



Numerical modelling of the effects of permeability contrasts on underground hydrogen storage in sandstone reservoirs

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Abstract: Hydrogen is an energy carrier that can balance the divergent variations in seasonal energy demand and energy supply from renewables. Underground hydrogen storage in porous formations, such as depleted gas sandstone reservoirs or saline aquifers, provides the capacities needed for large-scale, long-duration energy balancing. This paper reports on the fundamental behaviour of hydrogen in a model reservoir setup, involving a two-phase (H₂, water) system and a two well (injector, producer) setup placed at different depths in the reservoir. We specifically focus on the impact of natural heterogeneities, and associated permeability contrasts, on flow and efficacy of hydrogen injection and production. We found that positioning the wells, both injector and producer, at the top of the reservoir facilitates the highest hydrogen production. We also found that permeability contrasts of three to four orders of magnitude significantly affect hydrogen flow; however, factors affecting the pressure gradient also need to be considered. These factors include compartmentalization, the behaviour of co-existing fluids and the localized pressure gradient created by the hydrogen plume. Our research underlines the need to understand the architecture of the whole reservoir, from seismic to sub-seismic scales, not just the zones surrounding the wells and pathways in-between, as this controls capacity, pressure fluctuations and informs operational management decisions.

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Underground hydrogen storage (UHS) can provide large-scale energy storage suitable for applications such as industrial processes (including production of ammonia or steel), transportation, reconversion to electricity and domestic heating in some circumstances (IEA 2023a). Hydrogen can balance energy demand and supply from intermittent renewable energy generators and, as such, many governments have adopted hydrogen as part of their future energy mix (de Coninck *et al.* 2018; AusGov 2019; UKGov 2020; IEA 2021; USGov 2021).

To ensure sufficient capacity and availability of hydrogen, to balance seasonal supply and demand, the gas needs to be stored. Underground storage provides ample capacity, building upon decades of experience from subsurface natural gas storage, a proven technology for supplying methane at scale (Scafi *et al.* 2021). Even storing hydrogen gas in the subsurface is not new. Hydrogen is a key constituent of town gas (composed of hydrogen, methane, nitrogen and carbon monoxide) with historical underground reservoirs in Teesside (UK), Texas (US), Beynes (France), Lobodice (Czech Republic) and 7 sites in Germany (Hydrogen TCP-Task 42 2023). Near-pure (95%) hydrogen has been stored successfully in the subsurface in salt caverns, e.g. Teesside (UK) and Texas (US), but the HYBRIT project will expand UHS options by constructing a lined rock cavern (LRC), a purpose-excavated cavern lined with concrete and steel to ensure that it is gas-tight, with the gas used for major industrial processes (Pei *et al.* 2020; Hydrogen TCP-Task 42 2023). However, the volumes of gas that can be stored in salt caverns and LRCs limit the use of hydrogen or require a significant number of repositories to be constructed. For instance, the HYBRIT LRC is expected to store up to 100 GWh and it is estimated that 56 salt caverns will be required to store 8 TWh (Mouli-Castillo *et al.* 2021; LKAB 2022). For scale, by 2050 the UK Government predicts that between 250–460 TWh of hydrogen

will be needed to meet Net Zero targets. In contrast the expectation is that the worldwide demand would be over 13 PWh (UKGov 2021; IEA 2023b).

Sandstone reservoirs offer storage volumes that are up to two orders of magnitude larger than the largest salt caverns, and are geographically more widespread (Heinemann *et al.* 2021; Mouli-Castillo *et al.* 2021; Aftab *et al.* 2022). There are two types of sandstone storage, saline aquifers and depleted hydrocarbon reservoirs. Saline aquifers are less commonly used for gas storage and, as a result, lack geological data, which is both time consuming and expensive to acquire (Tarkowski 2019). Hydrocarbon reservoirs account for the bulk of global natural gas storage (80% of working volumes in 2019: Cedigaz 2020), benefitting from lower geological uncertainties and existing infrastructure that can be repurposed for transporting hydrogen (Tarkowski 2019; Kanaani *et al.* 2022). The first underground storage site to have 100% hydrogen injected into sandstone, utilizing a depleted gas field at Gampern (Austria), recently became operational in April 2023 (RAG 2023).

However, most of our current knowledge of gas storage in porous reservoirs is limited to methane and carbon dioxide. Hydrogen storage in porous media needs further exploration due to its different physical and chemical properties. Hydrogen is a smaller, more mobile molecule, and we do not fully understand how hydrogen behaves alongside other fluids present in a reservoir, particularly in relation to the heterogeneities within a potential sandstone reservoir. In addition, hydrogen has a lower energy density (energy per unit volume) than natural gas, requiring increased storage to accommodate the same quantity of energy so that the suitability of additional storage may need to be explored (Hashemi *et al.* 2021). Additional capacity is also necessary due to the requirements of balancing seasonal supply and demand (Gasanzade *et al.* 2021; Mouli-Castillo *et al.* 2021).

Further understanding of how hydrogen behaves when it is injected and stored in different media is required, particularly as it migrates through heterogeneous subsurface reservoirs. In this respect, we examine how heterogeneity, specifically contrasting permeabilities, affect the injection, plume development and recovery of hydrogen in UHS.

Potential effects of contrasting permeability

Permeability contrasts are created by both sedimentary and structural processes and can either define the reservoir by establishing its boundaries, such as a tight caprock or a sealing fault, or can create barriers or compartments within the reservoir. Sedimentary features can result in architecture of varying complexity and include interbedded (layer-cake), jigsaw or labyrinthine arrangements, and sedimentology can be a strong influence on fluid flow through such rocks. The more complex arrangements are characterized by adjoining sandstone layers, interspersed with non-continuous, low-permeability strata (Lawrence *et al.* 2006). Faulting is a structural feature that can have multi-scale impacts, affecting or defining part or the whole reservoir (decimetre to kilometre scale), whereas deformation bands are examples of structures that are more likely to have localized effects (millimetre to decimetre scale) but that still impact upon pressure, plume integrity and gas recoverability (Leveille *et al.* 1997; Wakefield *et al.* 2022). Some sedimentary and structural features can be resolved by seismic mapping or be detected from core data. However, many features that create permeability contrasts are below seismic scale and may be abundant within potential porous storage media, such as deformation bands within well-sorted, aeolian facies, or are more extensive than survey data suggests (Leveille *et al.* 1997; Wakefield *et al.* 2022).

Compartments can diffuse or trap fluids, affecting pressure and fluid movement and ultimately can reduce the effective storage volume and efficiency of the reservoir. The effects of compartmentalization have been recognized at both the large, reservoir or aquifer-scale (up to kilometre scale), and at the centimetre, core-scale for water, hydrocarbons and CO₂ but have not been studied in relation to UHS (Leveille *et al.* 1997; Mohamed and Worden 2006; Pourmalek *et al.* 2021). This study provides a gateway into the effect of features created by permeability contrasts at the metre to kilometre-scale.

Utilising Darcy's equation of flow, the low viscosity (μ) of H₂ indicates that the flow rate (u) remains relatively unaffected by pressure gradients (∇P) unless there is a significant change in permeability (k) by several orders of magnitude (equation 1):

$$u = -\frac{k}{\mu} \nabla(P) \quad (1)$$

This observation, eponymously called 'Flora's rule' by Ringrose and Bentley (2021), predicts three orders of magnitude variation in permeability to observe an impact upon hydrogen flow. We test that prediction using models that quantify the influence of reservoir heterogeneity in a gas-liquid-rock system. We simulate hydrogen storage in an aquifer, as a depleted hydrocarbon reservoir would also contain gas, adding a further dimension to the simulations, obscuring the outcomes.

Plume integrity, the ability of the gas plume to remain connected, is also potentially affected by heterogeneity. Maintaining a coherent plume is important because more hydrogen can be recovered and less will be lost to processes such as diffusion and dissolution (Amirthan and Perera 2022). Diffusion and dissolution are not included in this study, to reduce confounding variables when determining the effect of heterogeneity, but viscous fingering, the unequal progression of the injected fluid, is one of the processes being monitored. Viscous fingering leads to the loss of integrity of

the plume and is often predicted using the mobility ratio (M) of the two fluids involved. The mobility of each fluid is defined as the effective permeability for that fluid, the product of absolute permeability (k_a) and relative permeability (k_{rH_2} for hydrogen and k_{rw} for water), divided by its viscosity (μ_{H_2} for hydrogen and μ_w for water). This is used to create a ratio between the fluids, such that (Pan *et al.* 2021),

$$M = \frac{\{(k_a k_{rH_2}) / (\mu_{H_2})\}}{\{(k_a k_{rw}) / \mu_w\}} = \frac{k_{rH_2} \mu_w}{k_{rw} \mu_{H_2}} \quad (2)$$

Viscous fingering is therefore a function of both the fluid and rock properties. The former establishes that fingering is more likely to occur in two phase systems when there is a large viscosity difference between the fluids, such as hydrogen and water. The rock properties control the fluid interaction by modifying contrasting permeabilities, which in turn influence the relative permeabilities of the fluids. There are only two experimental studies that have observed hydrogen flow in a two-phase system with sandstone rock that includes a permeability contrast (Boon and Hajibeygi 2022; Jangda *et al.* 2023). Boon and Hajibeygi (2022) describe their layered sample in terms of its porosity and did not make specific findings about the effect of the low porosity on fluid flow; they measured relative permeability across the aggregate of the layers, although the water saturation images across the core during drainage and imbibition highlight some of the effects of low permeability. Jangda *et al.* (2023) found that preferential pathways are established through low permeability layers and that those layers can reduce storage capacity.

Permeability contrasts are integral to a number of UHS modelling studies, due to the reservoir architecture, particularly in feasibility studies or research utilizing studied rock formations (for instance, Pfeiffer *et al.* 2017; Lubon and Tarkowski 2020; Lysy *et al.* 2023). However, studies that systematically altered permeability contrasts to observe their impact upon hydrogen production are limited (Arekhov *et al.* 2023). Here, they undertook a sensitivity analysis of permeability contrasts to determine their effect upon diffusion within UHS. They found that diffusion increases with an increase in permeability contrasts.

We examine the effect of permeability contrasts in the context of UHS at the metre to kilometre scale to determine their effect on flow, plume development and hydrogen injection and recovery. This, in turn, will provide an insight into the reservoir architecture that impacts upon the efficacy of UHS and prescribe what information is pertinent when assessing potential reservoirs. It is our aim to determine the fundamental behaviours of hydrogen in a two-phase system in relation to permeability contrasts so that the findings can be applied to a range of UHS scenarios.

Method

Modelling concept

In this study, we use different combinations of well placements in a series of layered geological models with increasing permeability contrasts with the aim of understanding the effect of heterogeneity in a two-phase (H₂-water) reservoir. In addition to observing the fluid pathways, we quantify the effect of permeability contrasts using hydrogen and water production forecasts, average reservoir pressure and bottom-hole pressure (BHP). We particularly study how heterogeneity affects plume integrity and structural trapping, which both impact upon reservoir effectiveness (Aftab *et al.* 2022). We use the Computer Modelling Group (CMG) reservoir simulator (version 2021.10) to build the reservoir models and the GEM software to run the fluid flow simulations. The Peng-Robinson (Robinson and Peng 1978) equation of state is used to calculate the relationship between the fluids.

