

1 **Flow Regimes and Storage Efficiency of CO₂ Injected into**
2 **Depleted Shale Reservoirs**

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9 **Abstract**

10 Depleted shale reservoirs are potentially attractive targets to store carbon dioxide (CO₂) as
11 free and adsorbed phases. The time-dependent efficiency factors that depict dynamic
12 storage performance in shale are estimated as a function of key reservoir parameters,
13 shapes of stimulated reservoir volume, and injection scenarios. Efficiency of CO₂ storage
14 and flow regimes are determined dynamically as CO₂ is injected in a depleted shale
15 formation for a time period of 60 years. The most effective reservoir utilization for carbon
16 storage was achieved during the transition from predominant flow in the stimulated
17 reservoir volume to flow into unfractured zones. That transition occurs within first 15-30
18 years of injection depending on cases considered. The importance of adsorption as a
19 mechanism of storage is determined based on sensitivity, which indicates that the amount
20 of CO₂ stored by adsorption would be on average ~26% of the CO₂ stored as a free phase.

21 **Keywords:** carbon sequestration; flow regimes; shale; rate transient analysis.

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23 I. Introduction

24 Commercial production of hydrocarbons from shale formations began just over a decade
25 ago with the advancement of technologies that made producing hydrocarbons from these reservoirs
26 economical. Hydrocarbon production from shale formations in North America, especially in the
27 U.S., demonstrates a sharp rise since then due to drilling of hundreds of thousands of new wells in
28 several shale basins across the U.S. The rate of production from these reservoirs falls very rapidly
29 (generally by more than half within first year [1] compared to conventional reservoirs due to fast
30 depletion of hydrocarbons through fractures. This results in a relatively shorter production life (~5
31 years) [2] that can be extended to a maximum of ~20 years through enhanced recovery methods
32 [1]. Availability of depleted shale reservoirs presents a promising opportunity for storing CO₂
33 because of their extremely tight pore space that can act as both a storage reservoir and a seal, with
34 an added benefit of a large number of wells that can be easily converted into CO₂ injectors.
35 Although the research literature on carbon storage in shale is not as exhaustive as its storage in
36 saline aquifers, a few studies have investigated different aspects of storage in shale; sealing
37 integrity of the caprock [3], dynamic response and practicality of large amounts of CO₂ injection
38 in shale gas wells [4], storage capacity in shale [5], and contribution of organic content to storage
39 [6,7]. The outcome of all these studies suggests a possibility of large-scale CO₂ storage in depleted
40 shale gas formations. However, the transport processes by which CO₂ would be stored in depleted
41 shale stratum and their contribution to storage remain poorly understood. This issue has been
42 investigated either for simultaneous production of methane by CO₂ injection [5,8] or through
43 sorption isotherms alone, but it is likely that sorption isotherms alone may not accurately reflect
44 the storage estimates in shale [9]. Schettler and Parmely [5] estimated from sorption isotherms of
45 Devonian shales that contribution of gas storage by open porosity is about 50% and the remaining
46 50% of storage is intimately associated with adsorption on minerals and organic matter, although
47 this amount could vary with depth and from well to well that presumably change mineralogy or
48 the structure of the shale. Our recent study on this topic [10] investigated time-dependent estimates
49 of efficiency factors for prospective CO₂ storage in depleted shale as free phase and adsorbed
50 phase by accounting for variable properties of shale stratum. Efficiency factors were estimated
51 based on the assumption that CO₂ injected in fractured shales is expected to be stored by sorption
52 on organic matter and clay minerals [9] in addition to its free phase in permeable pores and
53 fractures.

