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Temperature Dependent Phase Behavior and Geomechanical Effects during Injection of Liquid and Supercritical CO2:

A Field-Scale Coupled Flow-Geomechanics-Geochemistry Simulator

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Background: Cold CO2 Injection and Challenges

Global Importance:

- Achieving net-zero emissions requires sub-surface CO2 sequestration. This means that CO2 injectivity, injection induced fracturing, thermal effects and phase behavior are important to understand, quantify and model.

Motivation:

- Lower compression costs achieved by injecting CO_2 at colder temperatures **(Samaroo et al., 2024)**.
- Enhance operational efficiency and reservoir performance.

Challenges:

- Thermal stresses from cooling raise the potential risk of fractures or caprock failure **(Vilarrasa, 2014)**.
- Long-term impacts on caprock sealing remain uncertain.

Knowledge Gaps:

- This study evaluates reservoir performance under varying injection conditions considering thermal impacts of cold injection.

4 Key Modeling Challenges for CO2 Injection

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1. EOS Compositional Model is Essential:

- CO_2 injection simulations must account for **multi-phase** and **multi-component** flow and transport.

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2. Thermal Model is Required:

- **Significant temperature variations** occur in convection-dominant scenarios.
- Fluid properties (CO_2 and water) are highly **sensitive to temperature changes**.

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3. Geomechanics and Fracture Propagation Must be Coupled:

- **Poro-elastic stress** must be considered to prevent reservoir sealing risks.
- **Thermal-induced stress** can arise from temperature differences between the reservoir and injected fluid.

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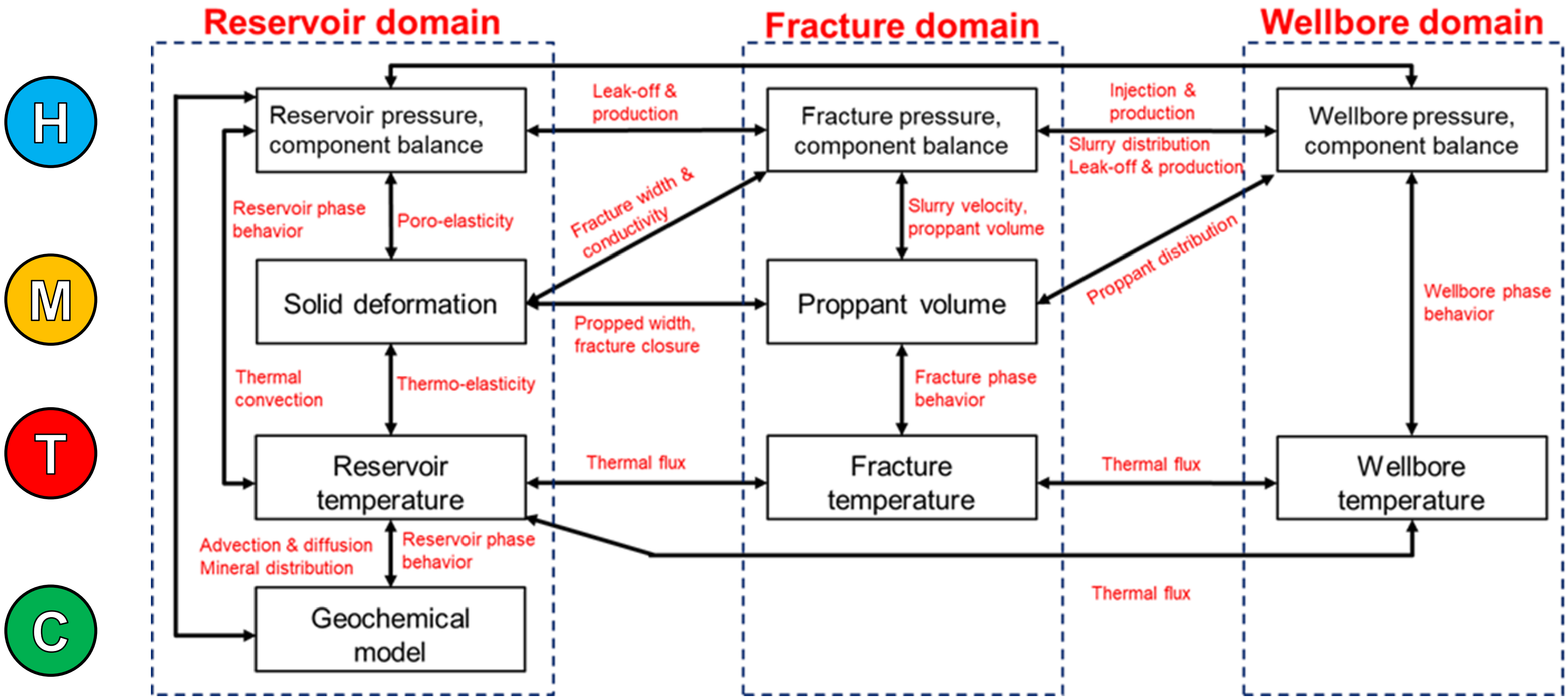
4. Geochemistry Plays an Important Role

- CO2 dissolves into the formation water, **increasing the acidity**.
- **Acidized formation water** can react with host rock, altering mineral composition, flow and geomechanical properties.

Numerical Approach of Multifrac-3D-GC

An advanced 3-D reservoir simulator fully integrating multiphase flow, geomechanics, and geochemistry.



(Mura & Sharma, 2024)

Incorporation of thermally induced fracture growth into MF3D

Energy balance for Black Oil Model including a propagating fracture, wellbore and reservoir, currently in the model:

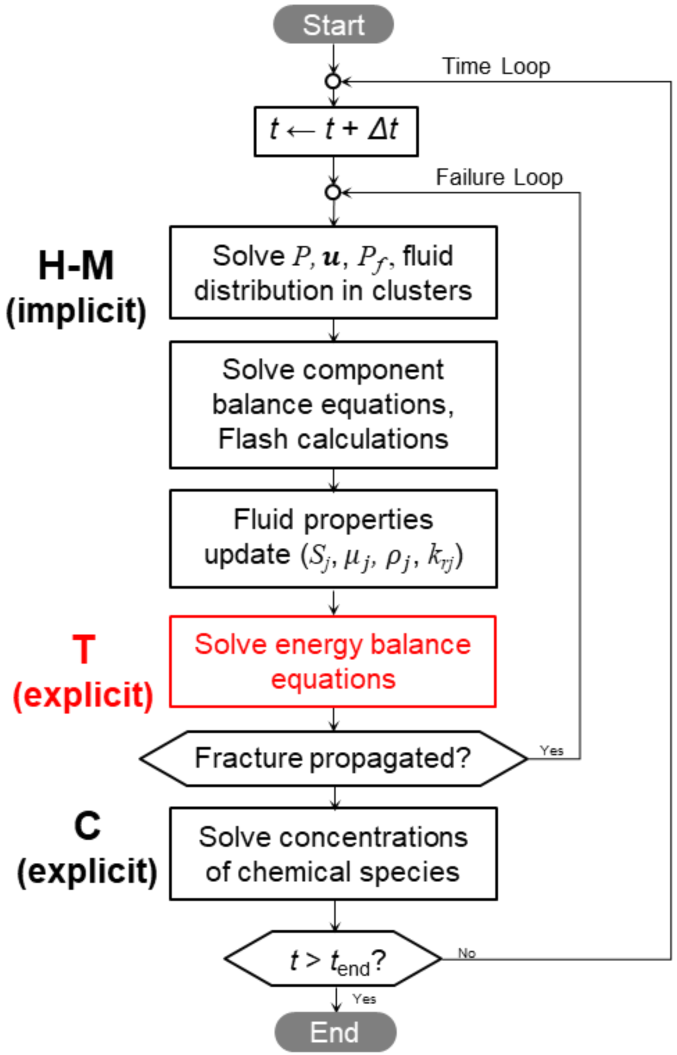
$$\rho_B C_{pB} \frac{\partial T}{\partial t} - \nabla \cdot (k_B \nabla T) + \sum_{j=1}^{n_p} \rho_j C_{pj} u_j \nabla T = \sum_{j=1}^{n_p} \frac{1}{V_b} \rho_j q_j C_{pj} (T - T_0)$$

