CO2 injection modeling in an aquifer: Phase transition study

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Abstract. This study analyzes the phase transition and corresponding effects of CO_2 injection in different states underground within the context of Carbon Capture and Storage (CCS). Using tNavigator software, we simulated CO_2 injection in a confined aquifer to reach the transition point at three different temperatures (20°C, 30°C, and 31°C , where the injected fluid is in a liquid state. The results revealed no free gas formation at 20°C. In comparison, gas formation occurred at 30°C and 31°C, with more significant gas formation at the latter due to the reservoir temperature being closer to CO_2 saturation temperature. These findings highlight the importance of temperature and pressure conditions in the safely and efficiently storing of CO_2.

Keywords: phase transition, injection modeling, reservoir, geological storage, carbon management.

1 Introduction

The IPCC's Sixth Assessment Report estimates the chances of exceeding the 1.5°C global warming threshold in the coming decades and concludes that unless there are immediate, rapid, and large-scale reductions in greenhouse gas emissions, limiting warming to around 1.5°C or even 2°C will be beyond reach [1].

Therefore, it is widely recognized that a broad portfolio of emission reduction and carbon management solutions is necessary to reduce and remove CO_2 from the system to meet future emission targets. Some of these technologies are controversial, such as carbon capture, utilization, and storage (CCUS) and carbon capture and storage (CCS). However, these technologies have evolved from primary technologies to become crucial for achieving net-zero emissions after several decades of experience with geological storage projects worldwide. As a result, these technologies have demonstrated that CO_2 can be stored safely under the right conditions with a shallow risk of leakage [2]. However, there is a necessity for simulating CO_2 injection, mainly due to the phase transition that the fluid may undergo during well closure. As pressure variations at the wellhead can influence the state of the injected fluid, when the injection process ceases, the fluid within the reservoir tends to return to the initial confinement pressure condition of the aquifer. Consequently, the pressure reduction can cause the transition of CO_2 from the liquid state to the gaseous state. Thus, liquid-phase CO_2 above a depth of ~300 m within the well will transition to the gaseous phase during the non-injection period [4]. Thus, this study aims to analyze the CO_2 injection process in different underground states by tracking phase transitions and their corresponding effects in the context of CCS when injected into a geological formation, quantifying the safety of the storage process and propagation efficiency [3].

2 Methodology

To investigate the phase transition phenomenon in a post-CO_2 injection scenario,a confined aquifer subjected to three different formation temperature scenarios was modeled: 20°C, 30°C and 31°C, the latter with the objective of reaching the supercritical CO_2 point. In order this, an aquifer model was used to simulate the CCS process, illustrated in Fig. 1 with initialization properties provided in Tab. 1. Pressure conditions along the injection plume were monitored before, during, and after CO_2 injection, considering different injection conditions relative to the reservoir temperature, using the tNavigator simulator. The injection was carried out with CO_2 in the liquid state. To simulate a confined aquifer, the boundary conditions applied over the aquifer bounds were an encroachment of the aquifer structure's water body. The model generated contains 130,174 cells, of which 21,142 actives.