54 The objective of this study is to investigate the time-dependent efficiency factors that depict
55 dynamic storage performance in shale [10] with the help of rate transient analysis (RTA).
56 Specifically, RTA is used to determine flow regimes and effective permeabilities of fractured shale
57 during injection, which are used to interpret changes in efficiency factors over the injection period
58 of 60 years. Unlike conventional reservoirs, permeability estimates for shale with hydraulically
59 fractured horizontal wells is not straightforward and is affected by induced and natural fracture
60 characteristics, besides other parameters [11-13]. RTA is widely used in the oil and gas industry
61 to predict permeability of a reservoir [14-20], where the unique advantage of the method lies in
62 the fact that it incorporates the in-situ conditions of the formation such as initial pressure, flowing
63 pressure, formation compressibility, etc. However, the original RTA in shale [20] was based on a
64 linear-flow theory that assumes constant compressibility, which is largely valid for liquids, but not
65 for gases or supercritical fluids like carbon dioxide. Further, fractured shale formations are affected
66 in their performance by several variables that include reservoir properties, horizontal well
67 completion, fracture geometry, etc. Therefore, correct representation of RTA in shale requires
68 accounting for non-linear fluid flow, and other parameters related to reservoir and well completion.
69 The RTA method used here accounts for non-linearity in fluid flow through a correction factor
70 term, whereas the effect of reservoir and well completion parameters on RTA is studied
71 exclusively through sensitivity analysis.

72

73 **II. Volumetric storage equation and associated efficiency terms**

74 A volumetric method incorporating petrophysical parameters and efficiency factors to
75 screen shale formations for prospective CO₂ storage was recently described in three studies [21-
76 23]. The general equation to estimate mass of CO₂ stored in shales is given as follows:

$$77 \quad G_{CO_2} = V_e [\rho_{CO_2} \phi E_\phi + \rho_{sCO_2} (1 - \phi) E_S] \quad (1)$$

$$78 \quad V_e = A_t E_A h_g E_h \quad (2)$$

79 where, G_{CO_2} is the CO₂ storage resource (mass) of the shale formation; V_e is the net effective volume of the formation;
80 A_t is the total area (map view) of the shale formation being assessed for CO₂ storage; h_g is the gross thickness of the
81 shale formation; E_A is the fraction of shale formation total area available for CO₂ storage; E_h is the fraction of shale
82 formation gross thickness available for CO₂ storage; ρ_{CO_2} is the density of CO₂ at the (averaged) pressure (\bar{P}) and
83 (averaged) temperature (\bar{T}) of V_e prior to production; ϕ is porosity; ρ_{sCO_2} is the maximum mass of CO₂ sorbed per unit

84 volume of solid rock, e.g., the asymptotic value of a sorption isotherm; E_ϕ is the fraction of the maximum volume of
85 CO₂ stored as a free phase; and E_S is the fraction of the maximum volume of CO₂ stored as a sorbed phase.
86

87 The basic principles and definitions used in the above referenced volumetric method,
88 including for storage in shale [10], are based on Society of Petroleum Engineers (SPE) Storage
89 Resources Management System (SRMS), which is a unified classification system for CO₂ storage
90 estimates [24]. In our previous work [10], we used numerical simulations of CO₂ injection into a
91 depleted shale reservoir to estimate efficiency factors, E_ϕ and E_S , for the above method. The
92 definition of dynamic efficiency factor for storage in pore space of shale is consistent with its
93 definition in saline formations [25,26], while the definition of efficiency factor for storage as an
94 adsorbed phase follows an analogous approach that is given as follows:

$$95 \quad E_\phi = \frac{V_i^{free}}{V_{max}^{free}} \quad (3)$$

$$96 \quad E_S = \frac{V_i^{sorb}}{V_{max}^{sorb}} \quad (4)$$

97 where V_i^{free} and V_i^{sorb} are the simulated CO₂ volumes stored in a reservoir volume contacted by the propagating CO₂
98 plume as a free gas and a sorbed phase, respectively; V_{max}^{free} and V_{max}^{sorb} are the maximum CO₂ volumes that can be
99 stored in the reservoir volume contacted by the CO₂ plume as a free phase and sorbed phase, respectively, at initial
100 (average) \bar{P} and \bar{T} conditions before gas production.

