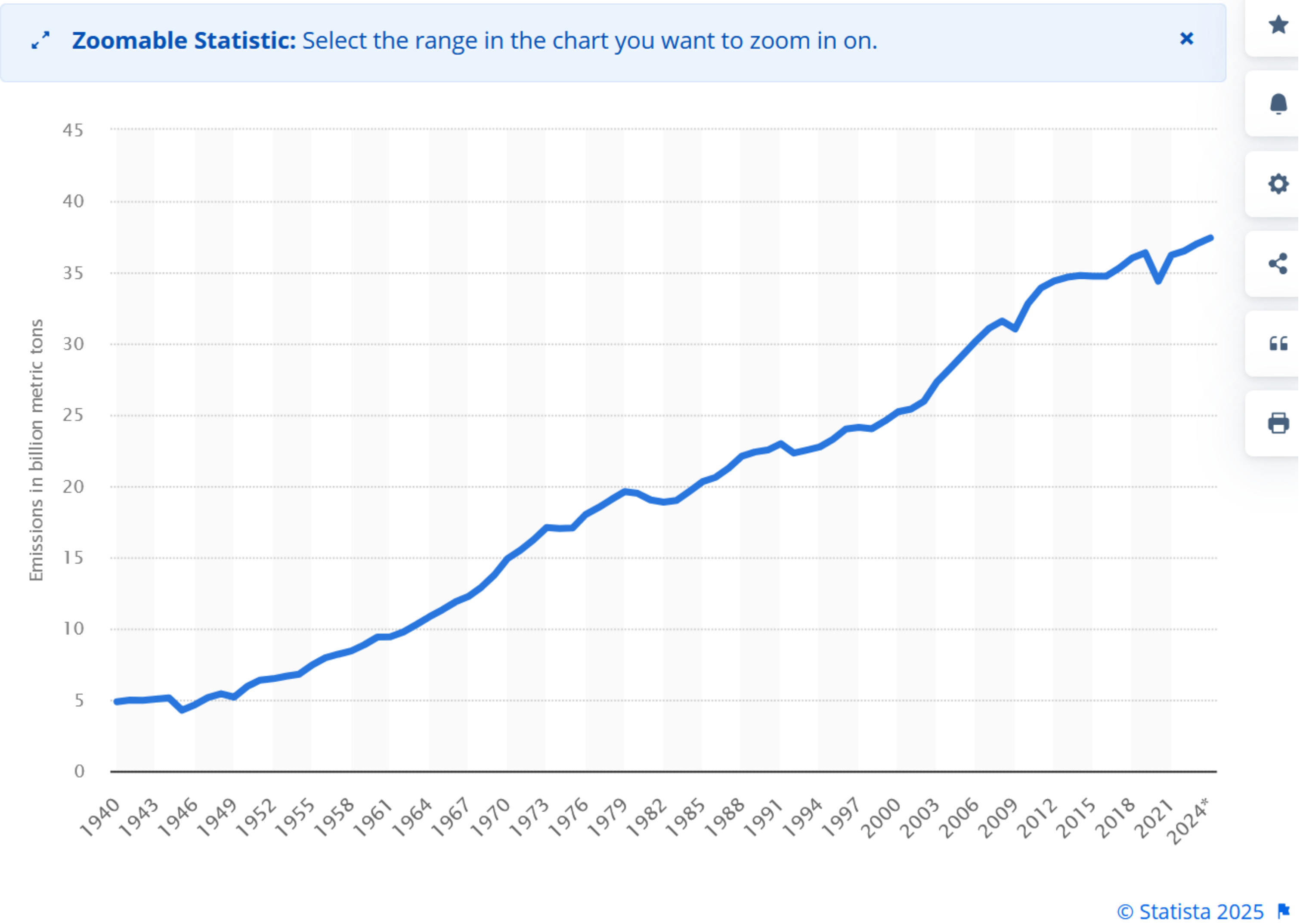
- Introduction
- Coupled multi-physical processes of CO_2 flow, transport and storage
- Modeling approaches for coupled processes
- Modeling example: CO_2 sequestration in depleted gas reservoirs
- Summary

