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The influence of impurities on CO_2 storage capacity within saline aquifers using 3-D simulation

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Summary

Investigating the uncertainty of carbon dioxide (CO_2) storage capacity is an essential prerequisite for de-risking geological carbon storage, as it directly impacts the success of CCUS projects. Due to impurities of CO_2 from different capture and separating processes, the density and viscosity of gas mixes varies, and the storage capacity is affected by the minor components. This study aims to analyze the phase variation of impurities in the CO_2 stream and their solubility in brines to identify actual sensitivities of CO_2 storage capacity. The main physical properties of CO_2 stream, e.g. density and viscosity, are investigated under different impurity scenarios. The PVTsim Nova CCS package is used to conduct the CO_2 phase behavior and brine solubility calculation, and co2lab module in the MRST package is added for the gas stream injection and migration simulation. We compared the output with previous laboratory experimental results to verify the reliability of simulation and then created three scenarios with different CO_2 impurities for sensitivity analysis. A reservoir model was created for analyzing the dynamic CO_2 storage mechanisms in saline aquifers. The total capacity and status components of three scenarios show the decrease of storage capacity and a higher ratio of free CO_2 plume as CO_2 concentration increases. The analysis of injection and migration simulations of different CO_2 mixes provides useful input for assessing an accurate CO_2 storage capacity and its reliability over the reservoir lifespan.

Background and Method

Using common assessment methods based on reservoir rock properties without considering phase variation of injected CO_2 stream will lead to a large uncertainty in the real storage capacity (IEA, 2011). Research on the dynamic variation of impurities in the CO_2 stream is needed to reduce the uncertainty in storage volume, and further numerical simulation on fluid properties in reservoir formations after CO_2 injection is an important step for long-term storage integrity.

In industrial operations, the captured CO_2 from different sources is impure, and includes various gases such as N_2, O_2, Ar, H_2O, and SO_2. These impurities negatively affect its phase property and thus reservoir storage capacity. In previous studies, the storage of impure CO_2 stream was discussed based on experiments and numerical simulation (IEA GHG, 2011; Wang et al., 2015). Wang et al. (2015) discovered the effect of impurities in oxyfuel flue gas on CO_2 storage with no-condensable impurity gases and studied the impact of impurities on the storage capacity of CO_2 in geological formations and density behaviors.

For short-to-medium periods of storage, deep saline aquifers provide the best CO_2 storage potential compared to other methods. In Canada, current estimate of carbon storage capacity in saline aquifers is around 360 Gt. Studying the physical properties of impurities and analyzing their impacts on the CO_2 stream will advance the understanding of gas impurities on regional storage capacity estimation in brine storage system. To better understand the problem, modelling phase change and simulating the injection/migration of an impure CO_2 stream for storage are necessary to make sure the CCUS system works seamlessly and is cost effective.

The fluid property simulation is conducted with PVTsim Nova CCS package for CO_2 impurity analysis, which was developed in response to growing industry demand for carbon capture and

storage (CCS) simulation technology. This CCS module offers specialized models to simulate and understand complex phase equilibrium problems related to CCS. It provides features that make a robust solution for modeling and evaluating CO_2-rich systems (e.g. pure CO_2, impact of impurities, CO_2 brine solubility), that supports nine variations of the Peng-Robinson (PR) and Soave-Redlich-Kwong (SRK) cubic equations of state (EoS) with constant or temperature dependent volume translation (Calsep, 2024). The models are thoroughly validated against experimental data relevant to CCS, ensuring the accuracy and reliability of the simulations for CCS applications.