101 The simulated storage efficiency factors are intended for dry gas shales characterized
102 predominantly by one phase flow in pore space and fractures. CO₂ injection was simulated over a
103 period of 60 years using selected time points, 5, 10, 20, 30, 40, 50, and 60 years to estimate
104 efficiency factors. As a formal requirement, CO₂ injection should be commercially and technically
105 viable on the time scale of site operation. At present, it is difficult to use a common approach to
106 evaluate a time frame required for CO₂ injection into shale reservoirs due large uncertainties in
107 relevant parameters.

108 The ranges of reservoir's matrix porosity and permeability, density of natural fractures, Langmuir
109 volumes for sorption isotherms, shale thickness, initial reservoir pressure, injection pressure of
110 CO₂, and shapes of stimulated reservoir volume (SRV) were considered to estimate the efficiency
111 factors. These parameters are considered to be the most important in controlling the fluid transport
112 in shale reservoirs [21, 27]. The values for these parameters were taken as measured or evaluated

113 quantities for the shale plays [10]. The NFFLOW code [28] used to conduct the simulations
 114 considers gas residing in the matrix as a free phase in pore space and fractures, and as a sorbed
 115 phase in rock matrix. Sorption is represented by the Langmuir isotherms, where a gas component
 116 behaves as a monolayer on a surface. The total amount of gas in each matrix block is considered
 117 to be the mass sum of free and sorbed gas. For convenience, the select parameters and the calculated
 118 efficiency factors are given in [Tables S1](#) (Supplemental Materials), respectively.

119

120 **III. RTA methodology**

121 RTA is broadly used to gauge well performance (and stimulated reservoir volume) by analyzing
 122 plots of pseudo rate (normalized by pressure) or pseudo pressure (normalized) vs square root of
 123 time [14-20]. The application of RTA allows identifying a specific flow regime prevailing at a
 124 particular injection time period. To investigate the well and SRV productivity, the method of
 125 Wattenbarger et al. [20] serves as an important diagnostic tool that provided the concept of
 126 transient flow in shale gas wells by the analysis of (pseudo) pressure-normalized rate versus the
 127 square root of time. The corresponding equation for linear flow at constant pressure condition is
 128 adapted here for the injection scenario with no skin effect (contribution of formation damage
 129 caused by the infiltration of drilling fluids into the pressure drawdown) as follows:

$$130 \quad x_f \sqrt{k} = f_{cp} \frac{1262 \cdot T}{h \sqrt{(\phi \cdot \mu \cdot c_t)_{wf}}} \frac{1}{m_{cp}} \quad (5)$$

131 where, x_f is the hydraulic fracture half-length, [ft]; k is the reservoir permeability, [md]; T is the
 132 reservoir temperature, [°R]; h is the net-pay reservoir thickness, [ft]; ϕ is the matrix porosity; μ is
 133 the injected carbon dioxide viscosity at flowing bottomhole pressure, [cP]; c_t is the total
 134 compressibility at initial conditions, [psia⁻¹]; m_{cp} is the slope of the fitted straight line obtained by
 135 plotting $\frac{m(P_{wf}) - m(P_i)}{q}$ vs \sqrt{t} , where $m(P_{wf})$ is the real gas pseudo-pressure at flowing bottomhole
 136 pressure, [psia²/cP]; $m(P_i)$ is the real gas pseudo-pressure at initial pressure, [psia²/cP]; q is the
 137 gas injection rate, [Mscf/d]; t is time. The real gas pseudo-pressure, $m(P)$, is calculated as:

$$138 \quad m(P) = 2 \cdot \int_0^P \frac{P}{Z(p) \cdot \mu(p)} dp \quad (6)$$

139 where $Z(p)$ – pressure-dependent non-ideality correction factor; $\mu(p)$ is the pressure-dependent gas
140 viscosity, [cP], P is pore pressure. The main purpose of pseudo-variables like $m(P)$ is to account
141 for the pressure-dependent variability in gas properties (Z -factor, viscosity, and compressibility)
142 in order to adapt the analytical solutions developed for liquid flow to compressible gas-flow with
143 single-phase [18]. The pseudo-pressure accounts for variation in Z -factor and viscosity of gas,
144 while the changes in gas compressibility are accounted through introduction of pseudo-time, $\sqrt{t_a}$
145 [29,30]. To address changes in compressibility with pressure, Nobakht and Clarkson [19] reported
146 a correction ($f_{cp} = \sqrt{\frac{(\mu \cdot c_t)_i}{\bar{\mu} \cdot \bar{c}_t}}$) to square-root of time in order to improve the values of $x_f \sqrt{k}$
147 calculated using the slope (m_{cp}) of the $1/q$ vs \sqrt{t} curve. Here, $\bar{\mu}$ and \bar{c}_t are averaged gas viscosity
148 and total compressibility in the region of influence [30]. Ibrahim and Wattenbarger [31,32] also
149 introduced an empirical correction factor (f_{cp}) for a constant flowing pressure conditions:

$$f_{cp} = 1 - 0.0825 D_D - 0.0857 D_D^2 \quad (7)$$

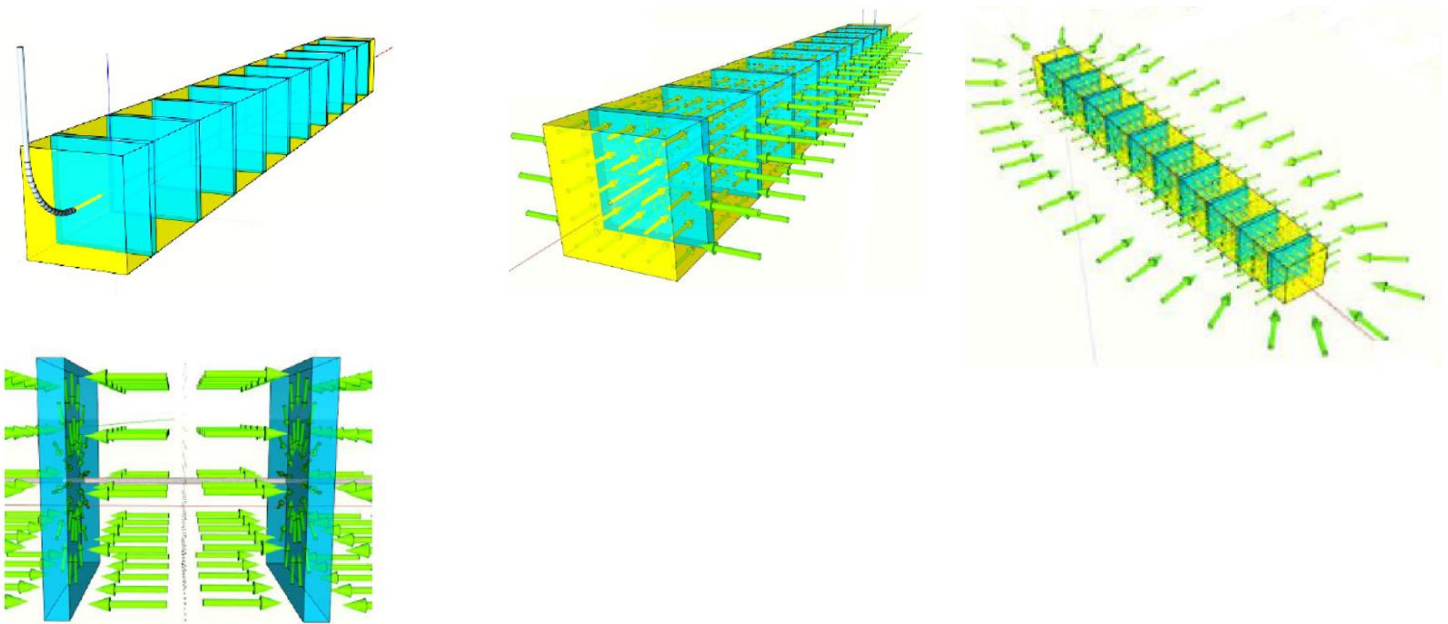
151 where, D_D is the drawdown parameter, which is related to pseudo-pressure at the flowing pressure
152 ($m(P_{wf})$) and initial pressure ($m(P_i)$):

