

1 A tool for first order estimates and optimisation of
2 dynamic storage resource capacity in saline aquifers.

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6 **Abstract**

7 The importance of carbon capture and storage in mitigating climate change has
8 emerged from the results of techno-economic or integrated assessment modeling, in
9 which scenarios of future energy systems are developed subject to constraints from
10 economic growth and climate change targets. These models rarely include limits im-
11 posed by injectivity, ultimate amounts, or the geographic distribution of storage re-
12 sources. However, they could if a sufficiently simple model were available. We develop
13 a methodology for the fast assessment of the dynamic storage resource of a reservoir
14 under different scenarios of well numbers and interwell distance. The approach com-
15 bines the use of a single-well multiphase analytical solution and the superposition of
16 pressure responses to evaluate the pressure buildup in a multiwell scenario. The injec-
17 tivity is directly estimated by means of a nonlinear relationship between flow-rate and
18 overpressure and by imposing a limiting overpressure, which is evaluated on the basis
19 of the mechanical parameters for failure. The methodology is implemented within a
20 tool, named CO2BLOCK, which can optimise site design for the numbers of wells and
21 spacing between wells. Given its small computational expense, the methodology can
22 be applied to a large number of sites within a region. We apply this to analyse the
23 storage potential in the offshore of the UK. We estimate that 25-250 GtCO₂ can be
24 safely stored over an injection time interval of 30 years. We also demonstrate the use of
25 the tool in evaluating tradeoffs between infrastructure costs and maximising injectivity
26 at two specific sites in the offshore UK.

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1 Introduction

Carbon capture and storage (CCS) is considered essential for mitigating climate change (IPCC, 2005). Several hundred Gt of CO₂ must be captured and permanently stored to achieve the net-zero CO₂ emission target by 2050 while approximately 220 MtCO₂ has been stored to date (IEA, 2017; IPCC, 2018; Global CCS Institute, 2017). The transition from megatonnes to gigatonnes of injected CO₂ requires the deployment of hundreds to thousands of large-scale projects with the commensurate potential for technical and economic limitations (Herzog, 2011). Emissions mitigation targets are estimated using a type of systems modelling known as techno economic or integrated assessment modeling (IPCC, 2018). These models rarely include limits imposed by the injectivity, ultimate amounts, or the geographic distribution of storage resources (Akimoto et al., 2004; Koelbl et al., 2014). However, these limitations can be accommodated by systems models should sufficiently simple models be developed to represent key aspects of CO₂ storage use.

There are different methods to estimate the amount of CO₂ that can be stored in a reservoir and the term "storage capacity" often refers to different concepts (see Bachu, 2015, for a complete review and discussion). Volumetric estimates are based on the available pore space in the aquifer that may be filled with CO₂. These estimates are often classified as "theoretical storage capacity" and they do not take into consideration constraints represented by the physical and chemical characteristics of the reservoir. Leading order limits on the use of subsurface saline aquifer resources may come from reservoir pressurisation, and plume migration towards leakage pathways (Szulczewski et al., 2012; Ringrose and Oldenburg, 2018). In practice, reservoir pressurisation is more often limiting over decadal timescales. With the exception of hydrocarbon reservoirs, reservoir pore space is already saturated by resident brine, and injected CO₂ leads to an increase in the pore pressure. This pressure build-up must be kept under certain limits to avoid reservoir fracturing, fault reactivation, or caprock failure, which can lead to felt seismicity, and in limited circumstances, CO₂ leakage from the reservoir (Bachu, 2008; National Academy of Science, 2012; Rutqvist et al., 2008; Rutqvist, 2012). Therefore, storage capacity should reflect the pressure-limited amount that can be safely stored and we adopt here this definition.

A number of simplified analytic models estimating the reservoir pressurisation have been developed and are potentially suitable for integration with techno-economic models (Neufeld et al., 2010; Krevor et al., 2019). The simplest involves approximation of the reservoir system as a closed volume and provides static estimates of pressure buildup based on the injected volume and compressibilities of rocks and fluids (Zhou et al., 2008). This is often overly conservative as it does not take into consideration the temporal evolution of the storage capacity and the permeability of reservoir bounding lithology which can serve as a pressure relief (Vilarrasa and Carrera, 2015). More accurate estimates are provided by models capturing the dynamic nature of both plume migration and reservoir pressurisation in response to the time evolution of storage resource use (Nordbotten et al., 2005; Dentz and Tartakovsky, 2009; Mathias et al., 2009, 2011; Vilarrasa et al., 2010; Azizi and Cinar, 2013). These models solve the governing multiphase flow equations for a problem geometry in which there is a single injection well in a reservoir. These single-well models have been extended to estimates of pressurisation during simultaneous injection through multiple wells by superposing their

70 solutions (Ganjdanesh and Hosseini, 2017; Huang et al., 2014; Joshi et al., 2016; Zakrisson
71 et al., 2008). While not mathematically rigorous, De Simone et al. (2019) show that the
72 error in the use of superposition is small for a wide range of injection scenarios relevant to
73 the development of regional subsurface storage resources, and a correction factor may be
74 applied in the case in which the error is significant.

75 This approximation allows for a consideration of the kinds of tradeoffs that may arise in
76 the comparison of scenarios considered in energy systems models. For example, on the one
77 hand, using multiple injectors may increase the reservoir injectivity, although this is highly
78 dependent on factors such as reservoir pressure, injection rates, and spacing between wells.
79 On the other hand, the construction and operation of wells is a significant contributor to
80 investment and operating costs, and may not always be justified by the increased volume of
81 CO₂ that may be stored.

82 In this paper we build on the analysis in De Simone et al. (2019) to develop a method-
83 ology to estimate CO₂ injection rates that maximise storage whilst not exceeding a limiting
84 pore pressure increase specific of the reservoir. A range of scenarios of injection well number
85 and inter-well distance is explored. The methodology has been implemented within an open
86 source software tool named CO2BLOCK. The computational expense of the estimation is of
87 the order of seconds in a normal desktop machine, which allows for an optimisation of well
88 numbers and spacing around an objective of interest such as storage capacity or net rev-
89 enue. We demonstrate two applications in the UK offshore system: estimates and sensitivity
90 analysis of the total storage resource of the offshore UK, and a net revenue estimate which
91 incorporates tradeoffs between injectivity and capital costs associated with injection wells for
92 site buildout at two specific sites.

93 2 Methodology

94 The tool, which is named CO2BLOCK, estimates the maximum rate of injection and ultimate
95 storage resource of a reservoir in which CO₂ is injected into a number n of vertical wells on a
96 geometrical grid with spacing d . This is done for a range of n and d such that the output can
97 be used as a basis for further optimisation. Overpressure, i.e., the pore pressure increase with
98 respect to the initial conditions, is assumed as the major constraint and it must be kept below
99 a critical value. We define the storage capacity as the maximum amount that can be stored
100 without exceeding the critical overpressure. The reservoir is assumed as homogeneous, with
101 the wells placed on a Cartesian grid and all operating with the same injection rate, which is
102 constant in time.

103 The workflow follows four steps following the input of data (Figure 1). First, the maxi-
104 mum sustainable overpressure in the reservoir is estimated according to the initial conditions
105 and the mechanical conditions for failure. Second, the tool predicts the pressure increase in
106 response to a reference CO₂ injection flow-rate. Third, the maximum sustainable injection
107 rate is estimated for the range of scenarios of well number and spacing by ensuring that the
108 maximum allowable overpressure is not exceeded. Fourth, three further constraints, related
109 to technical limitations and reservoir dimension, eliminate a number of scenarios. From this

110 information, scenarios may be identified according to defined optimization criteria, such as
 111 storage maximising scenarios, or revenue maximising scenarios. We provide an overview in
 112 the following, while further details are provided in Supporting Information.

113 The methodology is first applied to an illustrative example whose characteristics are
 114 detailed in Table 1. For the example case, the maximum interwell distance is set to 10 km
 115 and the maximum well number to 42 (a 6×7 grid). All properties are considered uniform
 116 over the reservoir and constant in time. Initial pressure and temperature, brine and CO₂
 117 properties, and geomechanical parameters may be provided as input, with values spanning
 118 over the typical ranges. If not provided, default values are assumed for compressibility and
 119 geomechanical properties, while fluid properties are calculated according to equations of state
 120 (see Table S3 in Supporting Information).