CCUS Related Publications at EMG

1. Zhou et al. "Review of Carbon dioxide utilization and sequestration in depleted oil reservoirs," ***Renewable and Sustainable Energy Reviews***, Vol. 202, 2024, 44 PGs
2. Zhao et al. "Fully coupled THM modeling of CO2 sequestration in depleted gas reservoirs considering the mutual solubilities in CO2-Hydrocarbon gas-brine systems," ***Geoenergy Science and Engineering,*** Vol. 238, pp. 2024.
3. Zhou et al. "Experimental study on dual benefits of improvement of CO2 enhanced oil recovery and its storage capacity for depleted carbonate oil reservoirs, ***Advances in Geo-Energy Research***, 2024
4. Wang et al. "Understanding the Multiphysical Processes in CO2-EOR Operations: A Numerical Study Using a General Simulation Framework," ***SPE Journal***, 2020
5. Zhang et al. "Hydrologic, Mechanical, Thermal, and Chemical Process Coupling Triggered by the Injection of CO2." In ***Science of Carbon Storage in Deep Saline Formations***, 2019.
6. Zhang et al. "Coupled geomechanical and reactive geochemical model for fluid, heat flow and convective mixing: application for CO2 geological sequestration into saline aquifer with heterogeneity," ***International Journal of Global Warming***, 2017
7. Zhang et al. "A fully coupled thermal-hydrological-mechanical-chemical model for CO2 geological sequestration," ***J. Natural Gas Sci. & Eng.***, 2016
8. Winterfeld et al. "Simulation of Coupled Thermal/Hydrological/Mechanical Phenomena in Porous Media," ***SPE Journal***, 2016
9. Zhang et al. "Sequentially coupled THMC model for CO2 geological sequestration into a 2D heterogeneous saline aquifer," ***J. Natural Gas Sci. & Eng.***, 2015
10. Huang et al. "Parallel simulation of fully-coupled thermal-hydro-mechanical processes in CO2 leakage through fluid-driven fracture zones," ***International Journal of Greenhouse Gas Control***, 2015

Introduction:

Total energy-related CO_2 emissions increased by 0.8% in 2024, hitting an all-time high of 37.8 Gt CO_2. The atmospheric CO_2 concentrations, **422.5 ppm, in 2024**, and 50% higher than pre-industrial levels.



Background

CO_2 geosequestration is one of the few options for addressing the issue of CO_2 atmosphere emissions and resulted climate change due to fossil energy consumption:

(a) Developed oil and gas reservoirs

(b) Unmineable coal seams/coalbed methane

(c) Deep saline aquifers

CO2 Storage Capacity in North America (NETL)

Atlas V CO_2 Storage Resource Estimates			
	Low	Medium	High
Oil and Natural Gas Reservoirs	186	205	232
Unmineable Coal	54	80	113
Saline Formations	2,379	8,328	21,633
Total	**2,618**	**8,613**	**21,978**