$$D_D = \frac{m(P_{wf}) - m(P_i)}{m(P_{wf})} \quad (8)$$

154 Both correction factors provide similar behavior over a range of the drawdown parameter under
155 assumption of constant viscosity and gas compressibility dominating total compressibility [19]. In
156 this study, we adopted the correction proposed by Ibrahim and Wattenbarger [31,32] because of
157 its simplicity that does not require estimation of averaged properties to calculate corrected pseudo-
158 time [19]. Equation 5 is a modified form of the original equation that was used for liquid, which
159 is based on linear-flow theory [20]. The original equation for liquid is based on the assumption of
160 constant compressibility of liquid, which is not valid for gases, so the original equation was
161 corrected to account for changing gas compressibility. Although at the bottomhole CO₂ injection
162 occurs at supercritical conditions where carbon dioxide behaves as gas in terms of its viscosity and
163 as liquid in terms of density [33]. Equation 5 is applicable to supercritical CO₂ because the value
164 of the correction factor (f_{cp}) is adjusted accordingly per the properties of CO₂ that are accounted
165 by the pseudo pressure term, which is a function of a compressibility factor term (Z) and viscosity.

166 The pseudo pressure will appropriately account for the properties of CO₂ irrespective of its state
167 that is expected to result in a reasonably accurate correction factor.

168 Flow regimes in unconventional reservoirs are affected by coupled effects of reservoir
169 properties, horizontal well completion, fracture geometry, etc. However, for simplicity and
170 illustrative purposes, we represent transient flow sequence only as a function of pressure
171 distributions within the reservoir model during injection. In case of a vertical well, the completion
172 parameter given by the product $x_f \sqrt{k}$ can be extracted from the linear flow analysis. For a multi-
173 fractured horizontal well, the fracture-half length, x_f , is modified to account for total fracture half-
174 length, *i.e.*, the summation of lengths of all hydraulic fractures $n \cdot x_f$ [18,19], where n is the number
175 of induced fractures spaced far enough to establish a linear transient flow regime within SRV. The
176 graphical representation of this flow regime perpendicular to hydraulic fractures is shown in Fig.
177 1a. The hydraulic fractures create highly permeable pathways for injected fluid that enters SRV
178 around the wellbore. Investigation of simulation results for the cases considered in this study shows
179 that such a flow regime dominates during early years of carbon dioxide injection. It shows that
180 clusters of fractures within a stage can be approximated as one combined conduit acting to inject
181 CO₂ into a stimulated volume between stages. The flow within SRV is defined here as Regime I.
182 As a result, the number of induced fractures (n) estimated from $n \cdot x_f \sqrt{k}$ is considered to be the
183 number of stages.



a) Regime I

b) Regime II

c) Regime III

184 **Fig. 1.** Simplified representation of flow regimes within a shale reservoir: **a)** transverse hydraulic fractures (cyan)
185 forming a rectangular SRV around a lateral (upper) and linear flow inside SRV towards hydraulic fractures (lower);
186 **b)** linear flow inside non-stimulated zone towards SRV; **c)** pseudo-steady radial flow affected by reservoir
187 boundaries inside untreated zone towards SRV (modified from Bahrami et. al. [34]). In case of injection the
188 direction of flow is the opposite.

