

UNRAVELING SALT PRECIPITATION MECHANISMS IN GEOLOGICAL CO₂ STORAGE: INSIGHTS INTO DOMINANT DRIVING FORCES

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ABSTRACT

This Supplementary Material provides additional information on the numerical model, the description of the cases, effect of capillary pressure function on salt precipitation, effect of the bond number (BO), effect of capillary pressure and salt precipitation on injection pressure, data extracted from literature, effect of heterogeneity, and data availability.

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1. NUMERICAL MODEL

This study employs TOUGH2^a, a versatile numerical simulator designed for the fluid flow of multiple components and phases. The formulation and implementation are extensively detailed in Pruess (4). TOUGH2 has been coupled by the ECO2N^b package, which serves as an equation of state (EOS) module. ECO2N accurately calculates fluid properties of individual phases and H₂O–NaCl–CO₂ mixtures, aligning closely with experimental values within the specified temperature, pressure, and salinity of interest (10°C ≤ *T* ≤ 110°C; *P* ≤ 600 bar; salinity up to full halite saturation) (5).

^a <https://tough.lbl.gov/software/tough2-mp-software/>

^b https://tough.lbl.gov/assets/docs/TOUGH2_ECO2N_Users_Guide.pdf



The *van Genuchten* equations are used to model relative permeabilities and capillary pressure in this context, and they are succinctly summarized in the following equations:

$$k_{rl} = \begin{cases} \sqrt{S^*} \{1 - (1 - [S^*]^{1/m})^m\}^2, & S_l < S_{ls} \\ 1, & S_l \geq S_{ls} \end{cases} \quad (S1)$$

$$k_{rg} = \begin{cases} 1 - k_{rl}, & S_{gr} = 0 \\ (1 - \hat{S})^2 (1 - \hat{S}^2), & S_{gr} > 0 \end{cases} \quad (S2)$$

$$S^* = \frac{S_l - S_{lr}}{1 - S_{lr}}, \quad (S3)$$

$$\hat{S} = \frac{(S_l - S_{lr})}{1 - S_{lr} - S_{gr}} \quad (S4)$$

$$P_c = P_0 ([S^*]^{-1/\lambda} - 1)^{1-\lambda} \quad (S5)$$

In the above formulations S_l is the liquid saturation, S_{lr} and S_{gr} are irreducible liquid and gas saturations, S_{ls} is a threshold value, P_0 is the entry pressure, and λ is a parameter depending on pore geometry.

The relative permeability and capillary pressure curves are illustrated in **Figure S1**. The corresponding values are summarized in **Table S1**. Conventional capillary pressure relationships are applied to model on the macroscale. However, these models have limitations in accurately describing capillary pressure at saturations below the irreducible water saturation, where dry-out and salt precipitation happen. This limitation introduces uncertainty, which will be addressed through alternative capillary pressure curves and sensitivity studies.

Salt precipitation in TOUGH2 is modeled by considering the solubility limit of NaCl as a function of temperature, with precipitated salt treated as a solid phase that reduces the porosity. Experimental studies have shown that small changes in porosity can significantly affect permeability, and various models have been proposed to describe this relationship (2, 3, 7). TOUGH2 offers three analytical options for describing permeability as a function of porosity reduction. This study uses the tubes-in-series model (6), which accounts for the converging-diverging nature of porous media.