**Data current as of November 2014. Estimates in billion metric tons.*

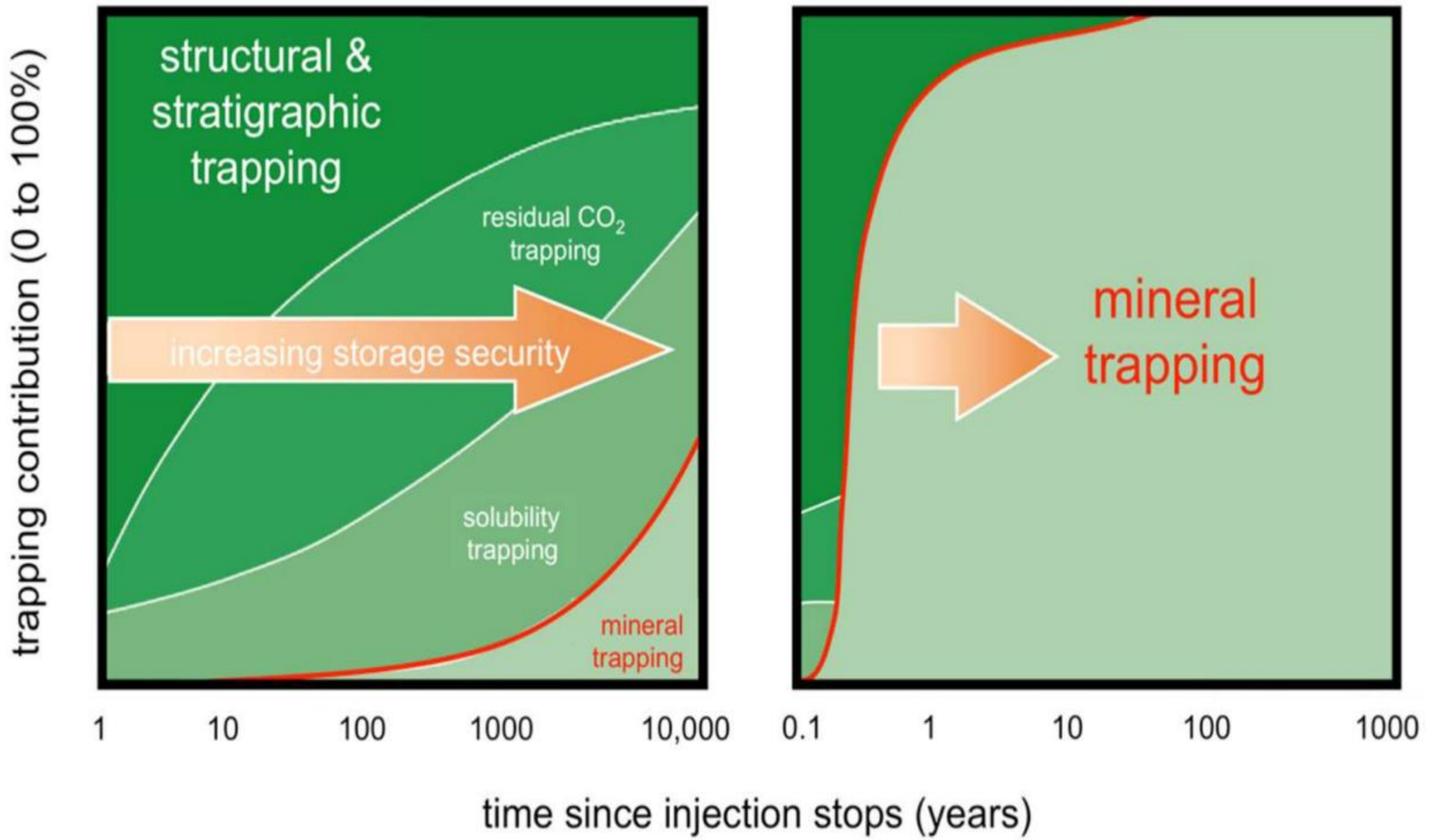


FIGURE 3 | Evolution of the extent of CO_2 trapping mechanisms with time. The extent of each trapping mechanism is highly site specific and depends on several parameters including the type of rock: carbonatitic and siliciclastic rocks (left panel), or mafic and ultramafic rocks that have the ability to react much faster with CO_2 to form carbonates (right panel) [from (National Academies of Sciences Engineering Medicine, 2019), Figure 6.7 and (Kelemen et al., under review), Figure 8, modified from (Benson et al., 2005); also see Figure 9 in (Snæbjörnsdóttir et al., 2017)].

TOUGH2-CSM: Incorporating CO2 Sequestration/Trapping Mechanisms

- Structural and Stratigraphic Trapping - as a separate phase trapped by impermeable rock
- Residual Trapping - CO2 plumes immobilized by capillary forces
- Solubility Trapping - dissolution of CO2 in the saline aqueous, and oil/gas phases
- Mineral Trapping - reaction of CO2 with minerals present in aquifer rock
- Minors: e.g., adsorption on rocks

All these are impacted by pressure, temperature, stress (THM), and chemical reaction (THMC)

Incorporate Flow and Transport Mechanisms:

- Advection of multiphase flow driven by pressure difference and gravity or buoyancy forces as well as regional water movement
- Molecular diffusion and mechanical dispersion
- ……

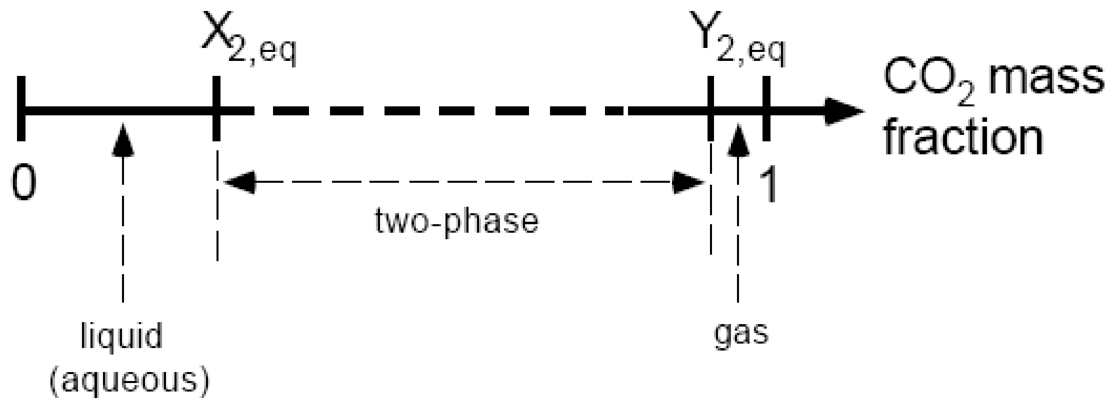
TOUGH2-CSM: Technical Approaches

- Based on TOUGH2-MP/ECO2N – most used CO2 sequestration simulator in the world!
- Numerical method: Integrated finite difference method
- H_2O-NaCl-CO_2 properties from ECO2N module
- ECO2M – new three-phase flow module
- CO_2 flow, transport and storage in saline aquifers
- Geomechanical processes occurring during CO_2 injection and storage
- Coupling geochemical reactions
- Parallel simulation
- General fracture conceptual model