I have incorporated an EOS-based energy balance:

$$\frac{\partial}{\partial t}\left[(1-\phi)H_r + \phi \sum_{j=1}^{n_p} H_j S_j\right] - \nabla \cdot \left[(1-\phi)k_r + \phi \sum_{j=1}^{n_p} k_j S_j\right] \nabla T$$

$$+ \sum_{j=1}^{n_p} \nabla \cdot (H_j u_j) = \sum_{j=1}^{n_p} \frac{q_j H_{j,inj}}{V}$$

Specific heat capacity (C_{po}, C_{pg}) for oil and gas phases are updated as a function of pressure, temperature, and composition.



(Mura & Sharma, 2025)

Numerical Models w/o Fracture

Model Dimension and Discretization

- 1.2 x 1.2 x 0.11 km(xyz) dimensions

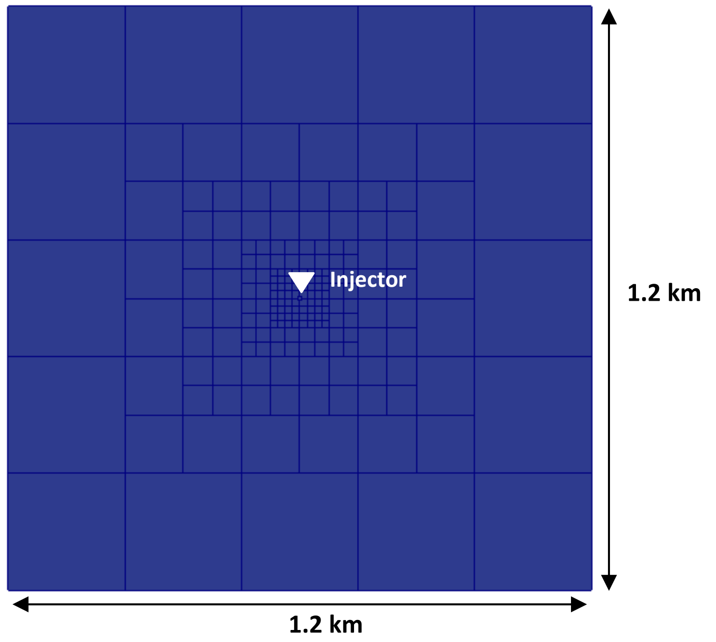
Rock Properties

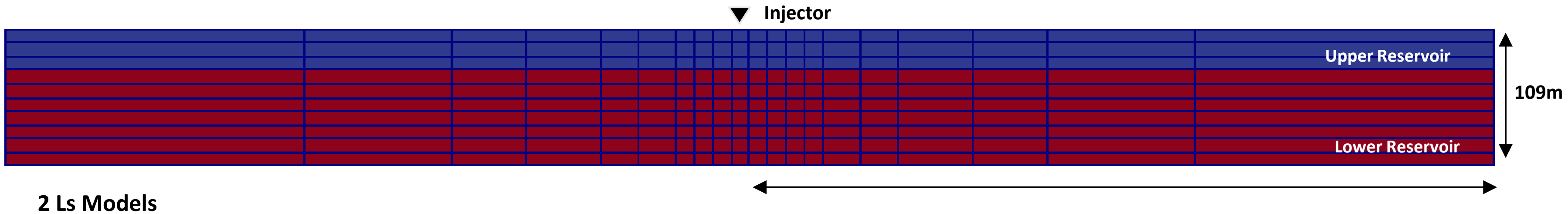
- Res. 1: H = 27 m, ϕ = 11.2 %, k = 66.6mD, S_w = 0.35
- Res. 2: H = 80 m, ϕ = 4.7 %, k = 4.7mD, S_w = 0.89

Initial Temperature, Pressure, and Stress

- P_{ini} = 25 bar (depleted gas reservoir)
- T_{ini} = 78oC
- S_{hmin} = 314 bar

2 Ls Model
(Top view)





Grid size
xy-direction: 6.25 ~ 200 m
z-direction: 4.7m

2 Ls Models
(Side view)

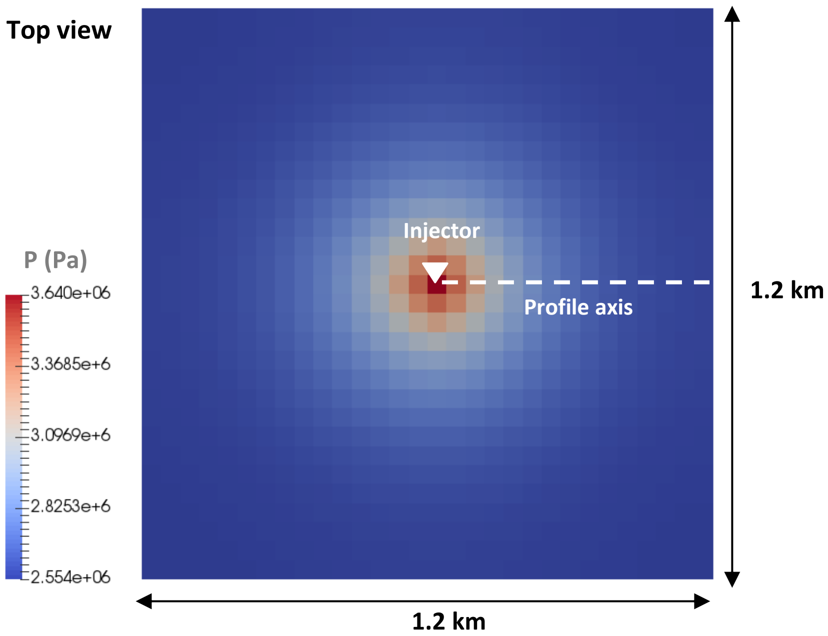
Simulation of HMTC Transport & Reservoir Impact Over Time

Speed of fronts:

