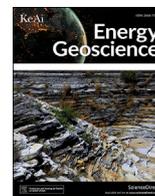




Contents lists available at ScienceDirect

Energy Geoscience

journal homepage: www.keaipublishing.com/en/journals/energy-geoscience

A numerical study to assess the effect of heterogeneity on CO₂ storage potential of saline aquifers

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ARTICLE INFO

Article history:

Received 23 March 2020

Received in revised form

26 March 2020

Accepted 26 March 2020

Keywords:

Aquifer

CO₂ storage

Heterogeneity

Numerical modeling

Performance

ABSTRACT

Many parameters have been indicated crucial for the selection of a saline aquifer as a carbon dioxide (CO₂) storage site. However, less attention has been given to the impact of heterogeneity on the performance of these storage media. Thus, the heterogeneity effect was evaluated in this paper by adopting a numerical modeling approach and the existing screening criterion developed for the aquifers was updated. The updated criterion for CO₂ storage purpose would enhance the confidence level during the selection of deep saline aquifer and thus, help to address the climate change issue. The numerical modeling was carried out via CO2STORE module of Eclipse300 Simulator to evaluate the effect of different levels of heterogeneity on CO₂ storage potential. Different degrees of heterogeneity from homogeneous systems to highly heterogeneous systems in the model were incorporated through the Lorenz coefficient. In this way, simulation of nine cases was carried out for three different aquifers with different porosity values. A comparison of these results showed that heterogeneity causes the aquifer to have lower storage capacity. On the trapping potential, dissolution trapping was significant and the amount of free gas in all cases was minimum. In addition, the aquifer with the highest level of heterogeneity (HLH) had a minimum fraction of residual trapping regardless of porosity. It was also found that final pressure at the end of 30 years is the same and high for low-level heterogeneity (LLH) and medium level heterogeneity (MLH) cases and low for HLH, while the injection rate stability duration is least for HLH and maximum for LLH. Based on the results obtained, it can be concluded that low to medium level heterogeneous aquifers with a good porosity can be a suitable choice for CO₂ storage.

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1. Introduction

Fossil fuel consumption has resulted in a significant increase of greenhouse gases in the atmosphere, depletion of the ozone layer

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<https://doi.org/10.1016/j.engeos.2020.03.002>

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and climate change (Raza et al., 2018, 2019a). Low-emission techniques might be a good replacement for conventional fuels but may need decades for implementation in countries such as India, USA, and China since the huge reserves of fossil fuels is remarkably contributing to economic growth (Blunt, 2010). To control this situation, many ways have been proposed to decrease the amount of CO₂ from the atmosphere including carbon capture and storage (CCS) method (IPCC, 2005) which has the ability to mitigate 17% of CO₂ emissions into the atmospheric by 2050 (Edenhofer, 2015). In 1977, it was suggested that CO₂ could be captured from the coal power plant and injected into suitable geological formations (Marchetti, 1977). In the last decade, the first CO₂ storage project was initiated in Statoil, Norway (IPCC, 2005). IEA stated that there

should be an initiation of more carbon capture and storage projects that would help to ensure the achievement of the targeted CO₂ emission reduction (IEA, 2020).

The CCS technology includes capturing CO₂ from the emissions sites such and power plants by post-combustion, pre-combustion, oxy-fuelling, or chemical looping, transport to the storage sites by the pipelines and inject in depleted reservoirs, saline aquifers or coal beds permanently (Bennaceur et al., 2008; IPCC, 2005; Leung et al., 2014; Moazzem et al., 2012; Raza et al., 2016; Songolzadeh et al., 2014). Given the important issue of climate change, the aim of this research is to unfold unaddressed areas in the CO₂ storage in the aquifer by investigating the effect of heterogeneity on CO₂ storage performance, and to update the existing screening criterion.

