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Quantitative Diagenesis for the Characterisation of CCUS Storage in Carbonates

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Abstract. Recent years have seen the growth of new techniques that combine conventional stratigraphic and observational approaches to characterising the type, scope, extent, timing, and effects of diagenetic processes with petrophysical measurements of their rock microstructure. These new Quantitative Diagenesis (QD) techniques can be used to predict post- and pre-dolomitisation porosities and permeabilities as well as track petrodiagenetic pathways. The objective of this paper is to use QD to calculate changes to the CO_2 storage of a CCUS target for the first time. These QD approaches include; porosity and permeability prediction resulting from varying degrees of dolomitisation, calculation of porosity and permeability of the host rock before dolomitisation, using petrodiagenetic pathways to track quantitatively the type, extent and timing of diagenetic processes, and methods for determining the impact of fractures (the Fracture Effect Index, FEI). This paper reports the impact of dolomitisation and fracturing on CO_2 storage by considering the Butmah and Shiranish formations (NE Iraq). The Butmah formation data shows that the CO_2 storage of the formation increased significantly 154.23 Mt (xx%) due to dolomitisation . The Shiranish Formation showed an increase in CO_2 storage of 144.23 Mt (x%) from the almost unfractured rocks of its U.1(A) lithofacies (FEI=0.31) to the highly fractured rocks of its U.4 lithofacies (FEI=15.55). The main scientific contribution of this paper is that it shows for the first time that QD techniques can be used to calculate very significant changes in CO_2

storage capacity concomitant upon fracturing, dolomitisation and precipitation. Such techniques should therefore be employed when judging any legacy reservoir or aquifer in carbonates the potential CCUS use.

Keywords: Petrophysics, quantitative diagenesis, dolomitisation, CO_2 storage. Butmah formation, Shiranish formation, reservoir quality, carbonate reservoirs, fracturing

1. INTRODUCTION

Direct CO_2 sequestration (taking CO_2 from the air) and indirect CO_2 sequestration (taking CO_2 from anthropogenic emissions) are suitable options for fulfilling the growing need to remove CO_2 from the atmosphere (Porcheron et al., 2011; Siqueria et al., 2017). However, there are several hazards associated with managing and storing a significant amount of CO_2, including CO_2 leaks (Buscheck et al., 2012; Harbert et al., 2016).

It is anticipated that injected supercritical CO_2 would undergo a number of phase transitions that might impact the long-term safety of subterranean storage, so both CO_2 behaviour during and after injection should be studied (Bildstein et al., 2009). Understanding the effects of phase changes as well as the part that geochemical and geomechanical effects play in the long-term storage of CO_2 is essential (Siqueria et al., 2017). It is important to understand the depositional and diagenetic textures and minerals, their impact on the petrophysical properties of the reservoir, and their spatial variability in order for accurate and efficient prediction of geologic carbon dioxide sequestration and the utilisation of the available pore space (Bowen et al., 2011).

Dolomitisation and hydraulic fracturing (e.g., Wang et al., 2019; 2020) are the primary mechanisms regulating CO_2 storage in carbonate reservoirs because they have an impact on the porosity and permeability of the reservoir rock. Carbonate reservoirs are recognised for being much more chemically reactive when CO_2 is present (Campbell-Stone et al., 2011; Siqueria et al., 2017; Stacey et al., 2024).

Consequently, this paper will briefly explain some of the main approaches to Quantitative Diagenesis (QD) that have been developed at the Petrophysics Research Group and Laboratory of the University of Leeds, including dolomitisation prediction, petrodiagenetic pathways, reservoir quality fields, and Fracture Effect Index (FEI), before examining how they can be used to ensure that the prospective CCUS target reservoir is sufficiently well characterised that effective reservoir modelling can take place, and that the volume, flow and trapping of CO_2 in the reservoir can be effectively calculated. It is worth noting that this study does not, in itself, provide data or modelling results to substantiate claims about enhanced porosity, permeability, or trapping efficiency, but applies previous work to the calculation of CO_2 storage in dolomitised reservoirs.

2 Study Data

The data of the studied formations in this work were collected in cooperation with the North Oil Company (NOC) in Iraq, including core plugs and geophysical log data from 4 boreholes from Ain Zalah and Butmah oilfields in northwestern Iraq (Figure 1). Table 1 illustrates the acquired data of this study in detail.

Table 1: The acquired data of the Shiranish and Butmah formations in northwestern Iraq.

Formation	**Oilfield**	**Well**	**Data**					
			Core plug	**Geophysical well log**				
				GR	Density	Neutron	Sonic	Resistivity
Shiranish	Ain Zalah	Az-16, Az-19, Az-29	35	√	√	√	√	√
Butmah	Butmah & Ain Zalah	Bm-15, Az-29	87	√	√	√	√	√

Figure 1: The location of the Ain Zalah and Butmah oilfields in north-western Iraq.

Some of the data we have used in this work has appeared previously in our papers (Mohammed Sajed and Glover, 2020; 2022; Mohammed Sajed et al., 2021; 2024a; 2024b; 2024c), but not for the analysis purposes it has been put to in this paper. The previous papers were concerned with the description of the two formations in various reservoirs, and the development of QD techniques to help the analysis of the core and well log data. This paper uses that analysis as a starting point, and applies every other day techniques for the purpose of predicting porosity and permeabilities in order to better judge the ability of those formations to host a significant CCUS storage resource, and in particular to recognise the change in storage that is associated with the progress of dolomitisation in the case of the Butmah formation, and the impact of fracturing in the Shiranish formation. While it is intuitive to recognise that dolomitisation will increase porosity generally and therefore leads to greater storage of carbon dioxide, it has not been previously known how carbon dioxide storage relies on the degree of dolomitisation, which is something this paper treats. In the case of fractures, fracturing increases both the amount of carbon dioxide that can be stored through the fracture porosity and by increasing the surface area of rock to which carbon dioxide can be adsorbed, as well as the extent to which the development of new flow pathways is engendered by fractures with different fracture effectiveness indices, again analysed in this paper.

2 Quantitative Diagenesis

Injection of CO_2 into a carbonate reservoir is known to be very sensitive to heterogeneities, especially those that result from diagenetic changes which can be very localised (Ringrose et al., 2022). The effectiveness of injection depends upon both porosity, which provides storage, and permeability, which describes gas transport. This section will briefly explain four of the main approaches to QD including prediction of porosity and permeability resulting from, and prior to, dolomitisation, as well as the quantitative use of petrodiagenetic pathways with reservoir quality zonation, and the quantification of how much impact fracturing has on rock properties using the Fracture Effect Index (FEI). Each of these QD techniques has uses in characterising the storage and flow properties of potential CCUS targets and provides data allowing injection into CCUS reservoirs to be modelled and flow-simulated.

2.1 QD dolomitisation porosity prediction

The large changes of porosity concomitant upon dolomitisation will have a significant effect upon the storage capacity of potential carbonate CCUS reservoirs. The following QD methodology is, consequently, likely to be of great use in the characterisation of such reservoirs. There are two aspects to predicting the change in porosity upon dolomitisation. The direct aspect arises from the difference in density between calcite and dolomite (Figure 2a, b). However, peri-dolomitisation change in porosity also depends on the progressive porosity, implying an indirect effect, which was thought to lead to a higher overall porosity (Rashid et al., 2022), but is now known to result in the same overall porosity increase.

This QD model does not include dolomite precipitation in new porosity. This is often referred to as overdolomitisation. However, we chose to not use the term because the process is not one of dolomitisation, but of dolomite precipitation. Nevertheless, it is noted that the QD methodology for predicting porosity consequent to dolomitisation could be modified to include it (Rashid et al., 2022).