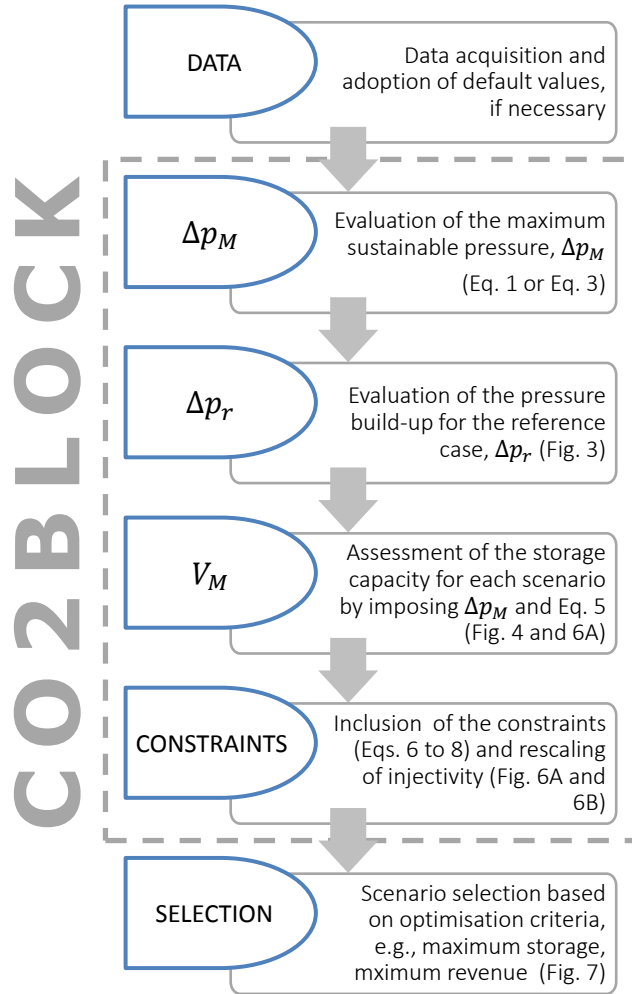


Figure 1: Methodology for the assessment and optimization of the CO₂ storage capacity using CO2BLOCK. Steps enclosed in the dashed rectangle are the steps taken within CO2BLOCK. Further details are provided in Supporting Information, Section S7.

Table 1: Parameters adopted for the case example.

Symbol	Parameter	Value	Units
Input parameters			
A	Reservoir surface area	900	km ²
BC	Domain boundary type	open	-
c_r	Rock compressibility	1×10^{-10}	Pa ⁻¹
c_w	Brine compressibility	1×10^{-10}	Pa ⁻¹
C	Cohesion	0	MPa
H	Thickness	250	m
k_0	Stress ratio	0.5	-
p_0	Initial pressure	15	MPa
Q_r^{tot}	Reference total injection rate	10	Mt/yr
Q_s	Technical limit to injection rate per well	2	Mt/yr
r_w	Well radius	0.05	m
S_0	Tensile strength	0	MPa
t	Injection time	40	yr
ζ_m	Average depth	1500	m
κ	Permeability	5×10^{-14}	m ²
μ_w	Brine viscosity	5×10^{-4}	Pa s
μ_c	CO ₂ viscosity	5×10^{-5}	Pa s
ρ_c	CO ₂ density	900	kg/m ³
σ_1	Maximum principal stress	40.5	MPa
ϕ	Porosity	0.2	-
φ	Friction angle	27	°
Output parameters			
p_M	Maximum sustainable pressure		MPa
Q_M	Maximum sustainable injection rate per well		Mt/yr
V_M	Maximum storage capacity		Gt

121 2.1 Limits to pressure build-up

122 A major technical constraint to storage comes from the geomechanical response of the reser-
123 voir to the pressure increase. The possibility of activating pre-existing faults or opening new
124 fractures is an issue of great concern, primarily due to seismicity, but also due to the potential
125 for CO₂ leakage back to the atmosphere (Zoback and Gorelick, 2012; Vilarrasa and Carrera,
126 2015; Ellsworth, 2013; National Academy of Science, 2012).

127 Rock failure may occur in either a tensile or shear mode (Jaeger et al., 2009). Tensile
128 failure is likely to occur along planes normal to the minimum principal stress, σ_3 , when the
129 pore pressure is greater than the sum of σ_3 and the rock tensile strength, S_0 . The limiting
130 pressure build-up for tensile failure, Δp_M^t , is given by

$$\Delta p_M^t = \sigma_3 - p_0 + S_0, \quad (1)$$

131 where p_0 is the initial pressure, often assumed equal to the hydrostatic pressure. It is common
 132 practice to assume $S_0 = 0$, which means that the fracture pressure is equal to the minimum
 133 principal stress.

134 Shear failure occurs along a given orientation when the shear stress, τ , overcomes the
 135 frictional forces, according to the Mohr-Coulomb failure criterion

$$\tau - [C + (\sigma_n - p) \tan \varphi] \geq 0, \quad (2)$$

136 where σ_n represents the stress acting normal to the orientation, φ is the internal friction
 137 angle, and C is cohesion, which many experimental data show to be often equal to $2S_0$
 138 (Jaeger et al., 2009). By assuming that failure occurs along the most critical orientations
 139 (i.e., the ones forming angles of $(\pi/4 \pm \varphi/2)^\circ$ with the direction of the maximum principal
 140 stress, σ_1), the limiting pressure build-up for shear mode, Δp_M^s , can be expressed by

$$\Delta p_M^s = \frac{k_0 - \theta}{1 - \theta} (\sigma_1 - p_0) + C \frac{\cos \varphi}{\sin \varphi}, \quad (3)$$

141 where $k_0 \leq 1$ is the ratio between the minimum and the maximum principal effective stresses,
 142 i.e., $k_0 = \sigma'_3/\sigma'_1 = (\sigma_3 - p_0)/(\sigma_1 - p_0)$, while $\theta = (1 - \sin \varphi)/(1 + \sin \varphi)$. The conservative
 143 assumption of $C = 0$ acknowledges that shear failure is likely to occur along planes of
 144 weakness, e.g., faults.

145 The difference between equations (1) and (3) indicates which of the two overpressure
 146 limits will be exceeded first,

$$\beta = \Delta p_M^t - \Delta p_M^s = \left(k_0 - \frac{k_0 - \theta}{1 - \theta} \right) (\sigma_1 - p_0) + S_0 - C \frac{\cos \varphi}{\sin \varphi}. \quad (4)$$

147 Positive values of β indicates that shear failure is more likely to occur than tensile
 148 failure and vice-versa. In the case of cohesionless rocks ($C = S_0 = 0$), failure mostly occurs
 149 in shear mode ($\beta > 0$), regardless of the stress conditions, since the first term on the right
 150 hand side of Equation (4) is always positive (Figs. 2A and C). Conversely, in the case of
 151 cohesive rocks, tensile failure is more likely to occur ($\beta < 0$) at shallow depths, where the
 152 effective stresses are smaller, even for small values of S_0 (Figs. 2B and D). This explains
 153 the processes of hydrofracturing performed in unconventional gas exploitation, where tensile
 154 failure is activated at depths less than 3 km in shale rocks with S_0 between 5 and 10 MPa
 155 (Chandler et al., 2016; Peduzzi and Harding Rohr Reis, 2013).