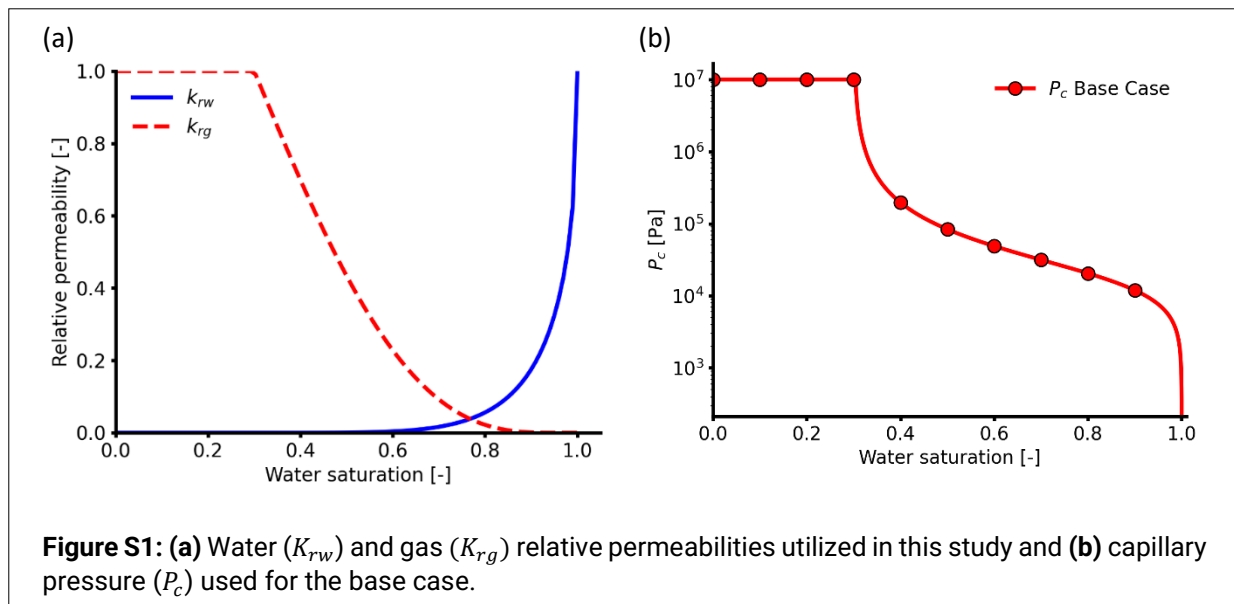


Table S1: List of values that are used to describe capillary pressure, relative permeabilities, and permeability reduction as a function of porosity reduction.

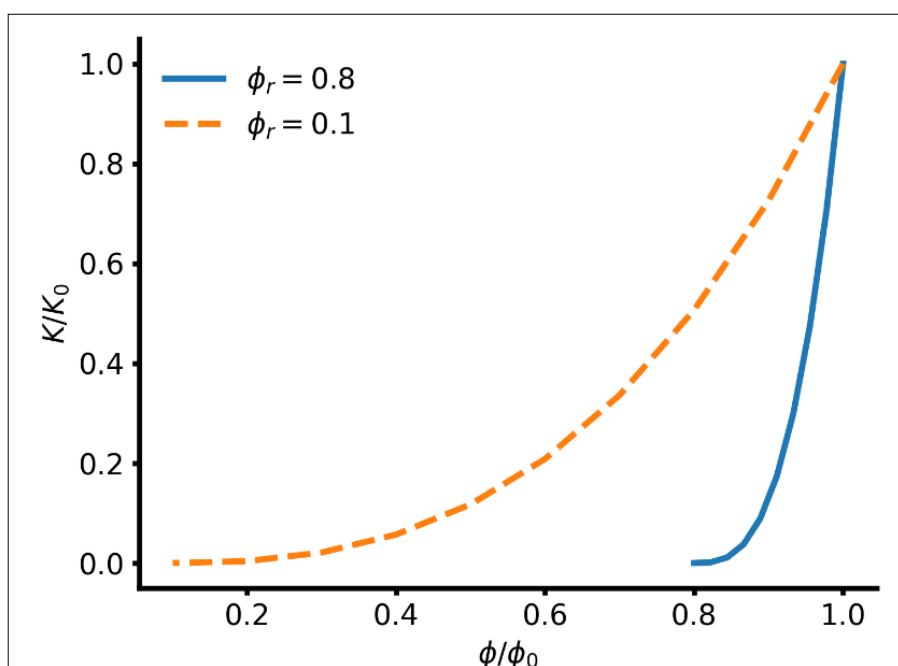
Parameters	Values
Irreducible liquid saturation (S_{lr}) [-]	0.3
Critical saturation (S_{ls}) [-]	1
Residual gas saturation (S_{gr})	0.05
Exponent coefficient (m, λ)	0.457
Capillary entry pressure (P_{cr}) [Pa]	19608
Maximum capillary pressure cut-off (P_{max}) [Pa]	1×10^7
Fractional length of the pore bodies (Γ) [-]	0.8
Fraction of original porosity (ϕ_r) [-]	0.1 and 0.8