Dolomitisation produces larger porosities because the mineral dolomite (2.87 g/cm^3) is denser than calcite (2.71 g/ cm^3). The resulting porosity can be calculated as a function of the degree of dolomitisation measured by the relative dolomite volume fraction in the rock. The reverse process can also be calculated, providing the initial porosity of the limestone before dolomitisation occurred, as expressed by the following equation;

$$\phi_{POST} = \frac{2M_{LMST}[\chi_{DOL}\rho_{DOL} + (1-\chi_{DOL})\rho_{LMST}\phi_o] - M_{DOL}[\chi_{DOL}\rho_{LMST}(1-\phi_o)]}{2M_{LMST}[(1-\chi_{DOL})\rho_{LMST} + \chi_{DOL}\rho_{DOL}]} \quad (1)$$

where, χ_{DOL} is the fractional degree of dolomitisation, ϕ_{POST} is the post-dolomitisation porosity, ϕ_o is the pre-dolomitisation porosity, M_{DOL} is the molar mass of dolomite, M_{LMST} is the molar mass of calcite, ρ_{LMST} is the density of calcite = 2.71 g/ cm^3 and ρ_{DOL} is the density of dolomite = 2.87 g/ cm^3. The same result is obtained whether this equation is applied directly to obtain the final porosity at the desired degree of dolomitisation, or applied incrementally and reiteratively, updating the porosity at the start of each incremental increase in dolomitisation fraction.

Setting χ_{DOL} = 1 (i.e., full dolomitisation), results in

$$\phi_{POST} = 1 - \frac{M_{DOL}}{2M_{LMST}} \frac{\rho_{LMST}}{\rho_{DOL}} (1 - \phi_O), \text{ and} \tag{2}$$

$$\phi_O = 1 - \frac{2M_{LMST}}{M_{DOL}} \frac{\rho_{DOL}}{\rho_{LMST}} (1 - \phi_{POST}), \tag{3}$$

Figure 2: (a) Post-dolomitisation porosity as a function of pre-dolomitisation porosity for different initial porosities. (b) Fractional increase in porosity on different degrees of dolomitisation.

Figure 2a shows the result of Eq. (1) giving post-dolomitisation porosity as a function of the fractional dolomitisation of the matrix for matrixes with various starting (pre-dolomitisation) porosities. It is worth noting that the fractional rise in porosity is greater for rocks with low initial porosities. This is clearer when the data is plotted as an increase in porosity percentage as a function of the fractional dolomitisation of the matrix which is shown in Figure 2b.

Since Eq. (3) is the reverse of Eq. (2), it may be used to calculate the porosity of the carbonate prior to dolomitisation (i.e., postdiction), together with an analogous equation in place of Eq. (1).

Once the predicted porosity is known, it is possible to use one of the existing methodologies for calculating the permeability. This is more difficult in carbonates than in clastic rocks because the processes of diagenesis decouple the functional interdependence that grain size and pore size have in clastic rocks (Glover and Walker, 2009; Glover and Dery, 2010) because they are formed by a process of comminution. The family of RGPZ equations are probably the most reliable in this regard (Glover et al., 2006; Rashid et al., 2015a; 2015b). However, the theoretical versions are not ideal for application to carbonates, and the generic or carbonate versions should be preferred (Rashid et al., 2015b; Al Khalifah et al., 2020). These are empirical versions of the theoretical base models by the addition of 2 and 1 fitting parameters for the generic and carbonate RGPZ models, respectively. The Kozeny-Carman approach (Rashid et al., 2015b) should be avoided in this case because it takes no account of dead-end pores and often overestimates permeability by several orders of magnitude.

Post-hoc calculation of permeability can be avoided completely by using the QD approach which predicts and postdicts both porosity and permeability in a single procedure, and is the subject of the next subsection.

2.2 QD poroperm prediction

While porosity prediction is useful in the characterisation, modelling, and simulation of potential CCUS target reservoirs, permeability is key. The following method allows the prediction or postdiction of both porosity and permeability from observed core and well-log data.

The QD poroperm prediction method enables both prediction and postdiction of porosity and permeability by building the generic RGPZ equation (Rashid et al., 2015b) into the porosity and permeability transformation. This approach has been implemented for carbonate rocks from the Butmah Formation in north-western Iraq (Mohammed-Sajed and Glover, 2022). The first step in the method is to ascertain the different petrofacies present in the formation so that the method can be applied independently to each. This process ensures that the method tailors the transformation to a facies of a specific type, and results in much better predictions. In the case of the Butmah Formation, 3 petrophysical fields were recognised; (a) diagenetically altered samples, (b) fractured and diagenetically-altered samples, and (c) fractured samples, all of which were characterised by distinct fields on a poroperm cross-plot, shown in Figure 3a-c, respectively (Mohammed-Sajed and Glover, 2022; Mohammed-Sajed et al., 2024a). For formations where clusters exist but are not so distinct, machine learning techniques can be used to separate the data into clusters (Glover et al., 2022).

Figure 3: Poroperm relationship of the 3 petrophysical fields in carbonate (limestone and dolomite), and the best power law fitting equations with coefficients of determination (R^2). (a) Diagenetically altered samples. (b) Fractured and diagenetically-altered samples. (c) Fractured samples (modified after Mohammed-Sajed et al., 2024a).

The method requires there to exist both the unaltered host rock (or one that can be considered analogous) and the dolomitised rock (or one that can be considered analogous). The post-dolomitisation poroperm properties can be calculated by using the scatter from the limestone measured orthogonally to the best power law fit to the host rock limestone data, and the power law fit to the existing dolomite following the steps shown by the arrows in Figure 4. (Please note that the generic form of the RGPZ equation has a power law form.) In the top row of this figure (Figure 4a-d), post-dolomitisation data (shown finally as green symbols in Figure 4d) are created from the initial blue symbols, which show the initial host limestone data. As expected, the post-dolomitisation data is shifted to higher porosities and permeabilities than the initial limestone data.

Figure 4: Prediction of the porosity and permeability of the limestone samples after the dolomitisation process (a-d) and *vice versa* (e-h) the dolomite samples are used to predict the pre-dolomitisation poroperm data (modified after Mohammed-Sajed et al., 2024a).

The lower row of Figure 4 (parts e-h) shows the opposite process, i.e., postdiction of the original limestone porosity and permeability from a dolomitised starting point. Resulting pre-dolomitisation data (again shown as green symbols in Figure 4h) are created from the initial pink symbols, which show the observed dolomitised data. The pre-dolomitisation data has, as expected, lower porosities and permeabilities than the observed data from the rock once it has been dolomitised.

While it is expected that this method will only work well when the limestones are non-dolomitised and the dolomitisation of those which have been dolomitised is full (Mohammed-Sajed et al., 2024a), there is no reason to believe the method would not work on partially dolomitised rocks providing the relevant dataset contains rocks that have all reached the same degree of partial dolomitisation.

2.3 QD petrodiagenetic pathways

The petrophysical qualities of a rock depend in a highly complex way on how the kind, style, amount, and timing of diagenetic processes change the microstructure of the rock and affect its measured petrophysical properties, whether they are purely geometrical such as porosity, or related to direction such as connectivity and permeability (Rashid et al., 2022). Although the interplay between the petrophysical qualities of the rock and the degree, type and amount of diagenesis is complex, we have attempted to describe it using a tool we call the petrodiagenetic pathway, which treats each diagenetic process separately, takes account of the degree to which that process affects the porosity and permeability of a rock, and allows the timing of diagenetic processes to be concurrent or consecutive mixture of both.

The petrodiagenetic pathway itself is a simple concept which associates each diagenetic process (or part of a diagenetic process) with a vector which exists in porosity permeability space and can be marked on a poroperm plot, such as the generic one shown in Figure 5.

Figure 5: (a) The impact of several diagenetic processes on tight carbonate rock poroperm expression (modified after Al-Khalifah et al., 2020). The contour lines in this case show the grain sizes obtained using the modified carbonate RGPZ model (Rashid et al., 2015b). The arrows corresponding to distinct diagenetic processes denote a random point on a curve, but they may also be applied to any point on any curve (Al-Khalifah et al., 2020). (b) The outcome of the text's specified petrodiagenetic route, which is a series of diagnostic processes on the plot (modified after Rashid et al., 2022). Pathways discussed fully in the main text.