Our aim is to conduct generic, non-site-specific research, so that the findings can be applied to understand the behaviour of hydrogen in different UHS settings. Although we use an analogue for porosity and permeability data for our geological models, our study is not intended to investigate the analogue formation's suitability for UHS and does not include a detailed analysis of its geology. The analogue we use is from the Jurassic Navajo sandstone at Green River, Utah, used previously for studying natural CO₂ accumulations (Kampman *et al.* 2014). Figure 1 shows the stratigraphy, porosity and permeability data of the Navajo sandstone from a borehole drilled near Crystal Geyser. The geological models replicate the thickness of the Navajo sandstone unit (85 m), although a hydrodynamically connected layer has been added at the base to simulate aquifer support (a further 10 m but the volume has been artificially increased). There are no-flow boundaries in all other directions. The plan-view area (2.25 km²) and the depth at which they are situated (1000 m at the top of the reservoir) were chosen to be similar to other hydrogen reservoir models to give them comparable representative reservoir properties such as temperature, pressure and capacity (Feldmann *et al.* 2016; Mahdi *et al.* 2021). In this study, the term 'reservoir' refers to the four zones, simulated from the properties of Navajo sandstone, above the aquifer-like zone. The approximate location of the zones, based upon the permeability properties and facies type of the Navajo sandstone, are shown in Figure 1.

The vertical heterogeneity of the models is increased by inserting a low permeability zone (LPZ) at one of two depths, in between zones 1 and 2 or zones 2 and 3, to maximize the permeability contrasts observed. The permeability range of the LPZs (10 – 10⁻⁵ mD) covers permeability from one order of magnitude below the highest permeability in the models to that of tight rocks like mudstones (Ringrose and Bentley 2021). The range also enables the

Flora's rule prediction (see above) to be tested as the lowest permeability is 4 orders of magnitude below the permeabilities of the least permeable layers in the basic models (0.24 and 0.32 mD); one order of magnitude more than the prediction. Although the lateral and continuous properties and uniformity of the LPZs are exaggerated they force the reservoir fluids to interact with the permeability contrasts. This enables us to observe and understand the effects of those contrasts.

In relation to the dynamic modelling, we use a universal Brooks–Corey, relative permeability relationship (described further below), as in the studies conducted by Pfeiffer *et al.* (2016), Lubon and Tarkowski (2020), Mahdi *et al.* (2021) and Chai *et al.* (2023), where they used either the Corey-type or Van Genuchten–Mualem relationships in their models. We also used a single drainage relative permeability relationship for both drainage and imbibition, so our results do not take account of effects that arise when different relative permeability relationships are used for the two processes (Lysy *et al.* 2023). After preliminary analysis we have not included capillary pressure data within our models as their effects on the simulation outputs were small, particularly in high permeability reservoirs, and other studies look at this phenomenon in more detail (for instance, see Wang *et al.* (2022) for the effects of capillary pressure on fluid flow and recovery factor).

Our flow simulations focus on addressing the impact of vertical permeability contrasts at the metre to kilometre scale on effective cyclical hydrogen storage for a single, central injection or production well, rather than optimizing reservoir performance in terms of well count, injection or production pressures, and hydrogen or water production. Therefore, we do not use pre-operational cushion gas as it would mask the effects of the permeability contrasts on hydrogen distribution in our geological models. As a result, we permit conditions which would otherwise be unrealistic

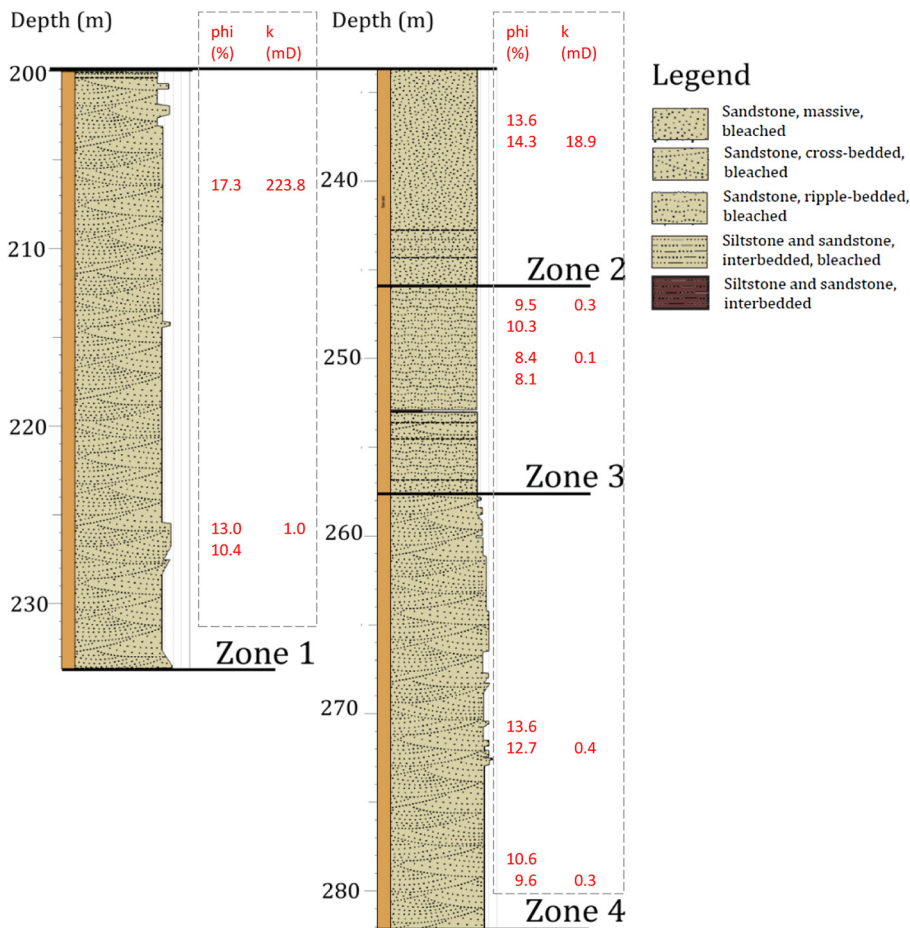


Fig. 1. Digitised core log of Navajo sandstone from borehole CO₂W55 with the approximate zonation of the analogue for the geological models shown. The approximate location of the porosity and permeability measurements, taken from core samples, are also shown (red writing within the dashed grey rectangle). Adapted from Kampman *et al.* (2014) © 2014, with permission from Elsevier. Porosity and permeability values were determined with a standard device using nitrogen as a working fluid. These values were the basis for the porosity and permeability values used in our geological models.

and uneconomic, such as allowing the BHP to increase to 1000 MPa during injection or reduce to atmospheric pressure during production. The former parameter, in relation to injection, enable the same amount of hydrogen to be injected into each reservoir simulation, so that simulation outputs can be directly compared. The latter limit allows the effects of the fluid flow in relation to the permeability contrasts to be observed, otherwise production well shut-in would be almost immediate for a number of scenarios, inhibiting the creation of pathways.

Previous studies have tested various operational strategies from a single three-year injection and one-year production cycle to ten cycles of eight months injection and four months production (Mahdi *et al.* 2021; Zamehrian and Sedae 2022). We chose four cycles, the first three mimic seasonal supply and demand and have an eight-month injection to four-month production period ratio. This provides sufficient time for the hydrogen to migrate into the reservoir and view the impact of permeability contrasts between zones. During the first three cycles, more gas is injected than recovered, resulting in an accumulation of gas until the last production period which showcases how heterogeneity within the reservoir can impact the distribution and availability of hydrogen in line with previous studies (Lysy *et al.* 2021; Kanaani *et al.* 2022; Zamehrian and Sedae 2022). To observe ultimate hydrogen recoverability, we chose a fixed final production period that prevented any models from maintaining a required production rate throughout the cycle. This consequence may also be observed in previous production cycles if insufficient gas is available to the producer, i.e. if it has been trapped or dispersed beyond the influence of the producer.

Chemical reactions and anaerobic digestion play a crucial role in ensuring the success of hydrogen storage but are not considered in this study. There are detailed discussions on these processes in publications by Pan *et al.* (2021), Aftab *et al.* (2022), Muhammed *et al.* (2022), and Miodic *et al.* (2023).

Reservoir model

To start we compare a basic heterogeneous model with a basic homogenous model. This comparison will show if there are any observable effects of metre-scale layering when cycling hydrogen through a reservoir. Both models have the same physical dimensions (Table 1 and Fig. 2) but where the basic homogenous model uses the formation arithmetic average values for porosity (11.64%) and permeability (35 mD), the basic heterogeneous reservoir has four layers with thickness, permeability and porosity

Table 1. Shared properties of the basic models

Parameter	Value
Dimensions	1500 m × 1500 m × 95 m
Cell number ($i \times j \times k$)	15 × 15 × 95
Cell volume multiplier for lowest 10 rows	10 000
Depth range	1000 – 1095 m
Initial pressure at 1000 m depth	10 MPa
Reservoir temperature	50°C
Rock compressibility	$5.8 \times 10^{-4} \text{ MPa}^{-1}$
Average porosity	11.64%
Average permeability (excl. low permeability layers)	34.96 mD
Initial water saturation	100%
Injection rate	$300\,000 \text{ Sm}^3 \text{ d}^{-1}$
Target withdrawal rate	$500\,000 \text{ Sm}^3 \text{ d}^{-1}$
Dip of strata	0° (horizontal)

The injection and production flow rates are based upon volumes at standard (atmospheric) pressure.

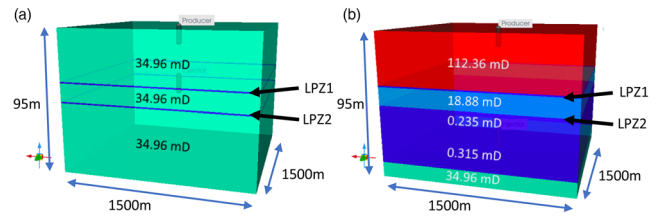


Fig. 2. 3D representations of the permeability distribution in the two basic models: (a) homogeneous and (b) heterogeneous. See Table 2 for more information about the zones. The dark blue horizontal lines indicate where the low permeability zones (LPZs) are positioned in the second part of the study, although only one LPZ is activated at a time.

reflecting those of the four main Navajo zones (Fig. 1 and Table 2). We use arithmetic average values for porosity and permeability within each zone of the basic heterogeneous model such that there are strong contrasts between zones, creating an array of vertical permeability contrasts but no grid-scale heterogeneity within each zone (Table 2). Both models have no-flow, Neumann-type boundaries on all sides and at the top of the reservoir, to represent a reservoir compartment with sealing faults and a low permeability caprock. In addition, we include a high-volume, bottom-drive aquifer, providing some pressure support and storage volume for displaced reservoir fluids (zone 5, Table 2). We generate the additional volume in the bottom 10 m of the reservoir by artificially increasing the capacity of each cell by a factor of 10 000, enabling the layer to accommodate a significant volume of fluid, which can potentially be exchanged with the adjacent layer, zone 4 (Table 2).