156 In our methodology the maximum sustainable overpressure, Δp_M , is evaluated as the
 157 lower value of the tensile and shear failure pressures, Δp_M^t and Δp_M^s . This evaluation is
 158 complicated by the uncertainty in the parameter values and by the reservoir heterogeneity.
 159 The relative magnitude and the orientation of the principal stresses defines the planes that
 160 are more likely to fail, as well as the critical overpressure. However, the *in situ* confining
 161 stress is often unknown. A common practice is to assume that one of the principal stresses
 162 is the vertical stress and is given by the lithostatic pressure. The other two principal stresses
 163 are therefore horizontal and can be estimated by the observations of wellbore compressive
 164 (breakouts) and tensile (drilling- induced) failures (Zoback et al., 2003). The lack of these

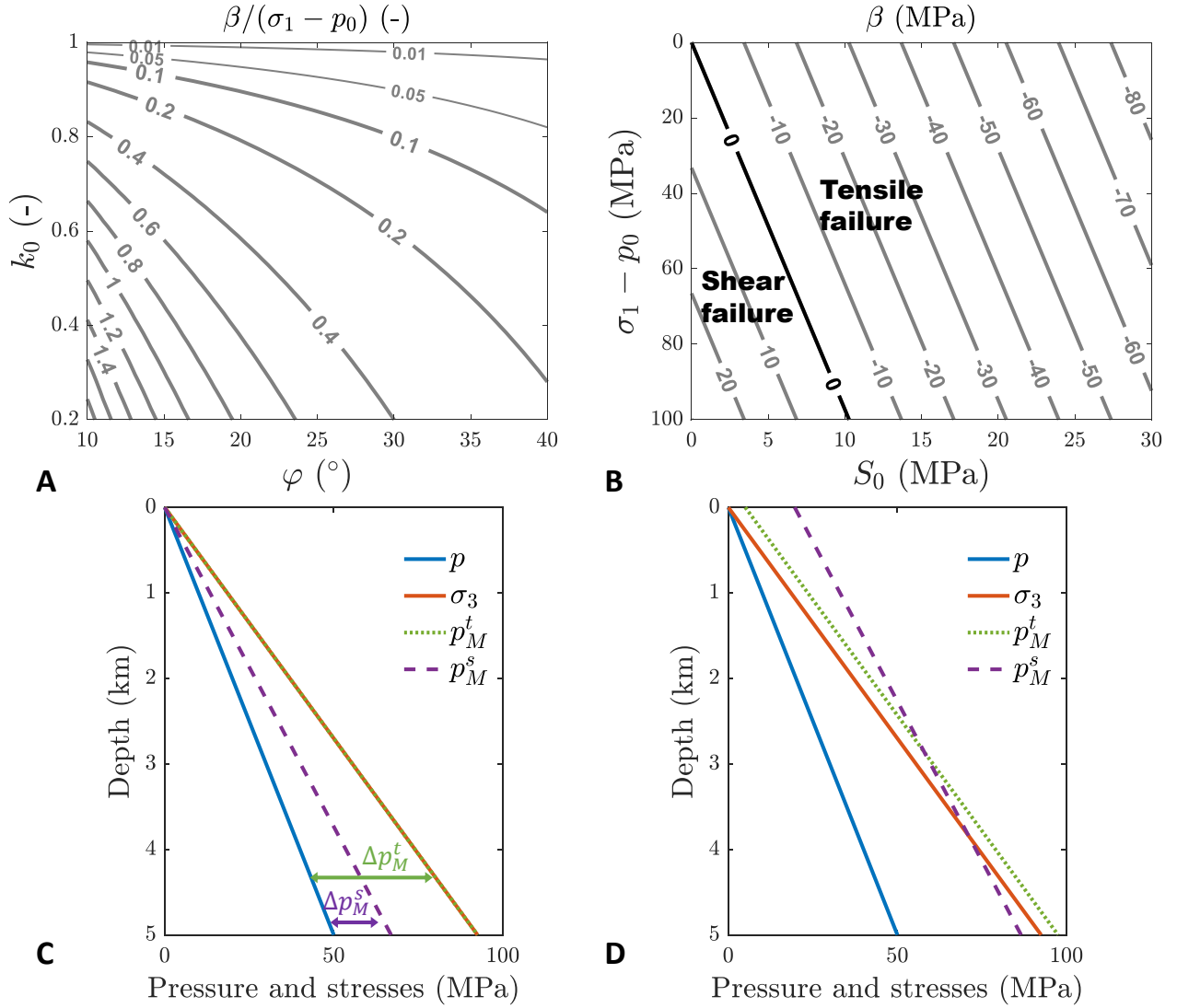


Figure 2: Example of potential for tensile and shear failure under different scenarios for cohesionless (left) and cohesive rocks (right). **A:** For cohesionless rock ($C = S_0 = 0$), the factor $\beta/(\sigma_1 - p_0)$ (eq. (4)) changes with the stress ratio k_0 and the internal friction angle φ , but it is always positive, which indicate that shear failure is more likely to occur over tensile failure. **B:** For cohesive rocks the values of β indicate that the failure mode is a function of the confining stress ($\sigma_1 - p_0$), as well as of the other parameters. In the example here, $C = 2S_0$, $\varphi = 27^\circ$ and $k_0 = 0.5$. **C and D:** Variation of pressure and pressure limits with depth for cohesionless and cohesive rocks, respectively. We assume that σ_1 is the vertical stress and that $\varphi = 27^\circ$ and $k_0 = 0.5$. Cohesion is $C = 2S_0 = 10$ MPa in the case of cohesive rock. Notice that the limiting pressure for tensile failure p_M^t coincides with σ_3 in the case of cohesionless rocks and it is greater than the limiting pressure for shear failure p_M^s for any depth. For cohesive rocks, the potential for tensile failure is greater than for shear failure at shallow depths (i.e., $p_M^t < p_M^s$), but the trend inverts for greater depths.

165 data generates large uncertainties in the evaluation of the pressure limit. Moreover, the pres-
166 ence of heterogeneity and planes of weakness is difficult to detect. We show how uncertainties
167 in input data may be evaluated in the applications in Section 3.1.

168 **2.2 Pressure build-up for a reference injection rate**

169 The next step is the prediction of the pressure buildup in response to a reference CO₂ injection
170 rate, over a specified time interval. This will be later used in the calculation of a maximum
171 possible injection rate, subject to constraints. Pressurisation is evaluated according to an
172 approach developed in De Simone et al. (2019). In summary, we adopt the solution to
173 single well CO₂ injection proposed by Nordbotten et al. (2005) with a modified version
174 for closed boundary domains (see Supporting Information, Section S1). The response to
175 the simultaneous CO₂ injection into multiple sites at a specified constant rate is estimated
176 as the superposition of single-well solutions, evaluated at the inner-most well, where the
177 overpressure is highest. The use of the superposition in the case of multiphase flow results in
178 an overestimate of the overpressure. The error is small for less than nine wells but becomes
179 significant with an increasing number of wells. With greater than nine wells, a correction
180 factor can be used to improve the estimate (supporting information, Section S3). This option
181 is available in the software tool that we provide but it is not used in the examples shown
182 here such that error is always in the direction of an overestimation of the pressure buildup,
183 corresponding to conservative estimates of CO₂ storage volumes.

184 The use of this approach allows us to evaluate various scenarios of well numbers and
185 interwell spacing for a total given injection rate into a reservoir unit. Figure 3 shows the
186 response to a reference total flow rate of $Q_r^{tot} = 10 \text{ Mt yr}^{-1}$ for 40 years in the case example
187 reservoir (Table 1). The pressure buildup decreases by increasing the number of wells and
188 increasing the distance between wells, but the response is non-linear. This allows for site
189 design subject to the constraint of maintaining pressure below the critical value, Δp_M .

190 **2.3 Estimating the maximum flow rate**

191 The pressure response to the reference injection rate can be used to estimate the maximum
192 sustainable flow rate, Q_M . This rate leads to a calculation of the maximum amount of CO₂
193 that can be continuously stored in a time interval, t , without exceeding the pressure limit,
194 Δp_M . In the case of single phase flow, the pressure build-up, Δp , increases linearly with the
195 injected flow rate, Q . Some authors have extended the linearity of the $\Delta p/Q$ relationship
196 to the case of multiphase flow (Szulczewski et al., 2012; Zhou and Birkholzer, 2011). This
197 allows them to estimate the maximum sustainable flow rate as $Q_M(t) = Q_r \Delta p_M / \Delta p_r(t)$,
198 where Δp_r is the pressure response to the injection of a reference flow rate Q_r , estimated at
199 the inner-most well. However, the nonlinearity of multiphase flow makes this approximation
200 valid only for small variations of flow rate, i.e., $Q_M \approx Q_r$.

201 For greater variations of Q , the variation of overpressure is strongly nonlinear, especially
202 for open domains and a small number of wells (Fig. 4, Supporting information Figs. S1 and
203 S2). This can give raise to significant errors in the estimation of the storage capacity. If the

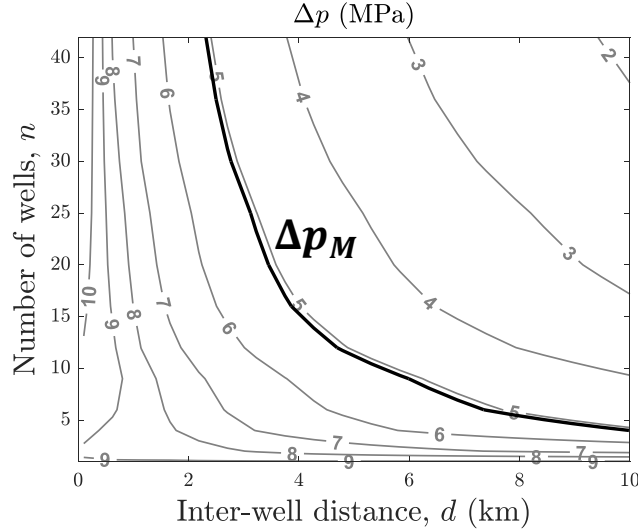


Figure 3: Pressure build-up at the inner-most well of the case example reservoir in response to 40 years of continuous injection under different scenarios of well number and spacing. The estimate is performed by superposition of single-well analytical solutions. The black solid line represents the maximum sustainable overpressure.