The length (magnitude) of each vector shows the effect of the diagenetic process on porosity (in the x-direction, with unit vector $\hat{x}$) and the permeability (in the y-direction, with unit vector $\hat{y}$). Vectors pointing to greater porosity or permeability indicate that the diagenetic process has increased porosity or permeability, respectively. Conversely, vectors pointing to smaller porosity or permeability indicate that the diagenetic process has decreased porosity or permeability, respectively. Consequently, the length of the vector (its magnitude) represents the extent of the diagenetic process. If the process affects porosity and/or permeability slightly, it will be short, and if the effect is large, it will be long.

In practice, the length and direction of vectors can either be obtained from core data, well log data or even by modelling. The direction and length of the vectors, as with all petrophysical quantities, will vary from lithology to lithology and also depend on the rock 's history and pressure and temperature conditions. Consequently, it will always be best to define the vectors specifically for the lithology and location in question. While it is beyond the scope of this paper to consider the exact steps taken to characterise the vectors of all diagenetic processes, it is possible to take one or two examples.

In the first, we consider dolomitisation. Porosity and permeability values are required before dolomitisation as well as after the degree of dolomitisation observed has taken place. Possibilities will depend upon the availability of rocks. If there is an outcrop nearby of undolomitised rock, then core analysis will provide coordinates of the base of the vector. If such rock is unavailable, then the processes described in sections 2.1 and 2.2 above can be used to calculate the porosity and permeability values of the un-dolomitised rock. A final possibility is that a suitable analogue rock is used. The coordinates of the point of the vector can be obtained from well logs or core analysis on samples representing the degree of dolomitisation required to be represented by the vector. Again, calculations in sections 2.1 and 2.2 above may be useful. One example of this is if one has the information to create a vector describing 50% dolomitisation using rock that has been dolomitised to this extent, but one wants to have a vector which describes the effect of 100% dolomitisation.

In the second example, we consider fracturing. This is a simpler situation in that the coordinates which represents the base of the vector are very often the porosity and permeability values associated with the unfractured rock, which can be obtained from core analysis or well logs. The coordinates which represent the point of the vector could in principle be obtained from core analysis, but commonly such core is sufficiently broken up not to provide a reliable estimate of its porosity and permeability. Under these circumstances, it is often more reliable to use measurements from well logs. The degree to which fracturing enhances porosity and permeability in a rock is described by the fracture effectiveness index (FEI), which is described below. This quantitative measure allows one to associate an increase or decrease in FEI with the length of the vector. In order to do this, we envisage, but have not carried out a calibration of vector length as a function of FEI. This should be the subject of future work.

The direction of the vector depends on the relative sizes of the porosity and permeability effect due to the diagenetic process. Each diagenetic process has a vector direction which differs from other process. For example, in Figure 5a, dolomitisation tends to increase both the porosity and permeability of a rock, so the vector points to the right (increasing porosity) and upwards (increasing permeability), while cementation tends to decrease porosity and permeability, resulting in a vector pointing down and to the left. The exact vector direction for each process will depend upon the local conditions and should be determined from local measurements. Sequential or contemporaneous occurrence of more than one diagenetic process can be described by the simple addition of vectors. Conversely, vector subtraction can be carried out if one wanted to remove the effect of a particular diagenetic process (say the most recent) to obtain the porosity and permeability of the rock before that process began.

Figure 5b shows two processes. In the first process a limestone, initially at Point A undergoes dolomitisation which increases its porosity and permeability. Dolomite is weak and brittle compared to limestone, and while the regional stresses may not have changed, local stresses may have altered because of the change in volume of the rock itself. Consequently, it is highly likely that fracturing then occurs (and this is observed in many locations around the globe (Mohammed Sajed et al., 2021)). The subsequent vector shows the result of this fracturing, increasing the permeability by a significant amount for only a small increase in (fracture) porosity. In this example, fracturing is followed by compaction and then cementation to reach a final rock expressed as Point B, which is of lower porosity, but the same permeability as its original form (Point A). The petrodiagenetic pathway represents a quantitative summary of the rock's diagenetic history, while the vector $\overrightarrow{AB}$ is the vector sum of its component vectors, vectors that each represent a single diagenetic process.

The second example (Point C to Point D) in Fig. 5b shows the simple case of dolomitisation followed by dolomite cementation (sometimes erroneously called overdolomitisation).

Dolomite cementation often diminishes reservoir quality by obstructing intercrystalline, interparticle, and fracture-associated pore networks. The deposition of dolomite cement reduces effective porosity and pore-throat connection, resulting in decreased permeability and impaired fluid-flow capacity (Figure 6B). The consequences are especially significant when cementation transpires late in the diagenetic sequence (Figure 6C). Conversely, early, restricted, or localised dolomite cementation may have little effects (Figure 6A) and, in exceptional instances, may reinforce the grain structure, marginally improving mechanical stability. In general, dolomite cementation is usually linked to considerable deterioration of reservoir quality (Machel, 2004; Mohammed Sajed and Glover, 2020).

Figure 6: Dolomite cementation effect on three different samples of the Butmah Formation; (A) early dolomite cementation with minimal effect on the pore space of the sample, Bm-15, 2450 m. (B) Late dolomite cementation with a moderate effect on the pore space of the sample, Bm-15, 2511 m. (C) Late dolomite cementation with a major effect on the pore space of the sample Bm-15, 2563 m. Yellow arrows indicate increased dolomite cementation in the pore space of the Butmah Formation.

The petrodiagenetic pathway method could easily be extended to 3 dimensions or more of data, if the data were available. For example, suppose characteristic grain size data were available. This could be represented on a z-axis placed orthogonally to the x- and y- axes. While more difficult to envisage, all the previous concepts still apply while the quantitative characterization of the diagenetic process would be more precise and distinguishable from other processes.

It should be noted that Figure 5 contains parametric lines representing the carbonate-RGPZ relationship between porosity and permeability for a variety of characteristic grain sizes to act as a reference grid for the vector dance. The base diagram can also be sectored to represent qualitative reservoir quality (in Figure 5a), or be sectored quantitatively (Mohammed-Sajed et al., 2024b). While the discussion above is done from the point of view of a single sample representing a rock, and may be carried out for individual rock samples, it is best carried out by calculating a petrodiagenetic pathway from the movement of the centre of gravity of a cloud of data representing a given distinct facies.

2.4 QD fracture effect index (FEI)

The existence of fractures influences how injected CO_2 flows in a CCUS reservoir. Not all fractures enhance or degrade fluid flow to the same extent. We have developed a Fracture Effect Index (FEI) to quantify the positive (flow enhancing), and negative (flow compartmentalising) effects of the fractures in a rock using the following equation (Mohammed-Sajed et al., 2024b);

$$FEI = \frac{k_{m\,Log} - k_{m\,Core}}{\phi_{m\,Log} - \phi_{m\,Core}} \quad (4)$$

where FEI is the Fracture Effect Index (unitless), $k_{m\,Log}$ is the mean permeability in a specific unit (mD) of fractured rock (from log measurements), $k_{m\,Core}$ is the mean permeability in a specific unit (mD) of unfractured rock (from core measurements), $\phi_{m\,Log}$ is the mean porosity in a specific unit (fraction) of fractured rock (from log measurements), and $\phi_{m\,Core}$ is the mean porosity in a specific unit (fraction) of unfractured rock (from core measurements).