A well is drilled through the centre of the reservoir and includes a dual completion for different stratigraphic injection and production zones, i.e. the same well can inject and produce H_2 from either the same or different zones of the reservoir. Each completion covers 12 meters of vertical stratigraphy so that we can place both the injection and production completions entirely within zone 2, which is important to observe the impact of the vertical heterogeneity on reservoir performance, including the additional heterogeneity incorporated in the complex models (see below). Completions are placed in one of three positions; at the top (between 1000 – 1012 m), middle (1035 – 1047 m) and base (1073 – 1085 m) of the reservoir. We avoid injecting into the aquifer layer (zone 5). Keeping the production well above or at the same level as the injection well, there are six completion designs for both the basic homogeneous and basic heterogeneous models (see Fig. 3). These 12 models are called the ‘baseline models’, against which we assess the impact of increased heterogeneity on reservoir performance.

For the next step, we create complex homogeneous and heterogeneous models. To do this heterogeneity is increased in the 12 baseline models by introducing a 1 m thick, low permeability zone (LPZ) at the base of zone 1 (1034 – 1035 m) or zone 2 (1047 – 1048 m) (Fig. 2). Only one LPZ is activated at a time in different

Table 2. Properties of zones 1–4 that act as the reservoir for the basic heterogeneous model

Zone	Thickness (m)	Porosity (%)	Permeability (mD)
1	35	13.55	112.36
2	13	13.95	18.88
3	7	9.07	0.235
4	30	11.61	0.315
5	10	11.64	34.96

Zone 5 is an aquifer-like zone at the base of the reservoir, in which the volume of the cells in zone 5 were enlarged by a factor of 10 000. The overall thickness, including the aquifer, was 95 m.

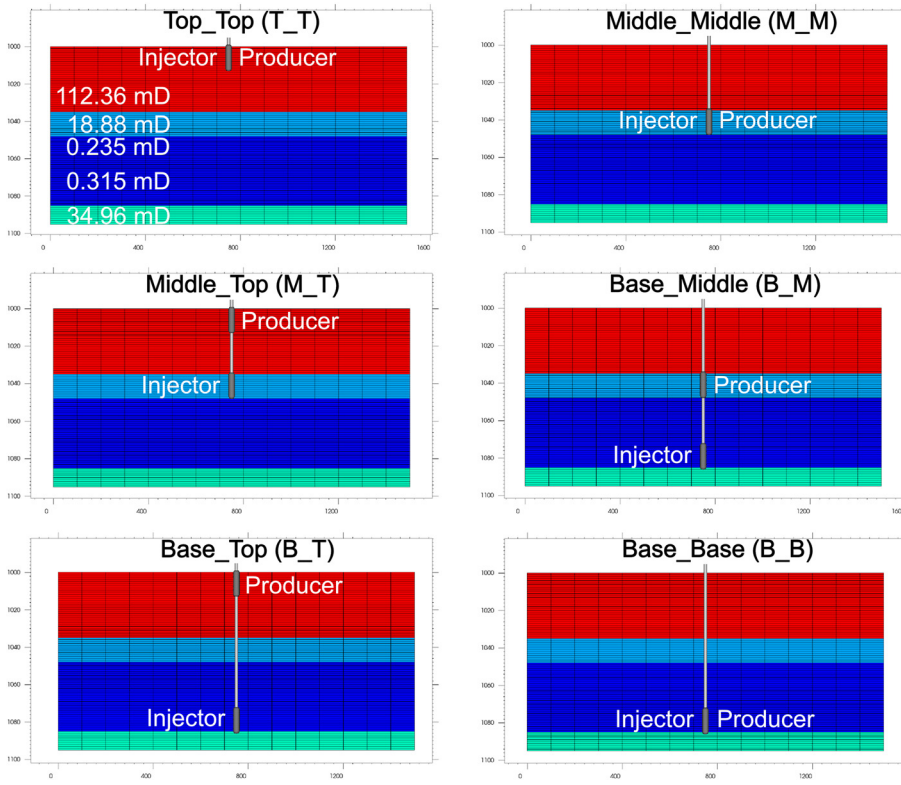


Fig. 3. Six configurations of the well positions shown in the basic heterogeneous model. The zonal colours relate to the permeability of each layer. The green zone at the base is zone 5, the aquifer-like zone.

simulations. The layers used for the LPZs are already incorporated into the basic reservoir models used to create the baseline models, so the overall reservoir thickness remains at 95 m. Only the permeability is altered so that the porosity in the LPZ layer and the overall pore volume of the reservoir remains the same as in the baseline models (Fig. 2).

The permeability of each LPZ is altered in 7 increments of one order of magnitude, from 10^{-5} to 10^1 mD while porosity is fixed at 11.61% for the complex homogeneous models and either 13.55% (LPZ1) or 13.95% (LPZ2) for the complex heterogeneous models. We ran a total of 180 simulations, constituting 15 scenarios for each of the 12 baseline models. The scenarios comprise of all seven permeability increments, for each LPZ position (the complex models) with an additional scenario without any LPZ (the baseline model) (Fig. 4).

Dynamic fluid model

In the absence of relative permeability data for the Navajo sandstone samples, we used a surrogate Brooks-Corey relative permeability relationship in this study (Fig. 5). The same relationship was used for both drainage and imbibition processes.

We inject the same hydrogen volume (at standard conditions) during each simulation over a four-year, four-month lifetime ($7.35 \times 10^8 \text{ Sm}^3$ per injection period, $2.94 \times 10^9 \text{ Sm}^3$ in total). This comprises three injection/production cycles of eight months injection/four months production plus a final eight-month injection/eight-month production cycle. The gas is injected at $300\,000 \text{ Sm}^3 \text{ d}^{-1}$ and the production target is $500\,000 \text{ Sm}^3 \text{ d}^{-1}$. To inject the required quantity of H_2 , the maximum injection BHP limit is 1000 MPa. The minimum BHP for production was set at atmospheric pressure to

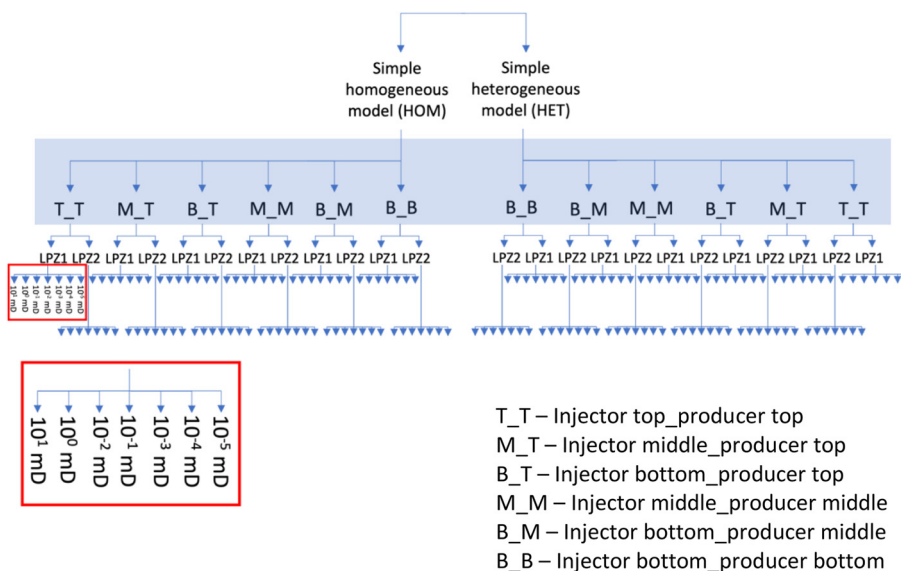


Fig. 4. Schematic of the 180 simulations run for this study. These include the 12 ‘baseline scenarios’ (highlighted in the shaded blue box) and 168 scenarios where either LPZ1 or LPZ2 is activated (the two ranks of downward pointing arrows at the base of the tree). The downward pointing arrows relate to each of the seven permeability options for the LPZ displayed in the box outlined in red (magnified in the larger rectangle, also outlined in red). Clarification of the nomenclature used throughout the study are also included in this figure.

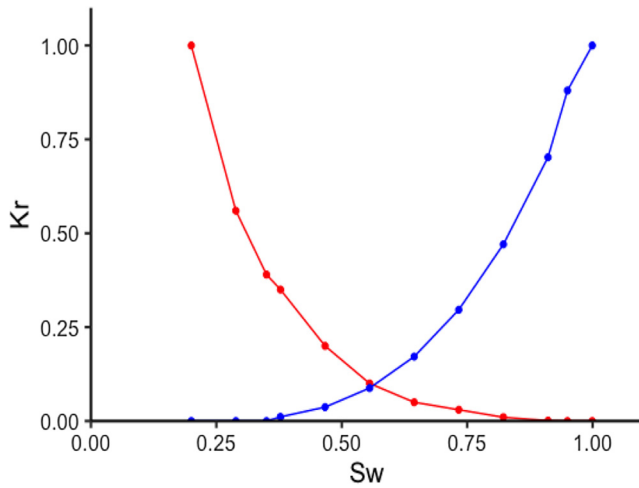


Fig. 5. Relative permeabilities of hydrogen (red line) and water (blue line) used in simulations. The same relative permeability relationship was used for both drainage and imbibition processes.

enable the movement of gas to be observed in simulations with lower permeability. Otherwise well shut-in would occur quickly in these circumstances and would be the main control on the scenarios. On violating the minimum BHP limit, production rates are reduced to ensure that the cycle maximizes the overall productivity but remains within the set operational limits.

Results

Baseline scenarios

The cumulative (a) hydrogen and (b) water production over the four cycles for the six well-completion options (Fig. 3) for each of the basic homogeneous and heterogenous models are shown in Figure 6. There are clear differences in the magnitude of H₂ production response with decreasing well depth. The basic homogeneous model demonstrates that the shallower the production well, the higher the cumulative recovery, with the top of the reservoir being the optimal position for the production well. This is expected and takes into account the way hydrogen moves between cycles due to buoyancy effects. However, due to the increased permeability in the upper zone of the basic heterogeneous model the maximum cumulative hydrogen production of $2.79 \times 10^8 \text{ Sm}^3$ for all the basic models results from the heterogeneous model with either both injector and producer at the top of the reservoir (HET_T_T – see Fig. 4 for a list of all nomenclature) or the injector in the middle position and producer at the top (HET_M_T) ($2.78 \times 10^8 \text{ Sm}^3$), about 55% larger than the volumes produced by the homogeneous models (1.80×10^8 and $1.79 \times 10^8 \text{ Sm}^3$, respectively).