189
190 After pressure buildup within SRV becomes sufficiently high, the next dominant linear flow
191 regime is established towards the reservoir volumes characterized with natural fractures and pore
192 space of rock matrix to transmit fluids outside of SRV (Fig. 1b). In order to estimate effective
193 (bulk) permeability k , the $n \cdot x_f h \sqrt{k}$ product in Equation 5 has to be replaced with the cross-
194 sectional area at well face [17] equal to $2 \cdot x_w h \sqrt{k}$, where x_w is the distance between the center of
195 the first stage and the last stage (762 m (2500 ft)). Next, the pseudo-steady radial flow shown in
196 Fig. 1c (Regime III) was observed at the late injection times and only for a limited number of cases
197 with low matrix porosity and low adsorption. For flow regime that experiences the presence of the
198 reservoir boundaries, $n \cdot x_f h$ is replaced by a reservoir drainage area, A_m [ft²], (1372 x 1372 m
199 (4500 x 4500 ft)) to calculate k [17,18]. It should be noticed that there are no clearly defined
200 boundaries between Regimes I and II, and II and III, instead the transitions to Regimes II and to
201 III occur over a few years.

202

203 IV. Results and Discussion

204 Bachu et al. [35] indicated that CO₂ storage capacity has a time dependency over the
205 lifetime of a CO₂ storage project and efficiency factors change both temporally and spatially. For
206 saline formations, Gorecki et al. [36] reported storage coefficients at the end of CO₂ injection and
207 as estimated between selected time points “dynamically through injection”. Table 1 lists the
208 efficiency factors at discrete times to account for dynamic nature of CO₂ storage per various flow
209 regimes in hydraulically fractured shale. In the beginning of injection, induced fractures and
210 natural fracture network act as the main conduit for CO₂ flow. Then, flow through matrix pore
211 volume characterized with permeability on the order of nano-darcy is expected to pick up. Because
212 of diminished permeability, the pressure slowly propagates through the matrix to the outer parts
213 of the reservoir, resulting in transient flow that lasts for a long period of time within a shale
214 reservoir as if it is infinite in size. Later, flow is expected to reach the reservoir’s boundaries and

215 proceeds at pseudo-steady state [17]. Thus, over time CO₂ flows through highly heterogeneous
 216 media where a dominant conduit can be induced or natural fractures, with diffusion in matrix pores.
 217

218 **Table 1**
 219 Ranges of E_ϕ and E_S efficiency factors for CO₂ storage in shales (Adapted from [10]).

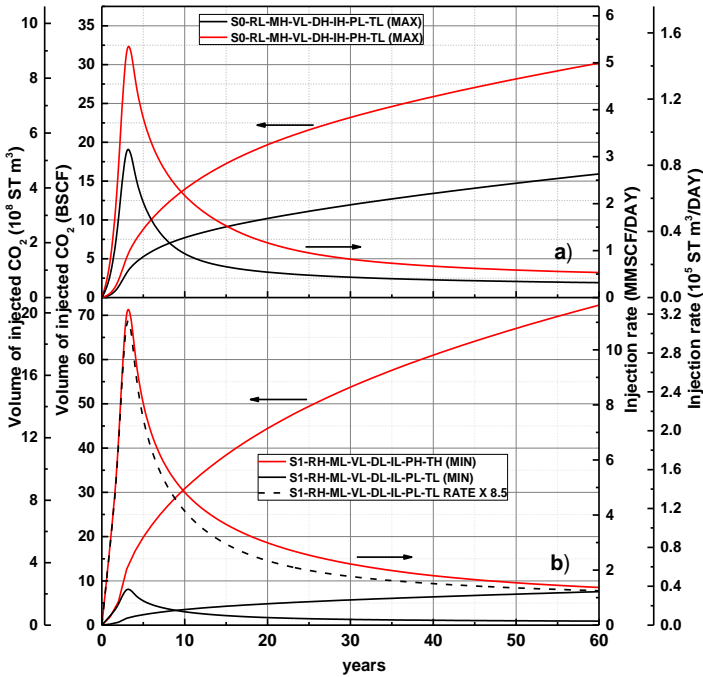
Years	E_ϕ			
	Minimum	Maximum	P ₁₀ [*]	P ₉₀ ^{**}
5	0.17	0.56	0.25	0.53 ²²¹
10	0.22	0.59	0.31	0.57 ²²²
20	0.27	0.60	0.34	0.59 ²²³
30	0.28	0.60	0.36	0.58
40	0.28	0.59	0.37	0.56 ²²⁴
50	0.27	0.58	0.34	0.55 ²²⁵
60	0.26	0.57	0.34	0.54 ²²⁶
E_S				
5	0.09	0.36	0.14	0.34 ²²⁷
10	0.13	0.48	0.16	0.44 ²²⁸
20	0.16	0.57	0.20	0.53 ²²⁹
30	0.15	0.59	0.20	0.56
40	0.15	0.58	0.21	0.57 ²³⁰
50	0.15	0.57	0.20	0.56 ²³¹
60	0.14	0.55	0.19	0.55 ²³²