2. Different aspects of CO₂ storage sites

Along with the various steps of the CCS process, the stage of site selection and characterization is mandatory to ensure that the site chosen has a (Bachu et al., 2009): (i) good storage capacity; (ii) favorable injectivity; and (iii) good containment (Bachu et al., 2009; Chadwick et al., 2008; Raza et al., 2016). Here, storage capacity depends on a number of factors including reservoir/aquifer characteristics, storage operation and regulatory constraints (Celia et al., 2015). For instance, aquifer characteristics, such as pressure, temperature, water salinity, depositional environment, lithology, porosity, permeability, heterogeneity, compressibility, areal extent, thickness, dip, topography and boundaries (open, semi-open, or closed) have a different impact on the fate on the storage capacity (Al-Khdheawi et al., 2018; Celia et al., 2015; Chadwick et al., 2008; Goater et al., 2013). Among these, the aquifer boundary condition is very important for the storage potential of open aquifers since their large lateral extent can are to store a huge amount of CO₂ compared to closed or semi-closed aquifers (Bachu, 2015). Low vertical permeability anisotropy hinders the upward movement of CO₂ (Bachu, 2015), and the water-wet formations are the best condition to store a large amount of CO₂ (Al-Khdheawi et al., 2018). On top of that, pore-throat size distribution affects the CO₂ distribution and thus CO₂ storage capacity is often high in the heterogeneous medium compared to a homogeneous medium due to dispersed flow paths (Hovorka et al., 2004).

Injectivity (ability to inject a fluid) is a time-dependent (flow rate) concept (Bachu et al., 2007). For injectivity, several factors need to be considered such as permeability of the aquifer, heterogeneity of the aquifer, pressure build-up, fracture pressure, capillary entry pressure, seal rock properties and integrity, injection rate, number and distribution of wells and types of wells (Birkholzer et al., 2009; Buscheck et al., 2012; Peysson et al., 2014; Raza et al., 2015b). A favorable permeability is a prime factor to achieve good injectivity. In low permeability reservoirs, the problem of high-pressure build-up can be resolved by increasing the number of wells (van der Meer and Yavuz, 2009) or by taking water production to increase the injectivity and storage capacity (Wessel-Berg et al., 2014). High heterogeneity in the pore-throat size distribution affects the CO₂ distribution and flooding processes (Wei et al., 2014). During injection, there are four main mechanisms through which the CO₂ is trapped in underground formations (IPCC, 2005). These mechanisms are classified as structural when CO₂ remains as free gas (Benson and Cole, 2008; Espie, 2005; Saeedi, 2012; Zhang and Song, 2014), residual when CO₂ is capillary trapped (Pentland et al., 2011; Zhang and Song, 2014; Zhao et al., 2014), dissolution when CO₂ is dissolved in resident fluid (Iglauer, 2011; Ketzer et al., 2012; Zhang and Song, 2014) or mineral, when dissolved CO₂ reacts with rock (Benson and Cole, 2008; Saeedi, 2012; Zhang and Song, 2014). The relative contribution of these

mechanisms, however, depends mainly on a number of factors. For instance, structural trapping depends on pressure, temperature conditions, heterogeneity, and pore geometry (Benson and Cole, 2008; Espie, 2005; Saeedi, 2012; Zhang and Song, 2014). Residual trapping is a function of rock and fluid properties as well as injection rate and reservoir conditions, particularly, heterogeneity (Raza et al., 2015a). Dissolution trapping is sensitive to the variation of pH and concentration of different ions in pore fluid (Solomon, 2006), the mineral trapping on the other hand depends mainly on pressure, temperature, pH, geochemical conditions, and activity of the cations dissolved in water (Ketzer et al., 2012).

Containment is the significant aspect that comes into play once CO₂ is injected. If proper sealing or containment is not present or injection pressure cross the threshold of sealing fracture pressure, then the injected gas can be leaked into other formations, causing environmental contamination or escape of CO₂ back to the surface (Raza et al., 2019b). Top surface topography (structural closures, channeling, and dipping) and caprock thickness also has a prevailing influence on the containment ability of the sealing rock (Goater et al., 2013). Different types of dissolution reactions occur in the caprocks while some of them provide further containment and some act opposite to the trapping ability. Dissolution of dolomite, K-feldspar and dehydration reactions of shale and slate mitigate the capability of the sealing rock to contain CO₂ (Rochelle et al., 2004). High permeability path in sealing rock will provide a path for saline water to escape through it and CO₂ will remain trapped due to higher capillary entry pressure (Birkholzer et al., 2009).

From the above studies, it is evident that a substantial amount of work is required to identify a suitable aquifer for CCS operation. Given the importance of heterogeneity on the storage capacity (Hovorka et al., 2004), trapping mechanisms (Raza et al., 2016), CO₂ distribution and flooding processes (Wei et al., 2014), the degree of storage potential for a relatively boarder spectrum influencing parameter such as geologic heterogeneity requires further investigation. The aim of this study is to assess the impact of heterogeneity on CO₂ storage potential by developing a numerical modeling approach.