Modeling Approach of TOUGH2-CSM for Saline Aquifers

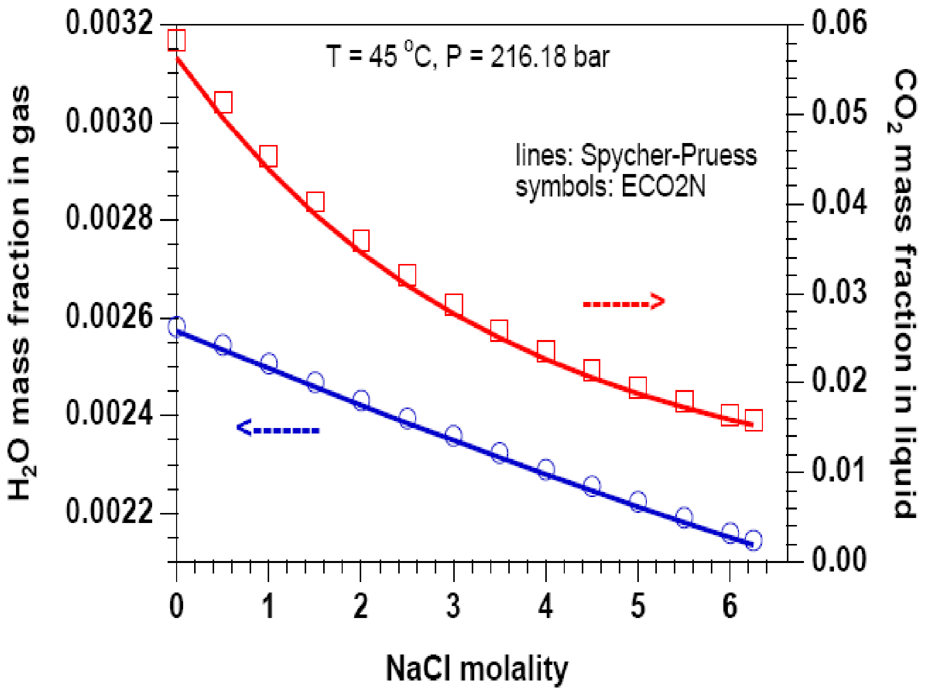
– Multiphase, Non-isothermal Compositional Modeling Approach

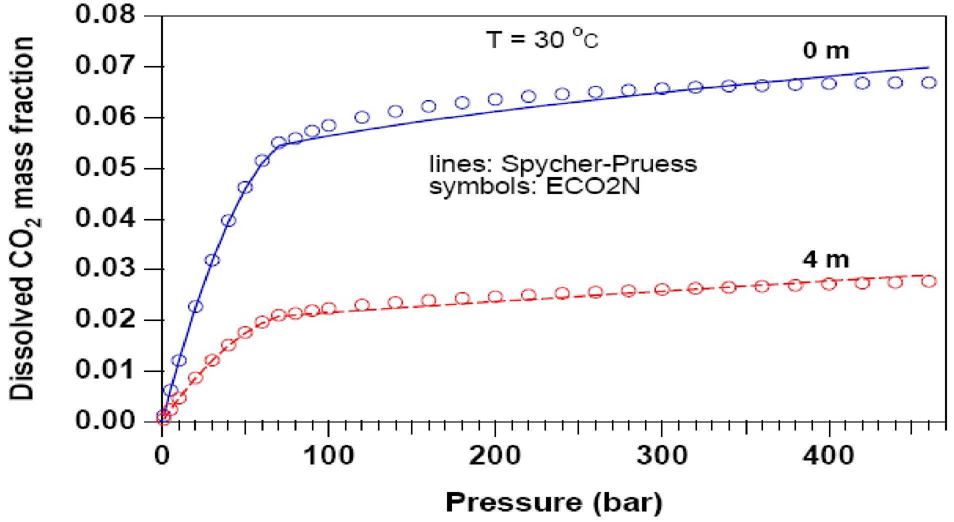
- Three components: Water, CO_2, and Salt as well as heat.
- Two phases: water-rich aqueous phase and CO_2-rich gas phase.

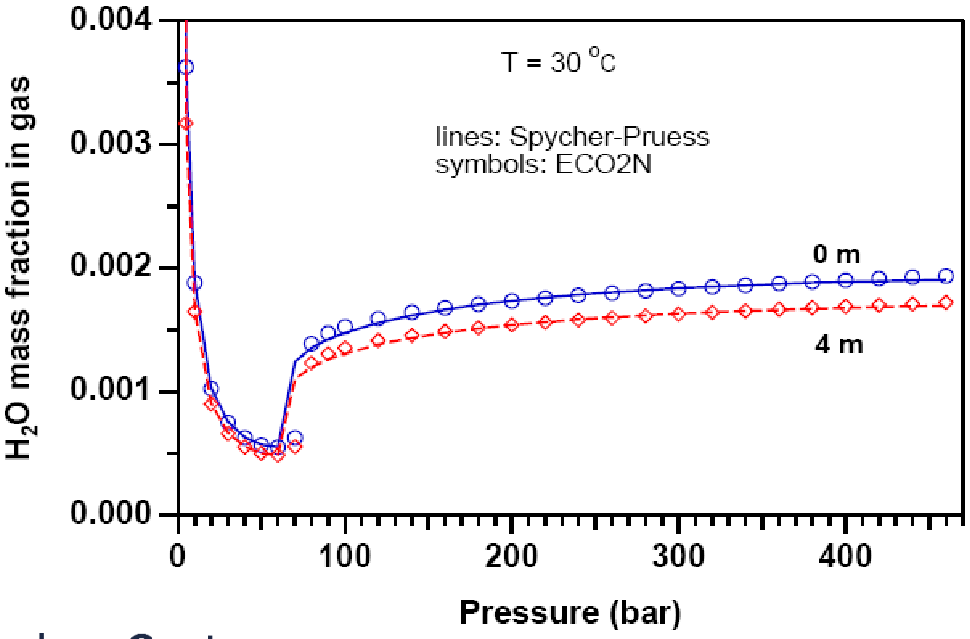


Modeling Approach-Continued

- The partitioning of H_2O and CO_2 between liquid and gas phases is modeled as a function of temperature, pressure, and salinity.