Pressure >> Salinity > CO2 Front > Temperature

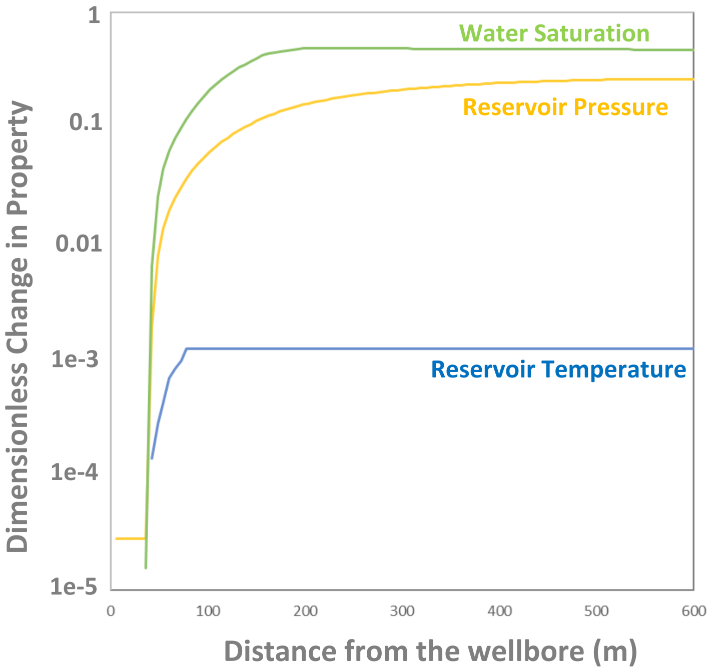
Reservoir Impact:

Pressure > Temperature ≈ CO2 Front >>> Salinity

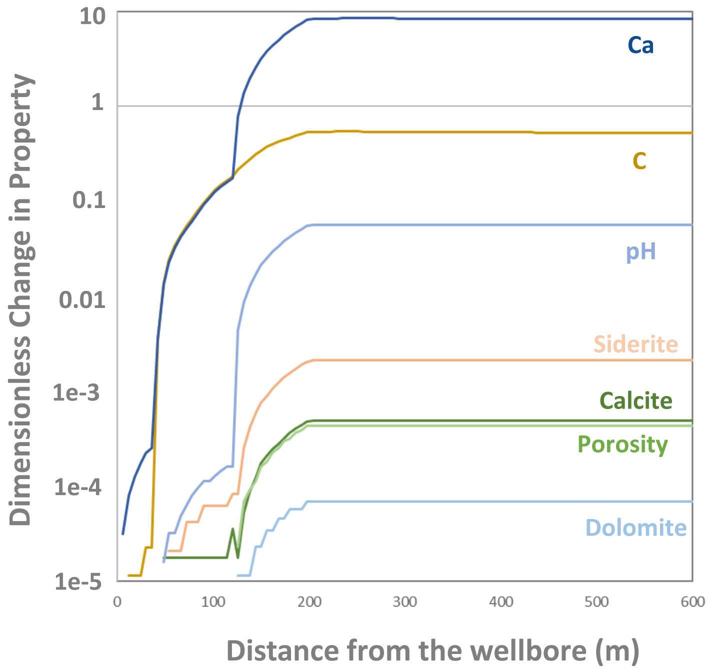


Pressure Distribution

100 Days After Injection



Physical Property Changes



Chemical Property Changes

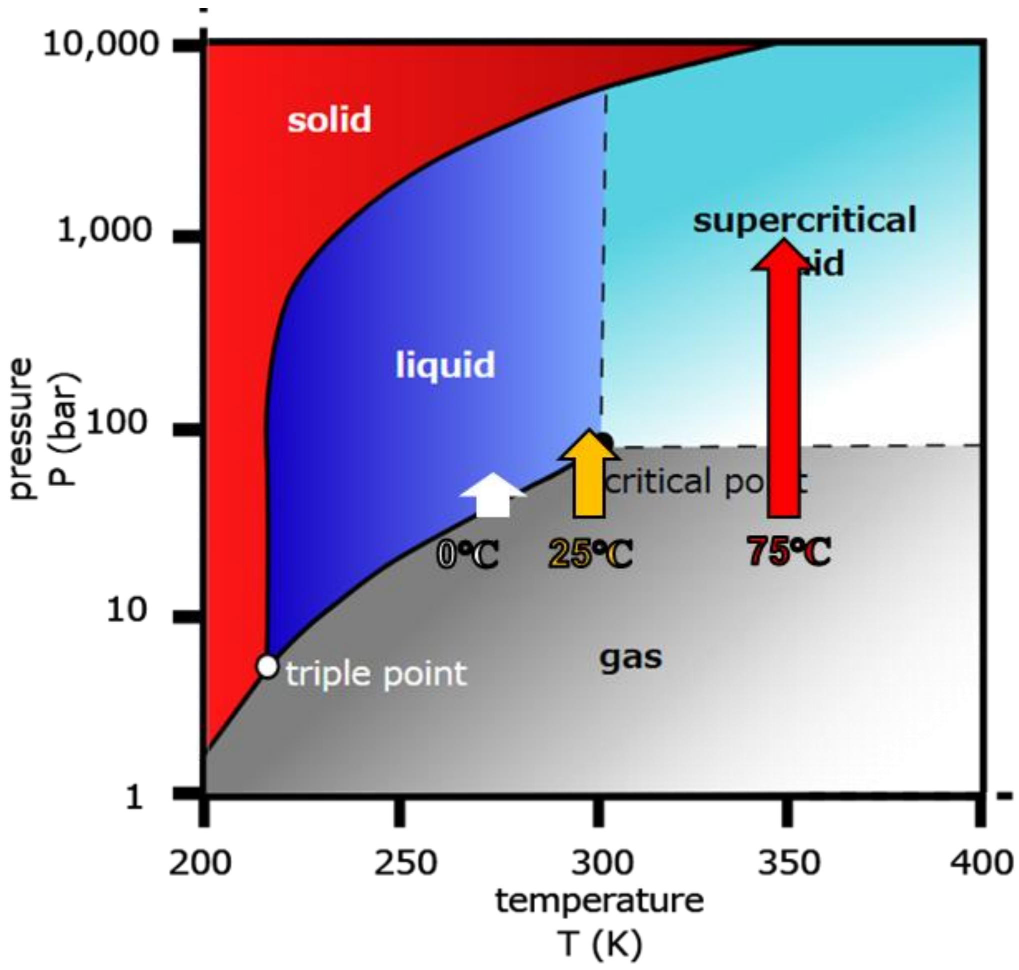
Numerical Wellbore Model: Compositional Flow (No Fracture)

Key Observations:

- Compare **supercritical** vs. **liquid CO2** injection.
- As BHT drops, volumetric flow rate decreases.
- Lower BHT reduces BHP.
- Injection rate: 750 tonnes/day CO2