3. Modeling of CO₂ storage in aquifer

3.1. Simulation approach

The purpose of this paper is to evaluate the effect of heterogeneity on different aspects of CO₂ storage sites. CO2STORE dynamic numerical modeling which is part of the Schlumberger Eclipse300 Simulator was used to carry out this study. CO2STORE module is

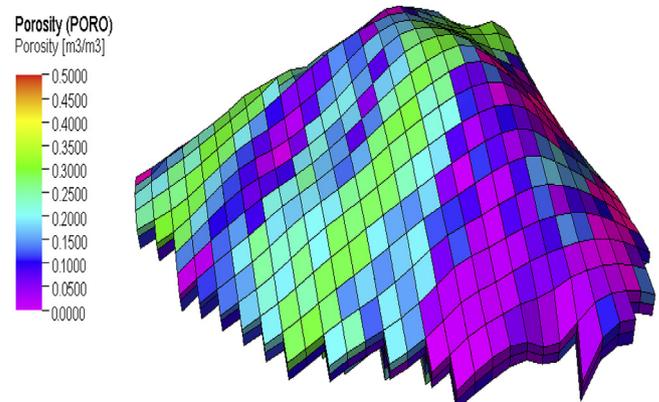
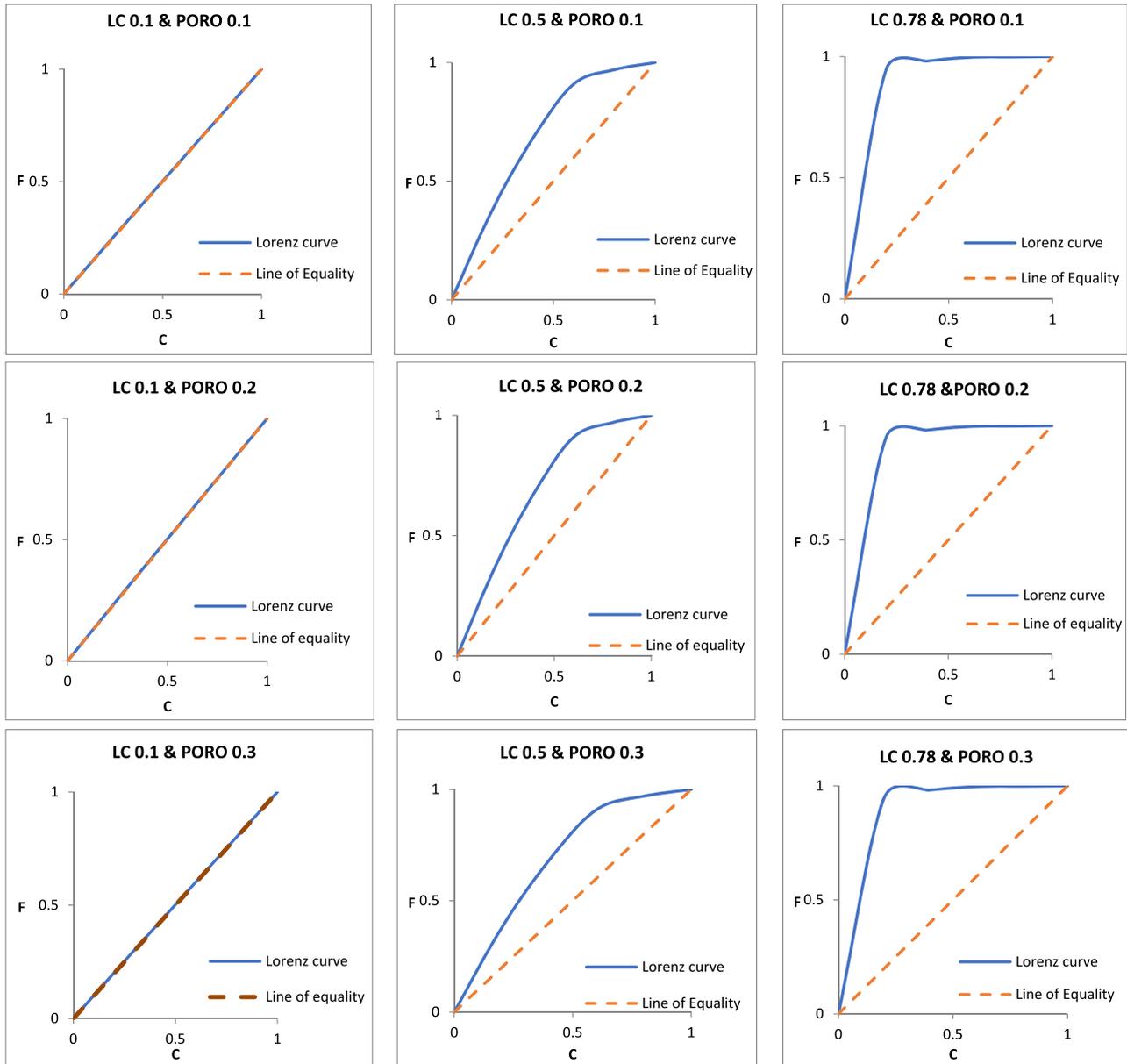


Fig. 1. Plot of porosity distribution in CO2STORE Model.