204 reference flow rate, Q_r , is smaller than the actual injectivity, Q_M , the linear assumption leads
 205 to an underestimate of the storage capacity. The adoption of a reference flow rate greater
 206 than the injectivity overestimates the storage capacity (Fig. 5).

207 We derive the exact relationship between overpressure and flow rate valid for both single
 208 and multiwell cases (Fig. 5 and Supporting Information, Section S2). This allows for the
 209 direct calculation of the maximum flow rate, given the overpressure response in a reference
 210 scenario,

$$Q_M(t) = -\frac{Q_r \widetilde{\Delta p}_M}{W\left(-\widetilde{\Delta p}_M \exp(-\widetilde{\Delta p}_r(t))\right)}, \quad (5)$$

211 where both the reference and the maximum sustainable flow rates refer to the mass injection
 212 into each well, $\widetilde{\Delta p}_y = \Delta p_y / (bQ_r)$, $b = (\mu_w - \mu_c) / (4\pi\kappa H\rho_c)$, κ is the absolute permeability, H
 213 is the reservoir thickness, ρ_c is the CO_2 density, μ_w and μ_c are the brine and CO_2 dynamic
 214 viscosities, respectively, while $W(x)$ represents the Lambert function for $x < 0$. This direct
 215 estimation provides a rapid assessment of the maximum sustainable flow rate for a number
 216 of scenarios (Fig. 6A). Note that density and viscosity are considered as constant during
 217 the injection. However, for both CO_2 and brine, density and viscosity increase with increas-
 218 ing pressure, especially in the case of CO_2 . Considering this variation would introduce an
 219 additional non-linearity in the relationship between overpressure and injected flow rate.

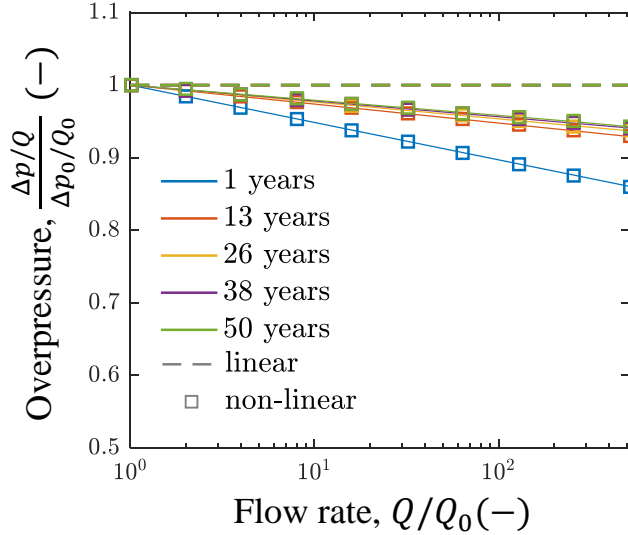


Figure 4: Maximum overpressure response normalized with respect to the injected flow rate under different flow rates of CO₂ injection. Values are non-dimensionalised with respect to the case of the smallest injection rate, Q_0 . Pressure build-up is evaluated at the inner-most well of the case example for the 16 wells scenario with interwell distance equal to 2 km. Colours correspond to different injection times (from 1 up to 50 years). Solid lines correspond to the solution calculated for each injection rate. Dashed lines, which all fall on the same line, represent the extrapolation of the pressure build-up from the response to Q_0 , by assuming a linear $\Delta p/Q$ relationship. Markers represent the extrapolation by means of the non-linear $\Delta p/Q$ relationship (see Eq. (S5) in Supporting Information). Note that the plot is represented in semi-log scale.

2.4 Constraints imposed by plume migration, reservoir dimension, and technical limitations to well injection rates

There are two constraints, a lower and upper, on the interwell distance. The first comes from the need to avoid CO₂ plume interference. This defines a lower constraint such that the half of the interwell distance is smaller than the plume average propagation distance, which gives

$$d > 2\sqrt{\frac{Q_M t}{n\pi\phi H\rho_c}}. \quad (6)$$

Note that plume intersection does not affect storage feasibility or safety. In this study, avoiding plume interference is a condition related with the assumptions underlying the adopted analytical model (see also section S1 and S2 in Supporting Information). Allowing plume interference would possibly imply a modification of the analytical solution and a verification/update of the error correction factor, which will be subject of future work and development of CO2BLOCK.

An upper constraint is defined by the reservoir surface area A , which limits the number of wells at a given spacing. Assuming that the well distribution is a Cartesian grid, and assuming a buffer area on the outer perimeter equal to $d/2$, the constraints imposed by the

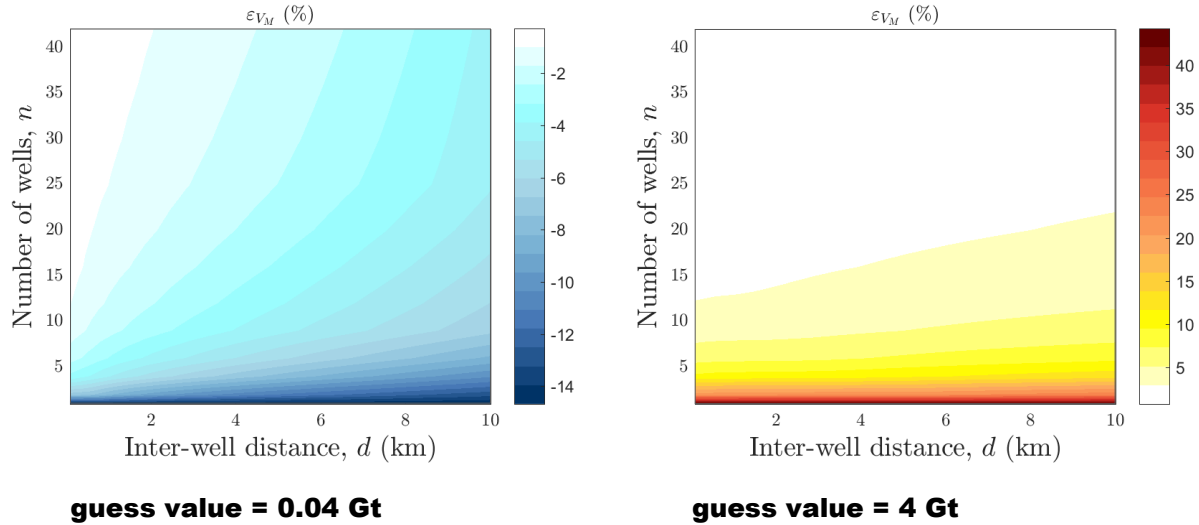


Figure 5: Relative error associated with the adoption of a linear $\Delta p/Q$ relationship for different well configurations of the case example adopted here, whose maximum storage capacity, V_M , is between 0.2 and 1.1 Gt for a 40 years injection (Fig. 6A). The linear approximation underestimates the storage capacity V_M if a small reference value is adopted (left), while it overestimates V_M if a greater reference value is assumed (right). The error is particularly high for small number of wells, according to the nonlinearity effects.

234 areal size of the reservoir is given by

$$d \leq \sqrt{A/n}. \quad (7)$$

235 There are technical limitations to the injectable flow rate per well and this is reflected
 236 by setting a value, Q_s , such that.

$$n \geq Q_M^{tot}/Q_s, \quad (8)$$

237 where Q_M^{tot} is the total injection rate, the sum of injection through the n wells. The storage
 238 resource use scenarios before and after these constraints are imposed are shown in Fig. 6A
 239 and Fig. 6B, respectively.