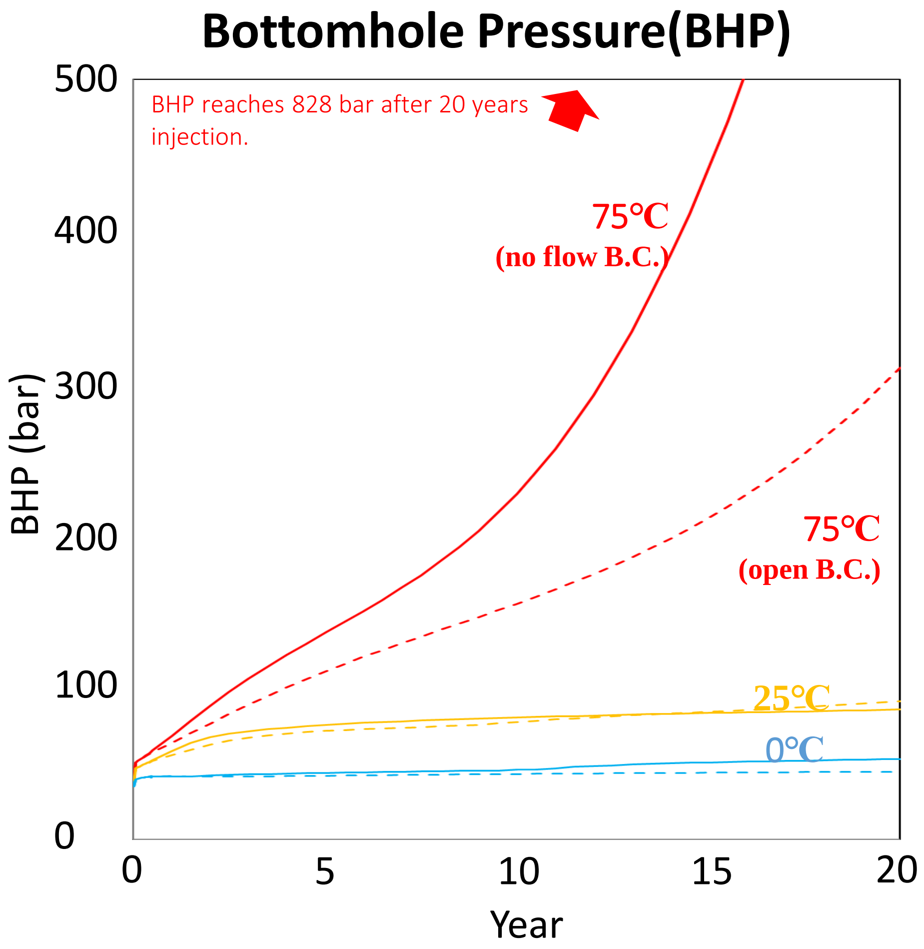
Simulation Features:

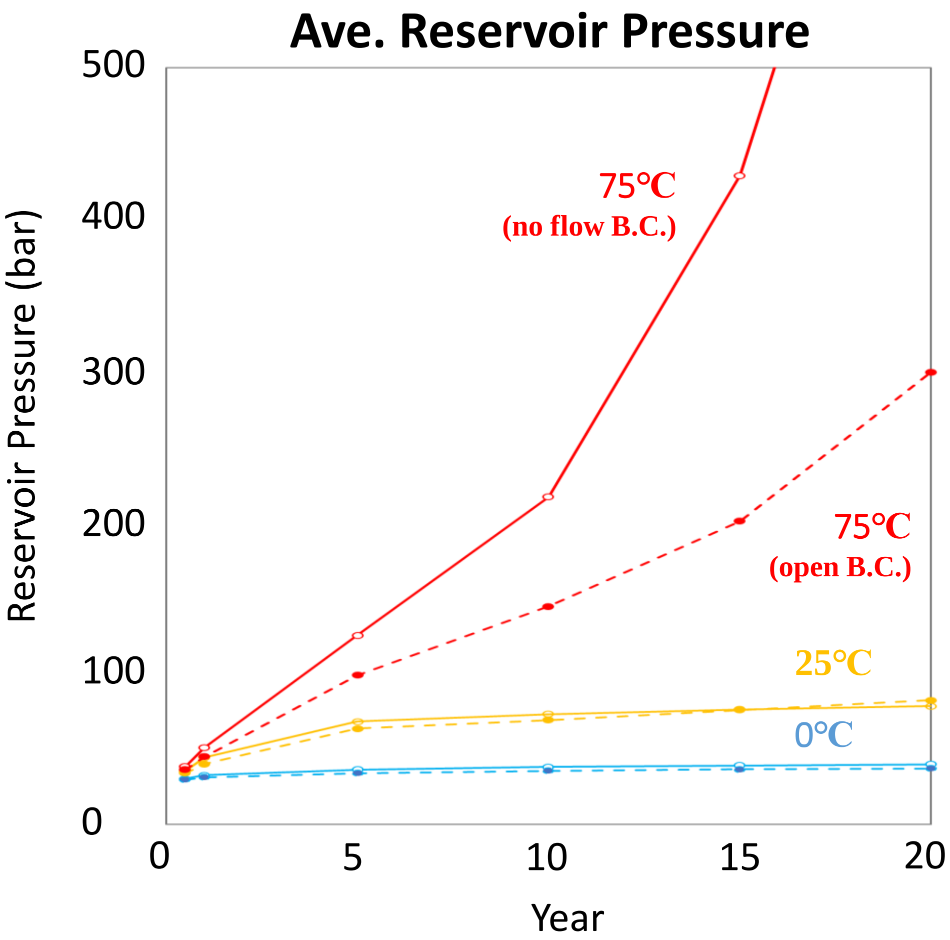
- 3 components: CO2, methane and C2+
- CO2 dissolved in water
- 3 phases (oil, gas, water)
- Geomechanics and thermo-elasticity
- No fracture propagation
- No geochemistry
- B.C.: No flow (case 1), open (case 2)



File:Carbon dioxide pressure-temperature phase diagram.svg - Wikipedia

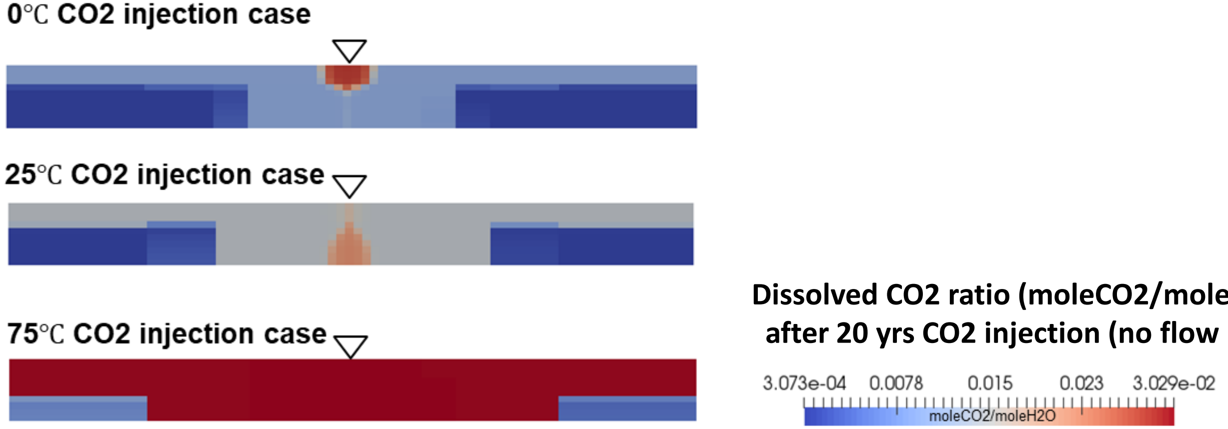
Supercritical vs Liquid CO2 Injection (No Fracture Propagation)



