Supporting information

Sensitivity analysis of CO_2 injection within saline aquifers for storage purposes in the form of hydrate using a reactive transport simulator

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1 Boundary conditions

Boundary conditions and layer properties are listed in Table S1 and Table S2, while material properties and CO_2 hydrate specifications are listed in Table S3. Table S4 shows the species that were used for geochemical reactions.

2 Fitting function coefficients

Table S5 shows the coefficients of the fitting functions that were used for each property.

Table S1: Boundary conditions used in our simulations.

Parameter	Top	Bottom
Pressure [MPa]	1	4
Temperature [K]	273.35	284
Mean stress [MPa]	2.33	8.76
CO_2 injection pressure [MPa]	4	-

Table S2: Properties of the reservoir layers used in our simulations.

Property	Aquifer	Cap rock	Fracture
Young's modulus [GPa]	0.5	0.5	0.5
Poisson's ratio	0.25	0.25	0.25
Zero stress porosity	0.3	0.03	0.5
Zero stress permeability [m^2]	10^{-13}	10^{-17}	10^{-10}
Van Genuchten's gas entry pressure (at zero stress)	0.0196	0.196	0.196
Van Genuchten's exponent [m]	0.457	0.457	0.457
Longitude dispersion factor [m]	11	11	11
Molecular diffusion [m]	10^{-10}	10^{-10}	10^{-10}

Table S3: Medium properties.

Property	Value	Unit
Thermal conductivity of saturated medium	3.1	W/(m·K)
Solid Phase Density	2163	kg/m^3
Specific heat of rock	874	J/(kg·K)
CO_2-hydrate molecular weight	1092	g/mol
CO_2-hydrate density	1021.47	kg/m^3
CO_2-hydrate specific heat	2200	J/(kg·K)
CO_2-hydrate reaction enthalpy	65.22	kJ/mol

Table S4: Chemical species in each of the phases of our simulations.

Phase	Species
Aqueous	H_2O
Primary	HCO_3^-
Species	OH^-
Aqueous	CO_2(aq)
Secondary	CO_3^{2-}
Species	H^+
Gas	CO_2(g)

Table S5: Coefficients of fitting functions of the form $\phi_n = ax^2 + bx + c$, where ϕ_n is the node porosity and x is the varied parameter. Time is denoted by t.

x	t [years]	a	b	c
Fracture permeability, K_f [m^2]	2	0.00593132	-0.0518282	0.306066
	3	0.00688892	-0.0476449	0.223582
	4	0.00345883	-0.0222389	0.170816
Fracture porosity, ϕ_f	2	0.0	-0.0160217	0.201777
	5	0.0	-0.0307548	0.148905
	8	0.0	-0.0331606	0.147837
Matrix porosity, ϕ_m	1	0.0	1.11151	-0.0483778
	2	0.0	1.2931	-0.195132
	4	0.0	0.736435	-0.0851356
	8	0.0	0.652205	-0.0667558
Injection temperature, T [°C]	3	0.0	-0.000120696	0.144909
	10	0.0	-0.0000682904	0.131124
	15	0.0	-0.0000881127	0.128459
Injection pressure, P [MPa]	1	0.0	-0.0502347	0.488066
	2	0.0	-0.0974598	0.576456
	2.5	0.0	-0.052548	0.356085
Water residual saturation, S_w	2	0.0	-0.184493	0.191728
	3	0.0	-0.0756166	0.142277
	4	0.0	0.0676153	0.135004