It should be noted that positive values of this index denote overall flow enhancement usually by open fractures, while negative values indicate flow degradation, usually by cemented fractures. However, networks of open fractures can also effectively compartmentalise some portions of reservoirs by diverting fluid flow away from blocks of unfractured rock, while sometimes cemented fractures can funnel fluid flow through blocks of matrix rocks allowing a better replacement of fluids therein. The FEI approach has been applied to the Shiranish Formation (deep fractured carbonate) in the north-western Iraq and the results are shown in Figure 7. The formation has 4 units, which plot as progressively better reservoirs (higher porosity and permeability) on the poroperm plot (Figure 7a). However, when the FEI is calculated (Figure 7b), only Unit 4 shows fractures which contribute significantly to overall flow, the improved poroperm values on Unit 2 and Unit 3 relative to those of Unit 1 being caused by better matrix porosity and connectivity rather than the effect of the fractures they may contain.

Figure 7: (a) Poroperm relationship for evaluation of the effect of the fracture on the petrophysical properties of the Shiranish Formation by comparison of the core plug samples with the wireline log data. (b) The fracture effect index in each stratigraphic unit of the Shiranish Formation (modified after Mohammed-Sajed et al., 2024b).

The introduction of the Fracture Effect Index (FEI) represents a promising step toward quantifying the complex influence of natural and induced fractures on CO_2 migration and trapping in subsurface storage formations. Nevertheless, the current conceptualisation and mathematical formulation of the FEI require more rigorous development before it can serve as a reliable diagnostic or predictive tool for CCUS applications. In particular, the present framework simplifies fracture–flow interactions and does not fully account for the multiscale geometric, hydraulic, and mechanical attributes that govern CO_2 behaviour in fractured media. Key properties such as fracture aperture variability, network connectivity, stress-dependent transmissivity, and matrix–fracture exchange are insufficiently represented, which limits the physical interpretability of FEI values.

Furthermore, the FEI has not yet been systematically calibrated or validated against high-fidelity simulations or empirical data. Without such benchmarking, the relationship between FEI and measurable flow responses remains uncertain. For the index to gain broader scientific and practical utility, its formulation must be grounded in demonstrable physical principles, supported by numerical modelling that explores a range of realistic fracture scenarios, and evaluated using laboratory measurements, wellbore-scale tests, and field-scale monitoring data. A strengthened theoretical basis, combined with transparent calibration and uncertainty quantification, is essential to ensure that FEI accurately reflects the dual role of fractures in enhancing or constraining CO_2 transport within heterogeneous geological storage systems.

Conventional FEI often uses fracture presence/intensity as a proxy for flow enhancement. To capture geometry, FEI should incorporate core geometric inputs including aperture distribution (mean and variance), fracture length/persistence, aspect ratio, roughness coefficients, orientation relative to flow direction/stress field, and Branching/intersections (network connectivity indices)

$$\text{FEI} = f(A, L, R, \theta, C, \chi),$$

where: A = aperture, L = length/persistence, R = roughness, θ = orientation factor, C = connectivity, and χ = petrophysical heterogeneity.

$$\chi = \frac{HI_k}{HI_\phi},$$

where HI_k is the permeability heterogeneity index (fractional), and HI_ϕ is the porosity heterogeneity index (fractional) (Mohammed-Sajed et al., 2024b).

In tight carbonates and especially fractured carbonates (e.g., Shiranish Formation), the FEI is dominated by aperture and connectivity, reflecting the capacity of even a small population of large, well-connected fractures to overwhelm matrix flow and produce disproportionately high $k_{\text{frac}}/ k_{\text{mat}}$ ratios. By contrast, sandstones and dolomite rocks exhibit a more balanced sensitivity structure, where aperture, fracture length, and connectivity share comparable influence, consistent with their more uniform pore–fracture interactions. Shales display the weakest FEI response overall, with roughness and aperture variability exerting greater relative control due to the inherently low matrix permeability and limited fracture transmissivity. Consequently, any application of FEI for reservoir screening, CO_2 migration prediction must explicitly account for lithology-dependent uncertainty.

In summary, there is a future in need for a rigourous calibration of FEI values against empirical flow data in order that FEI values can be interpreted correctly. Such an analysis should include a study of uncertainties when using the approach. Numerical simulation could not only be a beneficial tool to examine the interpretation of FEI values, but also would benefit from their use if rigorously calibrated.

3. CO_2 STORAGE CALCULATION

3.1. Scope and Assumptions

Assessing the carbon dioxide (CO_2) storage capacity is essential for determining the viability of geological carbon sequestration initiatives. Storage capacity estimates offer a preliminary evaluation of the volume of CO_2 that may be securely and efficiently stored inside a subterranean deposit over extended periods (Mohammed-Sajed et al., 2024c).

These estimations are often derived using volumetric approaches that incorporate essential reservoir parameters such as areal extent, thickness, porosity, and in-situ CO_2 density alongside efficiency factors that consider reservoir heterogeneity, trapping processes, and pressure constraints (Bachu et al., 2007; Szulczewski et al., 2012). Initial capacity estimates provide valuable screening metrics; however, more sophisticated computations account for dynamic reservoir behaviour, injection efficacy, and geomechanical limitations to more accurately depict true storage potential (Cavanagh & Ringrose, 2014).

The purpose of this calculation is to calculate the specific mass of carbon dioxide stored (i.e., mass per reservoir area and is per thickness of the storing formations) both before and after diagenesis, and hence to mark the change of storage concomitant on diagenesis. The calculations also convert these specific stored masses of carbon dioxide to absolute masses for each of the two fields (Butmah and Shiranish) for which both reservoir areas and thicknesses are known. Calculations are consistent with established frameworks from the DoE (NETL CO_2Screen), CSLF and IPCC but do not take account of site-specific geological constraints.

In this study, we have made some simplifying assumptions. First, that there is no residual oil phase in which the CO_2 can dissolve. While this trapping mechanism usually contributes little to the overall storage, it is only applicable to storage in legacy oil fields and depends on knowledge of the final oil saturation of the oil field. This data is not available for the Butmah and Shiranish fields because they are still active producers.

The second assumption is that we do not calculate the CO_2 adsorbed to the rock. This contribution is often significant, but to be carried out accurately requires knowledge of the adsorption process (e.g., Langmuir constants and pressure) and the mass fraction or internal area of the rock taking part in gas adsorption. Neither of these was available to us. Consequently, we have constrained ourselves to calculating the mass of CO_2 stored in the pores and fracture of the rock, and dissolved in the water within that pore and fracture space. This is an important issue because adsorbed carbon dioxide can make up a very significant proportion of the total carbon dioxide storage by reservoir. For example, an in-house calculation of total carbon dioxide storage (in pores, dissolved legacy oil, dissolved in water and adsorbed to matrix surfaces) for a Brent reservoir in the North Sea to be in the ratio 25:4:1:70 for pore storage: oil dissolution: water dissolution: matrix absorbance. The dominance of the adsorbed carbon dioxide indicates that it should not normally be left out of calculations even if, as is usually the case, this form of carbon dioxide storage is only developed over the medium timescale.

The results here represent the calculated expectation for how diagenesis will affect the amount of carbon dioxide that can be stored in a diagenetic altered limestone reservoir, that is not validated against empirical data because the two reservoirs studied are still producing hydrocarbons. Consequently, from one point of view, this study is a screening study that will help judge whether these two reservoirs will be of future use as a CCUS resource.

3.2 Calculation Methodology

Input data to the calculation models included the zoning of each reservoir, for each of which the mean areal extent, thickness, porosity and water saturation was associated. The density of the carbon dioxide was calculated from the carbon dioxide pressure and temperature in each zone. The dissolution constant of carbon dioxide in water was calculated knowing the pressure and temperature of the fluid in each zone. Since the reservoir is currently producing hydrocarbons, the decision was made to carry out the calculation at a time when hydrocarbon production had just stopped. Under these conditions any legacy oil is fully saturated with hydrocarbon gas, and so provides no dissolution storage for carbon dioxide. Consequently, carbon dioxide dissolution in residual oil has not been included in the calculations. The density is water and hydrocarbons in the reservoirs are known and used in the equations for carbon dioxide storage calculation.