240 2.5 Optimising storage design

241 There are a number of ways in which storage resource use might be optimised. In Figure
 242 7 we estimate the maximum storage achievable in the reservoir for all scenarios of injection
 243 well numbers. Figure 7 shows that the maximum capacity does not necessarily correspond
 244 to the maximum number of wells. For this location, there is a maximum storage resource
 245 use obtained with the deployment of 20 wells throughout the formation. It is notable that
 246 in this example the storage capacity increases with the well number until reaching a sort of
 247 plateau, which corresponds to scenarios in which the storage is constraint by the reservoir
 248 surface area (observe the red line in Fig. 6B). Therefore, nearly the same capacity can be
 249 achieved with 16 wells, possibly presenting greater value for money. In the following sections

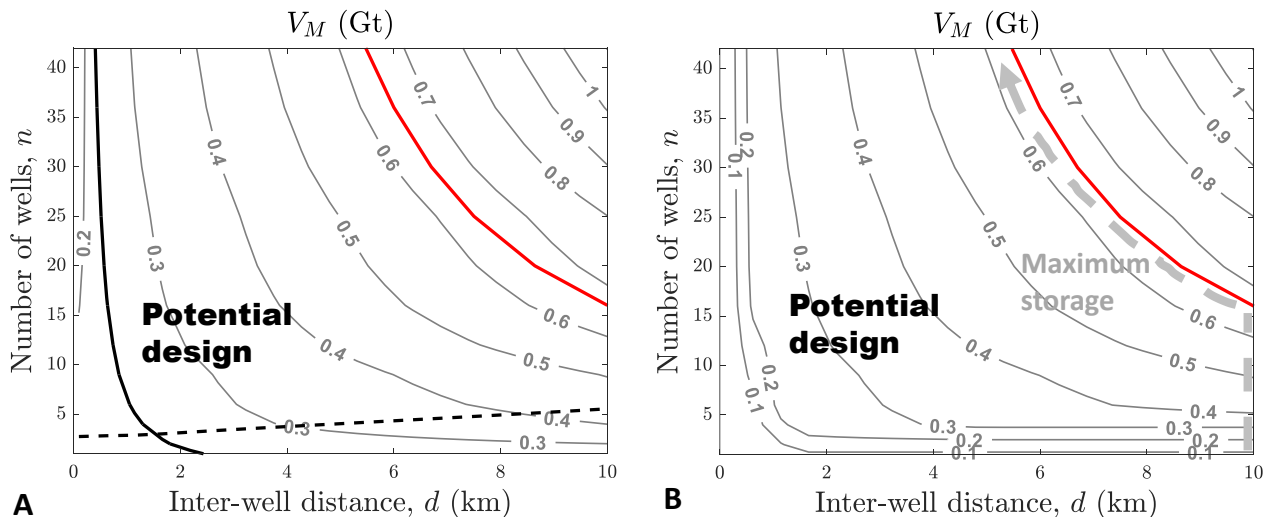


Figure 6: CO₂ storage capacity for the case example under different scenarios of well number and spacing and with 40 years of injection. **A:** pressure-limited storage capacity according to Eq. (5) and imposing the maximum sustainable pressure, Δp_M . The black solid line represents the lower constraint to avoid plume interference (Eq. (6)), the black dashed lines represents the lower constraints associated with technological limits (Eq. (8)), while the red solid line represents the upper constraint imposed by the reservoir dimension (Eq. (7)). **B:** Plausible storage capacity after the scaling out of those values of injectivity that fall out of the lower constraints (black solid and dashed lines in Fig. A). The dashed grey arrow defines the scenarios of maximum storage capacity, shown in Fig. 7.

250 we apply the tool for two targets - the assessment of the dynamic storage capacity of UK
 251 reservoirs, and optimising the use of specific reservoirs for maximum revenue.

252 3 Applications

253 3.1 Dynamic Storage Resources of the UK

254 We apply the methodology described in Section 2 (Fig. 1) to assess the maximum potential
 255 for CO₂ storage in the UK offshore system. All data have been collected from the CO₂
 256 stored database (Bentham et al., 2014; Energy Technologies Institute LLP, 2018), which
 257 contains information including geological data for nearly 600 potential CO₂ storage units
 258 located offshore UK. These include oil and gas reservoirs and saline aquifers.

259 We perform an initial screening to identify a subset of the sites with the most beneficial
 260 attributes for storage. Our analysis is limited to saline aquifers, representing about the 85%
 261 of the total storage capacity in the UK (Gammer et al., 2011; Pale Blue Dot Energy, 2016).
 262 The analysis is further restricted to formations where the caprock is deeper than 1 km in
 263 the subsurface, to ensure CO₂ remains in a supercritical state (IPCC, 2005). Only sites with
 264 permeability greater than 1 mD and porosity greater than 0.1 are considered. Finally, the
 265 aquifers with theoretical CO₂ storage less than 200 Mt are excluded. The screening reduces

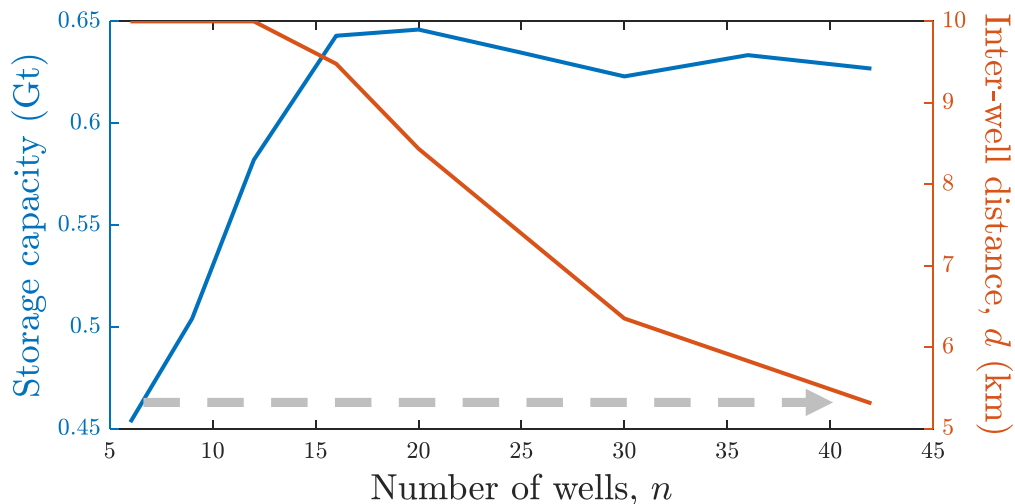


Figure 7: Maximum storage capacity for the case example for each scenario of well number (corresponding to the dashed grey arrow in Fig. 6B). The corresponding well spacing is represented by the orange line.

266 the consideration from 292 potential saline aquifer sites to 25, mostly located in the Northern,
 267 Southern or Central North Sea (see inset of Fig. 9 and Section S4 in supporting information
 268 for further details). They represent approximately 1/3 of the total theoretical capacity of 60
 269 Gt provided by the 292 saline aquifers.

270 The database does not provide information about the *in situ* stress conditions and the
 271 mechanical parameters, which are essential for the evaluation of the maximum sustainable
 272 pressure. We assume that the maximum stress is the vertical stress, σ_v , which implies that
 273 the minimum stress is horizontal, σ_h . For the mechanical parameters, we adopt the values
 274 detailed in Table S3 of Supporting Information. A sensitivity analysis for these parameters
 275 is performed in the following. We set the technical limit to injectable flow rate per well, Q_s ,
 276 to 5 Mt yr⁻¹ and we assume continuous injection for 30 years.

277 Figure 8 shows the injectivity for two of the most significant sites as examples. The
 278 Forties 5 has a very large area and open boundaries, which allows for the injection of huge flow
 279 rates without exceeding the critical pressure. However, the absence of structural confinement
 280 may lead to lateral migration of CO₂ (Bentham et al., 2014). For less than 10 injectors
 281 placed at large distance (see inset of the left panel), the cut-off constraint is represented by
 282 the maximum technological capacity of injection Q_s , which means that even greater flow rate
 283 might be injected in the case of further technological improvements. For larger number of
 284 injectors, plausible scenarios are limited by the reservoir surface area, i.e., the combination of
 285 well number and distance must be such that the well pad size does not exceed the reservoir
 286 surface area (eq. (7)). The maximum per well injectivity reduces with increasing number
 287 of injectors (scenarios close to the red line). This reduction is however compensated by the
 288 increasing number of injectors, resulting in a roughly constant storage capacity when the well
 289 number is greater than 200 (see Fig. S3A and B in Supporting Information). The Bunter
 290 Closure 28, as well as the other Bunter closures, are stratigraphic traps with relatively small
 291 volumes. However, the trapping topography makes them promising sites for storage. As a

292 consequence of the closed boundaries and the small surface area, increasing the well number
 293 does not compensate the reduction in the per well injectivity, thus storage is maximized with
 294 few injectors placed at large distance (see also Fig. S4A and B in Supporting Information).

