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Coupled Thermal-Hydrodynamic-Mechanical-Chemical (THMC) Processes for CO₂ Geological Sequestration in Deep Saline Aquifers

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Injecting CO₂ into deep saline aquifers is considered as a promising method to reduce the emissions of anthropogenic CO₂ to Earth's atmosphere, which is referred to as CO₂ geological sequestration (CGS). CGS thermal-hydrodynamic-mechanicalinvolves coupled chemical (THMC) processes, which are important for predicting migration and transformation of injected CO_2 , evaluating the reservoir performance, and assessing the risk associated. Based on the Terzaghi consolidation theory, a coupled mechanical module is developed and is incorporated into the existing simulator TOUGHREACT, which is a well-established code for THC processes in subsurface flow systems. We have performed numerical simulations of the coupled THMC processes during and after the CO₂ injection period using the modified simulation tool. Geological and geochemical conditions from the Orods CCS demonstration project are utilized.



Fig. 1 Approach for coupled THMC processes

The effects caused by variations in temperature, pressure, stress and strain, and rock chemistry have been investigated. The migration and transformation of CO₂ between different forms, effects of injection on reservoir porosity and permeability due to change in temperature and stress and water-rock-gas interaction, and its feedback to injection are analyzed. The results show that pressures increase in the system with more at the top of reservoir resulting from gravity-driven accumulation of CO₂ along the top of reservoir. The maximum pressure occurs in the vicinity of injection well after a few years' injection. The increase in pressure leads to decrease in effective stress, which alters the reservoir porosity and permeability. This stress-dependent permeability changes have a positive effect on the CO₂ injection because it's favorable for pressure dissipation. The reduction in effective stress also would induce possible rock shear-slip failure in the lower part of the caprock. The mechanical effect reduces after the injection period because the CO₂ spread and dissolution into formation water makes the pressure buildup decrease. However, the effect of water-rock interaction on CGS begins to increase with time. Gas trapping decreases, but solubility trapping and mineral trapping increase. The mineral trapping is sensitive to the



Fig. 2 Conceptual model and results comparison for one-dimension consolidation (a) Pressure (b) Displacement

primary minerals which contain significant Ca, Mg, and

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Fig. 3 Characteristic of Shiqianfeng-Liujiagou reservoir-caprock formations and conceptual model for THMC processes (a) Shiqianfeng-Liujiagou reservoir-caprock formations (b) Conceptual model for THMC processes

Table1. Governing equations for THMC coupled processes

Description	Main Equations	_ 1n-
Multiphase Fluid and Heat	$\frac{d}{dt} \int_{V_n} M^{\kappa} dV = \int_{\Gamma_n} \mathbf{F}^{\kappa} \bullet \mathbf{n} d\Gamma + \int_{V_n} q^{\kappa} dV$	-
Flow (TH)	Left-Hand: $M^{\kappa} = \sum_{\beta=A,G} \phi S_{\beta} \rho_{\beta} X_{\beta}^{\kappa}, \kappa = w, i, g$ $M^{\kappa+1} = (1-\phi)\rho_{R}C_{R}T + \sum_{\alpha} \phi S_{\beta} \rho_{\beta} u_{\beta}$	
Mechanics (M)	Right-Hand: $\mathbf{F}_{\beta}^{\kappa} = -k \frac{k_{r\beta} \rho_A}{\mu_{\beta}} X_{\beta}^{\kappa} (\nabla P_{\beta} - \rho_{\beta} \mathbf{g}) + \mathbf{J}_{\beta}^{\kappa}, \kappa = w, i, g \mathbf{F}_{\beta}^{\kappa+1} = -\lambda \nabla T + \sum_{\beta} h_{\beta} F_{\beta}$	
	Change in Effective Stress: $\Delta \sigma_x' = \Delta \sigma_y' = -\frac{v}{1-v} \alpha_P \Delta P + \frac{5K(1-2v)}{1+v} \alpha_T \Delta T$ $\Delta \sigma_z' = -\alpha_P \Delta P$	
	Change in Average Effective Stress: $\Delta \sigma_M' = \frac{1}{3} \frac{(1+v)}{(1-v)} \alpha_P \Delta P - \frac{2K(1-2v)}{(1+v)} \alpha_T \Delta T$ Vertical Strain: $\varepsilon_z = -\frac{1+v}{1-v} \alpha_T \Delta T - \alpha_P \Delta P \frac{(1+v)}{3K(1-v)}$	
Solute Transportation (C)	$\frac{d}{dt} \int_{V_n} M^{\kappa} dV = \int_{\Gamma_n} \mathbf{F}^{\kappa} \bullet \mathbf{n} d\Gamma + \int_{V_n} q^{\kappa} dV$ Left-Hand: $M_j = \phi S_1 C_{j1}$ Right-Hand: $F_j = u_1 C_{j1} - (\tau \phi S_1 D_1) \nabla c_{j1}$ $q_j = q_{j1} + q_{js} + q_{jg}$	
Geochemical Reaction	1.Definition of geochemical system: $S_i = \sum_{j=1}^{N_c} v_{ij} S_j$	
(C)	2.Conservation of component: $T_j = c_j + \sum_{k=1}^{N_x} v_{kj} c_k + \sum_{m=1}^{N_p} v_{mj} c_m + \sum_{n=1}^{N_q} v_{nj} (c_n^0 - r_n \Delta t_r) = T_j^0$	

Fe such as chlorite.

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Thermal-Hydrodynamic-Mechanical-Key words:



Fig. 4 Change in pressure induced by CO₂ injection



Fig. 5 Gas saturation after 20 years' CO₂ injection (a) Not considering Mechanical effect (b) Considering Mechanical effect

Chemical Processes, CO₂ Geological Sequestration, Numerical Simulation

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