The cumulative water production does not follow the same pattern as gas production for the basic models. Scenario HET_B_T

produces the most water ($3.04 \times 10^5 \text{ Sm}^3$) followed by HOM_B_B. The same configuration in the basic heterogeneous model (HET_B_B) produces the least water overall ($4.47 \times 10^3 \text{ Sm}^3$) (Fig. 6b). In the former two scenarios, with high water production (HET_B_T and HOM_B_B), the producer is positioned in a zone with high (HET, 112.36 mD) or reasonably high (HOM, 34.96 mD) permeability and low hydrogen availability, whereas the low water production (HET_B_B) is due to the low permeability (0.315 mD) in zone 4, where the producer is placed.

Bottom hole pressures and produced gas rate are shown in Figure 7 (basic homogeneous) and Figure 8 (basic heterogeneous) for the six possible well configurations. The maximum production rate ($500\,000 \text{ Sm}^3 \text{ d}^{-1}$) is sustained for longest in the basic heterogeneous model with both the injector and producer positioned at the top of the reservoir (HET_T_T, Fig. 8). The maximum production rate is not achieved in any of the four cycles in either the basic homogeneous or heterogeneous models with both the injector and producer at the base of the reservoir and in the basic heterogeneous model with the injector at the base and the producer in the middle position (Figs 7, 8).

The maximum injection BHP (1000 MPa) is reached in the basic heterogeneous models, all where the injector is placed in the layer that has the lowest permeability (zone 4, 0.315 mD) of the three completion positions (Fig. 8). Almost all scenarios violate the minimum production BHP (atmospheric pressure) in all production cycles. There are two exceptions, both for the basic heterogeneous model with the producer at the top and the injector either at the top or in the middle position of the reservoir (HET_T_T and HET_M_T). These scenarios only avoid the minimum BHP in the third cycle. It is perhaps predictable that the scenarios closest to meeting the required outputs involve the basic heterogeneous model when the layer with the highest permeability is utilized. However, the failures to achieve the target production rate in most of the scenarios highlight the need for additional H₂ or lower production targets for reservoirs with similar pore volumes to be run effectively.

Simulations with increased heterogeneity

The cumulative gas outputs of 108 scenarios are displayed in Figure 9. These include 12 baseline scenarios with no LPZs (utilizing the basic models) and 96 simulations with increased heterogeneity (either LPZ1 or LPZ2 activated – employing the complex models). The outputs of 72 simulations where the LPZs were either 0.1, 1 or 10 mD are excluded due to their similarity to the baseline scenarios, in particular the integral contrasts within the baseline heterogeneous models and do not provide additional insight into the effect of permeability contrasts on H₂-water flow. The maximum cumulative hydrogen production is $2.82 \times 10^8 \text{ Sm}^3$. This is observed in the complex heterogeneous model with the injector and producer at the top of the reservoir and a LPZ1 of 10^{-5} mD (HET_T_T_LPZ1(10^{-5}), Fig. 9b). The cumulative hydrogen production shows a minimal increase (1.4%) from the maximum production of the baseline HET_T_T, with no LPZs (Fig. 9b). The

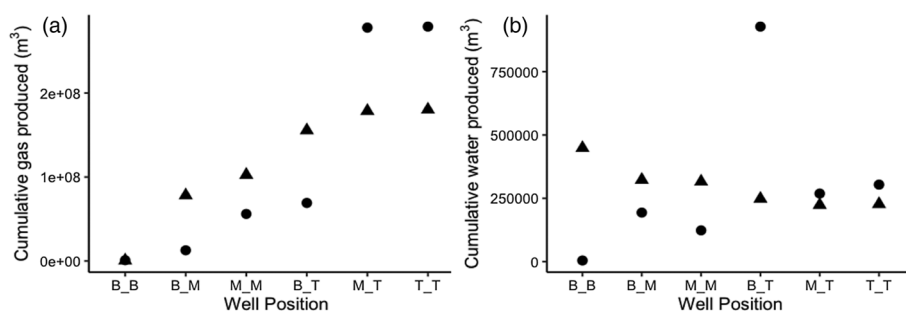


Fig. 6. Outputs from the baseline scenarios (a) cumulative gas and (b) cumulative water production. There were six variations of well position (B – Base, M – Middle and T – Top), the injector position is recorded first, for each of the homogenous (triangles) and heterogeneous (circles) models.

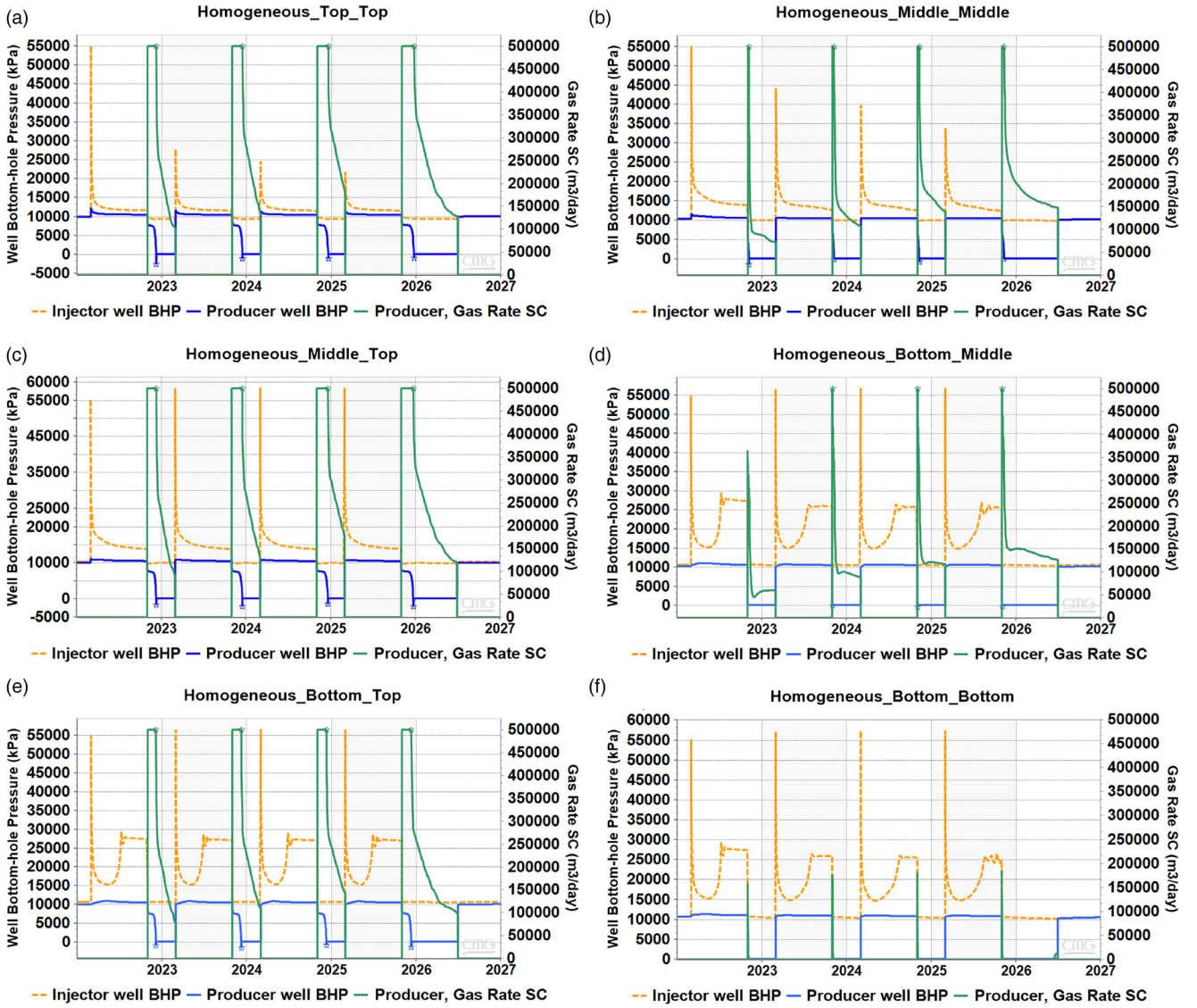


Fig. 7. Gas production rate, injection well bottom hole pressure (BHP) and production well BHP for the six baseline homogeneous models described by their injector position and then producer position. The hydrogen injection target was $300\,000\text{ Sm}^3\text{ d}^{-1}$ for 8 months in each of the four annual cycles.

highest cumulative hydrogen production in the homogeneous model is $2.78 \times 10^8\text{ Sm}^3$, also the T_T scenario with a LPZ1 of 10^{-5} mD (HOM_T_T_LPZ1(10^{-5}), Fig. 9a); more than 50% increase from the T_T baseline scenario ($1.80 \times 10^8\text{ Sm}^3$) (Fig. 9a).

In all scenarios with the injector and producer either side of the LPZ cumulative gas production is reduced when the LPZ $\leq 10^{-2}\text{ mD}$ (Fig. 10). Once the permeability of the LPZ is reduced to 10^{-5} mD there is no gas production (except in the HOM_B_M_LPZ2 scenario). There is also no gas production where the LPZ is 10^{-4} mD in the HOM_M_T_LPZ1, HOM_B_T_LPZ1 and HOM_B_T_LPZ2 scenarios (Fig. 10).

Discussion

Well position

Although well position was predominantly employed to determine the effects of the heterogeneity in the reservoirs, there are some relevant findings from their inclusion in the study. In the baseline scenarios, well position affects cumulative gas production (Fig. 6) and the position of the production well is more critical than the injection well. As a result, and due to H_2 buoyancy, the shallower production wells yield more gas. The relationship between the producer position and gas production is best demonstrated when

calculating mean production values for all 180 scenarios. These decrease from 1.73×10^8 to 0.93×10^8 and $0.22 \times 10^8\text{ Sm}^3$ for the top, middle and base position, respectively (Fig. 11).

In addition, shallower injection wells produce more gas for the same production well position; particularly compare the outcomes of HOM_T_T, HOM_M_T and HOM_B_T (producing 1.80×10^8 , 1.79×10^8 and $1.56 \times 10^8\text{ Sm}^3$ of H_2 , respectively), where permeability is not an additional variable (Fig. 6a). However, the difference between the outputs can be small when (i) both wells are in high permeability zones, (ii) the production well is near the top of the reservoir, and (iii) there are no low permeability barriers in between the wells. Similar outputs for M_T and T_T scenarios for both basic homogeneous and heterogenous models are obtained when all three conditions are fulfilled (Fig. 6a) in contrast to the outputs for the M_T models with and without LPZ1 activated (Fig. 10).