In this study, the mass of CO_2 capable of being stored in the pore volume was calculated using the following equation;

$$M_{FCO_2} = A\, h\, \phi (1 - S_w)\, \rho_{CO_2} \quad , \tag{5}$$

where; A = area of the reservoir (m^2); h = thickness of the reservoir (m), ϕ = porosity (fraction); S_w = water saturation (fraction); ρ_{CO_2} = density of CO_2 at reservoir conditions (kg/m^3).

Whereas the dissolved CO_2 in the water of the reservoir was given by;

$$M_{SCO_2} = K_{sol} A\, h\, \phi S_w \rho_{H_2O}, \tag{6}$$

where; K_{sol} = dissolution constant (kg/kg); ρ_{H_2O} = density of H_2O at reservoir conditions (kg/m^3).

Consequently, the total storage of CO_2 in the rock can be calculated by the following equation;

$$M_{VCO_2} = A\, h\, \phi \left[\, \rho_{CO_2}(1 - S_w)\right] + \rho_{H_2O}[K_{sol}\, S_w] \tag{7}$$

Initially, we calculate the effects of dolomitisation and fracturing on the mass of CO_2 stored in generic calculations, quoting the storage in Mt/m/km^2, which we will refer to as the specific mass of CO_2 stored. Subsequently, the results of applying previous equations to calculate the CO_2 storage in the Butmah and Shiranish formations will be calculated, initially also as specific mass of CO_2 stored in Mt/m/km^2, but finally in Mt by taking the area and thickness of horizons in the reservoirs into account.

3.3 Calculation Uncertainties

There is an uncertainty associated with all of the input parameters, and which will contribute to the uncertainty in the calculated final values. Parameter uncertainties were calculated from well log data as standard deviations whenever possible.

The uncertainty in the area was calculated based upon the uncertainty caused by the size of the Fresnel zone in the seismic data and was 3.3% and 4.6% for the Butmah and Shiranish fields, respectively. The area of the reservoir was assumed to be the same for all of its zones.

The uncertainty in zone thicknesses was taken to be equal to 5 ft. (about 1.5 m on the basis of the quality of the well logs). This provides a variable percentage uncertainty depending upon the thickness of each zone.

Although the mean porosities were taken from high quality core analysis data, there were not sufficient data (35 and 87 core plugs for the Butmah and Shiranish fields, respectively) for the core plugs to reasonably represent variability in the reservoir. Consequently, we used the standard deviation of the porosities calculated from the well logs in each zone of each field. Consequently, the resulting uncertainties vary as a percentage in each zone of each reservoir. The water saturations were taken from a reasonable estimation of the results of gas flooding in core plugs from the reservoirs.

All other data, which includes the densities of carbon dioxide, water and hydrocarbon as well as the solubility of carbon dioxide in water have been given and nominal 5% uncertainty, which is almost certainly larger than will exist in reality, that represents underlying uncertainties in the temperature and pressure at a given depth, which will provide such an overall uncertainty.

3.4 Generic calculations of the effect of QD on CO_2 storage

Application of the CO_2 mass storage equation (Eq. (7)) to the change in porosity concomitant upon dolomitisation allows the total CO_2 storage (Figure 8a) and increase in CO_2 storage (Figure 8b) to be calculated. In this figure the mass of stored CO_2 is given per metre thickness and per kilometre areal extent. While Figure 8a shows that there can be a significant extra storage capacity of CO_2 achievable for dolomitized rocks, Figure 8b shows that the greatest increment on the existing porosity and hence mass of CO_2 is associated with rocks which initially had low porosities.

Figure 8: (a) Post-dolomitisation storage of CO_2 (excluding oil dissolution and adsorption) as a function of degree of dolomitisation. (b) Increase in CO_2 storage (excluding oil dissolution and adsorption) as a function of degree of dolomitisation. Values also depend linearly on the value of S_w, which here is S_w=0.2.

3.2 Calculations of the effect of QD on specific CO_2 storage for the Butmah reservoir

Dolomitisation can augment porosity and permeability through the formation of intercrystalline pore networks and the superior resilience of dolomite to compaction relative to calcite (Lucia, 2007; Ehrenberg et al., 2009; Mohammed Sajed and Glover,2020). Significantly, although dolomite exhibits lower reactivity with CO_2-saturated fluids compared to calcite, hence decreasing the degree of mineral trapping, its stability allows improved structural and residual trapping mechanisms essential for the enduring confinement of CO_2 (Kaszuba et al., 2003; Machel, 2004). As a result, dolomitised carbonate deposits are frequently regarded as advantageous sites for CO_2 sequestration owing to their enhanced reservoir quality and mechanical integrity.

This section will present the results of applying QD poroperm relationship on the well log data of the Butmah formation with respect of the calculated CO_2 storage in this study for the main lithology, limestone and dolomite. The fractional degree of dolomitisation (χ_{DOL}) in the Butmah Formation was calculated using;

$$\chi_{DOL} = \frac{\rho_g - 2.71}{0.16} , \tag{8}$$

where ρ_g is the grain density in g/cm^3, 2.71 is the density of limestone (or different if known locally to be different), and 0.16 is the difference in density between dolomite and limestone (which may also vary locally). The grain density is given by

$$\rho_g = \frac{\rho_b - \phi_N \, \rho_f}{(1-\phi_N)}, \tag{9}$$

where ϕ_N is the neutron porosity (fractional) and ρ_b is the bulk density of rock from the density log (g/cm^3). The density of the fluid can be calculated as a linear mixing of the two known fluid densities providing S_w is also known. In this case the water saturation is known, and the individual fluid densities are ρ_{water} =1.0 g/cm^3, and ρ_{oil} = 0.8 g/cm^3.

$$\rho_f = S_w \rho_{H2O} \; + (1 - S_w) \, \rho_{Oil} \tag{10}$$

This method for calculating the fractional degree of dolomitisation assumes that the neutron log and density log are measuring the same apparent porosity of the rock. While this is valid to a first approximation for clean rocks, it is invalid in rocks containing shales and hence cannot be used in such rocks.

The improvement in the porosity and permeability caused by dolomitisation in the Butmah Formation is reflected as a change in the arithmetic mean of specific CO_2 storage capacity from 0.01273 Mt/m/km^2 in limestone (U.1, U.3, and U.5) to 0.0178 Mt/m/km^2 in dolomite (U.2 and U.4) and a change in the arithmetic mean of gross CO_2 storage capacity from 43.49 Mt in limestone (U.1, U.3, and U.5) to 197.72 Mt in dolomite (U.2 and U.4) (Figure 9).

Figure 9: The relationship between the total specific CO_2 storage in limestone and dolomite with (a) porosity, (b) water saturation, and (c) permeability, respectively. (d) Poroperm relationship with the mean of the specific CO_2 storage of the limestone and dolomite units of the Butmah Formation.

Figure 9 generally illustrates that dolomite has higher specific CO_2 storage compared to limestone, with a positive relationship between the total specific CO_2 storage with porosity and permeability and a reverse relationship with water saturation. The differences in the specific CO_2 storage capacity within the stratigraphic units of the Butmah Formation can be summarised in Table 2.

Table 1: The dolomitisation effect on the reservoir quality and specific CO_2 storage capacity of the Butmah Formation. Area assumed to be 72 km^2 (Mohammed-Sajed and Glover, 2022).