In this study, the PR-Peneloux equation of state (EoS) is used to predict the thermodynamic properties of the CO_2 stream with impurities. The PR EoS equation is expressed as: $P = \frac{RT}{V-b} - \frac{a(T)}{V(V+b)+b(V-b)}$, where R is universal gas constant, a and b are the parameters for the EoS (Peng and Robinson, 1976). The cubic plus association (CPA) is used by combining cubic EoS with an association term; and the Peneloux volume correction is added with a constant to tune density in operating region of PT space, $c = V^{SRK/PR} - V^{Exp}$. The components, N_2, Ar, O_2, H_2O are considered as CO_2 impurities and three different impurity levels are added to each scenario. Physical characteristics (density, viscosity) and effect of solubility to mixed impure CO_2 in brine saline aquifers are simulated with PVTsim, then the calculated fluid analysis data and reservoir parameters are used as initial inputs for reservoir simulation to estimate storage mechanisms and capacity.

The MATLAB Reservoir Simulation Toolbox (MRST) (Nilsen et al., 2015; Lie and Møyner, 2021), developed by a research group at SINTEF, was used for injection/migration simulation in this study. MRST is an open-source software that features multiple discretization schemes for simulating multiphase flow in porous media. The numerical simulation model is solved using the multiscale nonlinear finite volume method for stratigraphic and unstructured grids. This toolbox includes many features typically found in commercial simulators and workflow tools. MRST currently provides three main methods for simulating the long-term trapping in field-scale geologic carbon sequestration (GCS) sites: 1) Vertical-equilibrium (VE) models (co2lab-ve); 2) Full-scale solvers (ad-blackoil); and 3) Multi-model approaches (hybrid-ve) (Saló-Salgado et al., 2024). Fluid density, a thermodynamic property, is determined by solving the simultaneous pressure and temperature equation of state. In this study, we used the co2lab-blackoil module for simulations with a thermodynamic model to calculate PVT properties of CO_2-brine mixtures without considering mineralization.

Results

1. Property simulation of impure CO_2 stream

Focusing on the influence of physical properties, three scenarios with different CO_2 impurity levels (99.5%, 94.5%, 89.5%) are created for PVTsim simulation and comparison. Figure 1 illustrates the relationship between the physical properties of CO_2 streams, temperature, and pressure. The top row shows density variation, and the bottom row displays viscosity variation. The first column is the generated pressure-temperature phase diagram of density and viscosity for pure CO_2, other three columns are the differences with three scenarios. One can see the density and viscosity decrease as impurity from high-purity to low-purity, the average variation at pressure 300 bar is around 10%. Additionally, the CO_2 mix is highly sensitive to changes of reservoir temperature and pressure at certain points. Based on the analysis of property variation, impurities will affect CO_2 storage capacity in geological formation and cause a large reduction at specific temperature and

pressure points. The CO_2 solubility is plotted at the pressure 300 bar with temperature range of 15 ºC to 150 ºC (Figure 2). In general, the CO_2 solubility decrease along with the impurity increasement at same temperature, which would affect solubility trapping in brine.

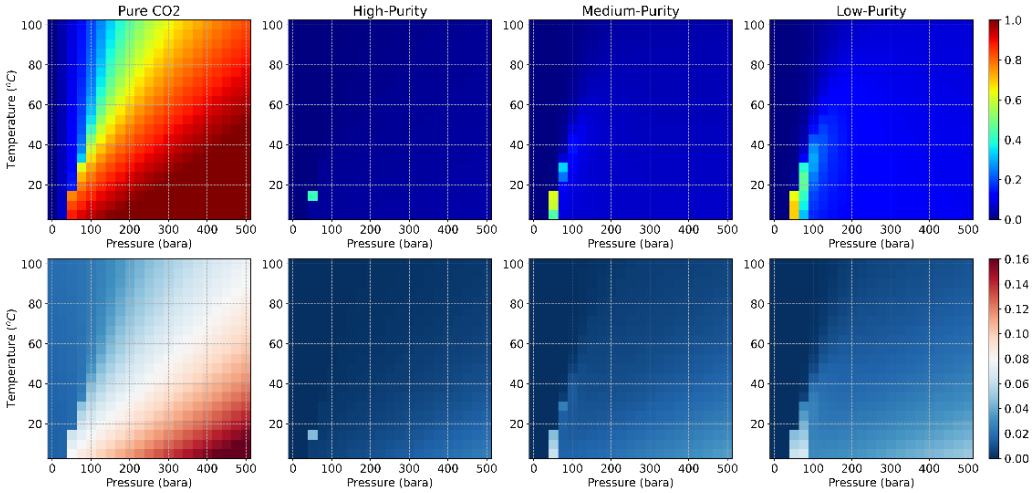

Figure 1. Calculated density (top) and viscosity (bottom) with different pressure-temperature of impure CO_2 (units: g/cc and mPas).