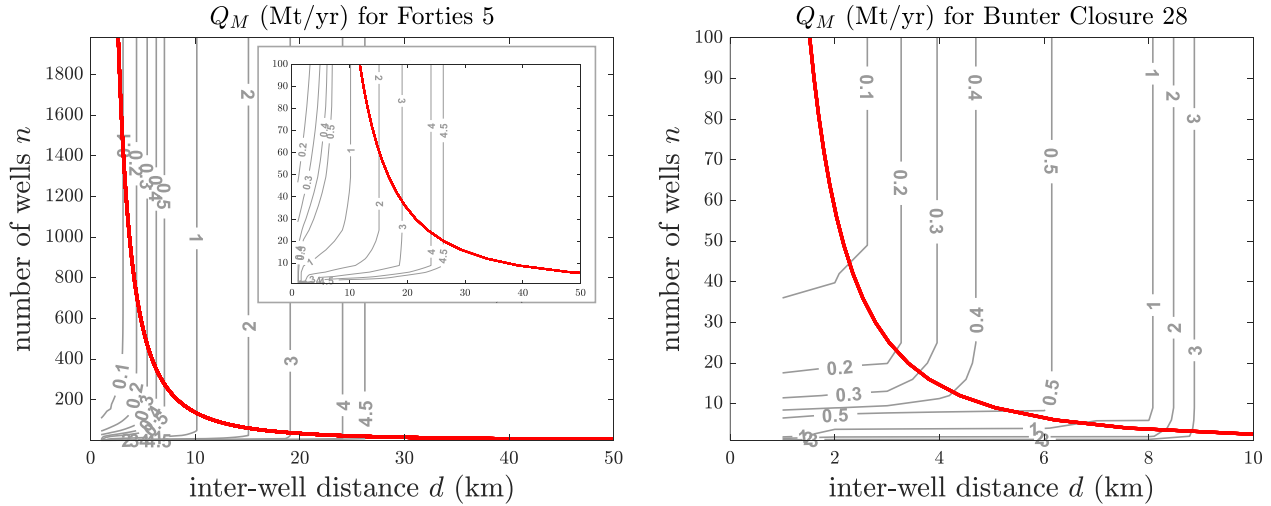


Figure 8: Examples of the per well injectivity estimated for an open (left) and a closed (right) reservoir. Contours show the maximum sustainable flow rate per well for 30 years of injection. The red lines show upper limits imposed by the reservoir area, i.e., plausible scenarios are to the left of the red lines. See text for further details.

295 For the Forties 5 the maximum storage is achieved with a very large number of wells
 296 (around 1300, see Fig. S3B in Supporting Information), which may be unfeasible due to
 297 other practical limitations not considered by the tool. However, for reservoirs with these
 298 characteristics (large reservoirs with open boundaries), the storage capacity is essentially
 299 constrained by the reservoir surface area, thus it becomes approximately constant for well
 300 numbers greater than a certain value, and the maximum storage estimate may reflect a
 301 local maximum. We thus limit the well number to 200, but we also analyze the cases with
 302 maximum well number equal to 2000 and 50.

303 Figure 9 shows the total mass that can be stored in the UK reservoir system over a
 304 period of 30 years. Numerical values and corresponding scenarios are detailed in Table 2.
 305 The total storage capacity provided by the 25 selected sites is approximately 140 Gt over 30
 306 years, which corresponds to a total injection rate of 4.7 Gt yr^{-1} . If the maximum well number
 307 is capped at 2000, then the storage mass is 165.5 Gt, while if the well number is limited to
 308 50, the storage resource is reduced to 68 Gt (see Table S1 in Supporting Information). This
 309 reflects that the storage capacity is approximate constant for $n > 200$ for most reservoirs in
 310 this example.

311 The greatest storage resource is provided by the Mey 5, Maureen 2 and several Cormorant
 312 sites, each providing more than 10 Gt of storage. These sites reveal the huge storage resource
 313 potential of the Central and Northern North Sea. A similar storage capacity is provided by
 314 the Collyhurst formation in the East Irish Sea. Note that for some of these sites the storage
 315 capacity is capped by the maximum number of wells, i.e., they are not pressure limited in
 316 our evaluation. Another significant source is provided by the Forties 5, which we estimate to

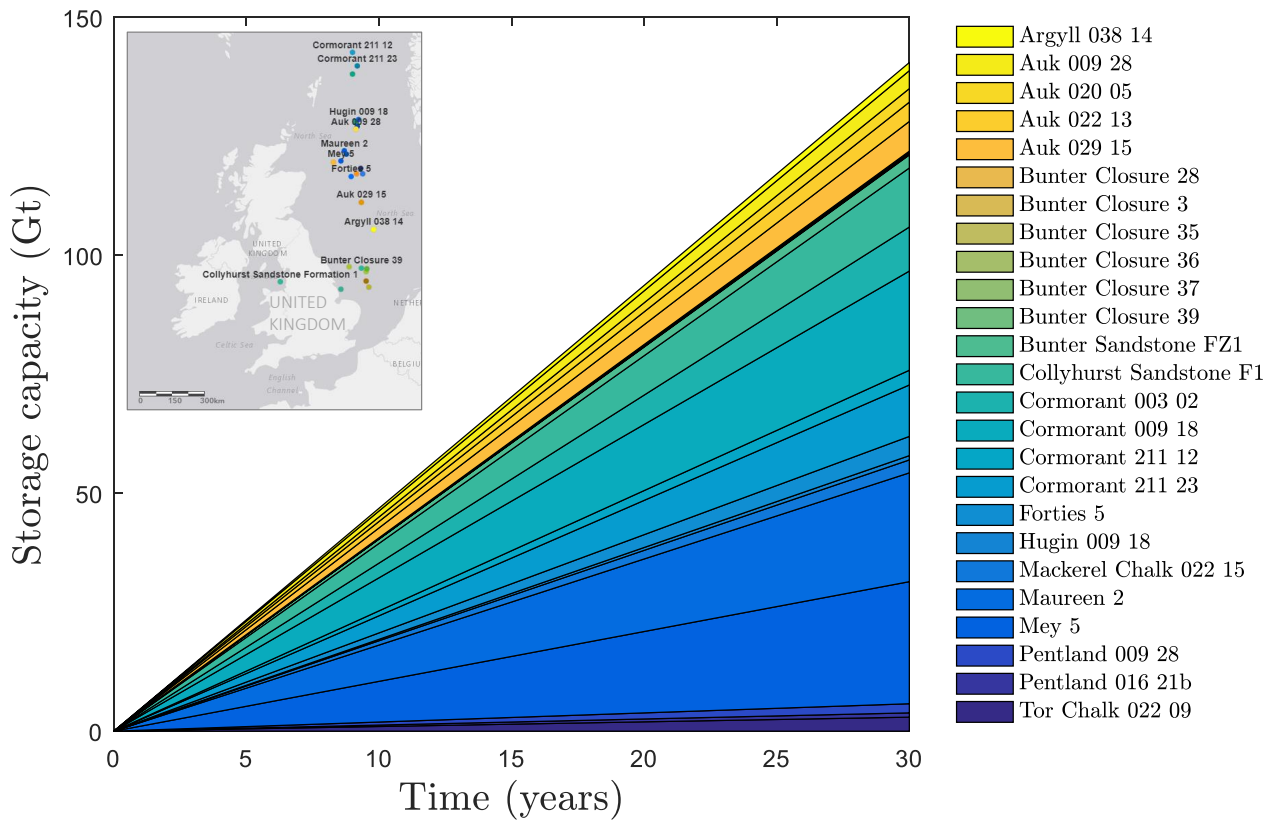


Figure 9: Maximum storage capacity of the selected UK sites for 30 years of continuous injection and maximum well number equal to 200.

317 be able to store 4 Gt in 30 years using 196 injectors.