Lorenz coefficient 0.1 showing low level of permeability heterogeneity

Lorenz coefficient 0.5 showing medium level of permeability heterogeneity.

Lorenz coefficient 0.78 showing high level of permeability heterogeneity.

Fig. 2. Lorenz coefficient showing different levels of permeability heterogeneity in the aquifer models.

specifically designed for CO₂ operation.

The aquifer was a 3D model from our previous study (Raza et al., 2017) as shown in Fig. 1. This aquifer was assumed to be an anticline model with no-flow boundaries. It consists of five layers of equal thicknesses (5 m). The aquifer was composed of 2660 cells, 19 in the X direction, 28 in the Y direction and 5 in the Z direction. The x and y dimension of each block is 180 m. The top of the aquifer was at 2000 m to achieve the supercritical condition for carbon dioxide. Porosity and permeability considered are assigned to model after Lorenz coefficient calculations. Injection well was in the middle of the aquifer. The temperature of the aquifer was 100°F while the initial pressure was 278 bars at 2000 m. Carbon dioxide was injected in the aquifer for a period of 30 years at the initial rate of 5.66 million Sm³/day. The aquifer model used in this study has the compressibility of $5 \times 10^{-4} \text{bar}^{-1}$. Gas and brine densities (effect of

salt and CO₂) were also determined by the utilization of equations of state and Ezzokhi's methods. Molecular diffusion was considered at the beginning of injection for the creation of the diffusive flow (Schlumberger, 2014).

The relative permeability and capillary pressure curves were generated using the Corey and van Genuchten correlations as expressed by Eqs. (1)–(3) (Raza et al., 2017).

$$k_{rw} = \left(\frac{S_w - S_{wr}}{1 - S_{wr}} \right)^4 \quad (1)$$

$$k_{rg} = k_{rg-\max} \left(1 - \frac{S_w - S_{wr}}{1 - S_{wr} - S_{gr}} \right)^2 \quad (2)$$

Table 1The criteria proposed by (Chadwick et al., 2008) and modified by adding parameters in Sr. 11–12 to screen aquifer for CO₂ storage.

| Sr. No. | Parameters | Positive Indicators | Cautionary Indicators |
|---------|--------------------------|--|--|
| 1 | Total Storage Capacity | Total Capacity of reservoir estimated to be much larger than the total amount produced from the CO ₂ source | Total capacity of reservoir estimated to be similar or less than the total amount produced from the CO ₂ source |
| 2 | Depth | 1000–2500 m | <800m or >2500m |
| 3 | Thickness (net) | ≥ 50m | <20m |
| 4 | Porosity | >20% | <10% |
| 5 | Permeability | >300mD | 10–100mD |
| 6 | Salinity | >100 g/L | <30 g/L |
| 7 | Seal Properties | | |
| 8 | Lateral Continuity | Un-faulted | Laterally Variable Faults |
| 9 | Thickness | >100 m | <20 m |
| 10 | Capillary Entry Pressure | Much greater than buoyancy force of maximum produced CO ₂ column high | Similar to buoyancy force of maximum produced CO ₂ column height |
| 11 | Aquifer boundary | Open Aquifer | Closed or semi-closed Aquifer |
| 12 | Aquifer heterogeneity | -Low to medium level heterogeneous aquifer having good porosity (upto 30%) is better for storage of CO ₂ | - High heterogeneous aquifer having low porosity (upto 10%) is less efficient for storage purpose. |

$$P_c = P_o \left[\left(\frac{S_w - S_{wr}}{1 - S_{wr}} \right)^{\frac{1}{\lambda} - 1} - 1 \right]^{1-\lambda} \quad (3)$$

In the above equations, k_{rw} and k_{rg} are the water and gas relative permeability, respectively, S_w is the water saturation, S_{wr} is the residual water saturation, S_{gr} is the residual gas saturation, k_{rg-max} is the maximum gas relative permeability, P_c is the capillary pressure, P_o is the capillary entry pressure and λ is the capillary pressure exponent.