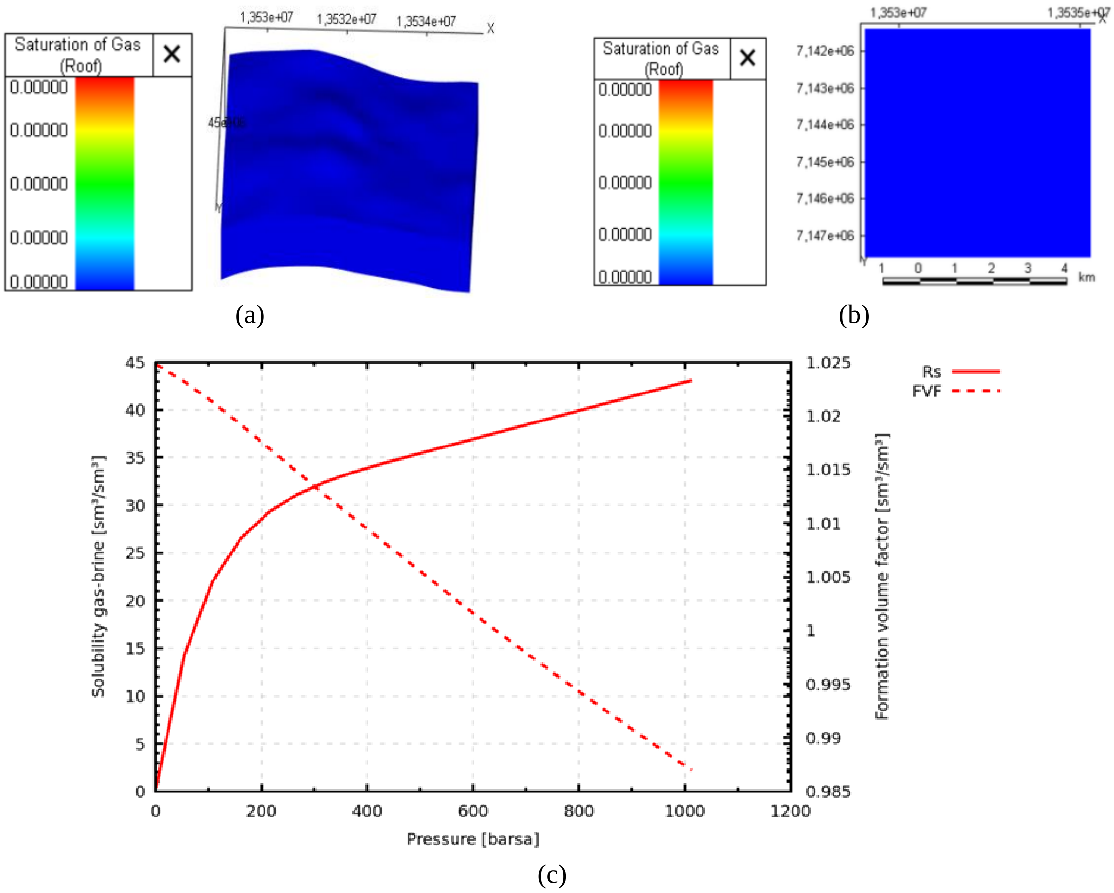


Figure 1. Aquifer Model: (a) Permeability profile, (b) Porosity profile, (c) PVT properties brine and CO_2 in Saturation of Gas Scales.

For our study, the software simulates the two-phase flow of CO_2 and brine, including dissolution at the CO_2-brine interface, using the isothermal compositional model, with thermodynamic properties obtained from the NIST webbook by Linstrom & Mallard, 2024 [5], see Fig. 1(c). Additionally, the process is considered isothermal, with the reservoir temperature in the first scenario being 20°C, in the second scenario 31°C, and in the third scenario 35°C (i.e., CO_2 in the reservoir conditions is in the liquid, liquid, and supercritical states, respectively). The injection rate for the nine injector wells is constant at 10^6 m³/day. The simulation began on March 1, 2013, with wells placed on fifth day of the same month and closed six months after the start of injection. Phase transition analysis occurs during this period after closure until the end of the simulation, assessing whether free gas is generated or not. For the three scenarios simulated at different temperatures reservoir conditions indicated zero gas saturation immediately after closing all wells, as depicted in Fig. 2.