Formation	Strati-graphic unit	Number of Measure-ments (-)	Coverage (%)	Thickness (m)	Lithology	χ_{DOL} (-)	MCO_2 stored in pores (Mt/m/km^2 (%)*)	Uncertainty in MCO_2 stored in pores (Mt/m/km^2 (%)§)	MCO_2 stored in water (Mt/m/km^2 (%)*)	Uncertainty in MCO_2 stored in water (Mt/m/km^2 (%)§)	MCO_2 stored in total rock (Mt/m/km^2 (%)*)	Uncertainty in MCO_2 stored in total rock (Mt/m/km^2 (%)§)
Butmah	1	106	66.25	48	Limestone	0.0775	0.0106 (94.69%)	0.00116 (10.94)	0.000593 (5.31%)	6.49×10^{-5} (10.94)	0.0112 (100%)	0.001226 (10.94)
	2	170	75.00	68	Dolomite	0.6120	0.0139 (97.32%)	0.001472 (10.58)	0.000383 (2.68%)	4.06×10^{-5} (10.58)	0.0143 (100%)	0.001514 (10.58)
	3	99	87.35	34	Limestone	0.0909	0.0128 (95.69%)	0.001409 (11.01)	0.000578 (4.31%)	6.36×10^{-5} (11.01)	0.0134 (100%)	0.001475 (11.01)
	4	96	13.58	212	Dolomite	0.8409	0.0209 (97.98%)	0.002308 (11.04)	0.00043 (2.02%)	4.75×10^{-5} (11.04)	0.0213 (100%)	0.002352 (11.04)
	5	33	30.94	32	Limestone	0.0842	0.0130 (95.59%)	0.001694 (13.03)	0.000598 (4.41%)	7.79×10^{-5} (13.03)	0.0136 (100%)	0.001772 (13.03)

Notes: The * indicates the percentage is a percent of the fraction of CO_2 stored in either the pores or dissolved in the water. The § indicates the error percentage of the pertaining measurement.

Table 2 shows that the highest specific mass of CO_2 stored in total rock was in the dolomite lithology represented by U.4 (212 m) with 0.0213 Mt/m/km^2, followed by U.2 (68 m) with 0.0143 Mt/m/km^2, whereas the lowest specific mass of CO_2 stored in total rock was in the limestone lithology represented by U.5 (32 m) with 0.0136 Mt/m/km^2 and U.3 (34 m) with 0.0134 Mt/m/km^2, respectively. U.1 (48 m) showed the lowest specific mass of CO_2 stored in total rock with 0.0112 Mt/m/km^2. Table 2 also illustrates that the positive relationship between the calculated χ_{DOL} and the specific mass of CO_2 storage for the Butmah Formation; i.e., the storage capacity increases as χ_{DOL} increases.

3.3 Calculations of the effect of QD on gross CO_2 storage for the Butmah reservoir

While it is useful to consider specific storage for the purposes of comparing the CO_2 storage efficacy for individual samples and lithofacies, as in the last subsection, for any particular reservoir a total final gross predicted CO_2 storage is required. Consequently, we have taken the mean values of the individual core data that was shown in Figure 9 and converted the data to provide a total gross CO_2 storage value for each lithofacies of the Butmah reservoir, and assumed a constant reservoir area of 72 km^2. This data is shown in Table 3.

Table 3: The dolomitisation effect on the reservoir quality and gross CO_2 storage capacity of the Butmah Formation.

Formation	Strati-graphic unit	Number of Measure-ments (-)	Coverage (%)	Thickness (m)	Lithology	χ_{DOL} (-)	MCO_2 stored in pores (Mt (%)*)	Uncertainty in MCO_2 stored in pores (Mt (%)§)	MCO_2 stored in water (Mt (%)*)	Uncertainty in MCO_2 stored in water (Mt (%)§)	MCO_2 stored in total rock (Mt (%)*)	Uncertainty in MCO_2 stored in total rock (Mt (%)§)
Butmah	1	106	66.25	48	Limestone	0.0775	50.77 (94.69%)	5.55 (10.94)	2.85 (5.31%)	0.312 (10.94)	53.61 (100%)	5.87 (10.94)
	2	170	75.00	68	Dolomite	0.6120	68.20 (97.32%)	7.22 (10.58)	1.88 (2.68%)	0.199 (10.58)	70.08 (100%)	7.42 (10.58)
	3	99	87.35	34	Limestone	0.0909	43.66 (95.69%)	4.81 (11.01)	1.96 (4.31%)	0.216 (11.01)	45.62 (100%)	5.02 (11.01)
	4	96	13.58	212	Dolomite	0.8409	318.80 (97.98%)	35.20 (11.04)	6.56 (2.02%)	0.724 (11.04)	325.36 (100%)	35.92 (11.04)
	5	33	30.94	32	Limestone	0.0842	29.85 (95.59%)	3.89 (13.03)	1.38 (4.41%)	0.180 (13.03)	31.23 (100%)	4.07 (13.03)

Notes: The * indicates the percentage is a percent of the fraction of CO_2 stored in either the pores or dissolved in the water. The § indicates the error percentage of the pertaining measurement.

Table 3 shows that the highest gross mass of CO_2 stored in total rock was in the dolomite lithology represented by U.4 (212 m) with 325.36 Mt, followed by U.2 (68 m) with 70.08 Mt, whereas the lowest gross mass of CO_2 stored in total rock was in the limestone lithology represented by U.5 (32 m) with 31.23 Mt and U.3 (34 m) with 45.62 Mt, respectively. U.1 (48 m) showed moderate gross mass of CO_2 stored in total rock with 53.61 Mt.

The final predicted gross tonnage of CO_2 for the reservoir is 525.9 Mt, which is reasonable given that oil solution trapping and adsorption trapping have not been included in the calculations.

3.4 QD fracture effect and CO_2 storage

Fractures inside subsurface formations significantly impact the efficacy and security of geological CO_2 storage. Fractures can improve injectivity by creating high permeability channels for CO_2 migration (Mohammed-Sajed et al., 2024c; Rutqvist et al., 2010; Birkholzer et al., 2015). Conversely, they may serve as conduits for leakage if they compromise the integrity of sealing caprocks or connect to overlying permeable units (Doster et al., 2013). Moreover, the geomechanical stress field and fluid–rock interactions are influenced by CO_2 injection, which can reactivate pre-existing fractures, induce new fracture propagation (Kim and Hosseini, 2014).

The effect of fracturing on the stratigraphic units of the Shiranish Formation was clear, especially in Unit 4. The fracturing effect improved the total CO_2 storage capacity by 461 Mt between the low fractured rocks of U.1 (Part A) (187 Mt) and the high fractured rocks of U.4 (648 Mt). The highest fracturing effect was represented by U.4 and U.1 (B), and a moderate fracturing effect was noticed in U.2 and U.3, whereas U.1 (A) showed the lowest fracturing impact in the formation. Figure 10 illustrates the fracturing effect on the stratigraphic units of the Shiranish Formation through a comparison of the identified units from the perspective of the relationship between total CO_2 storage and porosity, permeability, and water saturation.

It is clear that there is a positive relationship with porosity and permeability and, as expected, a reverse relationship with water saturation.

Figure 10: Comparison examines the total CO_2 storage in rock based on porosity (a, b, c), water saturation (d, e, f), and permeability (g, h, i) across three categories: low fractured U.1 (A), moderately fractured U.2 and U.3, and highly fractured U.1 (B) and U.4.

The improvements in the CO_2 storage capacity in the Shiranish Formation can be summarised in Table 4.

Table 4: The fracturing effect on the reservoir quality and specific CO_2 storage capacity of the stratigraphic units of the Shiranish Formation. Area assumed to be 100 km^2 (Mohammed-Sajed et al., 2024c)

Formation	Strati-graphic unit	Number of Measure-ments (-)	Coverage (%)	Thickness (m)	Lithology	FEI (-)	MCO_2 stored in pores ($kt/m/km^2$ (%)*)	Uncertainty in MCO_2 stored in pores ($kt/m/km^2$ (%)§)	MCO_2 stored in water ($kt/m/km^2$ (%)*)	Uncertainty in MCO_2 stored in water ($kt/m/km^2$ (%)§)	MCO_2 stored in total rock ($kt/m/km^2$ (%)*)	Uncertainty in MCO_2 stored in total rock ($kt/m/km^2$ (%)§)
Shiranish	1 (Part A)	345	54.19	191	Marly limestone	0.31	2.95 (91.88%)	0.377 (12.79)	0.261 (8.12%)	0.0333 (12.79)	3.21 (100%)	0.410 (12.79)
	1 (Part B)	309	59.04	157	Limestone	1.09	9.3 (93.54 %)	1.246 (13.39)	0.643 (6.46 %)	0.086 (13.39)	9.95 (100%)	1.333 (13.39)
	2	392	94.84	124	Marly limestone	0.43	7.16 (94.47%)	1.024 (14.3)	0.42 (5.53%)	0.060 (14.3)	7.58 (100%)	1.084 (14.3)
	3	459	99.78	138	Limestone	0.85	8.35 (94.89%)	1.158 (13.86)	0.449 (5.11%)	0.062 (13.86)	8.8 (100%)	1.219 (13.86)
	4	230	71.88	96	Marly limestone	15.55	28.2 (94.65 %)	4.386 (15.55)	1.59 (5.35 %)	0.247 (15.55)	29.8 (100%)	4.634 (15.55)

Notes: The * indicates the percentage is a percent of the fraction of CO_2 stored in either the pores or dissolved in the water. The § indicates the error percentage of the pertaining measurement.