The model involves two parameters: Γ (fractional length of the pore bodies with two different radii) and ϕ_r (fraction of original porosity defined as $\frac{\phi}{\phi_0}$). Equation S6 to Equation S8 describe the tube-in-series model. The parameters used here are $\Gamma = 0.8$ and $\phi_r = 0.8$, indicating that when 20% of porosity is lost, permeability approaches zero. These values are the standard for most scenarios used in this study, but in sensitivity studies where salt precipitation is uncertain, $\phi_r = 0.1$ is used to avoid early reservoir blockage. Corresponding curves are illustrated in Figure S2. This correlation, which is a key uncertainty in this study, can significantly impact the injectivity assessment.

$$\frac{k}{k_0} = \theta^2 \left[\frac{1 - \Gamma + \Gamma \omega^{-2}}{1 - \Gamma + \Gamma \left(\frac{\theta}{\theta + \omega - 1} \right)^2} \right] \quad (S6)$$

$$\theta = \frac{1 - S_s - \phi_r}{1 - \phi_r} \quad (S7)$$

$$\omega = 1 + \Gamma^{-1} / (\phi_r^{-1} - 1) \quad (S8)$$

**Figure S2:** Correlation between porosity (ϕ) and permeability (K) reduction due to salt precipitation.

2. DESCRIPTION OF CASES

Table S2: Description of all cases used in this study.

Case Name	K [mD]	Rate [kg/s]	P _{cr} [kPa]	S _{lr}	λ	g [m/s ²]
Base case	150	11	20	0.3	0.457	10
Effect of capillary-saturation model choice						
1A_Pc-Log	150	11	20	0	0.3	10
1B_Pc-Slr-neg	150	11	20	0	0.457	10
1C_NoPc	150	11	***	***	***	10
1D_NoPc_No-Kred *	150	11	***	***	***	10
* In addition to neglecting capillary pressure effect, the effect of salt precipitation on permeability reduction is also neglected						
*** Capillary pressure has been neglected so the parameters related to the capillary pressure curves are omitted.						
Capillary number (Ca) test cases						
Ca1_0.1R	150	1.1	20	0.3	0.457	10
Ca2_0.01R	150	0.11	20	0.3	0.457	10
Ca3_0.1K	15	11	20	0.3	0.457	10
Ca4_10K	1500	11	20	0.3	0.457	10
Ca5_0.1R_0.1K	15	1.1	20	0.3	0.457	10
Ca6_0.1R_10K	1500	1.1	20	0.3	0.457	10
Ca7_0.01R_0.1K	15	0.11	20	0.3	0.457	10
Ca8_0.01R_10K	1500	0.11	20	0.3	0.457	10
Gravity number (Gr) test cases						
Ca1_0.1R_Gr1	150	1.1	0.2	0.3	0.457	10
Ca1_0.1R_Gr2	150	1.1	0.002	0.3	0.457	10
Ca1_0.1R_Gr3	150	1.1	20	0.3	0.457	1
Ca1_0.1R_Gr4	150	1.1	0.2	0.3	0.457	1
Ca1_0.1R_Gr5	150	1.1	0.002	0.3	0.457	1
Ca1_0.1R_Gr6	150	1.1	20	0.3	0.457	0
Ca1_0.1R_Gr7	150	1.1	0.2	0.3	0.457	0
Ca1_0.1R_Gr8	150	1.1	0.002	0.3	0.457	0
K = Absolute Permeability; Rate = Injection rate; P _{cr} : entry capillary pressure; S _{lr} = Irreducible Liquid Saturation; λ : Exponent coefficient in van Genuchten equation; g = Gravitational acceleration coefficient.						