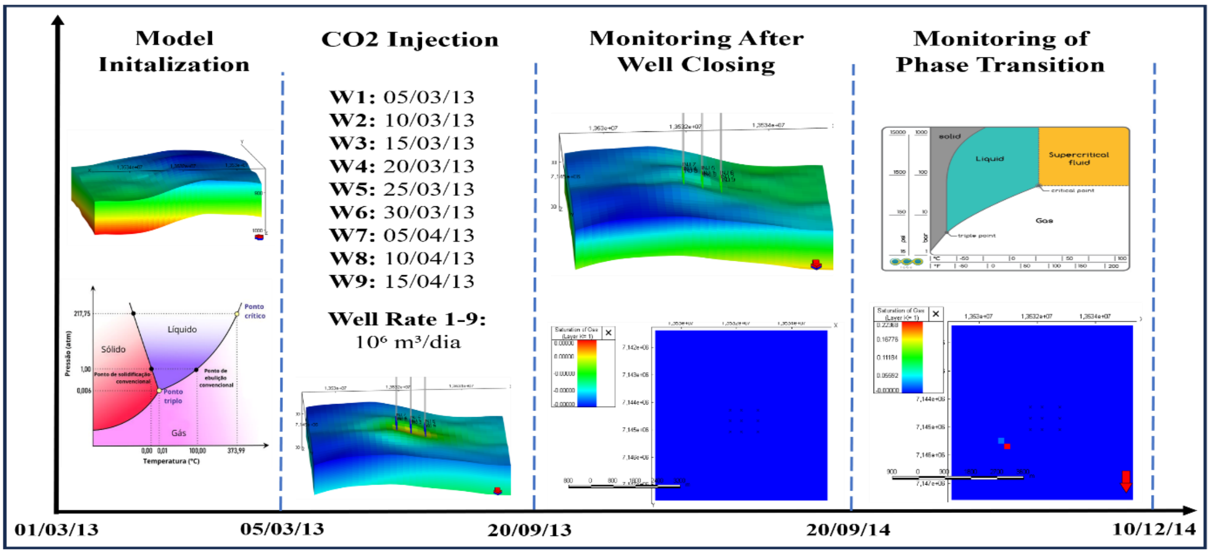


Figure 2. Timeline for First Scenario Simulation

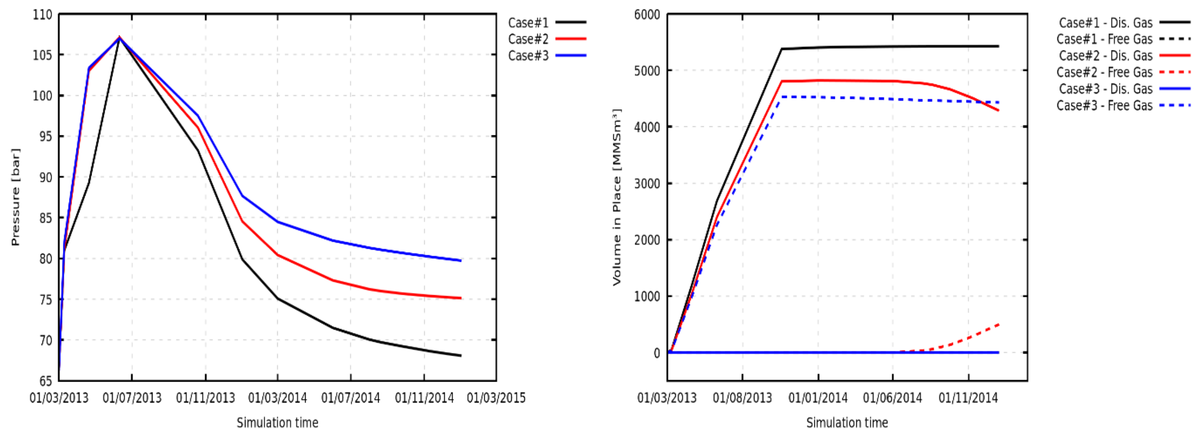
Based on the reservoir and fluid parameters outlined in Tables 2 and 3, an analysis was conducted regarding the pressure behavior within the aquifer after cessation of CO2 injection.

Table 1. Aquifer and CO_2 Properties

Properties	Value
Depth (m)	840 m
Thickness (m)	47,49 m
Pressure (bar)	65 bar
Permeability (mD)	300 mD
Porosity	0,35
Compressibility (bar^{-1})	10^{-6} bar^{-1}
Inner Radius (m)	27000 m
Salt Concentration (g/cm³)	0
CO_2 properties (compositional parameters)	
Phase	Liquid
Critical Pressure (bar)	73,82
Critical Temperature (°C)	304,19
Critical Molar Volume (m³/mol)	0,094
Z Factor	0,2743667
Molecular Weight (g/mol)	44,01
Acentric Factor	0,228