General Framework Model (THM)

Mass Balance

for Component κ

$$M^\kappa = \sum_\beta \phi S_\beta \rho_\beta X_\beta^\kappa + R^\kappa$$

$$G^k = \lambda_k \left(\phi \sum_\beta \left(\rho_\beta S_\beta X_\beta^k \right) + R_\beta^k \right)$$

$$F^k = -\sum_\beta \nabla \bullet \left(\rho_\beta X_\beta^k \mathbf{v}_\beta \right) + \sum_\beta \nabla \bullet \left(\underline{D}_\beta^k \bullet \nabla \left(\rho_\beta X_\beta^k \right) \right)$$

Energy Balance

$$M^h = (1-\phi)\rho_R C_R T + \phi \sum_\beta S_\beta \rho_\beta u_\beta$$

$$F^h = -\left[(1-\phi) K_R + \phi \sum_\beta S_\beta K_\beta \right] \nabla T + \sum_\beta h_\beta F_\beta$$

Stress Equilibrium

$$M = 0$$

$$F_j = \left[\Delta\sigma_{1j} \quad \Delta\sigma_{2j} \quad \Delta\sigma_{3j} \right]^T$$

$$\Delta\sigma_{ij} = 2G\varepsilon_{ij} + \delta_{ij}\lambda\varepsilon_v + 3\delta_{ij}\beta K \Delta T + \delta_{ij}\alpha\Delta P$$

$$\frac{d}{dt}\int_{V_n} \mathbf{M}^\kappa dV_n = \int_{\Gamma_n} \mathbf{F}^\kappa \bullet \mathbf{n} d\Gamma_n + \int_{V_n} G^\kappa dV_n + \int_{V_n} q^\kappa dV_n$$

TOUGH2-CSM and MSFLOW-CO2:
for CO2 EOR and geosequestration in depleted oil/gas reservoirs)

Fluid/Heat Governing Equation:

$$\frac{\mathrm{d}\boldsymbol{M}^{\kappa}}{\mathrm{d}\boldsymbol{t}} = \nabla \cdot \boldsymbol{F} + \boldsymbol{q}^{\kappa}$$

Mass Balance Equation

$$\mathbf{F}^{k} = \sum_{\beta} \mathbf{F}_{\beta} x_{\beta}^{k} - m_k D_k \nabla y_k, \quad \beta = L, G, A, \quad k = 1,..,N_C$$

$$\boldsymbol{F}_{\boldsymbol{\beta}} = -K_a \frac{K_{r\beta}\rho_{\beta}}{\mu_{\beta}} (\nabla P + \nabla P_{c,\beta} - \rho_{\beta}\mathbf{g})$$

$$M^k = \phi S_L \rho_L L^k + \phi S_G \rho_G G^k, \ldots\ldots k = 2, \ldots, nc + 1$$

Energy Balance Equation

$$\mathbf{F}^{N+1} = -k_t \nabla T + \sum_{l} h_l \mathbf{F}_l$$

$$M^k = (1-\phi) C_r \rho_r T + \phi \sum_{l} S_l \rho_l U_l$$

Mechanical governing equation:

$$\sigma_{kk} - \left[\alpha P + 3\beta_T K_B \left(T - T_{ref}\right)\right] = \lambda_L \varepsilon_v + 2G\varepsilon_{kk}, \quad k = x, y, z$$

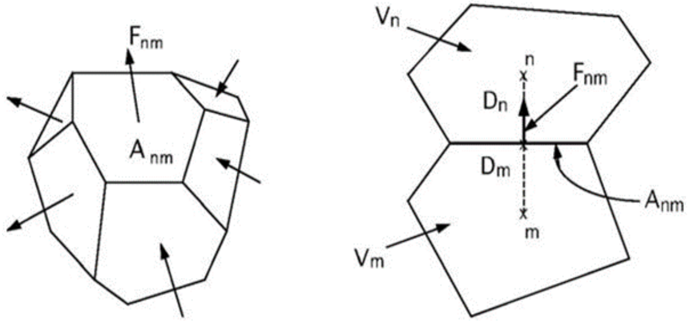
$$\nabla \cdot \left[\nabla(\alpha P + 3\beta K T) + \frac{\lambda + 2G}{K} \nabla(\sigma_{mean} - \alpha P - 3\beta K \Delta T) + \overline{F}_b\right] = 0$$

Winterfeld, P. H., & Wu, Y. S. (2016), "Simulation of coupled thermal/hydrological/mechanical phenomena in porous media," *SPE Journal*.

Zhao et al. (2024) "Fully coupled THM modeling of CO2 sequestration in depleted gas reservoirs considering the mutual solubilities in CO2-Hydrocarbon gas-brine systems," *Geoenergy Science and Engineering.*

Numerical Discretization and Formulation: TOUGH2-CSM and MSFLOW_CO2

Integrated Finite Difference Method (TOUGH2 Methodology!)