Scenarios that do not have the producer at the top of the reservoir produce less gas because buoyancy pushes H_2 above the well position. However, in the scenarios with the producer at the base of the reservoir, the basic heterogeneous model produced more hydrogen than the basic homogeneous model as the low permeability of zone 4 inhibits upward H_2 migration, resulting in $9.8 \times 10^5\text{ Sm}^3$ (HET_B_B) compared to $6.2 \times 10^5\text{ Sm}^3$ (HOM_B_B) (Fig. 6a). However, the low permeability of zone 4 in the heterogenous model (0.315 mD) significantly hampers hydrogen injection, requiring an

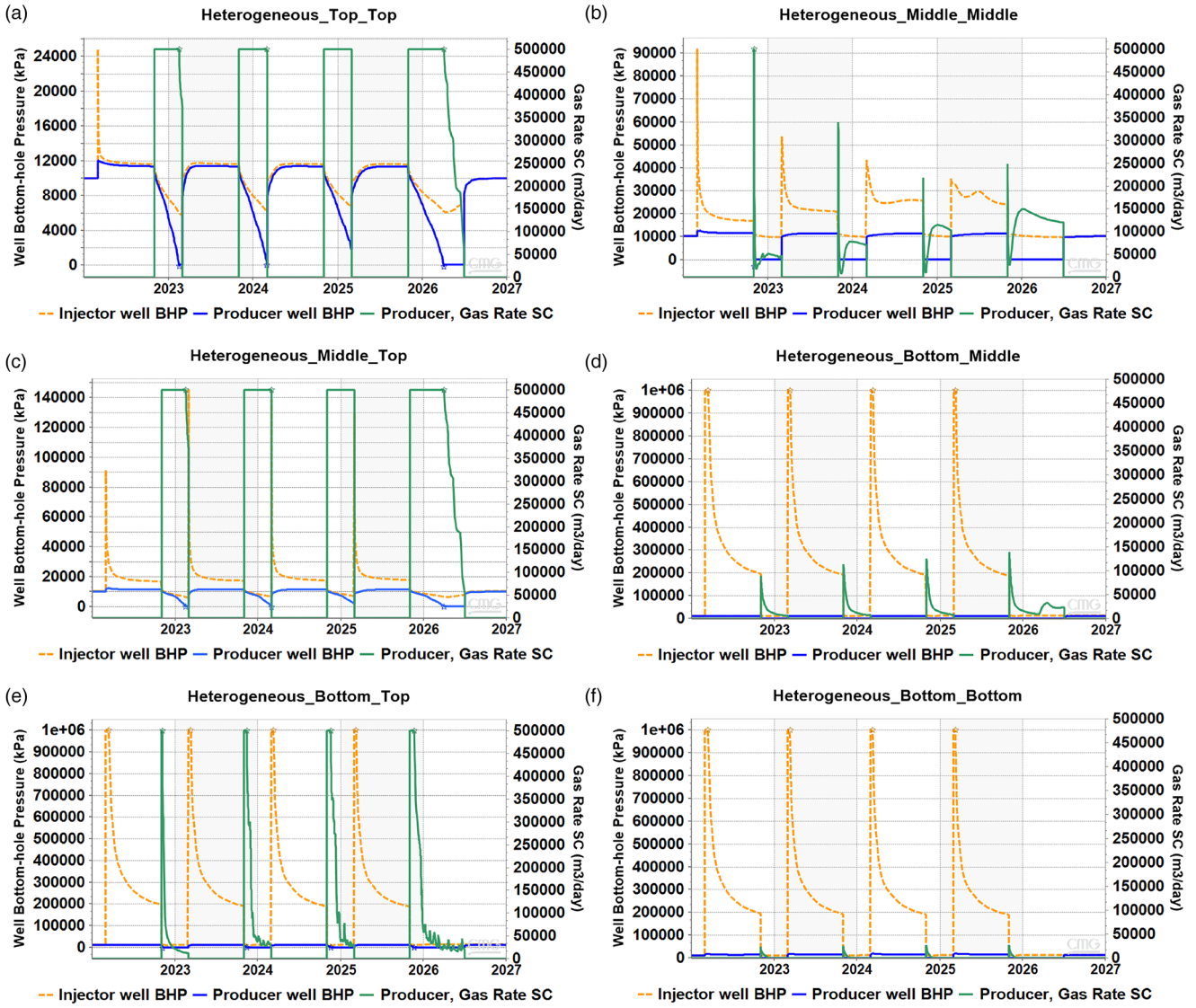


Fig. 8. Gas production rate, injection well BHP and production well BHP for the six baseline heterogeneous models described by their injector position and then producer position. The hydrogen injection target was $300\,000\text{ Sm}^3\text{ d}^{-1}$ for 8 months in each of the four annual cycles.

unrealistic maximum injection well BHP of 10^3 MPa to inject the required volume of hydrogen. In addition, when hydrogen is injected into the base of the reservoir, a significant proportion flows into the aquifer beneath and is prevented from returning to the reservoir by the low permeability of zone 4 at the base of the heterogeneous model.

Contrasting permeabilities

In our models, hydrogen migration is disrupted by permeabilities of 10^{-2} mD (Fig. 10). This suggests that even minor heterogeneities in a sandstone reservoir (one order of magnitude in HET_B_T), particularly if they are laterally continuous and extensive, will affect flow, plume development and the withdrawal of hydrogen when cycled. Such heterogeneities could be created by subtle changes in depositional layering, such as fine or silty interdunes in a succession dominated by aeolian dune bedding, or structural features, including zones of deformation bands, which may extend up to hundreds of metres, with permeabilities several orders of magnitude lower than the main reservoir rock (Krystinik 1990; Mountney 2011; Pourmalek *et al.* 2021). Permeabilities of $\leq 10^{-4}$ mD create sealing or near sealing layers under the conditions investigated (Fig. 10), although in some circumstances there is still some flow across LPZs of 10^{-5} mD, indicating that pressure gradient is having an effect in these scenarios.

We find that a permeability contrast of three to four orders of magnitude is needed for reduction in flow, due to the relationship between permeability and viscosity (equation 1). This is similar to what has been proposed by Ringrose and Bentley (2021). There is a stepped reduction in flow in the M_T_LPZ1 model when the barrier permeability decreases from 10^{-2} to 10^{-3} mD. This transformation point corresponds to a contrast of three and four orders of magnitude lower than the preceding permeability in the reservoir (34.96 and 18.88 mD in the homogenous and heterogeneous models, respectively) (Fig. 10). When LPZ1 is 10^{-2} mD, over 90% of the heterogeneous baseline ($2.53 \times 10^8\text{ Sm}^3$, compared with $2.78 \times 10^8\text{ Sm}^3$ (HET_M_T)) and over 70% of the homogeneous baseline model total ($1.28 \times 10^8\text{ Sm}^3$ compared with $1.79 \times 10^8\text{ Sm}^3$ (HOM_M_T)) of hydrogen is produced. An activated LPZ1 of 10^{-3} mD reduces flow to 30% of the heterogeneous and 4% of the homogeneous baseline hydrogen production totals, respectively. Therefore, this decrease in permeability can significantly affect reservoir performance.

The relationship between permeability and viscosity (equation 1) also implies that permeability contrasts do not affect all fluids equally. Although the simulations with the LPZ beneath the injector in either the M_T or T_T scenario generally produce more hydrogen as the LPZ permeability decreases, the results for the simulations with a LPZ of 10^{-3} mD do not fit this pattern (Fig. 12). This

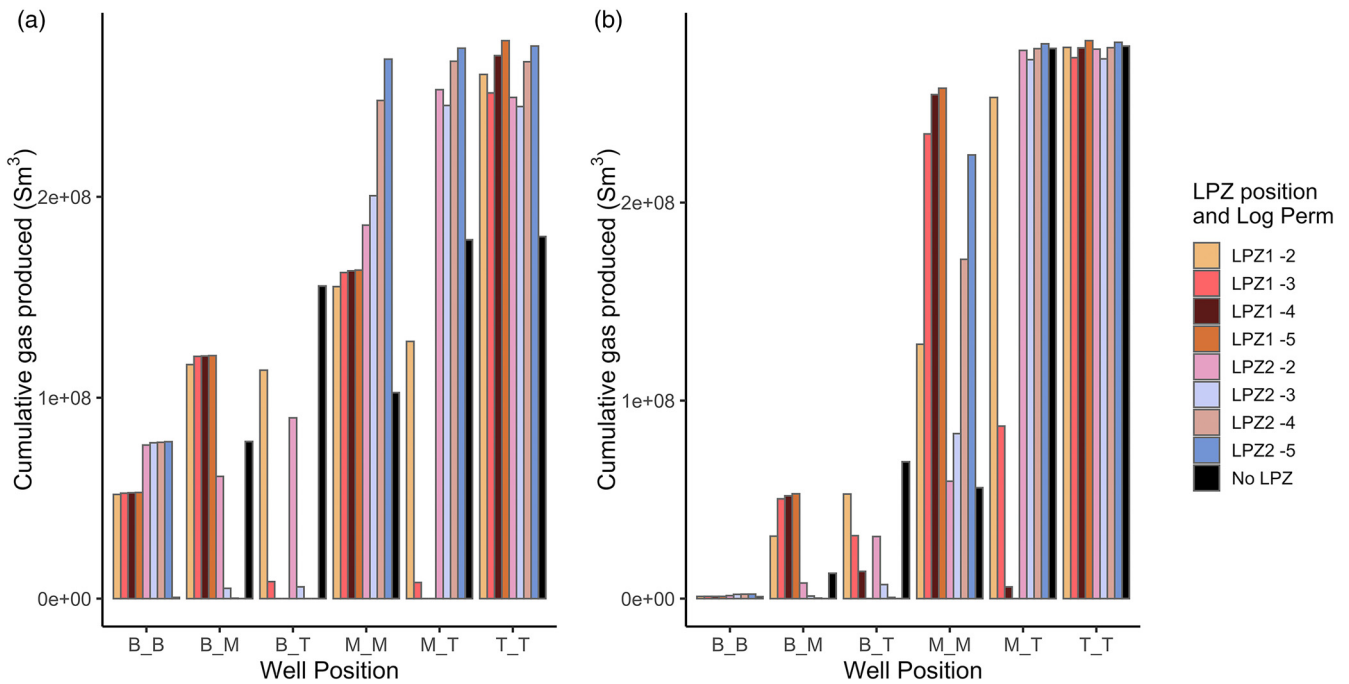


Fig. 9. The cumulative gas outputs of 54 simulations each for (a) the homogeneous model and (b) the heterogeneous model. Note that these charts do not include the outputs for the simulations where the low permeability zones are either 0.1, 1 or 10 mD. For comparison, the black bar marked as ‘No LPZ’ in the legend corresponds to the baseline scenarios.

seeming anomaly is created by the flow of fluid across the lower LPZ. In the simulation where the LPZ is 10^{-2} mD, both water and hydrogen can flow across the LPZ so that pressure is dissipated as hydrogen is injected and maintained as hydrogen is produced, creating smaller fluctuations in overall pressure (Fig. 13). When LPZ permeability is reduced to 10^{-3} mD, water is not able to flow through the barrier easily, so pressure fluctuations are larger as hydrogen is injected and produced (Fig. 13). As the pressure reduces more quickly than in the 10^{-2} mD simulation, the producer violates the BHP constraint (atmospheric pressure) earlier in the production

cycles in the 10^{-3} mD simulation, hence less hydrogen is produced. The comparison of the 10^{-2} and 10^{-3} mD scenarios highlight the importance of understanding the flow of all fluids in the reservoir and the timing of injection and production is crucial in balancing reservoir pressure and therefore how it performs in the successive cycles. If the 10^{-3} mD scenario arose it may require a costly recompletion of the well to prevent similar capacity, injection and potential storage security problems as experienced at the Snøhvit CCS and In Salah CCS demonstration projects (Ringrose *et al.* 2013; Jenkins *et al.* 2015).