233 ^{*}P₁₀ is 10th percentile; ^{**}P₉₀ is 90th percentile;

234 **Table 1** shows that the efficiency factors display maxima after 20-40 years of injection. A
 235 hypothesis considered in this work suggests that during continuous active transport from the
 236 wellbore into the SRV, the efficiency factor terms increase. Later, when flow moves to
 237 unstimulated zones through natural fracture network, flow regime changes and efficiency factors
 238 start to decline. Thus, the presence of the maxima on efficiency factor curves indicates the change
 239 in flow regime from SRV dominated flow to flow in unstimulated zones. To test this hypothesis,
 240 RTA was used as described in the Methodology section.

241 **Fig. 2a** and **Fig. 2b** show total volume of injected CO₂ with their corresponding rates of
 242 injection for the four cases that define the maximum and minimum boundaries of the efficiency

243 factor, E_{ϕ} , listed in Table 1. In the description of the cases, the **R** (Reservoir pressure), **M** (Matrix
 244 permeability), **V** (Langmuir Volume), **D** (Density of natural fractures), **I** (Injection pressure), **P**
 245 (matrix Porosity), **T** (shale Thickness) symbols define input parameters given in Table S1 and are
 246 used in a combination with **L** or **H** designating the lower and upper boundary, respectively.
 247 Additional symbol, **S** (Shape), indicates SRV and is used with three numbers corresponding to
 248 three shapes of SRV [10]. The general shape of the injection rates and volumes is similar for the
 249 cases considered and we focus here on those defining limiting values of the efficiency factor, E_{ϕ} ,
 250 for free phase storage in fractures and matrix pore space.



251
 252 **Fig. 2.** Total volumes of carbon dioxide injected and injection rates
 253 as a function of time for **a)** the S0-RL-MH-VL-DH-IH-PH-TL and
 254 S0-RL-MH-VL-DH-IH-PL-TL cases and **b)** the S1-RH-ML-VL-DL-
 255 IL-PH-TH, S1-RH-ML-VL-DL-IL-PL-TL cases.

256 As shown in Fig. 2a and Fig. 2b, the injection rates experience peaks after 3 years of injection,
 257 beyond which the injection pressure is decreased monotonically until the end of injection period.
 258 The reason of the peak appearance after 3 years of injection is connected to a step-wise increase
 259 of the injection pressure during first three years. The injection wells used for geologic CO₂
 260 sequestration into deep rock formations are designated as Class VI [37], which requires protecting
 261 underground sources of drinking water (USDWs). Hydraulic fractures provide direct preferential