Permeability heterogeneity can be found by a dimensionless factor named as Lorenz coefficient (Schmalz and Rahme, 1950). To do that, permeability values for different layers of subsurface formations need to be arranged in descending order. Then the product of permeability and thickness of each layer is calculated which is known as flow capacity (kh). Similarly, volume capacity is calculated which is the product of porosity and thickness. A plot of normalized cumulative flow capacity (kh) and normalized cumulative volume capacity (ϕh) is plotted on a Cartesian plot. There is a line of equality and a line of Lorenz curve on the plot. The area between the two lines shows the value of the Lorenz coefficient which is ranging from 0, for a completely homogeneous system, to 1 for a completely heterogeneous system (Ahmed, 2018). Permeability heterogeneity was then added to the aquifer model Level of heterogeneity was depicted by the values of Lorenz coefficients in each case which is 0.1 for the least heterogeneous aquifer, 0.5 for the intermediate one and 0.78 for the highly heterogeneous system. For three aquifer models, Lorenz coefficients were calculated to find the degree of heterogeneity as a total of nine cases shown in Fig. 2. After the calculation of Lorenz coefficients, simulation of the aquifer model was done for three cases of heterogeneities with three levels of porosities i.e., Case A-0.1, Case B-0.2 and Case C-0.3 fractions as illustrated in Table 1.

4. Results and discussion

4.1. Sensitivity analysis at a different level of heterogeneity

In this section storage capacity, trapping mechanisms, injection rate stability time, and pressure buildup for all three cases of heterogeneities are compared at different levels of porosities in the aquifer model. Fig. 3 shows the result obtained from these three cases of heterogeneities at the porosity of 0.3. As it is seen, the total

amount of CO₂ injected varies with heterogeneity level and goes high in the medium-level heterogeneity (MLH) while stays low in the high-level heterogeneity (HLH). On the trapping potential, dissolution trapping is a significant and a minor fraction of free gas was observed in all cases. Comparatively, residual trapping potential is high in the LLH medium with a value of 89.5 million kg-mole, dissolution trapping is high in the MLH with 359 million kg-mole, and free CO₂ fraction is very high (57.6 million kg-mole) in the MLH medium. In addition, the aquifer which has the highest level of heterogeneity has the minimum fraction of residually trapped. It was also observed that the final pressure at the end of 30 years is the same at 479 bar for the LLH and MLH cases while the injection rate stability duration is low for the HLH which shows the impact of heterogeneity on the storage capacity.

Fig. 4 shows the result of the three cases of heterogeneities at porosity 0.2. From the figure, it is seen that there is not a such significant effect of heterogeneity at the porosity of 0.2 on the storage capacity. However, the trend of storage capacity and trapping mechanism is the same as the one presented earlier for the porosity of 0.3. The fraction of mobile gas is different but as the years of injection passes, the free gas fraction declines gradually for all the cases. Free gas is low in the LLH medium and high in the HLH medium. Oppositely, capillary trapped CO₂ has the highest fraction in the aquifer with the LLH and the HLH aquifer has a comparatively minimum amount of immobile gas. As for the Lorenz coefficient of 0.1, the fraction of trapped carbon dioxide was 66.6 million kg-mole while it was 43.7 million kg-mole in the Lorenz coefficient of 0.78. Solubility trapping plays a very vital role in the storage of injected gas. For the homogenous aquifer, solubility has the least value, but have the higher amount of trapped CO₂ in the solution with MLH and HLH. For the solubility trapping, there is only a small difference among aquifers with different levels of heterogeneity. It was also evident from Fig. 4 that the final pressure at the end of 30 years and the injection rate stability duration trends are the same as the one reported for the porosity of 0.3.

Fig. 5a shows the result of the three cases at the porosity of 0.1. From the figure, it is seen that there is not a significant effect of heterogeneity at the porosity of 0.1 on the storage capacity. Total CO₂ injected varies with the heterogeneity level and goes low in the LLH scenario and high in the HLH case. However, the trend of trapping mechanisms is the same as the one presented earlier. The amount of free gas is low for the LLH and high for the HLH but with minor differences. Residual trapping was high in the LLH model and low in the HLH model. The amount of dissolved CO₂ for the highly