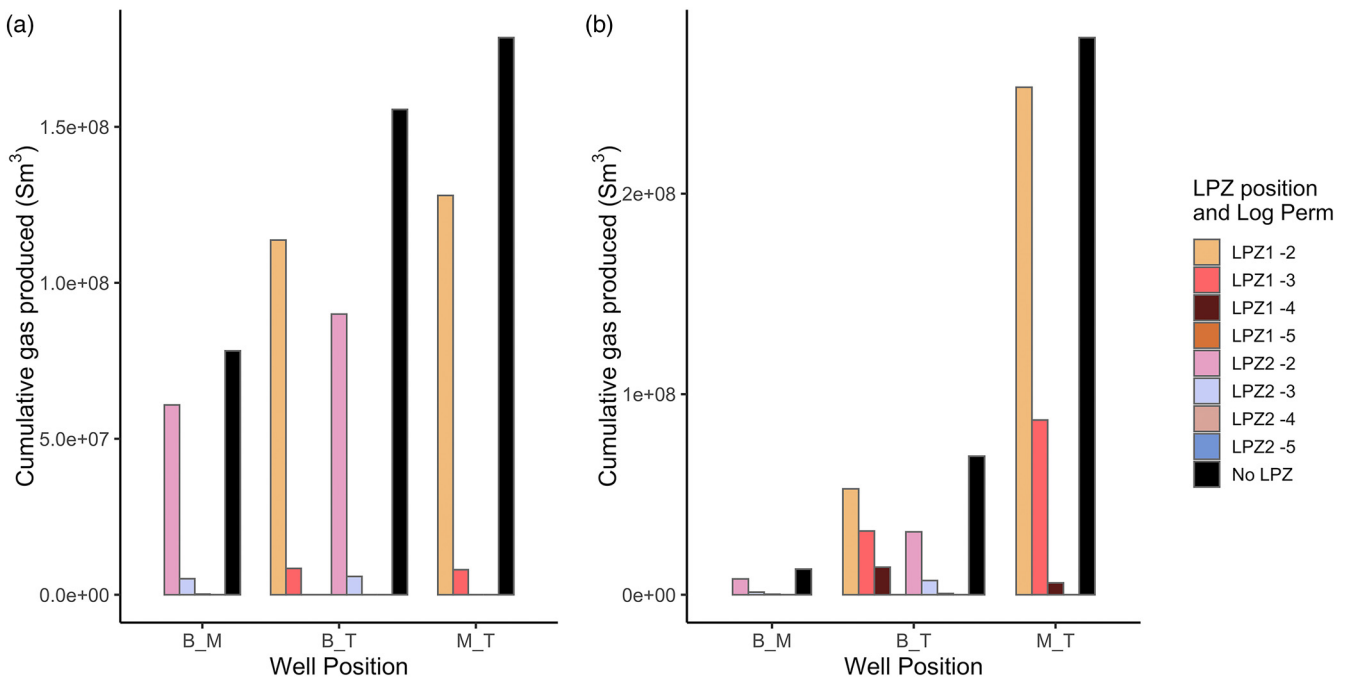


Fig. 10. Outputs of the simulations where the LPZ is in between the injector and producer (B_M_LPZ2, B_T_LPZ1 and LPZ2, M_T_LPZ1) for (a) the homogeneous and (b) the heterogeneous model. For comparison, the black bar marked as ‘No LPZ’ in the legend corresponds to the baseline scenario.

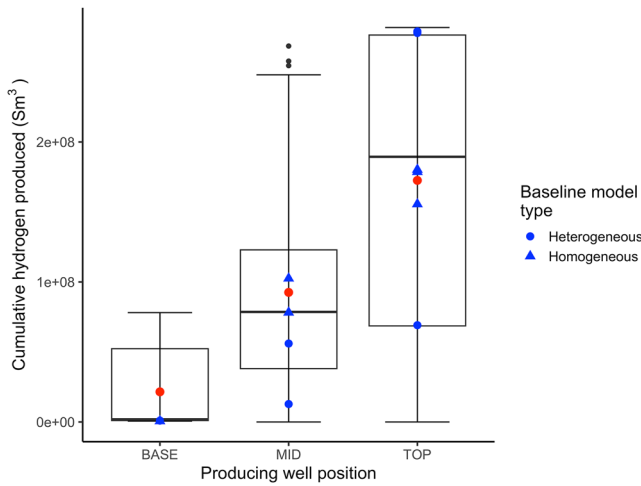


Fig. 11. Distribution of the cumulative hydrogen production from all simulations in relation to the position of the producing well. Red points indicate mean values; black horizontal lines are median values; whiskers are 1.5 times the standard deviation; black points are outliers. The blue shapes highlight the outcomes from the baseline models.

Compartmentalization

The combination of low permeability layers and features can create compartments, ranging from reservoir-defining, kilometre-scale structures (e.g. created by faults) to metre-scale features, including

deformation bands, with sedimentary processes spanning this scale range (Griffiths *et al.* 2016; Medici *et al.* 2019). Our results suggest that compartmentalization also needs to be considered in relation to the effectiveness of UHS within porous media. The scenarios with the LPZ below both injector and producer (i.e. wells within the same structural compartment), show that activating a LPZ of $\leq 10^{-2}$ mD increases the cumulative gas produced in almost all scenarios for both the homogeneous and heterogeneous models (Fig. 12). However, the increase in H₂ production is more dramatic in the homogeneous models. This is because the basic heterogeneous model already acts as a compartmentalized reservoir, with the low permeability of zones 3 and 4 (0.235 and 0.315 mD, respectively) restricting fluid movement (Fig. 14). This demonstrates the need for a holistic understanding of reservoir structure as fluid flow and plume development are affected by permeability and thickness of all surrounding facies in the reservoir and not just those on the immediate flow paths.

In scenarios that did not have any flow barriers below the injector, we observe that in addition to upward migration, hydrogen flows downwards during injection, even though the well is perforated laterally and gas is injected radially (Fig. 14). This indicates that when the injector is placed at the base of the reservoir some H₂ flows into deeper aquifer layers (zone 5). We also find downward flow in the basic heterogeneous model by constructing a model with higher permeability in zones 3 and 4. This is because some of the injected H₂ is forced downwards as the cells surrounding the upper portion of the well completion become saturated making lateral and downward movement the most energy efficient pathway. The

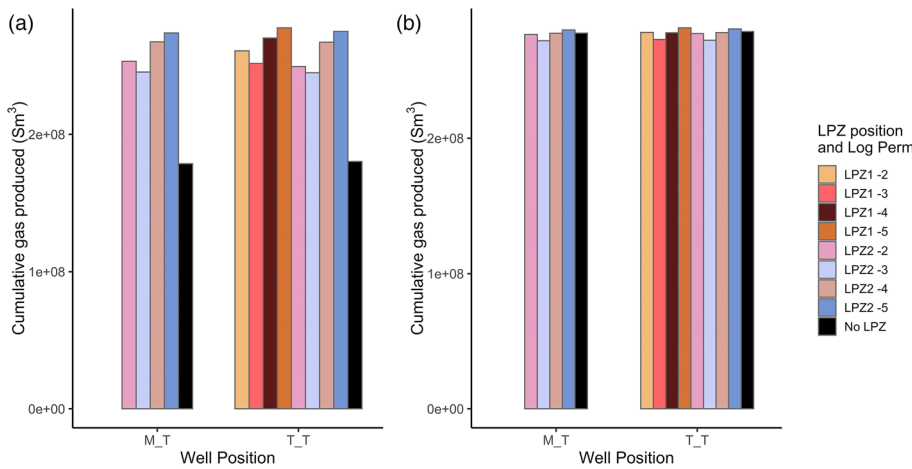


Fig. 12. Outputs of the simulations where the LPZ is below the injector and producer (M_T_LPZ1 and T_T_LPZ1 and LPZ2) for the (a) homogenous model and (b) heterogeneous model. For comparison, the black bar marked as ‘No LPZ’ in the legend corresponds to the baseline scenario.

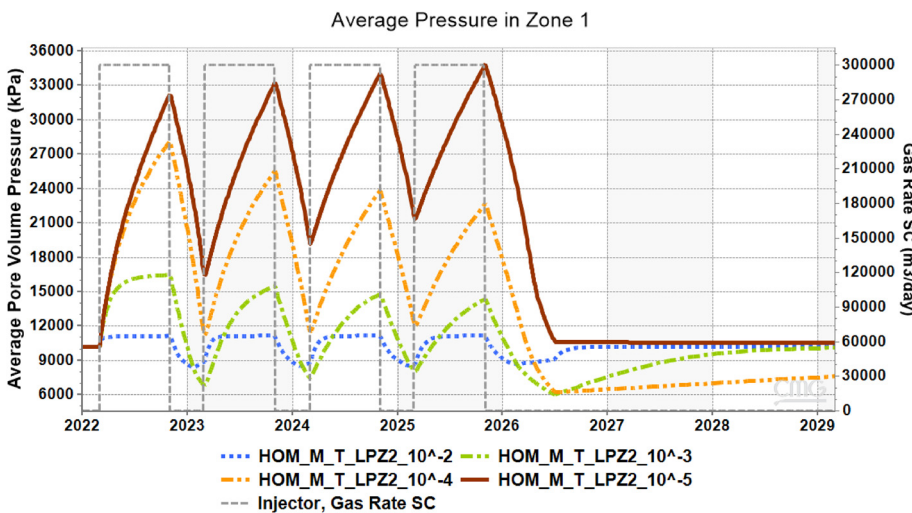


Fig. 13. Pressure fluctuations in homogeneous model with injector in the middle position and producer at the top with LPZ2 activated (M_T_LPZ2). As the permeability of the LPZ decreases from 10^{-2} to 10^{-5} mD, the pressure fluctuations increase. The grey dashed line shows the periods of hydrogen injection.