General formulation: $$\frac{\partial M^k}{\partial t} = \nabla \cdot \overline{F}^k + q^k$$

Integral form: $$\frac{\partial}{\partial t}\int_{V_n} M^k dV = \int_{\Gamma_n} \overline{F}^k \cdot n d\Gamma + \int_{V_n} q^k dV$$

Discretization: $$\left[M_n^k\right]^{l+1} - \left[M_n^k\right]^{l} - \frac{\Delta t}{V_n}\left[\sum_m A_{nm}F_{nm}^k + V_n q_n^k\right] = 0$$

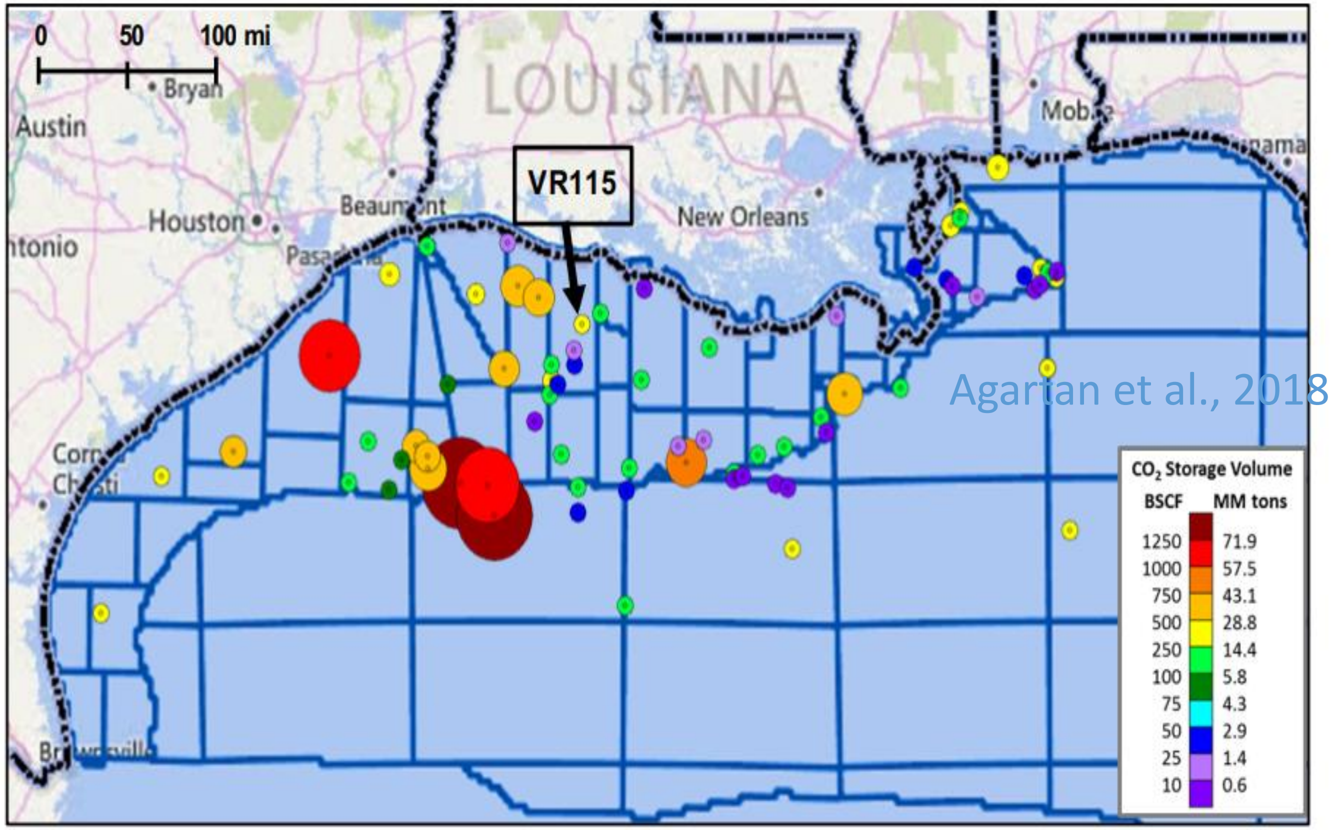
Newton's method (gradient based searching)

$$\mathbf{J_f}(\mathbf{x}) = \frac{d}{d\mathbf{x}}\mathbf{f}(\mathbf{x}) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_N}{\partial x_1} & \cdots & \frac{\partial f_N}{\partial x_N} \end{bmatrix}$$