318 For the Bunter Sandstone Formation 1 we estimate a maximum storage of 2.74 Gt,
 319 which is achieved by injecting CO₂ into 144 wells placed at a spacing of 6 km. The storage
 320 capacity is not dissimilar (2.6 Gt) if we inject into 42 wells (see Table S1 in Supporting
 321 Information). For the same region and timescale Heinemann et al. (2012) estimate a greater
 322 storage capacity, 7.8 Gt. The different estimates may be explained as a consequence of two
 323 major discrepancies. On the one hand, the authors use a formation area nearly a factor of 10
 324 greater than in this study (56 660km² vs 5 126km²). Countering this, however, Heinemann
 325 et al. (2012) approximate the overpressure by means of numerical simulation of single well
 326 injection into a closed domain with radius equal to half the interwell distance. This incurs an
 327 overestimation of the overpressure. In contrast, Noy et al. (2012) perform multiwell numerical
 328 simulations in a 3D domain and find that just 1 Gt can be stored in the Bunter Sandstone
 329 Formation by injecting into 12 locations for 50 years. The discrepancy may be related with the
 330 adoption of different mechanical parameters or failure criteria, or with limiting the number
 331 of wells to 12, as the use of numerical simulations hinders the exploration of a large number
 332 of scenarios.

333 The Pale Blue Dot Energy (2016) report estimates a storage resource in the Bunter
 334 Closure 36 of 280 MtCO₂ with injection over 40 years. For this site we estimate a lower
 335 potential, with a value of 90 Mt stored in 30 years. We think the discrepancy is clerical. The

Table 2: Maximum storage capacity, per well injectivity and corresponding scenario of number of wells n and interwell distance d for each of the selected UK sites. We consider 30 years of continuous injection and a maximum of 200 wells.

Site name	V_M (Gt)	Q_M (Mt/yr)	d (km)	n
Argyll 038 14	1.70	0.29	6.0	196
Auk 009 28	3.77	0.64	4.2	196
Auk 020 05'	2.85	0.48	4.0	196
Auk 022 13	4.05	0.69	6.8	196
Auk 029 15	6.25	1.06	7.5	196
Bunter Closure 28	0.20	3.32	8.8	2
Bunter Closure 3'	0.08	1.29	5.1	2
Bunter Closure 35	0.18	3.02	7.3	2
Bunter Closure 36	0.09	1.53	4.9	2
Bunter Closure 37	0.13	2.09	5.3	2
Bunter Closure 39	0.12	2.03	4.9	2
Bunter Sandstone FZ1	2.74	0.63	6.0	144
Collyhurst Sandstone F1	12.41	3.76	6.2	110
Cormorant 003 02	9.26	3.43	3.8	90
Cormorant 009 18	20.84	3.55	2.9	196
Cormorant 211 12	3.10	1.43	2.5	72
Cormorant 211 23	10.81	2.13	3.6	169
Forties 5	4.04	0.69	8.3	196
Hugin 009 18	0.90	5.00	7.0	6
Mackerel Chalk 022 15	2.72	0.50	3.8	182
Maureen 2	22.87	3.89	13.3	196
Mey 5	25.65	4.70	11.4	182
Pentland 009 28	1.92	1.77	4.5	36
Pentland 016 21b	0.90	2.50	6.2	12
Tor Chalk 022 09	2.95	0,50	4,2	196

336 parameters reported in the report, as well as the aquifer surface area, appear more similar
337 to the values of Formation 4 comprising closure units 35, 36, 37, and 39. The cumulative
338 storage that we evaluate for the Bunter Closures 35, 36, 37 and 39 is around 500 Mt.

339 A detailed site characterization is not usually available and there are significant un-
340 certainties in the storage resource estimates. The greatest uncertainty is related to the
341 geomechanical parameters, which are often difficult to estimate. Given the lack of informa-
342 tion about these parameters in the CO₂ stored database, we explore here the sensitivity of
343 the storage capacity to the values of the geomechanical parameters by assuming a range of
344 possible values. The ratio of the average horizontal stress to the vertical stress, $\overline{\sigma}_h^t/\sigma_v$, varies
345 over a range between 0.5 and 2 (Brown and Hoek, 1978). Values smaller than 1 correspond to
346 the case of a normal faulting regime (extensional), whereas values greater than 1 correspond
347 to a reverse faulting regime (compressional). Values of the friction angle, φ , vary between 25°
348 and 35° (Jaeger et al., 2009). We vary cohesion, C , from 0 up to 10 MPa. The lower value

349 corresponds to the presence of pre-existing faults, the upper to the case of a well-compacted
 350 rock. We also consider the uncertainty of the permeability, κ , by increasing and decreasing
 351 the reference value for each site, κ^* , by one order of magnitude.

352 Figure 10 shows the variation of the total storage capacity with the values of parameters
 353 considered. Storage capacity increases with C and φ as the limiting overpressure increases,
 354 reflective of an increasing strength of the rock. A similar increase in the limiting overpressure,
 355 and thus storage capacity, is observed with increasing $\overline{\sigma'_h}/\sigma_v$. This represents an increase in
 356 the *in situ* average stress, as the vertical stress is fixed, and moves the stress condition
 357 away from the failure condition. The response is more sensitive to the stress ratio $\overline{\sigma'_h}/\sigma_v$
 358 than to the strength parameters. A reduction of $\overline{\sigma'_h}/\sigma_v$ from 0.7 to 0.5 means a loss of
 359 storage capacity greater than 50%. The response is also very sensitive to permeability, which
 360 affects the overpressure response to the injection. An increase in permeability of one order
 361 of magnitude results in a reduction of the overpressure such that the total storage increases
 362 by almost 70%. Overall, the range of plausible system parameters results in a variation in
 363 injectivity from 0.8 - 8.6 Gt y^{-1} around the baseline of 4.7 Gt y^{-1} .

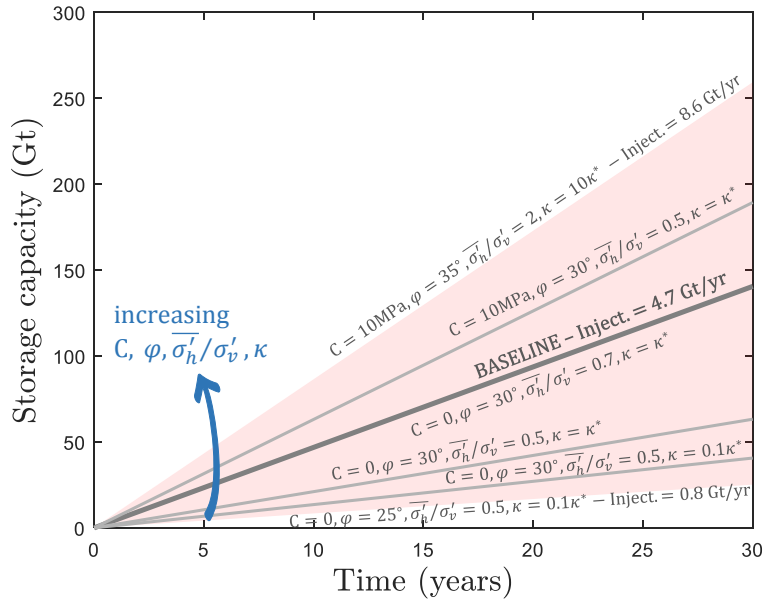


Figure 10: Uncertainty of the total UK storage resource for 30 years of continuous injection and a maximum of 200 wells per site. We explore the impact of changing the permeability, κ , and the geomechanical parameters, such as the cohesion, C , the ratio of the average horizontal stress to the vertical stress, $\overline{\sigma'_h}/\sigma_v$, and the friction angle, φ .

364 3.2 Optimising storage resource use for revenue

365 We now provide a simple example of the use of CO2BLOCK for the economic optimization
 366 of site use. Given revenues associated with CO₂ disposal and costs associated with well
 367 construction, we evaluate the tradeoff between cost and revenue for different scenarios of
 368 well numbers in the Bunter Closure 28 and Forties 5 sites. For each well number scenario,

369 we consider the maximum allowable well distance (close to the red lines in Figure 8), which
370 maximizes the storage.

371 Following Carneiro et al. (2015) and Mathias et al. (2015), the storage cost in deep
372 offshore saline formations is calculated as the sum of the following components: drilling cost
373 = k€26 per meter length of well, fixed cost per well = k€8200 per well, cost for the surface
374 facilities on the injection sites = k€6120 per well, cost of site development = k€24 097, and
375 cost of monitoring equipment = k€1530, plus a 5% for additional operating, maintenance,
376 and monitoring costs. A cost of 50 €tCO₂⁻¹ for capture costs is assumed, but this can range
377 widely (Rubin et al., 2015; IPCC, 2005). Transportation cost ranges between 1-8 €tCO₂⁻¹
378 for a pipeline of 250 km, depending on the terrain conditions and whether the pipeline is
379 onshore or offshore (IPCC, 2005). A total value of 10 €tCO₂⁻¹ is assumed for both sites.
380 We disregard the presence of existing oil and gas infrastructure and facilities that might be
381 re-employed, with consequent cost reduction. For the revenue, five scenarios are considered
382 with revenue between 5 and 200 €tCO₂⁻¹, reflecting values from simple tax credits to revenues
383 from enhanced oil recovery (Kolster et al., 2017). Detailed equations and a summary table
384 are provided in Supporting Information, Section S6.