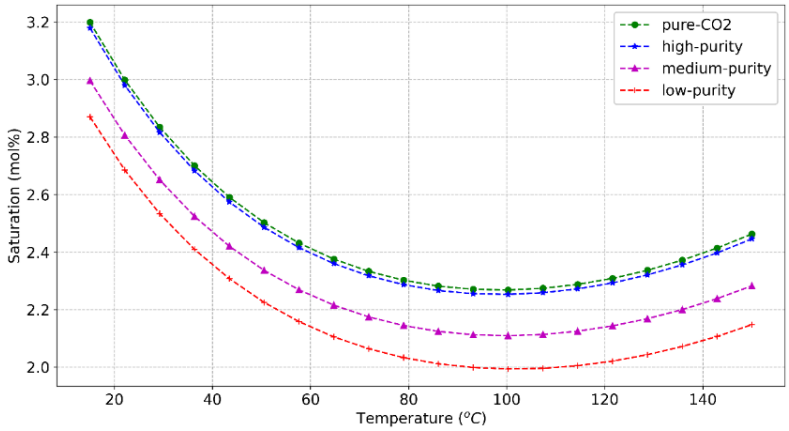

Figure 2. Solubility with different CO_2 impurity levels (pressure 300 bar).

2. Storage mechanisms and capacity simulation

Based on the physical properties from PVTsim simulation with previously defined impurity parameters, the initial fluid phase models are created. The three scenarios are used to simulate the reservoir model. The model size is 5 km by 10 km, with a variable cell size for mesh gridding, and two faults are incorporated into the model. Some reservoir parameters are based on the Deadwood Formation in the Williston Basin (Hau et al., 2024). The average reservoir depth is 3.0 km with a thickness of 150 meters; porosity is 0.1; permeability is 100 mD with anisotropy vertical-to-horizontal permeability ratio 0.1 kv/kh; initial viscosity is 0.05 mPas; the reference pressure and temperature are 300 bar and 95 ºC; initial injection rate 60 cubic liter per second for 25 years, and 100 years migration period.

Figure 3(a, b, c) displays the CO_2 distributions at different time points including the initial injection, end of injection, and post-injection migration via buoyancy. The CO_2 saturation varies as

supercritical CO_2 migrates along the formation. During post-injection period, the free plume rises to the top of the reservoir due to its lower density. Figure 3(d) displays the storage trapping mechanisms from the median-purity, that shows around 30% CO_2 are residual trapped. The total storage capacity ratios for the different scenarios are listed in Table 1. The storage ratios are 4.1%, 4.42%, and 4.73%. The high purity CO_2 stream occupies more pore space because of its denser property. The effective porosity for scenario-3 is larger than the scenario-1, and the lower density and viscosity result in faster updip plume migration because carbon dioxide becomes less mobile. The CO_2 impurities in the investigated range had negative effect on plume migration, impacting the front depth of CO_2 migration in the reservoir.