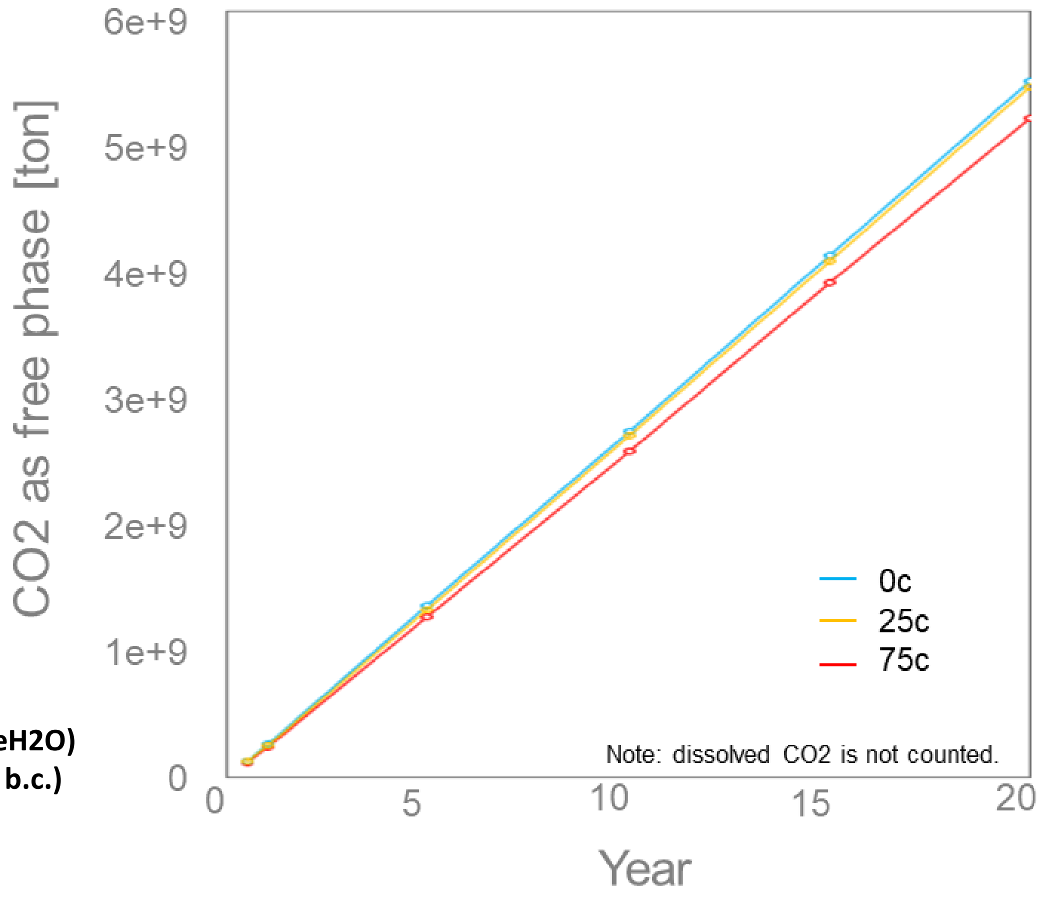


CO2 State in the Reservoir under 750 tpd CO2 Injection

- Confirmed, CO_2 in the reservoir is the same for all cases.
- CO_2 state varies with temperature and pressure.
    - CO_2 dissolves more in water in 75 C case due to high pressure.

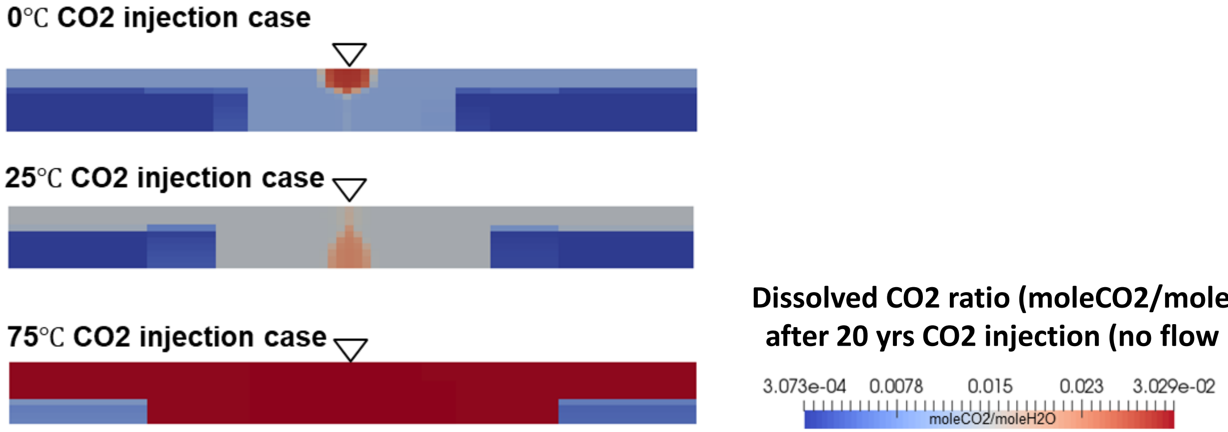


Dissolved CO2 ratio (moleCO2/moleH2O) after 20 yrs CO2 injection (no flow b.c.)



Supercritical vs Liquid CO2 Injection: CO2 Solubility in Water

- CO2 solubility is obtained as a function of pressure and temperature.
- Salinity is not considered in this model.



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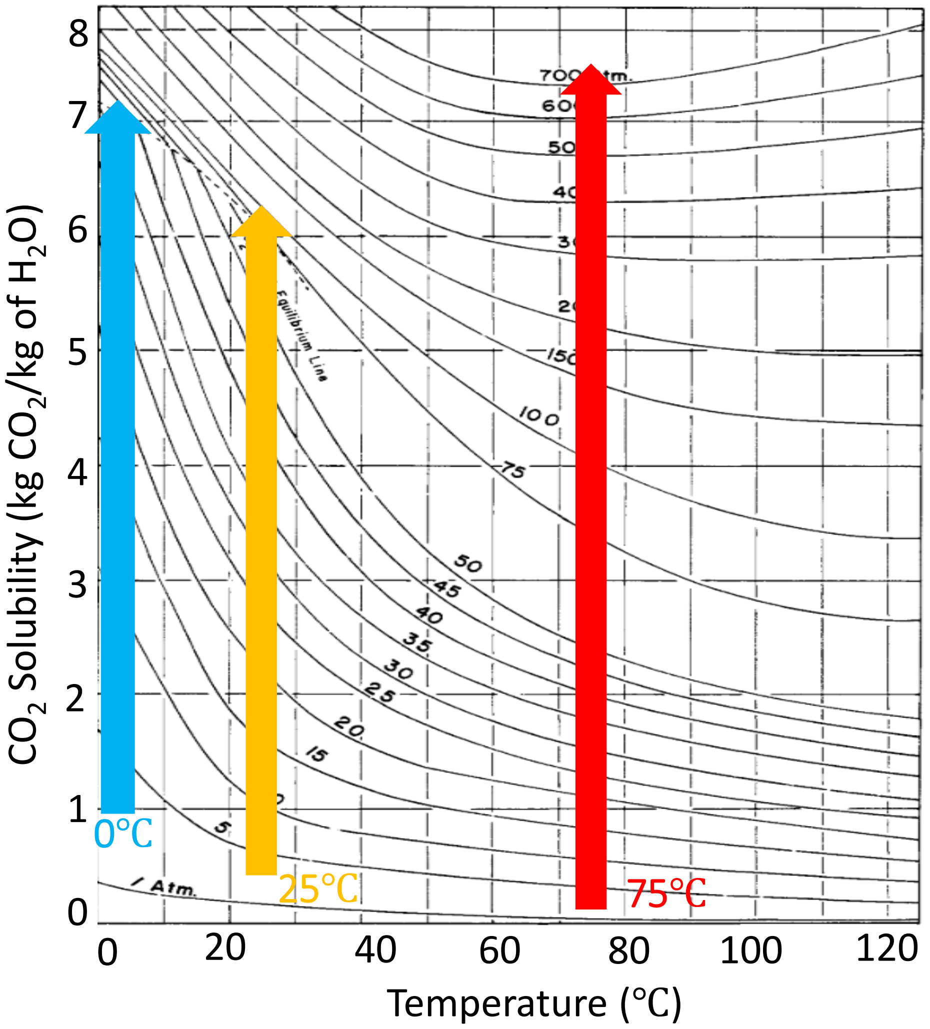