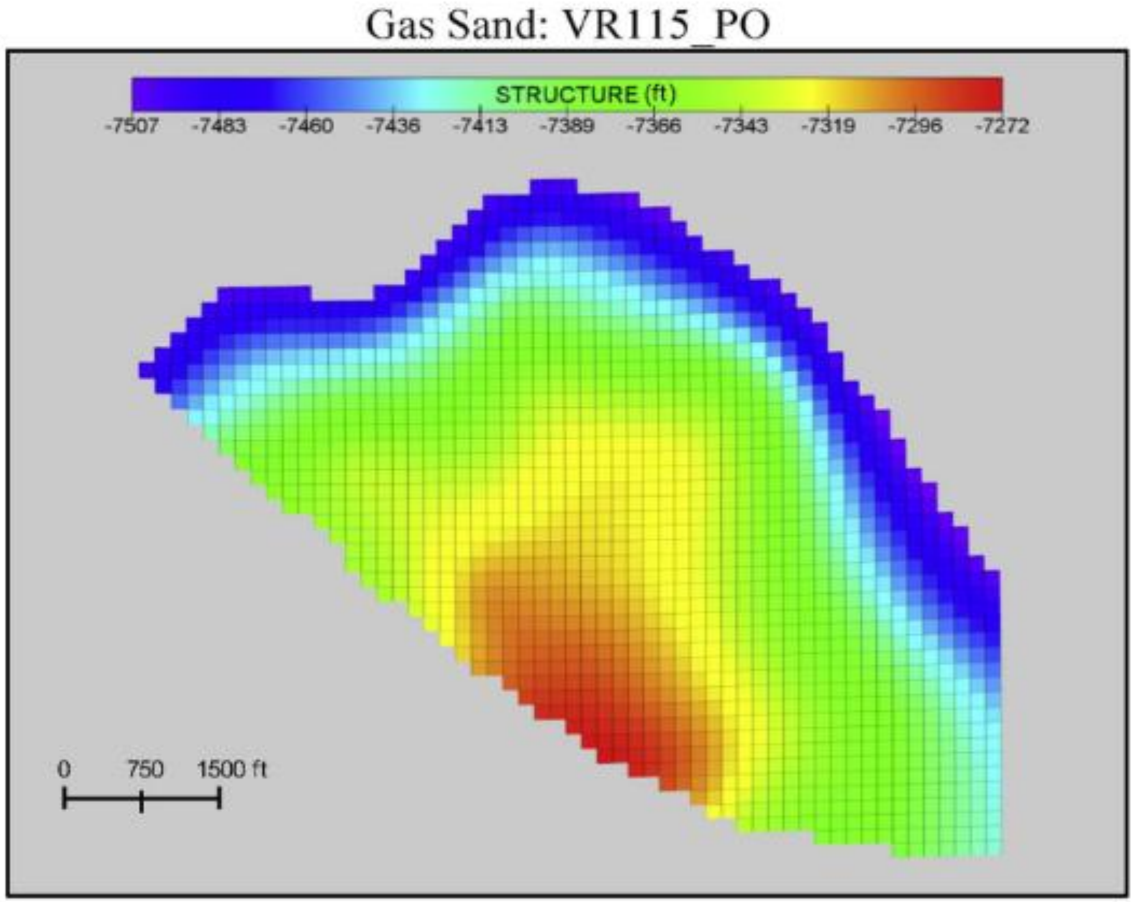
$$\delta \mathbf{x} = \mathbf{J}(\mathbf{x})^{-1}[\mathbf{f}(\mathbf{x} + \delta \mathbf{x}) - \mathbf{f}(\mathbf{x})] = -\mathbf{J}(\mathbf{x})^{-1}\mathbf{f}(\mathbf{x})$$