3. EFFECT OF CAPILLARY PRESSURE FUNCTION ON SALT PRECIPITATION

As previously mentioned, conventional capillary pressure curves are inadequate for accurately representing capillary pressure values at water saturations below the irreducible level, which is critical for modeling the dry-out region. To address this limitation, two alternative capillary pressure models are considered in addition to the conventional curve. These are illustrated in [Figure S3](#).

The effect of changing the capillary pressure model on salt precipitation profiles is illustrated in [Figure S4](#).

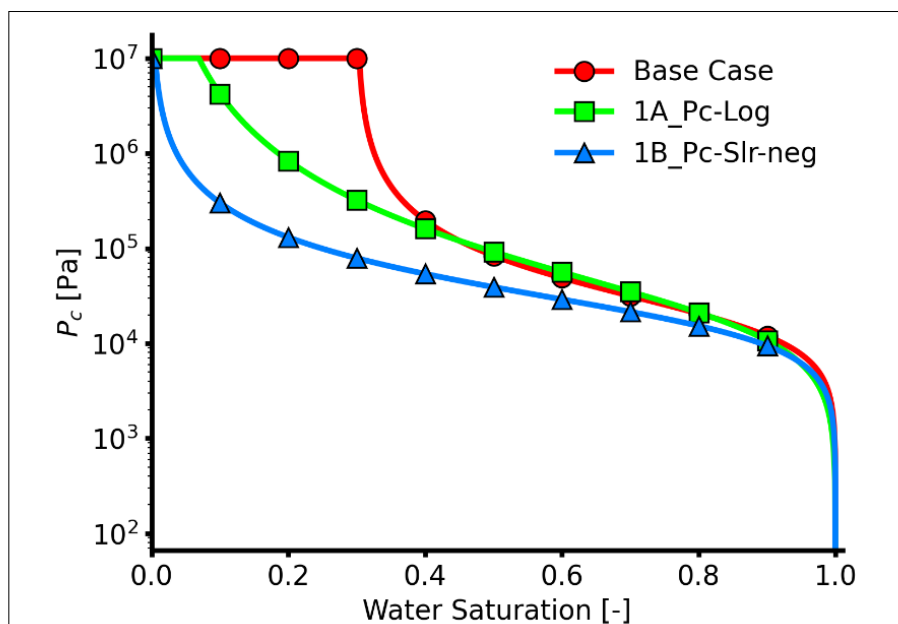


Figure S3: Capillary pressure curves utilized in the Capillary force analysis.

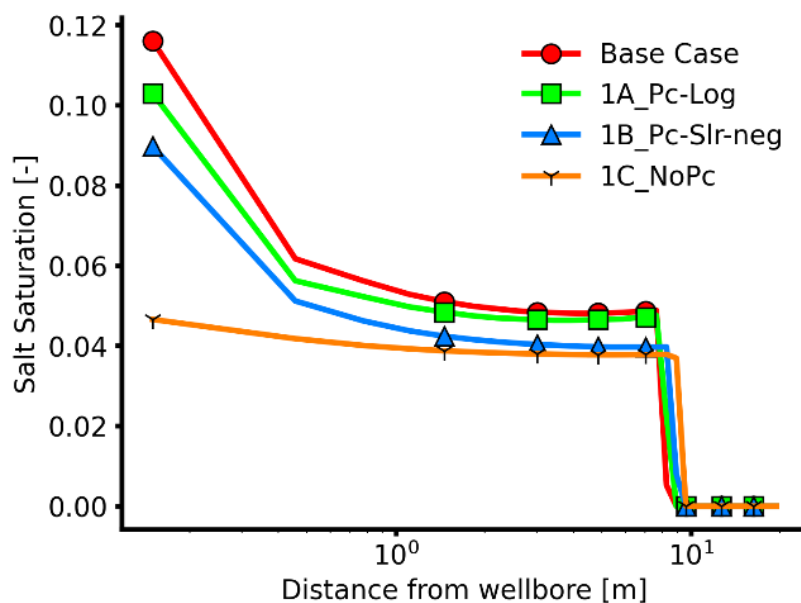


Figure S4: Effect of different capillary functions on salt saturation profile along the bottom line of the reservoir.