(Dodds et. al, 1956)

Supercritical vs Liquid CO2 Injection: CO2 Density

Temperature of injected CO2 influences the CO2 density significantly.

- CO2 density becomes more than 10 times the initial value in 75 C case while CO2 density is stable in other cases at the wellbore.

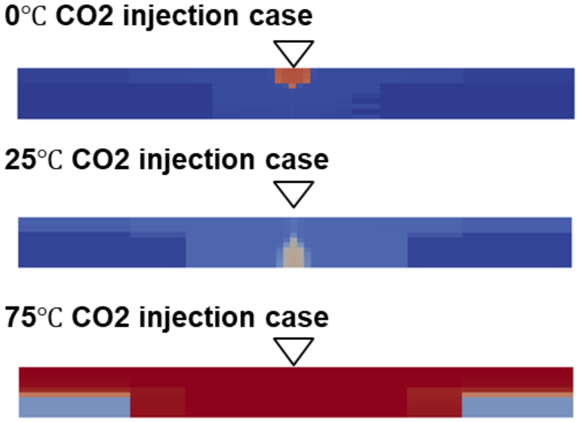
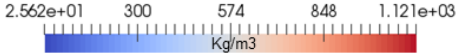


Fig. CO2 density after 20 yrs CO2 injection (no flow boundary condition)



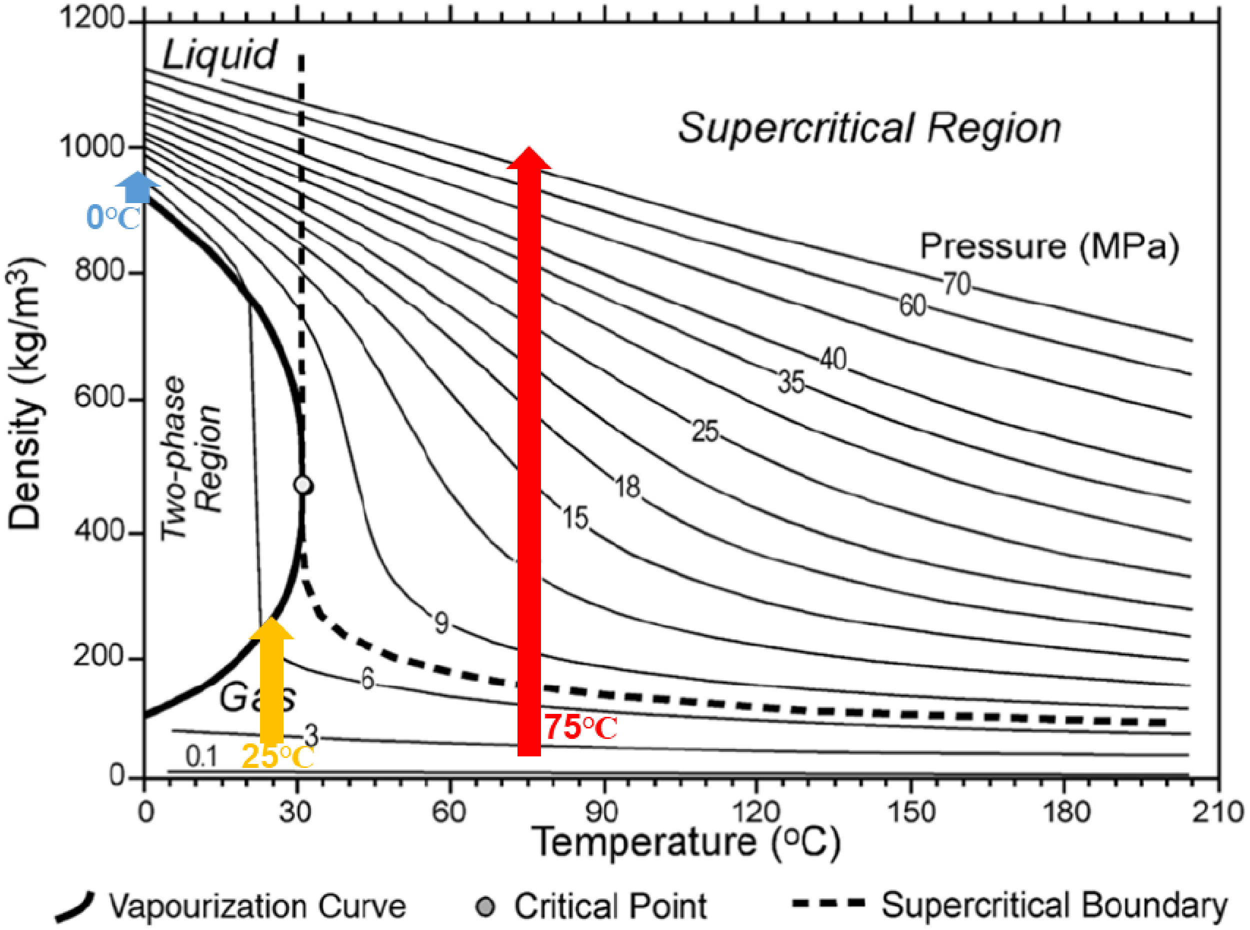


Figure AI.2 Variation of CO_2 density as a function of temperature and pressure (Bachu, 2003).

Supercritical vs Liquid CO2 Injection: CO2 Viscosity

Temperature of injected CO2 influences the CO2 viscosity significantly, but the variation range is smaller than CO2 density.