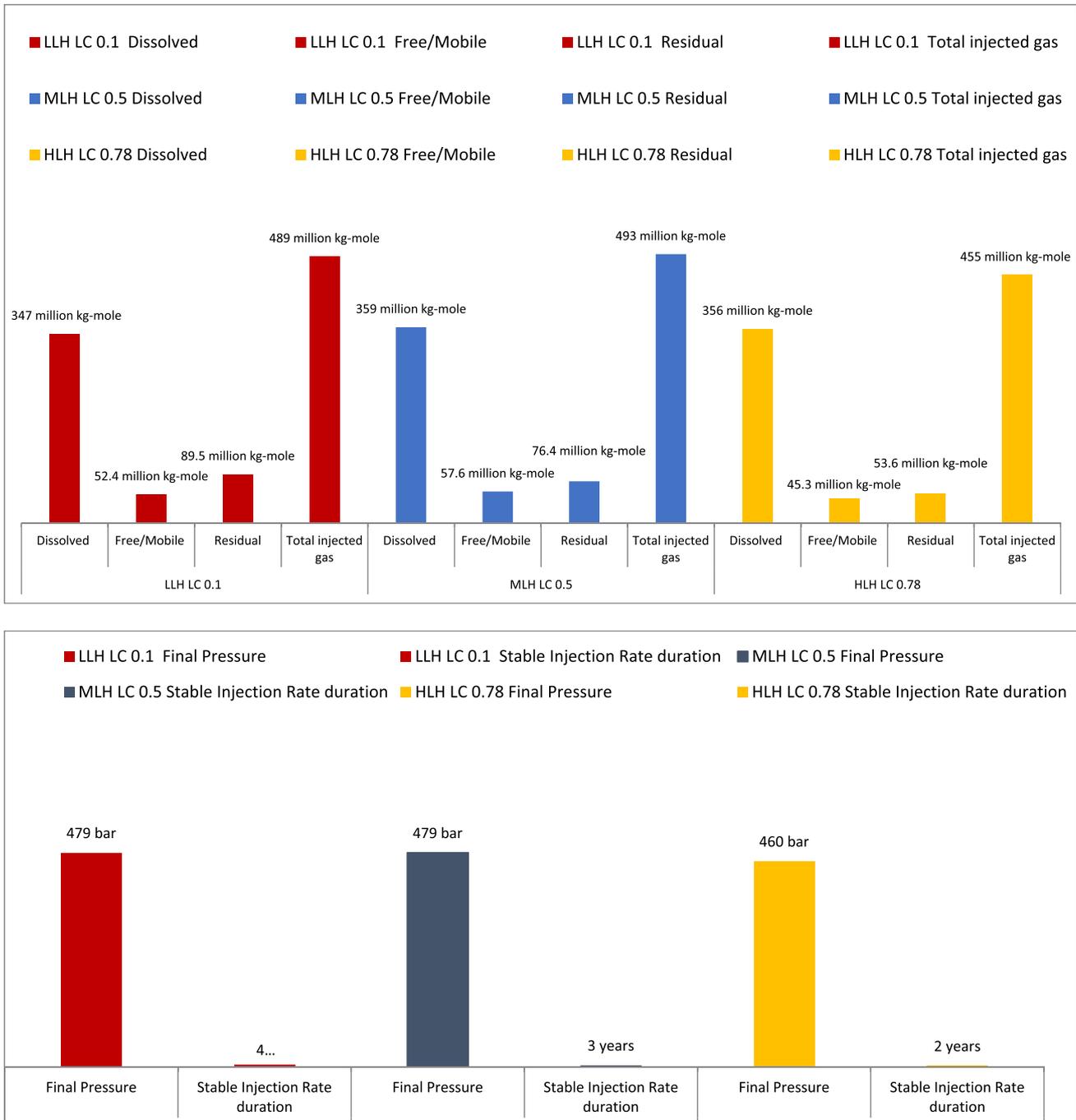


Fig. 3. Comparison of the storage capacity, trapping mechanisms, fraction of the final pressure and injection rate stability for different levels of heterogeneities in the aquifer with the porosity of 0.3.

heterogeneous aquifer (HLH) was also high while the opposite observed in the aquifer with the LLH. It was also observed that the final pressure at the end of 30 years and the injection rate stability duration trends are the same as the previous cases but with a lesser threshold.

5. Updating existing screening criteria

The screening criterion proposed by Chadwick et al. (2008) was the first one distinguishing different aquifers for the storage purposes. It was a very useful criterion, but there is a need to update this screening criterion by including the aquifer boundary and

heterogeneity aspects. This updated criterion covers most of the parameters based on the literature review as given in Table 1. The updated criterion for CO₂ storage purpose would enhance the confidence level during the selection of deep saline aquifer and thus, may contribute to addressing the climate change issue.