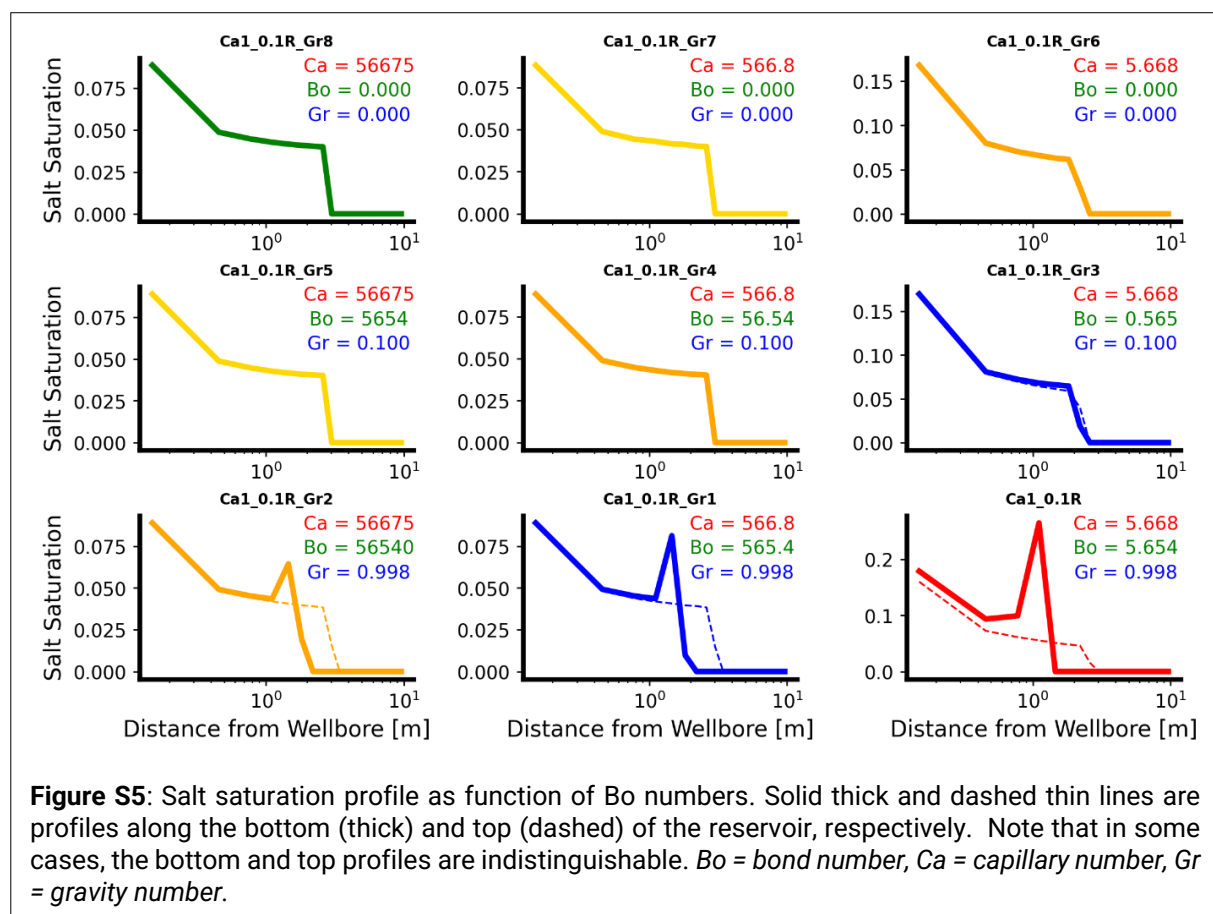
4. EFFECT OF BOND NUMBER (BO)