Table 4 shows that the highest specific mass of CO_2 stored in total rock was in the U.4 (96 m) with 0.0298 Mt/m/km^2, followed by U.1(B) (157 m) with 0.00995 Mt/m/km^2, whereas the lowest specific mass of CO_2 stored in total rock was represented by U.1(B) (32 m) with 0.00321 Mt/m/km^2. U.2 (124 m) and U.3 (138 m) showed the lowest specific mass of CO_2 stored in total rock with 0.00758 Mt/m/km^2 and 0.00880 Mt/m/km^2, respectively.

Table 5: The fracture effect on the reservoir quality and gross CO_2 storage capacity of the Shiranish Formation.

Formation	Strati-graphic unit	Number of Measure-ments (-)	Coverage (%)	Thickness (m)	Lithology	FEI (-)	MCO_2 stored in pores (Mt (%)*)	Uncertainty in MCO_2 stored in pores (Mt (%)§)	MCO_2 stored in water (Mt (%)*)	Uncertainty in MCO_2 stored in water (Mt (%)§)	MCO_2 stored in total rock (Mt (%)*)	Uncertainty in MCO_2 stored in total rock (Mt (%)§)
Shiranish	1 (Part A)	345	54.19	191	Marly limestone	0.31	56.30 (91.88%)	7.201 (12.79)	4.98 (8.12%)	0.637 (12.79)	61.28 (100%)	7.838 (12.79)
	1 (Part B)	309	59.04	157	Limestone	1.09	146.08 (93.54 %)	19.567 (13.39)	10.09 (6.46 %)	1.351 (13.39)	156.18 (100%)	20.920 (13.39)
	2	392	94.84	124	Marly limestone	0.43	88.84 (94.47%)	12.703 (14.3)	5.20 (5.53%)	0.744 (14.3)	94.05 (100%)	13.448 (14.3)
	3	459	99.78	138	Limestone	0.85	103.59 (94.89%)	14.360 (13.86)	5.57 (5.11%)	0.772 (13.86)	109.16 (100%)	15.132 (13.86)
	4	230	71.88	96	Marly limestone	15.55	194.53 (94.65 %)	30.253 (15.55)	10.99 (5.35 %)	1.709 (15.55)	205.51 (100%)	31.961 (15.55)

Table 5 shows that the highest total CO_2 storage was in U.4 and U.1 (B) with 205.51 Mt and 156.18 Mt, respectively, followed by U.3 (109.16 Mt) and U.2 (94.05 Mt) as moderate CO_2 storage, then U.1 (A) as the lowest CO_2 storage capacity with 61.28 Mt. The results in Table 4 align with those of the Fracture Effect Index, which highlights the importance of Quantitative Diagenesis (QD) in estimating CO_2 storage capacity in carbonate reservoirs.

Figure 11 illustrates the porosity-permeability relationship with the total CO_2 storage in the stratigraphic units of the Shiranish Formation.

Figure 11: Poroperm relationship with the mean of the CO_2 storage capacity in the four stratigraphic units of the Shiranish Formation.

4 DISCUSSION

Due to their high reactivity and tendency to create very heterogeneous reservoirs, carbonate minerals are highly susceptible to major changes upon CO_2 injection. These changes may have an impact on injectivity and integrity and, ultimately, storage safety (Bildstein et al., 2009; Mohammed-Sajed and Glover, 2020, 2022; Mohammed-Sajed et al., 2021; Glover et al., 2022). The relationship between chemical interactions porosity and permeability is a well-known problem needing a challenging solution. This association is essential to comprehending the effects of CO_2-induced geochemical processes (Luquot et al., 2014). Consequently, it is crucial to characterise thoroughly any storage location before the injection phase, and it is crucial to look at the interactions between CO_2 and water-rock in these kinds of reservoirs and how they affect gas emplacement (Gaus, 2010).

Dolomitisation and fracturing are the most important factors, which control CO_2 storage in carbonate reservoirs by influencing the reservoir rock porosity and permeability (Campbell-Stone et al., 2011; Siqueria et al., 2017; Stacey et al., 2024). Carbonic acid, which is created when CO_2 is fed into a reservoir, and dissolves in *in situ* aqueous pore fluids, influences porosity both directly through dissolving and indirectly through altering the dynamics of the dolomitisation process (Siqueria et al., 2017; Stacey et al., 2024).

In this paper, we have presented two quantitative diagenetic (QD) techniques which allow the post- and pre-dolomitisation porosities and permeabilities to be calculated. These techniques also help to understand the petrodiagenetic pathways of the changing rock via many diagenesis phases that might transform a poor-quality carbonate reservoir into one of high quality, or *vice versa* (Mohammed-Sajed et al., 2024a). These new quantitative diagenetic techniques are very important for previous characterisation of any reservoir before CO_2 injection stage. Applying QD techniques on the well log data of the Butmah Formation shows that the CO_2 storage of the formation increased 154.23 Mt as the lithology transferred from limestone to dolomite, whereas the CO_2 storage capacity improved 144.23 Mt between the low fractured rocks of U.1 (A) and the high fractured rocks of U.4 in the Shiranish Formation. Moreover, we have also explained briefly a new parameter for calculating the fractional degree of dolomitisation (χ_{DOL}) and the effectiveness of fractures in improving fluid flow, the Fracture Effect Index (FEI). Understanding the effect of dolomitisation and existing and induced fracturing is one of the most important aspects of judging porosity and permeability for any carbonate reservoir, before assessing whether the reservoir shows potential as a prospective CCUS target reservoir. Figure 12a shows the positive relationship between the storage mass of CO_2 in the Butmah Formation with fractional degree of dolomitisation (χ_{DOL}). Hopefully, further data from other formations will allow a better empirical relationship to be derived in future. Figure 12b illustrates the storage mass of CO_2 the FEI indicating the fracturing effect on the stratigraphic units of the Shiranish Formation.

In each case, five units is not sufficient data to which to fit a mathematical relationship with high confidence. This is particularly the case for Figure 10a, where three datapoints are near χ_{DOL}=0 and one rock unit (data point) approaches χ_{DOL}=1, with only one other datapoint in between. Consequently, we have fitted a single linear relationship of the form

$$MCO_2 = 0.0091\,\chi_{DOL} + 0.0177 \tag{11}$$

which has R^2=0.7274, and which indicates that the expected specific storage of CO_2 in limestone (without adsorption) is 0.0177 Mt/m/km^2. However, we accept that logarithmic and power law fits might also exist, and this will become clear as more data for different rock units can be added to the figure and the fit.

For Figure 12b the data is more evenly distributed, and it is clearer that a power law fit is most appropriate with R^2=0.9811, but a linear fit also works well.

All of the QD techniques are useful with regard to the necessary characterisation, modelling and flow simulation that would then need to be carried out in order to ensure that CO_2 could be injected effectively and stored safely in the CCUS reservoir.