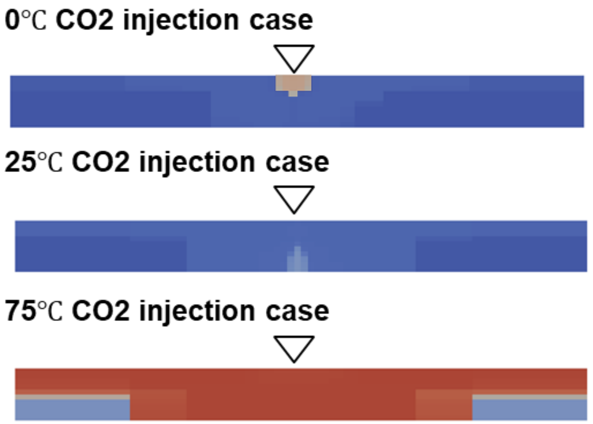
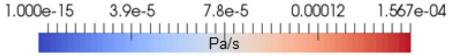


Fig. CO2 viscosity after 20 yrs CO2 injection (no flow boundary condition)



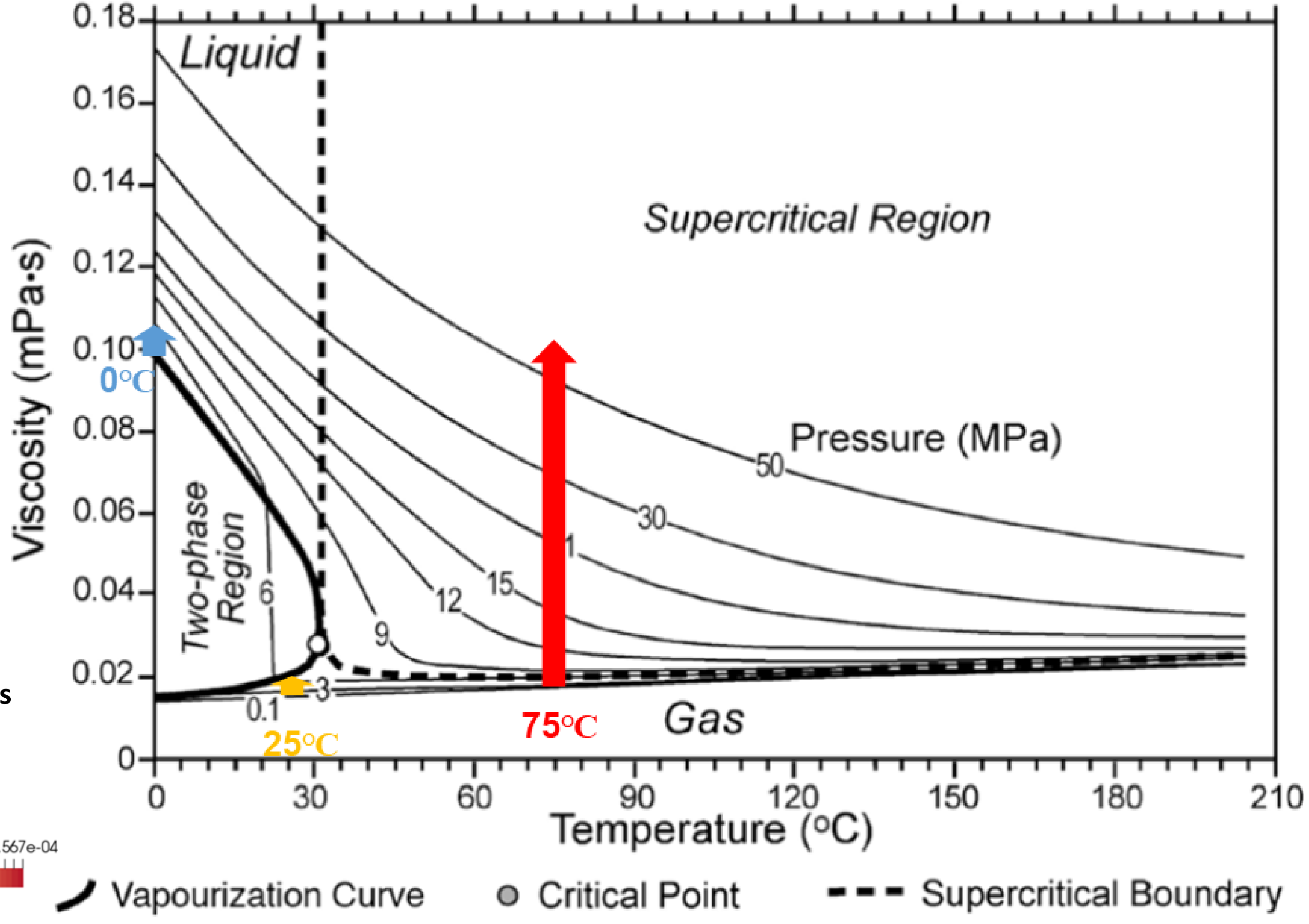
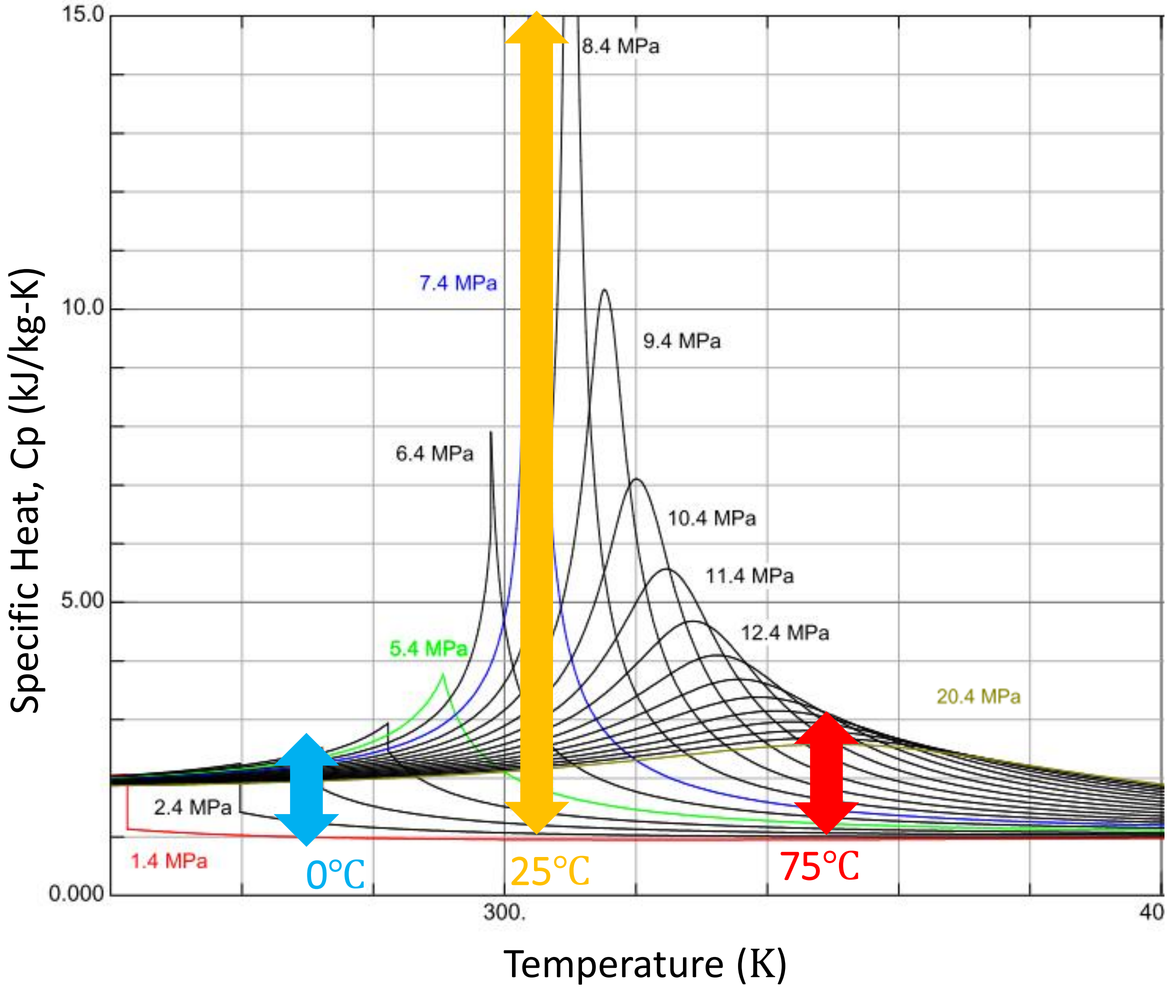


Figure AI.4 Variation of CO_2 viscosity as a function of temperature and pressure (Bachu, 2003).