Investigating scenarios that isolate the influences of gravity and capillary forces while keeping the viscous force constant can provide valuable insights. In several case studies, although the Bo numbers are constant, significant variations in salt precipitation patterns and amounts are observed. This section focuses on the effect of the Bo number on salt precipitation, particularly using the base case with a reduced injection rate (Ca1_0.1R), where modifications to capillary entry pressure and gravitational acceleration are implemented. This specific case is chosen due to the presence of a peak in salt precipitation away from the wellbore.

Figure S5 reveals a discernible pattern within each column and row: in each column, the Ca number remains constant while the Bo number increases from top to bottom. Conversely, the Bo number remains constant across each row, while the Ca number decreases from left to right. Throughout these variations, the viscous force remains unchanged due to consistent velocities.

Figure S6 illustrates a consistent decline in salt precipitation near the wellbore and a secondary peak further away as the Ca number increases (with Bo held constant). This trend aligns with the relationship concerning backflow, indicating that higher Ca numbers result in a decreased salt precipitation near the wellbore.

As the Bo number decreases (indicating stronger gravitational effects), salt precipitation near the wellbore remains largely unchanged, while the secondary peak away from the wellbore diminishes. This suggests that gravity primarily influences salt deposition farther from the injection point. The Ca number strongly affects salt precipitation at the inlet, but no consistent trend is observed for its impact on localized salt deposition. Similarly, the effect of the Bo number on localized precipitation remains inconclusive. Notably, despite constant Bo numbers, localized salt precipitation occurs in multiple cases, whereas reducing the Bo number while maintaining a

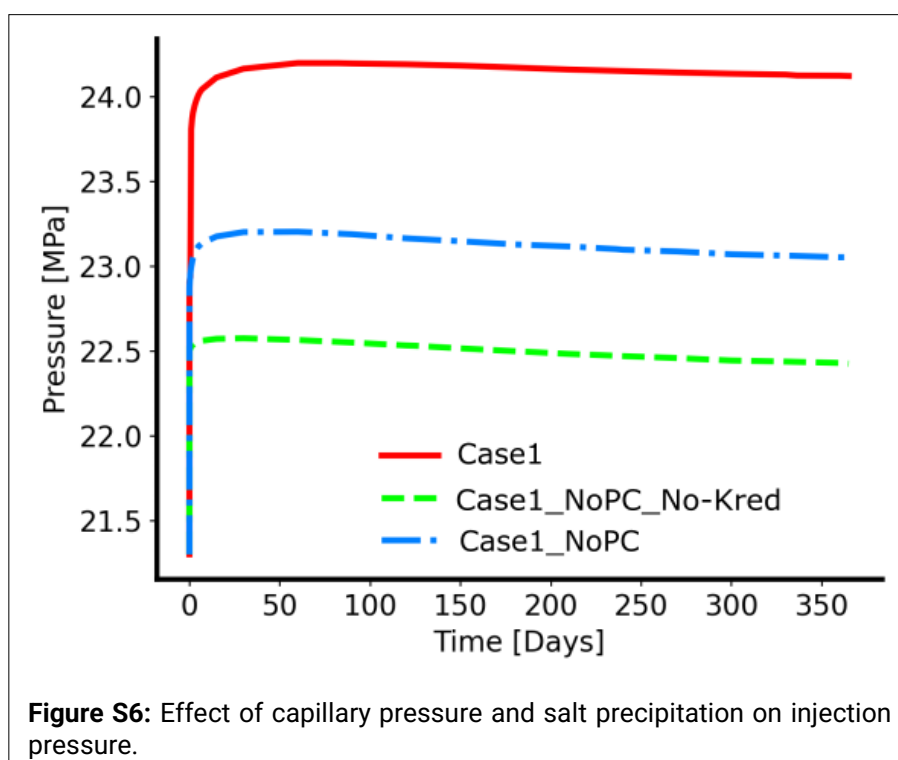


constant Ca number leads to diminished localized precipitation. These findings indicate that Ca and Bo alone are insufficient to fully describe localized salt precipitation dynamics.