Modeling CO_2 sequestration in depleted gas reservoirs – Simulation Example

Modeling CO_2 Storage in VR115_PO gas sand

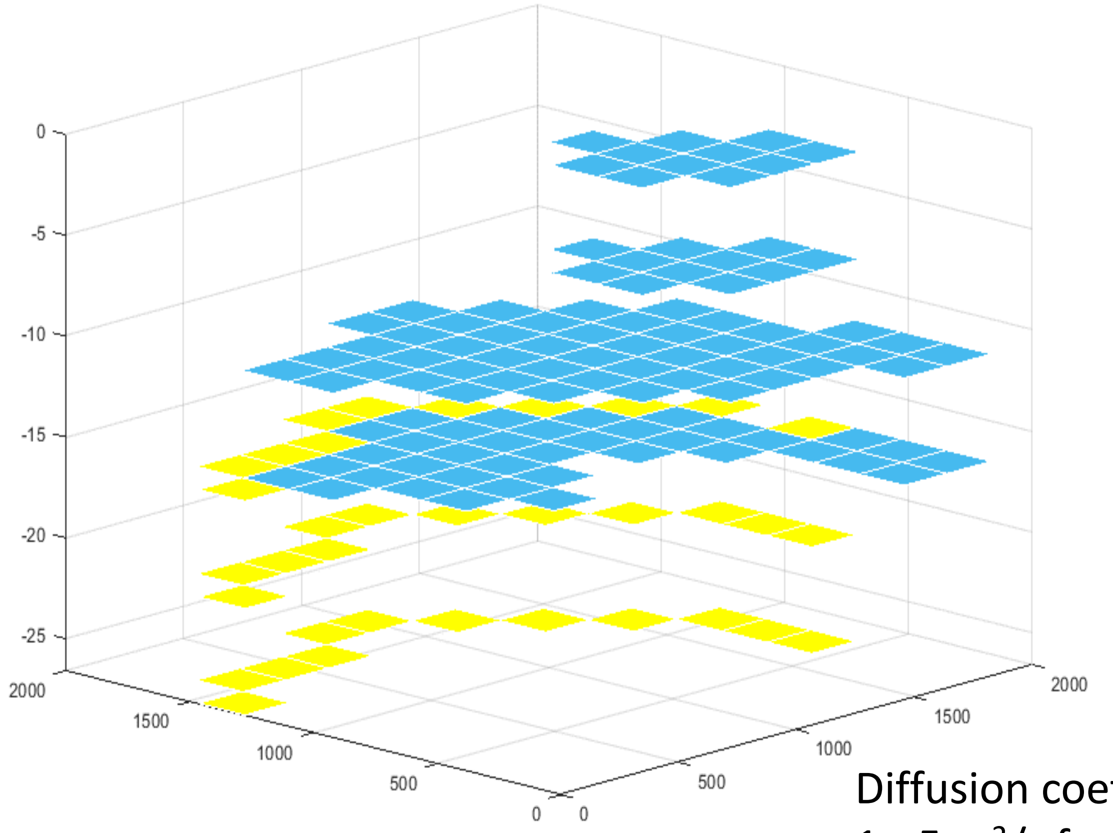


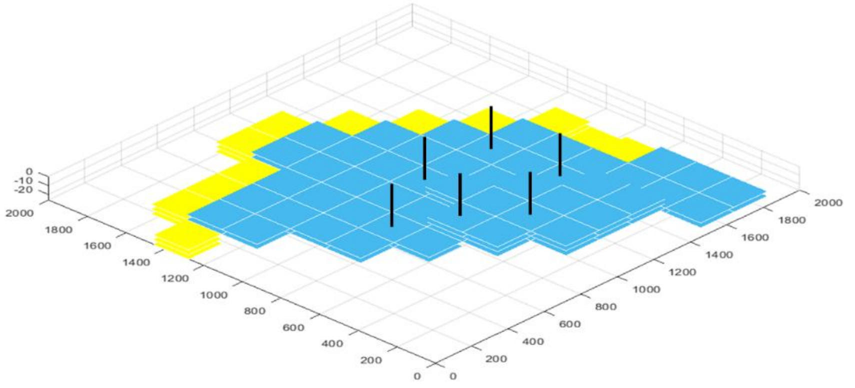
Agartan et al., 2018



Result and Discussion

❑ CO_2 Storage in VR115_PO gas sand





Parameters	Value
Original gas in place (OGIP) (m^3)	1.1015E+09
Cumulative gas production (m^3)	4.9554E+08
Cumulative water production (m^3)	5.6634E+06
Subsea depth (m)	2225
Gas zone average depth (m)	11.9
Total area (m^2)	1.6E+06
Porosity (frac.)	0.31
Residual water saturation (frac.)	0.16
Permeability (m^2)	1.23E-12
Initial Pressure (bar)	252
Initial Temperature (℃)	74
Total completions in the reservoir	6
Initial gas formation volume factor	0.044

Diffusion coefficient:
1e-5 m^2/s for gas
1e-10 m^2/s for aqueous

Result and Discussion

❑ CO_2 Storage in VR115_PO gas sand

- Aquifer size: 4.623×10^7 m^3, 8 times the reservoir size.
- The output of this matching was used as the input for the base case.

Depletion pressure: 146 bar

Base case

- 1.6 billion tonnes stored
- Noticed $CO_{2,aq}$ is much less than the equilibrium solubility. Aquifer still has great potential.

Injection strategy

Scenario 1: Cyclic injection.

Scenario 2: Reducing injection rate.

Same pressure limit

Scenario	CO_2 injection (billion tonnes)
Base case	1.6651
Scenario 1	1.6684
Scenario 2	1.6698

Result and Discussion

❑ CO_2 Storage in VR115_PO gas sand

- Deepen the injection:

Scenario 3: Deepen the injection by a layer.

Scenario 4: Directly inject into the aquifer.

Scenario 3: No much improvement.

Scenario 4: Improvement is significant. Injecting the same amount, the reservoir pressure is 20 bar lower than the pressure limit

Scenario 5: On the basis of Scenario 4, increase the injection rate to reach the pressure limit

Scenario	Final reservoir pressure (bar)	CO_2 stored in the aquifer (billion tonnes)	Overall CO_2 storage (billion tonnes)
Base case	252.13	0.03779	1.6651
Scenario 3	252.01	0.03953	1.6651
Scenario 4	232.37	1.59045	1.6651
Scenario 5	252.06	1.78452	1.9343

Summary

- CO_2 geosequestration (CCS, CCUS) is one of the few promising, viable technologies, but has not been implemented on industry scale.
- The best option for carbon management or near-term implementation in next decades (~50 years): - EOR/EGR and storage in developed gas/oil reservoir formations.
- New modeling tools, reservoir simulators, coupling multi-physics, for modeling CO_2 sequestration in depleted oil/gas reservoir have been developed in EMG.
- Reservoir simulation studies will play a critical role for field application of CO_2 sequestration, because of large spatial and time scale.
- We are looking for collaboration in the area of modeling, laboratory and field studies of CCUS.

Acknowledgements: Dr. Phil Winterfeld, Xinrui Zhao, Shihao Wang, Ronglei Zhang, and Cong Wang

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Halliburton Service

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