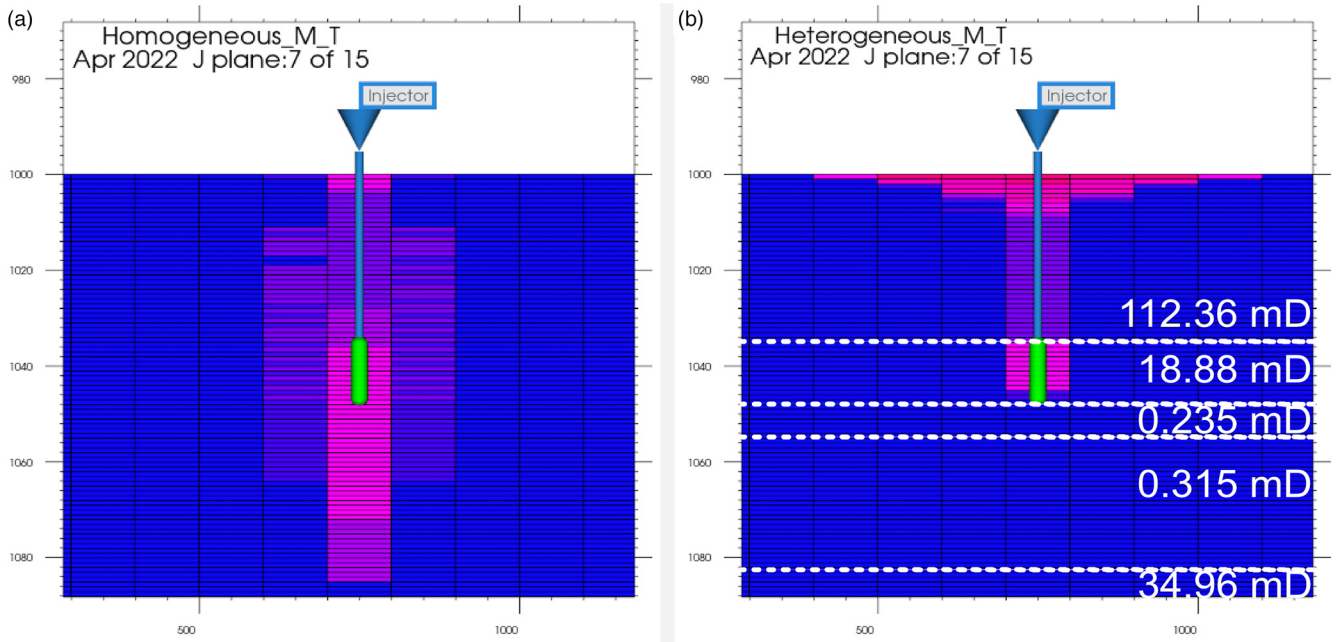


Fig. 14. Plume development during the first month of the first cycle of hydrogen injection in the (a) basic homogeneous and (b) basic heterogeneous model where the injector is placed in the middle of the reservoir. Blue indicates water and the intensity of the pink indicates the saturation of hydrogen in each cell. The white dashed lines indicate the different layers within the heterogeneous model.

downward migration is accentuated in our simulations because of the discrepancy in the horizontal and vertical cell size, 100 and 1 m, respectively. Downward movement of hydrogen was also identified by *Lysy et al. (2021)* by simulating injection of hydrogen into gas and oil zones. A consequence of the initial downward movement of hydrogen is increased lateral plume development. The additional lateral movement is generated when hydrogen alters its direction of movement, from downward to upward flow, when buoyancy pressure overcomes downward forces from injection. At the turning point hydrogen encounters the downward-flowing hydrogen, forcing it to move laterally into the adjacent cells as this is the path of least resistance.

The simulations where injector and producer are in the same structural compartment produce the most hydrogen: the highest cumulative quantities of hydrogen are produced by T_T_LPZ1 (10^{-5}), amounting to $2.78 \times 10^8 \text{ Sm}^3$ for the homogeneous and $2.82 \times 10^8 \text{ Sm}^3$ for the heterogeneous model. However, the compartmentalized scenarios also experience some of the highest zonal pressure fluctuations, which increase as the LPZ permeability decreases (Fig. 13). Pressure fluctuations can facilitate high hydrogen production but also increase stress and strain on the reservoir. This potentially affects subsequent injection and production cycles and might impact on caprock integrity (*Fu et al. 2017; Zhou et al. 2023*). As such, pressure needs to be carefully monitored within UHS, particularly as many features that form compartments are below the limits of seismic detection. Use of depleted hydrocarbon fields may mitigate against this potential issue as the structure of a field and flow pathways are better understood, particularly if they have been subject to secondary or tertiary recovery.

Where injector and producer are not in the same compartment, low permeability layers will form a barrier to fluid flow. This will lead to dissipation of the hydrogen plume and gas trapping where there is insufficient column height to create the excess pressure required to migrate across the barrier (see below). The hydrogen trapping may be exacerbated by the low permeability layers preventing the flow of other fluids, potentially creating additional baffles. The effect on other fluids is not only an important consideration in the use of aquifers for UHS but when other fluids, such as methane, carbon dioxide or nitrogen are considered for use

as cushion gas (*Kanaani et al. 2022; Zamehrian and Sedaei 2022*). Therefore, if the wells are separated by LPZs, the compartments influence the availability of hydrogen and pressure in the reservoir by regulating the flow of fluids through its barriers. As such, in reservoirs affected by compartmentalization it may be prudent to use the same well for injection and production (*Lubon and Tarkowski 2020*).

Pressure and hysteretic effects

Effects on pressure have been discussed in relation to the migration of different fluids across a barrier. However, the pressure gradient is also the impetus for fluid flow, indicated by the migration of hydrogen across a LPZ of 10^{-5} mD (above). The factors controlling the differential either directly relate to the gas pressure gradient below the LPZ, affecting the quantity and focus of H_2 present, or indirectly affect the gas pressure gradient by regulating the presence and production of other fluids, affecting overall reservoir (or compartment) pressure.

The antecedent gas column height controls the pressure gradient below the LPZ. Comparison of the B_T scenarios shows that in both the complex homogeneous and heterogeneous models more hydrogen is produced when LPZ1, rather than LPZ2, is activated (Fig. 10). We demonstrate the reason the LPZ1 simulation has a higher cumulative hydrogen production using the homogeneous model (so the LPZ creates the only permeability contrasts) with LPZs of 10^{-2} mD (as water flow is less affected), where the LPZ1 simulation has a higher total gas production of $2.37 \times 10^7 \text{ m}^3$. When LPZ2 is activated, less hydrogen is available to the producer in zone 1 (Fig. 15) because when the plume encounters the LPZ earlier, it has an increased lateral spread (Fig. 16). As a result, hydrogen concentration is lower in the centre of the reservoir and there is more hydrogen at the periphery of the plume (Fig. 16b, d). As such, more hydrogen becomes trapped below LPZ2 as the hydrogen column height at the margins of the reservoir is too low to create a sufficient pressure gradient for hydrogen to migrate across the LPZ. Conversely, if the LPZ is shallower, and therefore further away from the injector (Fig. 16a, c), hydrogen predominantly remains in the centre of the reservoir until it reaches the LPZ. In this scenario, a

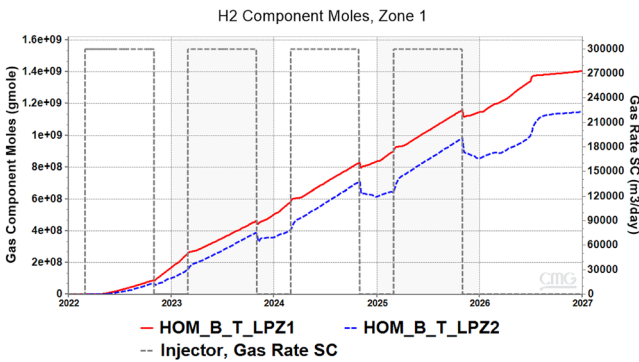


Fig. 15. Hydrogen available to the producer (zone 1) in the homogeneous model where the injector is at the base and the producer is at the top of the reservoir (B_T). The solid red line shows the simulation with LPZ1 activated and the blue dashed line shows the simulation with LPZ2 activated. In both instances the LPZ has a permeability of 10^{-2} mD. The grey dashed line shows the injection cycles, for reference.

greater gas column height results in a higher pressure gradient beneath the LPZ. The scenario with LPZ1 activated is then in a better position to take advantage of the biggest pressure drop across the LPZ during the production cycle. Figure 15 shows that during the production cycles in the LPZ1 scenario, the hydrogen in zone 1 is replaced quicker than it is produced in cycle 1 and nearly as quickly as it is produced in the other cycles, whereas in the LPZ2 scenario there is a greater drop in hydrogen volume in zone 1 during production cycles. It may be that the column height phenomenon is lessened by numerous cycles, when the eventual accumulation of gas in the LPZ2 case creates enough pressure to migrate across the barrier, or by longer shut-in periods in-between the injection and

production cycles, as the gas will rise and equilibrate below the LPZ prior to production.

In addition to the increased pressures caused by the gas column height, there is an increased hysteretic effect in the LPZ1 scenario. This is because the cells across the LPZ experience higher hydrogen saturation, enabling the hydrogen flow rate across the LPZ in successive migration to be maintained at lower pressures (Fig. 5). This form of hysteresis may be crucial to UHS as Wang *et al.* (2022) found that the piston-like movement of cushion gas during H₂ production, referred to as sweep efficiency, was not the main mechanism by which H₂ was recovered. Instead, the hydrogen migrated back along the flow paths utilized during injection, increasing the importance of processes, such as hysteresis, that affect the gas permeability along these pathways.

Implications for UHS optimization

In addition to the relationship between permeability and viscosity, local pressure factors governed by gas column heights, environmental pressures controlled by compartmentalization and the flow and production of other fluids in the reservoir, as well as hysteretic effects explain the behaviour of gas in relation to the permeability contrasts encountered in our reservoir simulations. The results show that it is not sufficient to consider permeability contrasts in isolation and the reservoir system must be viewed holistically to understand how flow patterns control plume development.

Overall, when the LPZs are introduced, there are some broad similarities in responses of the complex homogeneous and heterogeneous models; all simulations produce less gas than the baseline scenarios when the LPZ is in between the wells and almost all simulations produce more gas than the baseline scenarios when the reservoir is compartmentalized and the wells are in the same