5. EFFECT OF CAPILLARY PRESSURE AND SALT PRECIPITATION ON INJECTION PRESSURE

Increasing capillary pressure increases injection pressure, thus decreasing injectivity through two mechanisms: **(a)** it raises the pressure needed to penetrate the porous media, and **(b)** it enhances salt precipitation near the wellbore, which reduces permeability. We recall that the degree of permeability reduction due to salt precipitation is governed by the parameters in Equation S6, which defines the relationship between porosity reduction and permeability.

In Figure S6, injection pressure over one year is depicted for three scenarios to illustrate the effects of capillary pressure and salt precipitation on injectivity, maintaining all parameters consistent with the base case. In Case1_NoPC_No-Kred, the influences of capillary pressure and salt precipitation on permeability reduction are disregarded. Case1_NoPC excludes only capillary pressure. The comparison between Case1_NoPC and Case1_NoPC_No-Kred highlights the effects of permeability reduction due to salt precipitation. Conversely, the difference between Case1 and Case1_NoPC illustrates the combined effects of capillary pressure and permeability reduction from salt precipitation, showing a greater pressure difference than in the previous comparison. This indicates that injectivity loss is most sensitive to capillary pressure effects in this case.



6. DATA EXTRACTED FROM LITERATURE

Parameters extracted from Kim et al. (1) and all cases used for the calculation of Ca, Bo, and Gr numbers are summarized in **Table S3**.

Table S3: Summary of parameter values extracted from Kim et al. (1). The width of the reservoir is 100 m. P_{cr} is 1.96e3 [Pa], g is 10 m/s², porosity is 0.2, viscosity is 4.76e-5 Pa.s, and density is 629 kg/m³.