6. Conclusions

The degree of reservoir heterogeneities has a major impact on the storage potential. Heterogeneity calculation was performed using the Lorenz coefficient by numerically simulating three levels of heterogeneities (low, intermediate and high) for CO₂ storage in

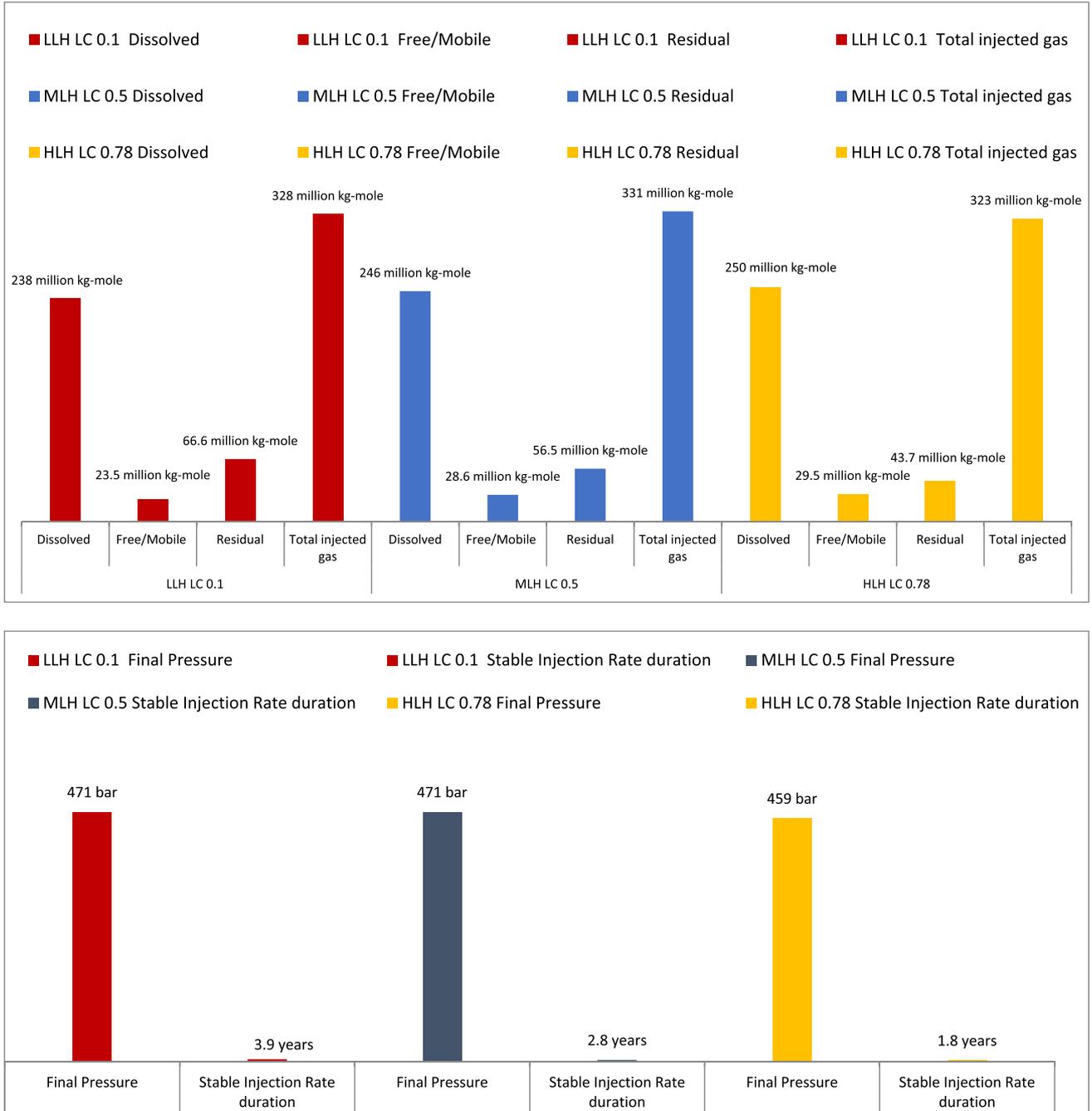


Fig. 4. Comparison of storage capacity, trapping mechanisms, fraction of final pressure and injection rate stability for different levels of heterogeneities for aquifer with porosity 0.2.