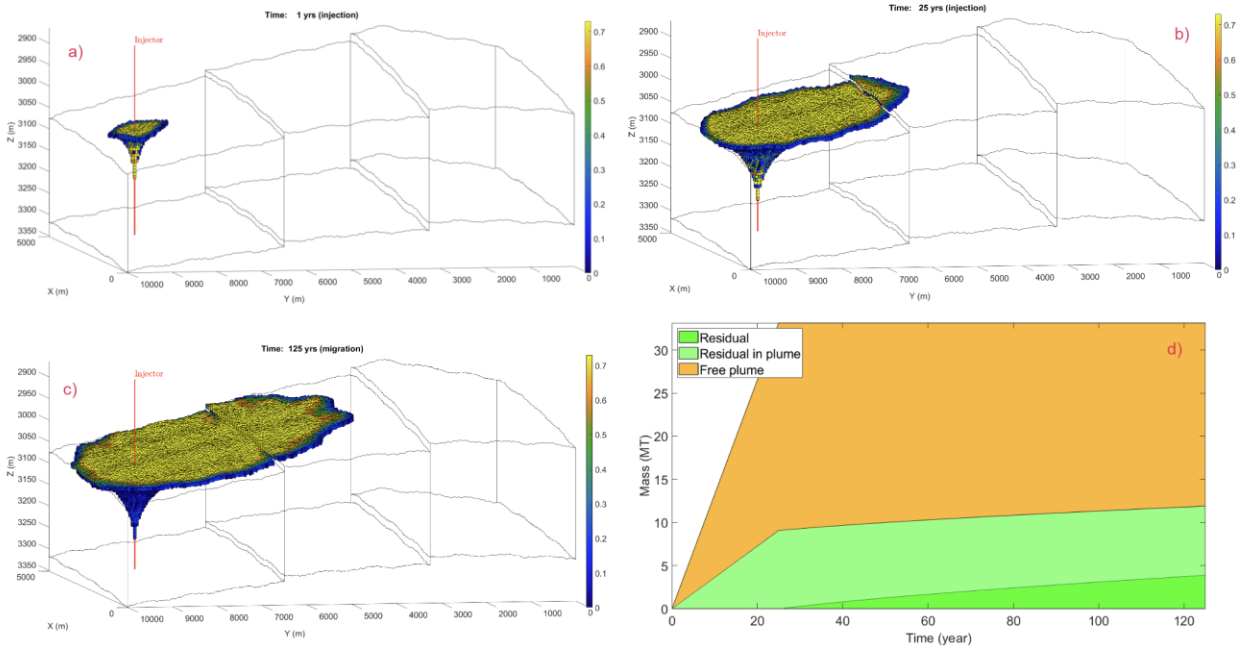

Figure 3. The reservoir modelling results, (a, b, c) CO_2 saturation at 1, 25, and 125 years); (d) the final main storage mechanism.

Table 1. The PVTsim parameters and simulated output with MRST toolbox.

CO_2 (%)	P (bar)	T (°C)	Density (g/cc)	Viscosity (mPas)	MRST simulation results		
					Residual (kg)	Total storage (kg)	Storage ratio (%)
89.5	300	95	0.5814	0.0469	0.3841e+10	3.0768e+10	4.10
94.5	300	95	0.6220	0.0505	0.3884e+10	3.3135e+10	4.42
99.5	300	95	0.6476	0.0534	0.3915e+10	3.5502e+10	4.73

Conclusions

PVT numerical simulation results in this study indicate both density and viscosity increase with the increasing CO_2 concentration in the scenarios, and the CO_2 solubility in the brine decreases slightly. The impurity of CO_2 will affect dynamic variation of its physical properties that influences the CO_2 stream injection/migration, storage mechanisms ratios, and the total storage capacity. The reservoir simulation output using MRST toolbox and scenario comparison shows the total storage capacity increases with higher purity. The free CO_2 plume decreased during the post-injection, and the trapped volume continues increasing during migration period. The bottom boundary of the free plume is deeper relatively and the 'replaceable volume' in the reservoir increases in the purer CO_2 scenario. The total storage capacity decreases around 13.32%. This

is a preliminary analysis workflow for analyzing CO_2 impurities effect on carbon storage capacity. Further comparison study is necessary by considering the pressure variation as optimizing injection rates and the dynamic variation of storage mechanisms over time for long term storage period in a real geological formation, which will help create more accurate storage prospectivity maps.

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