385 The investment cost, the sum of transport, capture and storage costs, is usually dom-
386 inated by the capture and transportation cost, which increases linearly with the injected
387 volume. However, storage costs can be significant for scenarios with large numbers of wells
388 providing marginal enhancement in injectivity (see Figures S3C and S4C in Supporting Infor-
389 mation). Revenue also increases linearly with the injected volume (Supporting Information,
390 Figs. S4D and S3D), and thus net revenue (the difference between revenue and cost) mostly
391 depends linearly on the total injected volume and the difference between the tax revenue and
392 the sum of capture and transport costs (Fig. 11). For 30 years of injection, the transport
393 and capture costs dominate and most of the fields in this example become profitable at a
394 CO₂ incentive of 70 €tCO₂⁻¹.

395 In the case of the Forties 5, the net revenue is monotonic with the number of wells;
396 once a threshold CO₂ incentive is provided, the project is most profitable with around 200
397 injection sites. In the case of the Bunter Closure 28, the net revenue is maximised with
398 two wells. The behavior is a consequence of the variation of the storage capacity with the
399 number of wells. In the case of the Forties 5, the storage capacity monotonically increases
400 with the number of wells until reaching a plateau for $n > 200$, where the storage capacity
401 oscillates around a constant value (Supporting Information, Fig. S3A and B). Net revenue
402 follows the same trend but it diverges for large well numbers, where the impact of the storage
403 cost on the total cost is greater. As a consequence, the maximum revenue corresponds to an
404 intermediate number of wells. The behavior is similar for the Bunter Closure 28, but in this
405 case both the maximum capacity and the maximum net revenue are achieved with two wells
406 placed at very large distance (Supporting Information, Fig. S4A and B).

407 This is a simple example, intended to be illustrative, of the use of this tool in considering
408 financial analysis of storage resource development. Far more sophisticated models could
409 as easily make use of the underlying representation of storage resource use provided by
410 CO2BLOCK, e.g., accounting for more infrastructure components and operational costs and
411 financial issues like depreciation, borrowing, and insurance costs.

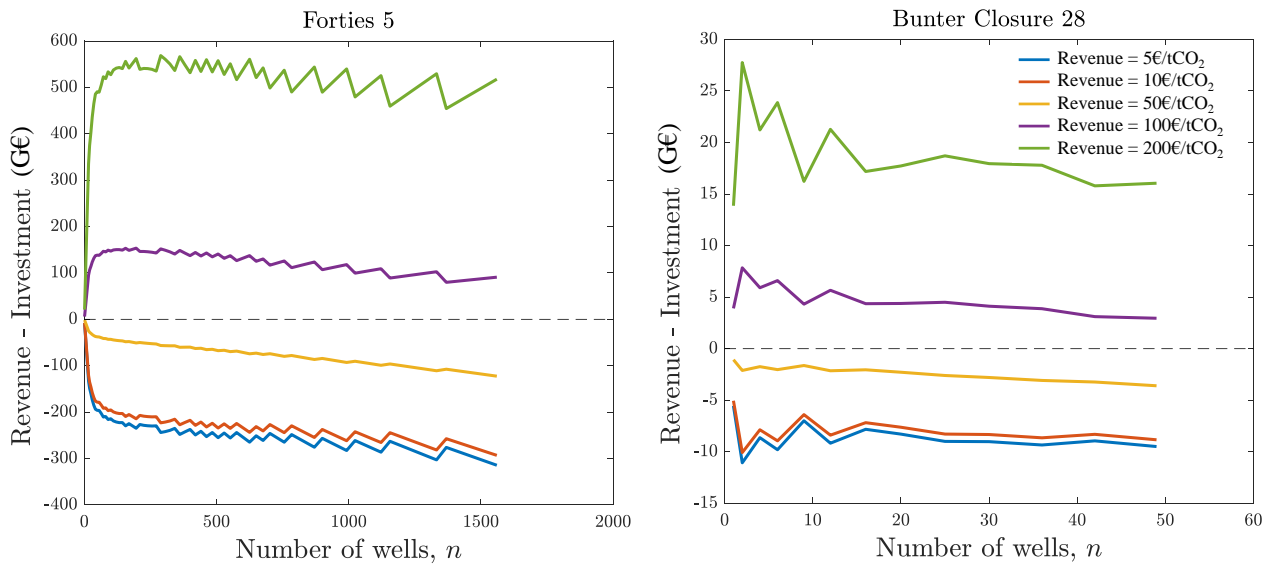


Figure 11: Net revenue (revenues minus investment) for the Forties 5 (left) and the Bunter Closure 28 (right) sites calculated by means of a simplified economic analysis. We assume the case of 30 years of continuous injection under different scenarios of well numbers and revenue values.

4 Discussion and Conclusions

In this paper we have presented CO2BLOCK, a tool for the preliminary evaluation of the CO₂ storage potential of geologic formations under different configurations of well numbers and distance. The procedure reflects the dynamic nature of pressure limitations on storage resource use, which provides a more realistic storage resource assessment than the static estimates (Zhou et al., 2008; Bachu et al., 2007; Bachu, 2015), adopted by other storage simulator tools (e.g., Burruss et al., 2009; Brennan et al., 2010; Poulsen et al., 2014; Gorecki et al., 2009). The simultaneous injection into multiple wells is an efficient strategy for pressure management and our tool analyses different multiwell scenarios with the pressure build-up evaluated as the superposition of single-well analytic models. This approach is also adopted in a similar software, EasiTool (Ganjdanesh and Hosseini, 2017, 2018), but CO2BLOCK includes a correction factor for the superposition error. From the output, optimisation may be performed, for example, to consider tradeoffs between costs and maximising injection volumes in a storage resource.

We demonstrate the use of CO2BLOCK to perform an estimate of the maximum storage resource in the UK offshore system, including an uncertainty analysis. Neglecting consideration of any regulatory and economic constraints, we estimate that around 140 Gt of CO₂ can be safely stored in 30 years through injection into 25 sites in UK identified through a screening for advantageous reservoir properties. Uncertainty from leading order geological parameters alone result in an order of magnitude range in the estimate, from 25 - 250 Gt of resource potential.

We also present a simple example of using CO2BLOCK for the economic optimization of site use. The design of this tool is intended to allow for the optimization of site development in

435 more complex techno-economic energy models so that they may identify possible limitations
436 in the deployment of CCS from injectivity and geography.

437 Although subject to simplifications, this rapid, yet accurate, estimate of storage capac-
438 ities is ideal for a first screening process at the basin or regional scale. The accuracy of the
439 solution under different scenarios of parameters depends on the sensitivity of the adopted
440 analytical model (Nordbotten et al. (2005) - see also the discussion in Vilarrasa et al. (2010))
441 and on the superposition correction. De Simone et al. (2019) show that this approach pro-
442 vides accurate predictions under typical parameter values. The impossibility to reproduce
443 heterogeneity is compensated by the possibility of performing sensitivity and uncertainty
444 analysis around all the parameters in a reasonable computation time. However, more ad-
445 vanced analyses of the resource at the reservoir scale require the use of numerical simulations
446 with a more complex and detailed reconstructed geological domain.

447 **Acknowledgements**

448 The authors acknowledge financial support from the MESMERISE-CCS (Multi-scale En-
449 ergy Systems Modelling Encompassing Renewable, Intermittent, Stored Energy and Car-
450 bon Capture and Storage - EP/M001369/1) and the UKCCSRC 2017 (UK Carbon Cap-
451 ture and Storage Research Centre 2017 - EP/P026214/1) projects funded by the Engi-
452 neering and Physical Sciences Research Council (EPSRC). All data are detailed in the
453 manuscript or in the Supporting Information. CO2BLOCK is available at the repository
454 <https://github.com/co2block/CO2BLOCK> or at <http://doi.org/10.5281/zenodo.4313311>).

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