Figure 12: (a) The positive relationship between the specific CO_2 storage capacity and the calculated χ_{DOL} of the Butmah Formation, (b) the relationship between the specific CO_2 storage capacity and the fracture effect index (FEI) in the four stratigraphic units of the Shiranish Formation.

Carbon capture and storage in deep saline aquifers and legacy oil reservoirs primarily differences in the methodologies employed for calculating and verifying the amount of stored CO_2. In saline aquifers, which are filled with brine and not associated with hydrocarbon extraction, nearly all injected CO_2 is deemed stored unless leakage is identified. Storage capacity is often assessed by evaluating reservoir volume, porosity, and efficiency parameters, while also accounting for constraints imposed by pressure accumulation and fracture risk (Zhou et al., 2008). Aquifers gradually sequester CO_2 through residual trapping, brine dissolution, and ultimately mineralization, processes that enhance long-term storage security (Neufeld et al., 2010).

Conversely, legacy oil reservoirs function as "open systems" where in injected CO_2 engages with hydrocarbons and is partially extracted with oil and gas during enhanced oil recovery (EOR) (Birkholzer et al., 2009). This indicates that net storage must be meticulously calculated as the injected CO_2 minus the quantity produced and exported, with further adjustments for surface recycling. Consequently, Storage estimations are contingent upon the reservoir's hydrocarbon pore volume and pressure management procedures, rendering them more site-specific and path-dependent compared to aquifer predictions (Szulczewski et al., 2012). Saline aquifers prioritize pressure-constrained volumetric capacity and inherent trapping processes, whereas oil reserves focus on precise mass accounting, production oversight, and recycling management. Both need rigorous measurement, monitoring, and verification (MMV) to validate long-term confinement (Birkholzer et al., 2009; Szulczewski et al., 2012).

Overall, this work indicates that the potential for diagenesis to enhance CO_2 storage is great. However, it is worth noting that there are several aspects of this paper which mean that it cannot be seen as a definitive statement on the issue, but a strongly suggestive statement nevertheless. The first is that we were unable to include calculations for CO_2 disolved in the remaining oil or CO_2 adsorbed to the rock matrix.

The first lacuna arises because the two fields concerned are not yet at the end of their production life so that the residual oil saturation is not known. However, when it is known such calculations must take account that the remaining oil is already saturated with hydrocarbon gases or flooding gases if gas-flooding has been used. It is likely, therefore that there will be negligible opportunity for further CO_2 to be stored dissolved in the residual oil.

The second lacuna is that insufficient information is currently known about the fields to calculate the mass of gas adsorbed per mass of rock. Even a simple treatment of this, say using a Langmuir isotherm, would require the maximum specific adsorption (q_{max}) and Langmuir pressure (P_L) to be used together with the CO_2 fluid pressure at depth. These two values depend on lithology and if known (here for limestone, dolomite, shale and anhydrite) can be mixed linearly. This would clearly be an important research route for the future, given that the mass fraction of calcite and dolomite change significantly during dolomitisation.

However, the interaction between CO_2 and both calcite and dolomite is complicated by reactions with CO_2, dissolution and precipitation, changes in wettability (Wang et al., 2013), the formation of nanobubbles on the surface (Yao et al., 2025) and competitive adsorption

(Tang and Ripepe, 2025) that makes the use of a Langmuir approach too simple and results in a lack of knowledge of the parameters for these systems because the values would be over-simplistic. Instead, an equation of State approach would need to be followed which is outside the scope of this paper. We have searched for scientific papers using this approach with no result. However, another approach is to use molecular modelling, where some studies are available on both calcite (Guo et al., 2023; Ravipati et al., 2021; Le et al., 2020) and dolomite (Yao et al., 2025; Li et al., 2024 ; Reischl et al., 2019), and may form the basis of CO_2 adsorption calculations.Another problem which the calculation of stored CO_2 mass shares with the conventional calculation of the volumes of hydrocarbon in place is that of uncertainties in the calculation input parameters. A wide range of statistical tools has been developed to handle the financial risk associated with such uncertainties in the hydrocarbon industry, which will be very applicable to the calculation of mass storage. These approaches include ensemble-based and history-matching approaches (Tuczyński and Stopa, 2023), deterministic and probabilistic approaches (Justine et al., 2024), Bayesian and geological scenario uncertainty (Demyanov et al., 2019), other Bayesian approaches (Ruiz Maraggi et al., 2022; Rotondi et al., 2006), and comparing probability point estimate methods with conventional Monte-Carlo approaches (Algdamsi et al., 2019). Application of any of these approaches to the uncertainties present in the input data, as shown in this paper, will help minimise uncertainties in the final calculated values.

5 CONCLUSIONS

Injection of CO_2 into carbonate reservoirs (as during CCS operations) is known to enhance dolomitisation, increase porosity and permeability and instigate new fracturing. In this paper, we have described four recent quantitative diagenesis techniques, which are useful in the provision of quantitative parameters for CCUS reservoir modelling and simulation. Two of the techniques allow the prediction of porosity and permeability after different degrees of dolomitisation and postdiction of host carbonate porosity and permeability before dolomitisation. Applying this technique to the Butmah Formation shows that the potential

CO_2 storage of the formation improved by 154.23 Mt (0.0051 Mt/m/km^2) as the lithology transferred from limestone to dolomite. However, only an unknown fraction of this value will take part in storage in reality, it must be considered to be an upper limit to the CO_2 storage enhancement.

The third technique maps the diagenetic evolution of a rock through many types of diagenetic process as a petrodiagenetic pathway, which also has the potential for prediction and postdiction of porosity and permeability as well as comparison of the rock at each diagenetic stage with a predefined assessment of reservoir quality.

Finally, the FEI parameter is a measure of the effectiveness of how fractures enhance or degrade fluid flow. This is an important QD parameter for CCUS in carbonate reservoirs because injected CO_2 can modify fracture networks. Carbon dioxide dissolves to produce carbonic acid in aqueous pore fluids, which can enlarge fracture apertures, increase porosity in the matrix in the proximity of the fracture, enhancing reservoir storage. The carbonic acid decreases the pH of the pore fluid, impacting the dynamics of the dolomitisation process. Consequently, the CO_2 storage capacity in the Shiranish Formation improved 144.23Mt (0.0266 Mt/m/km^2) between the low fractured rocks of U.1 (FEI=0.31) and the high fractured rocks of U.4 (FEI=15.55). As always, the implications for changes in FEI on CCUS mass storage depends on the accurate calibration of FEI values against the actual effect on flow. Since the FEI concept is still very recent (Mohammed-Sajed et al., 2024b), this has not yet been carried out. However, comparison of FEI values with empirical flow data and numerical simulations is required for heterogenous carbonate reservoir rocks in order that the FEI approach can be considered to be robust.

Quantitative diagenesis is still in the early stages of development, but the techniques available are already finding applications and it is expected that further quantitative ways of characterising reservoirs for CCUS will be developed as data becomes available. Although this study does not, in itself, provide data or modelling results to substantiate claims about enhanced porosity, permeability, or trapping efficiency, but applies previous work to the calculation of CO_2 storage in dolomitised reservoirs, it has been suggested that a more rigorous, data-driven comparison between dolomite and calcite systems would be beneficial to our understanding of the system, and is the focus of future work.

This work does not address the potential geomechanical risks (e.g., fracturing, leakage pathways) or long-term stability of the altered formations because that is not its goal. However, these are important aspects for researchers in the field to consider.

Overall, it is fair to say that the qualitative observations and quantitative calculations in this work clearly show that diagenesis improves significantly the potential of limestone reservoirs for use storing carbon dioxide underground, and the improvement can be calculated quantitatively the help of QD tools. However, it is clear that a more detailed study would be beneficial, preferably on a reservoir where CCUS has been implemented, allowing the calculations to be to some extent validated, and including site-specific geological constraints such as pressure limits, caprock integrity, and residual trapping mechanisms. This will also test the scalability and the degree to which calculations such as those carried out in this paper can be carried out effectively.

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