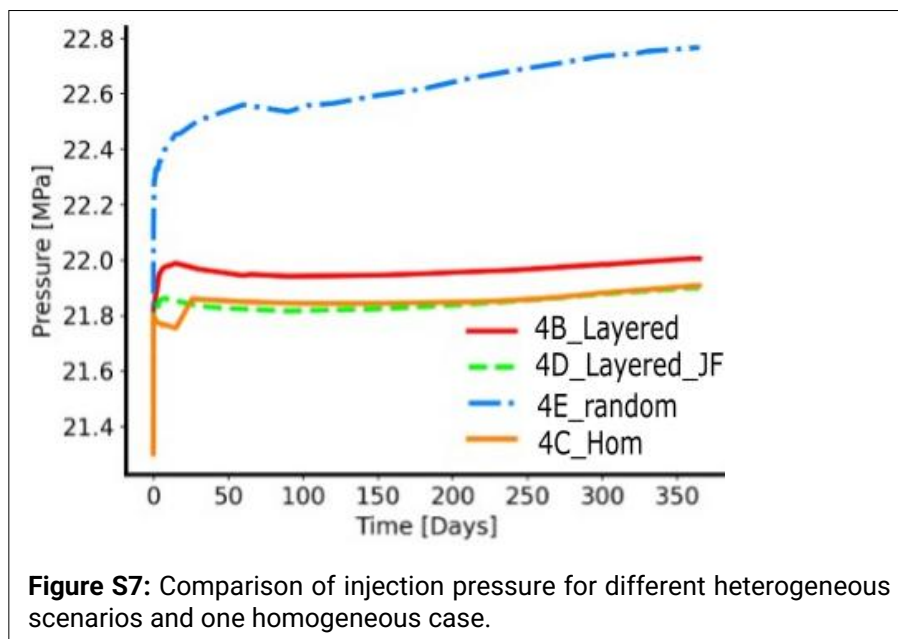
Case Name	Rate [kg/s]	Permeability [mD]	Vcr [m/s]	Ca	Bo	Gr	Localized Salt-precip.
Case1_kim	1	10	1.26514e-4	3.07E+02	8.33E+01	2.71E-01	No
Case1-1_Kim	2	10	2.53029e-4	6.14E+02	8.33E+01	1.36E-01	No
Case1-2_kim	3	10	3.79543e-4	9.22E+02	8.33E+01	9.04E-02	No
Case1-3_kim	4	10	5.06057e-4	1.23E+03	8.33E+01	6.78E-02	No
Case1-4_kim	5	10	6.32571e-4	1.54E+03	8.33E+01	5.42E-02	No
Case2_kim	2.5	50	3.16286e-4	1.54E+02	8.33E+01	5.42E-01	Yes
Case2-1_Kim	5	50	6.32571e-4	3.07E+02	8.33E+01	2.71E-01	Yes
Case2-2_kim	10	50	1.26514e-3	6.14E+02	8.33E+01	1.36E-01	No
Case2-3_kim	20	50	2.53029e-3	1.23E+03	8.33E+01	6.78E-02	No
Case2-4_kim	30	50	3.79543e-3	1.84E+03	8.33E+01	4.52E-02	No
Case3_Kim	3	100	3.79543e-4	9.22E+01	8.33E+01	9.04E-01	Yes
Case3_1_Kim	5	100	6.32571e-4	1.54E+02	8.33E+01	5.42E-01	Yes
Case3-2_Kim	10	100	1.26514e-3	3.07E+02	8.33E+01	2.71E-01	Yes
Case3-3_Kim	20	100	2.53029e-3	6.14E+02	8.33E+01	1.36E-01	No
Case3-4_Kim	30	100	3.79543e-3	9.22E+02	8.33E+01	9.04E-02	No
Base Case	11	150	2.68e-3	57	0.1	5.7	No
Ca1_0.1R	1.1	150	2.68e-4	5.7	1	5.7	Yes
Ca2_0.01R	0.11	150	2.68e-5	0.57	0.01	5.7	No
Ca3_0.1K	11	15	2.68e-3	570	0.01	5.7	No
Ca4_10K	11	1500	2.68e-3	5.7	1	5.7	Yes
Ca5_0.1R_0.1K	1.1	15	2.68e-4	57	0.1	5.7	No
Ca6_0.1R_10K	1.1	1500	2.68e-4	5.7	1	5.7	No
Ca7_0.01R_0.1K	0.11	15	2.68e-5	0.57	10	5.7	Yes
Ca8_0.01R_10K	0.11	1500	2.68e-5	0.06	100	5.7	No
Ca1_0.1R_Gr1	1.1	150	2.68e-4	570	1	570	Yes



Ca1_0.1R_Gr 2	1.1	150	2.68e-4	56700	1	56700	Yes
Ca1_0.1R_Gr 3	1.1	150	2.68e-4	5.7	0.1	0.57	No
Ca1_0.1R_Gr 4	1.1	150	2.68e-4	567	0.1	56.7	No
Ca1_0.1R_Gr 5	1.1	150	2.68e-4	56700	0.1	5670	No
Ca1_0.1R_Gr 6	1.1	150	2.68e-4	5.7	0	0	No
Ca1_0.1R_Gr 7	1.1	150	2.68e-4	570	0	0	No
Ca1_0.1R_Gr 8	1.1	150	2.68e-4	56700	0	0	No

Vcr = Darcy Velocity, *Bo* = bond number, *Ca* = capillary number, *Gr* = gravity number.

7. EFFECT OF HETEROGENEITY



8. DATA AVAILABILITY

The TOUGH2 input files used to generate the results presented in this paper can be found at <https://github.com/cssr-tools/saltprctough2>.

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