Supercritical vs Liquid CO2 Injection: CO2 Heat Capacity

Temperature of injected CO2 influences the CO2 heat capacity significantly.

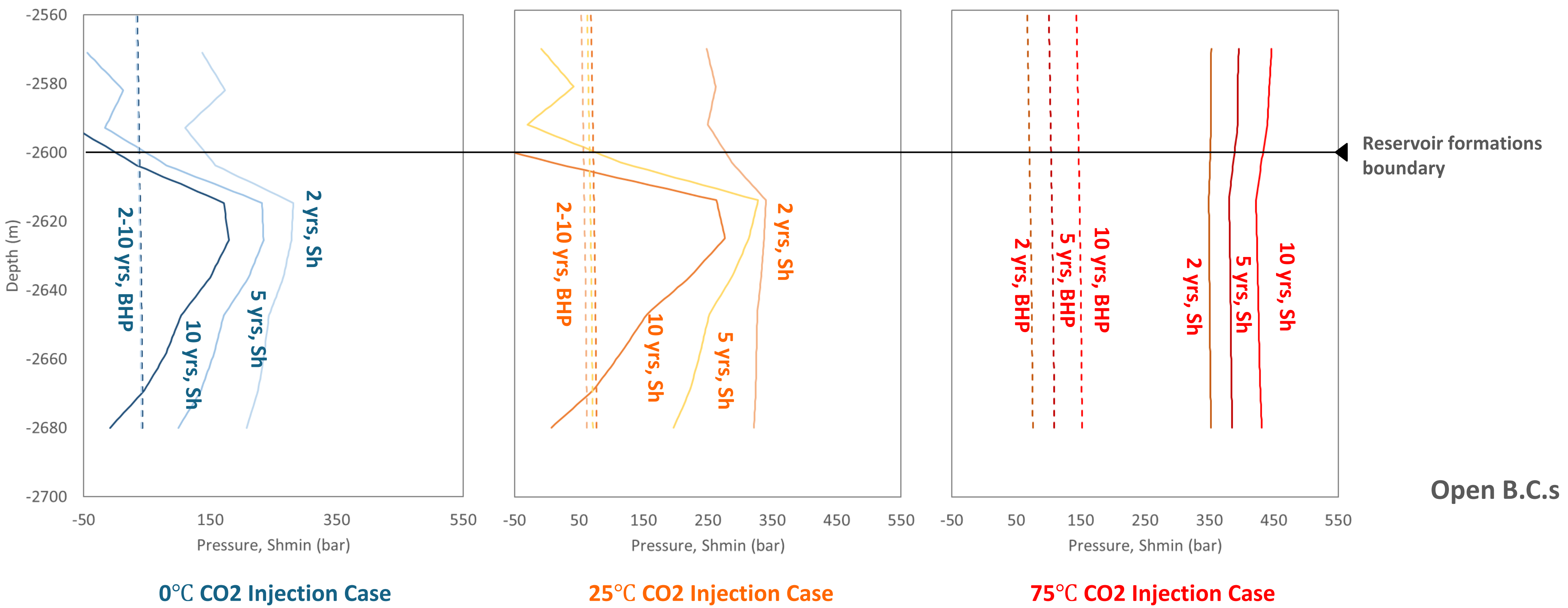
- The variation range is smaller than CO2 density if state-change is ignored.
- Heat capacity has peak value for the dynamic change in CO2 phase.
- Conductivity also varies with T and P but has minor impact under the convection dominant scenarios.



(Tumer et. al, 2014)

Prediction of Fracture Propagation: Timing and Location

- Stress reduction due to cold CO_2 may cause a fracture in both reservoirs.
  - Fracture initiates first in the upper reservoir (more permeable than lower reservoir).
- No fracture initiation was indicated in the case with res temp CO_2.



Conclusion

Cold CO_2 injection

Benefits:

- Lower transport costs.
- Higher injectivity due to increased CO_2 density.
- Induces thermal fractures, enhancing permeability and well stimulation.

Disadvantages:

- Higher fracture risk from rock thermal contraction and stress changes.
- Potential well integrity issues due to rapid temperature fluctuations.
- Requires long-term assessment of stress evolution and fracture propagation.

Supercritical CO_2 Injection

Benefits:

- Minimizes thermal stress effects, reducing uncertainty in reservoir response.
- Enhances miscibility with hydrocarbons, aiding EOR.

Disadvantages:

- Higher transport and compression costs.
- Increased BHP, potentially limiting injectivity.
- Risk of poro-elastic stress-induced fractures affecting integrity.

Reservoir & Fracturing Simulator Comparison

Fracture Propagation & HMTC Capabilities for CO_2 Injection

Simulator	Type	Hydro-Mechanical	Fracture Propagation	Thermal	Chemical	Research Reliability
Visage + INTERSECT (SLB)	Commercial	🟢 Strong	🟡 Limited (via UFM)	🟡 Full but Fixed Thermal Properties (EOS-based is Limited to E300)	🟡 Basic (Limited to E300, not INTERSECT)	🟡 Public Documentation
CMG GEM (CMG)	Commercial	🟢 Strong	🟡 Simplified	🟢 EOS-based Thermal Properties	🟢 Extensive library	🟡 Public Documentation
REVEAL (Petroleum Experts)	Commercial	🟢 Integrated	🟢 Explicit	🟡 Full but Fixed Thermal Properties	🟡 Partial (Production and EOR chemistry)	🟢 Direct discussions with users
ResFrac (ResFrac Corp)	Commercial	🟢 Integrated	🟢 Advanced	🟡 Full but EOS-based is In Development	🔴 Limited (Simple reactions only)	🟢 Direct discussions with developers
TOUGH Suite (LBNL)	Academic	🟢 Via FLAC/ROCMECH	🟢 Via Coupling	🟢 EOS-based Thermal Properties (via ECO2N module for CO_2-brine systems)	🟢 TOUGHREACT (For coupled reactive transport)	🟡 Public Documentation
MOOSE Framework (INL)	Academic	🟢 Flexible	🟢 Multiple Methods	🟢 EOS-based Thermal Properties (via PorousFlow for brine-CO_2 modeling)	🟢 Integrated	🟡 Public Documentation
Multi-Frac-3D (UT Austin)	Academic	🟢 Fully Coupled	🟢 Primary Focus	🟡 Full but EOS-based is In Development	🟢 Integrated	🟢 Strong

Notes: HMTC = Hydro-Mechanical-Thermal-Chemical processes. Capability indicators: 🟢 Full/Strong capability, 🟡 Partial/Limited capability, 🔴 Minimal capability

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