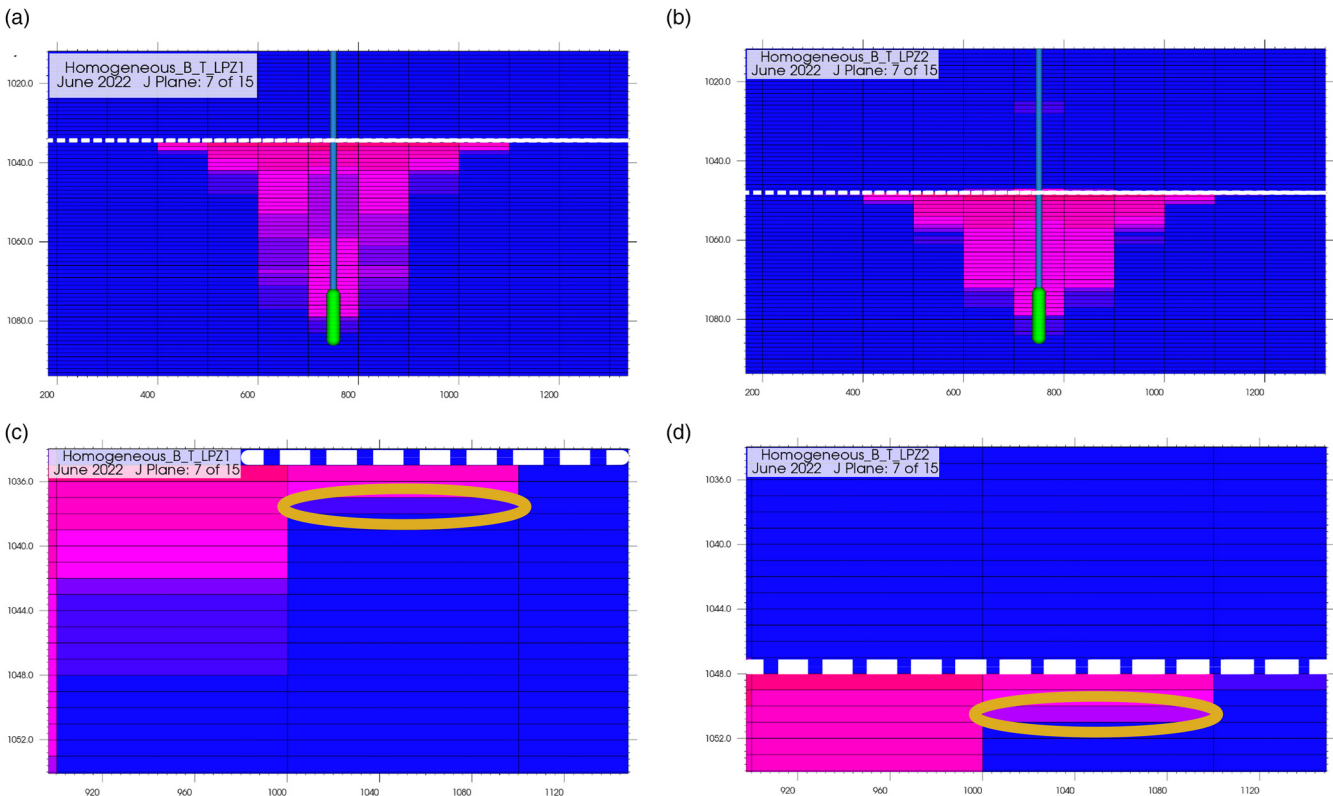


Fig. 16. Comparison of lateral hydrogen plume migration during the first injection cycle in the homogeneous simulations, where the injector is at the base and the producer at the top of the reservoir (HOM_B_T). Both simulations have a LPZ of 10^{-2} mD. (a) LPZ1 is activated; (b) LPZ2 is activated. (c) and (d) are expanded segments of (a) and (b), respectively, and the orange ellipse highlights the lateral movement of hydrogen in the equivalent cell below the LPZ. Blue indicates water and the intensity of the pink indicates the saturation of hydrogen in each cell. The white dashed line illustrates the position of the activated LPZ.

compartment. However, due to the combination of permeability contrasts, the LPZs also amplify some of the differences in the homogeneous and heterogeneous reservoir structures. For instance, the cumulative gas outputs reflect the usage of the respective higher permeability layers of the reservoirs, such that, the reservoirs based upon the homogeneous model produce more hydrogen when the base of the reservoir is utilized for one or both of the wells, whereas the complex heterogeneous simulations recover more gas when the top of the reservoir is utilized for one or both of the wells.

The M_M scenarios also reflect the permeability differences. Of the two LPZ positions, the complex homogeneous models produce more hydrogen in the LPZ2 scenarios and the complex heterogeneous models produce more gas in all LPZ1 simulations. In both scenarios, the higher permeability above the wells, or surrounding the well when the well is at the effective reservoir top in the M_M_LPZ1 scenario, allows increased lateral plume spreading so that less gas is available for production. The lower H₂ production for the homogeneous reservoir in the LPZ1 scenario is compounded by more gas being able to flow downwards into the base layers. This explains why the HOM_M_M_LPZ1 gas outputs are similar for the four LPZ permeabilities, as similar quantities of gas flow downwards, then migrate back upward (mechanism described above) and can be produced over the four cycles. However, the heterogeneous reservoir (HET_M_M_LPZ1) acts more similarly to the homogeneous T_T scenarios with either of the LPZs activated and produces increasingly more gas as the compartment becomes tighter (Fig. 9).

In relation to the compartmentalized scenarios, the cumulative gas outputs are very similar for the lowest permeability (LPZ of 10⁻⁵ mD) T_T_LPZ1/2 and M_T_LPZ2 scenarios, despite the homogeneous model having just over a quarter of the permeability in zone 1, i.e. 35 mD compared with 112 mD (Fig. 12). This suggests that for pre-set production rates there are diminishing yields for hydrogen production once permeability has increased above a certain level (tens of mD in this study for a production rate of 500 000 Sm³ d⁻¹), provided that pore volume is sufficient to accommodate the required hydrogen. Therefore, it may be possible to operate UHS in lower permeability storage sites if the required hydrogen production rate is reduced. However, compartmentalization also impacts upon effective reservoir size, potentially causing problems similar to those experienced at the CO₂ storage test site at Snøhvit and ultimately reducing storage capacity (Jenkins *et al.* 2015). Some of these issues can be mitigated by injection-production regime, as discussed below.

As we have shown, heterogeneity affects the pressure experienced in a reservoir by affecting fluid movement. This creates a circular relationship because pressure gradient dictates how the fluids interact with permeability contrasts. Operational tools, such as the length of the injection and production cycles, including any shut-in periods, and the injection and production rates, along with the use of cushion gas (not discussed in this study), can be used to overcome some of the pressure issues and control flow within the reservoir (Lubon and Tarkowski 2020; Mahdi *et al.* 2021). These mechanisms can also be used to manage the storage facility, either recovering the maximum amount of hydrogen (recovery factor), ensuring a timely meeting of energy demand, or managing the purity of the recovered H₂ (Lubon and Tarkowski 2020; Kanaani *et al.* 2022; Wang *et al.* 2022; Bo *et al.* 2023). It will be necessary to decide which of these three, potentially competing, outputs from a reservoir is the overarching objective to implement the most effective management strategy. It may be that a range of reservoir management strategies can be produced, based-upon the nature or timeliness of end use, which can then be tailored to each reservoir.

Although our models are not sufficiently complex to induce viscous fingering, we can infer that coupling of some of the observed processes may create this effect in a more heterogeneous

reservoir. For instance, the lateral plume development from the downward injection initially reduces the plume's intensity. If this plume, with lower gas concentration, then encounters low permeability features, it is less likely to be able to migrate across them, creating further lateral movement. This is particularly the case if there is better lateral than vertical connectivity. In an anisotropic reservoir with multidirectional plume development and numerous permeability contrasts, the hydrogen plume is likely to lose its integrity, creating different pathways as it migrates upwards. Multiple pathways increase the likelihood of trapping, as the pressure gradient is reduced if the plume is separated. However, much of the plume coherence may be recaptured if hydrogen accumulates at the top of an anticlinal structure (Zamehrian and Sedaei 2022; Bo *et al.* 2023). In general, it is most effective for both the injector and producer to be placed at the top of the reservoir. However, having a separate injector may prove beneficial to regulate pressure around the wells, so that it is not necessary to inject hydrogen into a smaller volume at the top of an anticline, although there is obviously a cost implication to having separate wells.

In addition to selecting the most appropriate well location for the reservoir structure, our findings from the simple models with escalating heterogeneities underline the need to understand the sedimentary and structural geology that create the permeability contrasts throughout the entirety of the reservoir. This study demonstrates that features that are lateral and continuous will affect the fluid flow and therefore the efficacy of a potential storage system. As discussed, the features affecting permeability within the reservoir can either be sedimentary or structural. Some of the reservoir architecture will be detected by seismic surveys, however, many impactful features are below seismic detection limits, such as thin beds within a layer-cake architecture or zones of deformation bands (Ringrose and Bentley 2021; Wakefield *et al.* 2022). Further work is needed to determine how fluid flow is impacted by this range of features to determine whether they significantly affect the efficacy of UHS in clastic reservoirs. Answers arising from this research will inform the type and frequency of sampling needed to obtain the resolution required, or in other terms, the complexity needed for effective modelling and the day-to-day operational management of the reservoir.

Finally, in this study we show that hysteretic effects prove beneficial to hydrogen flow, allowing the gas to flow more easily along previously established pathways. In addition, it may be that hysteretic effects over multiple cycles prevent plume dispersal, improving the recovery factor (Zhang *et al.* 2023). However, several studies using different relative permeability relationships for drainage and imbibition and incorporating trapping into subsequent cycles, have predicted that hysteresis reduces working gas capacity, H₂ recovery factor and has a negative effect on injection and production rates (Wang *et al.* 2022; Bo *et al.* 2023; Lysy *et al.* 2023; Pan *et al.* 2023). This is because the phases trapped in the reservoir at the end of the injection and production cycles are immobile. Nonetheless, this may not substantially impact upon the hydrogen recovery (Wang *et al.* 2022). More experimental work is needed in relation to this process and its effects.

Conclusions

By introducing increasing heterogeneities into simple reservoir models, we found that, due to the buoyancy of H₂, wells placed higher up in the reservoir produce more gas. In addition, permeabilities of $\leq 10^{-2}$ mD disrupt the flow of H₂ and lower permeability of $\leq 10^{-4}$ mD create near-no flow barriers.

Similar to predictions, permeability contrasts of three to four orders of magnitude significantly affect flow, however, factors affecting the pressure gradient also needed to be considered. These factors include compartmentalization, the effect of permeability on

the flow of co-existing fluids (which in themselves can create additional baffles) and the localized pressure gradient created by the H₂ plume. We have demonstrated some of the fundamental processes of fluid pathway development using simple models, providing insights that can be applied to more complex UHS investigations.

We have shown that reservoirs with lower permeability (35 mD) can work almost as effectively as storage with higher permeability (112 mD) if injection and production demands are not too high and there is sufficient pore space for fluid storage. Lower permeability also reduces lateral spreading and may improve the hydrogen recovery factor. Likewise, some of the issues created by permeability contrasts, such as dispersal of the hydrogen plume and structural trapping, can be mitigated by operational reservoir management, such as well placement, controlling injection and production rates or shut-in times. Although not studied in this research, the use of cushion gas is another tool that can assist in managing the reservoir effectively. However, our research underlines the need to understand the architecture of the whole reservoir, not just the zones surrounding the wells and pathways in-between, as this controls capacity, pressure fluctuations and informs operational management decisions. It also highlights the need for further research about how heterogeneities across different scales, particularly those that are below sub-seismic detection, affect fluid flow and therefore the efficacy of UHS in sedimentary reservoirs.

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Author contributions **DS**: conceptualization (lead), formal analysis (lead), methodology (lead), visualization (lead), writing – original draft (lead), writing – review & editing (equal); **AB**: conceptualization (supporting), methodology (supporting), supervision (lead), writing – review & editing (equal); **DA**: conceptualization (supporting), methodology (supporting), supervision (supporting), visualization (supporting), writing – review & editing (equal); **EH**: supervision (supporting), writing – review & editing (equal)

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Data availability The datasets generated and analysed during the current study are not publicly available as they are files particular to the commercial software used in the study but are available from the corresponding author on reasonable request.

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