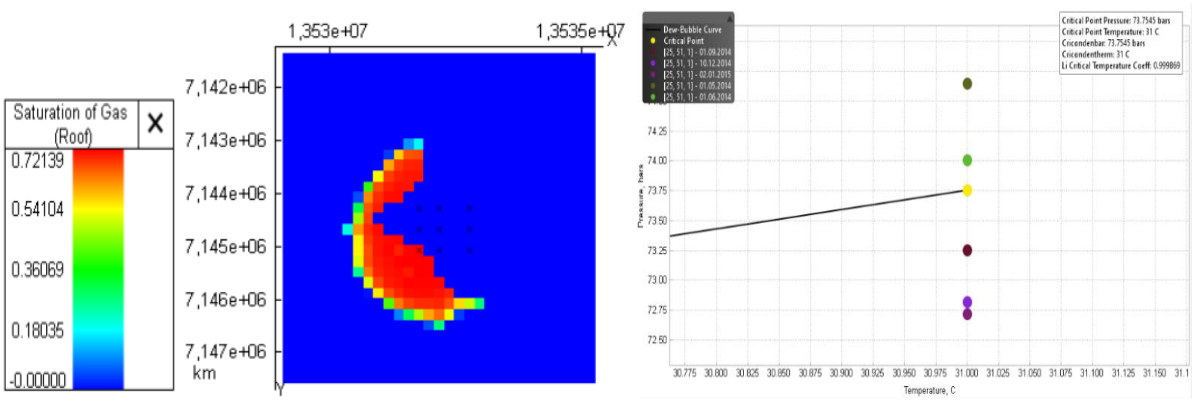
3 Results and discussions

Based on the reservoir and fluid parameters outlined in Tab.1, an analysis was conducted regarding the pressure behavior within the aquifer after cessation of CO_2 injection. The analysis revealed that pressure values within the aquifer decreased significantly after well closure, enabling CO_2 to reach its critical pressure state in two out of three scenarios. This directly correlates with its phase change to the gaseous state, as depicted in Fig. 3.In the postinjection period (i.e., curtailment of CO_2 injection), combined with the restrictions imposed on the aquifer border (water inflow condition), the aquifer pressure tends to return to the confined condition. Thus, the transition from the liquid phase to the gaseous phase is observed through the graphs presented in Fig. 3 for scenarios 1, 2 and 3, considering all the simulation time. According to the PVT analysis, there was no gas formation in scenario 1 (temperature 20°C); despite the confining condition imposed on the aquifer limits, the pressure did not reach the transition point of the bubble/dew point curve. However, in scenarios 2 and 3 (at 31°C and 35°C, respectively), the gas phase appeared at the end of the simulation, as illustrated in Fig. 4 and 5, respectively. The formation of gas is evident through the indication of gas saturation. Due to the difference in the aquifer temperature in scenario 3 (35°C), it was closer to the critical CO_2 temperature than in scenario 2 (31°C). Despite the difference being 4°C, we can say that the temperature and pressure (i.e., type of aquifer: confined or open) are parameters that must be taken into consideration when analyzing the risk of leakage, as such variables facilitate or prevent the liquid gas phase transition phenomenon from occurring earlier.



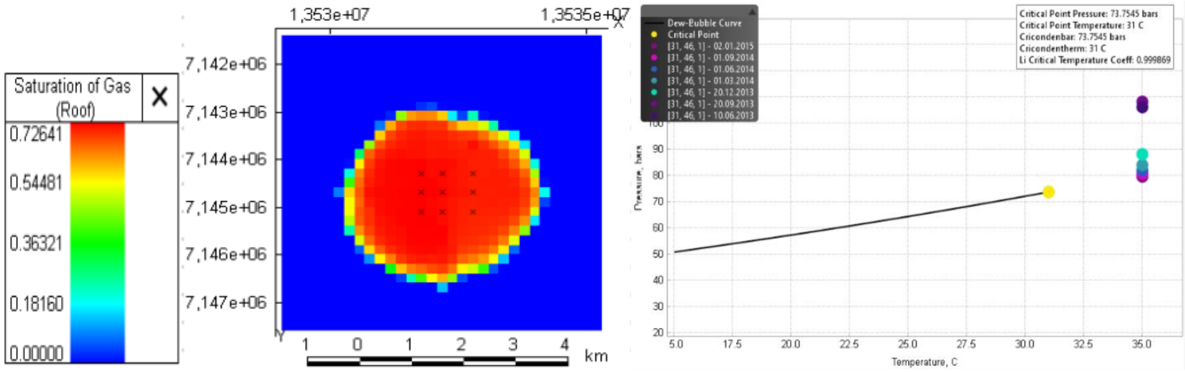
(a) (b)

Figure 3. Transition from the liquid phase to gaseous phase: (a) Pressure Graphs, (b) Volume in Place Graphs.



(a) (b)

Figure 4. Scenario #2: (a) Gas formation in the aquifer at time 02-01-2014 (b) Phase diagram showing phase transition.



(a) (b)

Figure 5. Scenario #3: (a) Gas formation in the aquifer at time 02-01-2014 (b) Phase diagram showing phase transition.

4 Conclusions

In this work, the phase transition of CO_2 from liquid to gas state was evaluated, which occurred due to the reduction in pressure within the confined aquifer, leading to surpassing the critical pressure as depicted in the CO_2 phase diagram. After one year and three months from well closure, concluding injection, free gas formation occurred within the reservoir in scenarios 2 and 3, where the reservoir temperatures were 31°C and 35°C, respectively. This condition arose because the fluid was injected in its liquid state, facilitating the transition. Importantly, injecting in the supercritical state would have resulted in more free gas formation, as the critical pressure to be achieved in the reservoir would have been higher, allowing the reservoir to adjust to this pressure more rapidly after well closure. Another significant factor contributing to this phase change was the constant reservoir temperature in each scenario; the fluid's transition from the bubble\dew point curve to gas phase depended solely on pressure.

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