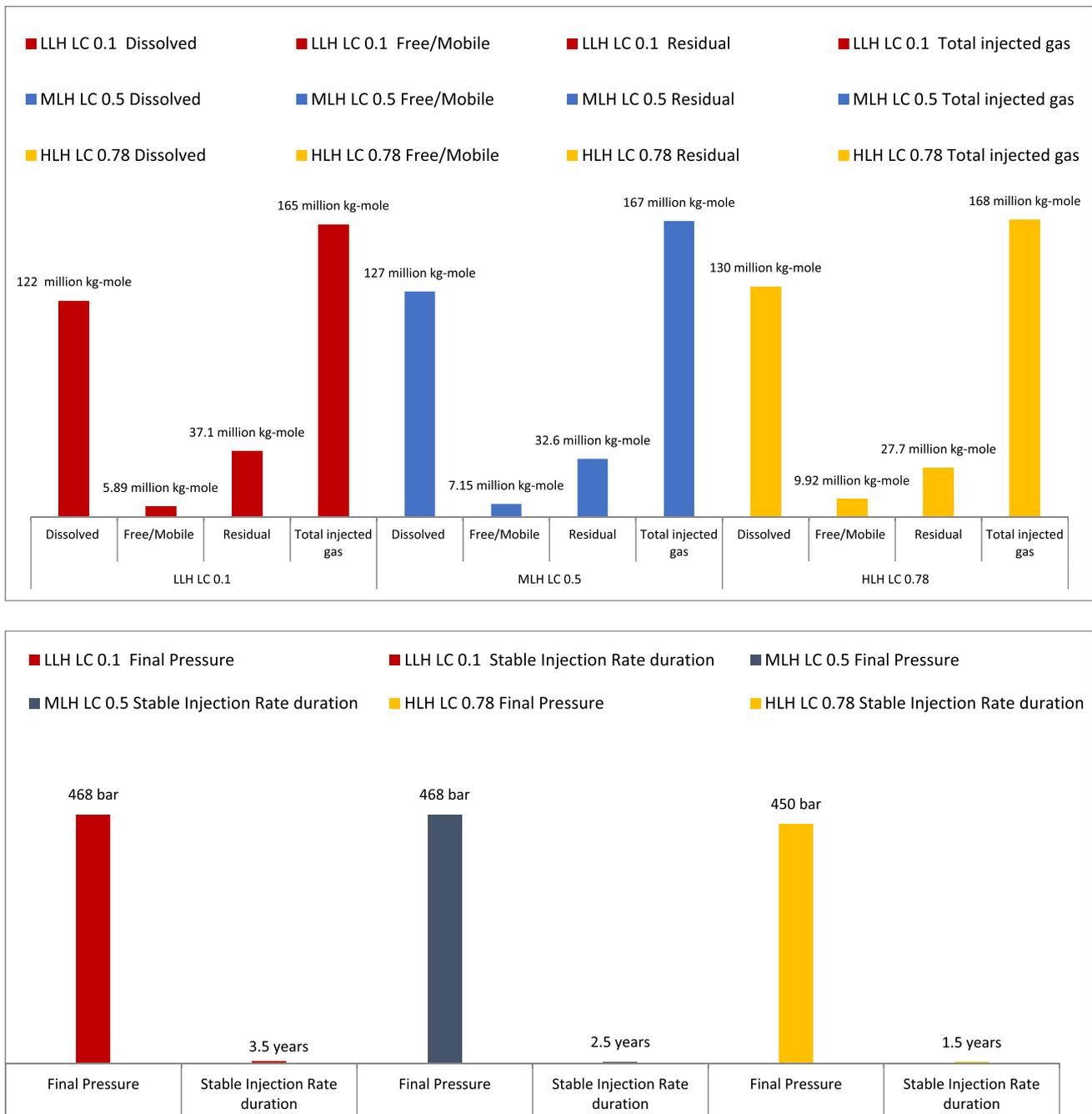


Fig. 5. Comparison of storage capacity, trapping mechanisms, fraction of final pressure and injection rate stability for different levels of heterogeneities for aquifer with porosity.

an aquifer model. A comparison of these results showed that heterogeneity causes the aquifer to have lower storage when porosity changes. It was also observed that the dissolution trapping is significant with the least amount of free gas in all models. In addition, the aquifer which has the highest level of heterogeneity could have a minimum fraction of residually trapped gas. It was also found that final pressure at the end of 30 years is the same and high for low-level heterogeneity (LLH) and medium level heterogeneity (MLH) cases and low for HLH, while the injection rate stability duration is least for HLH and maximum for LLH. It was concluded that a good porosity (>20%) aquifer with low-level or medium level of heterogeneities is suitable for CO₂ storage.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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