262 pathways for upward fluid migration in shale-dominated strata located hundreds of feet above the
263 hydraulically fractured layers [38]. The risk to USDW contamination could arise if the injection
264 pressure is immediately set at the target values because of further hydraulic fracture propagation.
265 To prevent that possibility in a field injection scenario, in this study the injection pressure is
266 initially kept at 6.89 MPa during the first year, which is increased to 13.79 MPa for the second
267 year, followed by the target pressure from the third year to the rest of the injection period (Table
268 S1). Noticeably, cases with low porosity experience faster rate drop before leveling out after
269 approximately 30-40 years (the dashed black line represents the 8.5 times increase in injection rate
270 for the case with the low porosity value and is shown in Fig. 2b for convenience to compare against
271 the high porosity case). The cases depicted in Fig. 2a and Fig. 2b indicate that low/high matrix
272 permeability, low/high natural fracture density, low/high injection pressure, and high/low initial
273 reservoir pressure are the main drivers of low/high reservoir efficiency. Besides, it appears that the
274 regular SHAPE 0 / irregular SHAPE 1 (representing enlarged fractures at the heel and the toe of
275 the lateral [10]) represents the most/less effective induced fracture distribution among three
276 considered. This finding agrees with conclusion of another study [14], which showed that the
277 analytical methods using only regular shaped SRVs [29,39] cannot accurately describe the well
278 performance.

279 Fig. 3a and Fig. 3b show pressure distributions for the two cases that give minimum
280 efficiency factors (Fig. 2b) at the end of the injection period. Because of the heterogeneous nature
281 of the natural fracture network, the pressure distributions are non-uniform. Certain areas
282 demonstrate a more pronounced flow reflecting better fracture connectivity (an analysis using
283 several natural fracture realizations was performed for selected cases to ensure that every
284 stochastic distribution provides statistically close results).

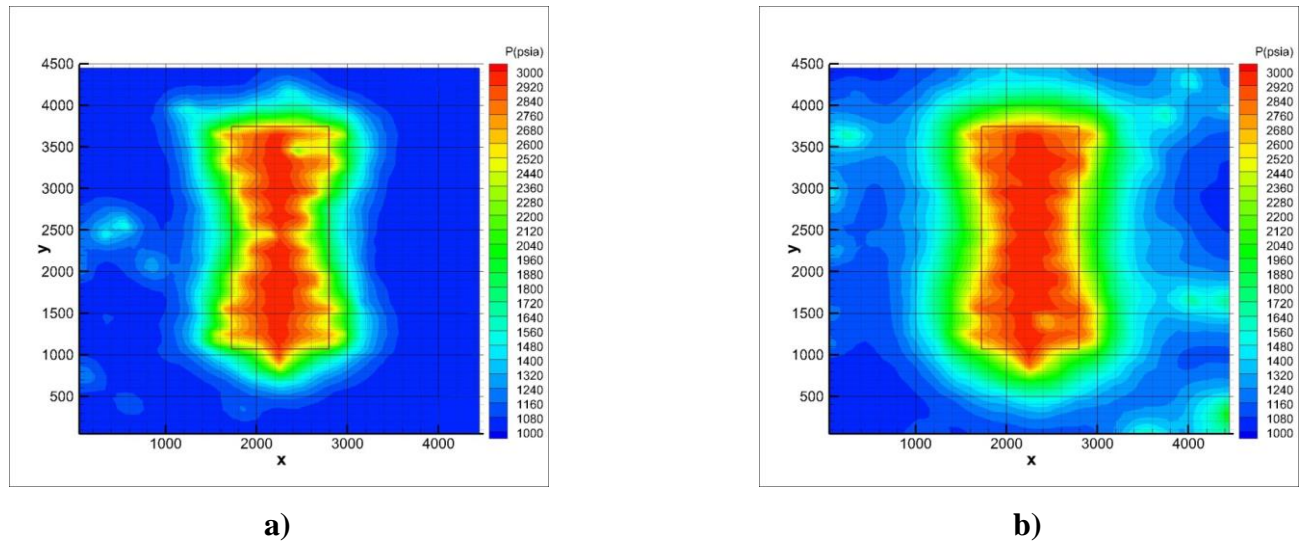


Fig. 3. Pressure distributions in the middle horizontal plane of the shale reservoir after 60 years of injection for the **a)** S1-RH-ML-VL-DL-IL-PH-TH and **b)** S1-RH-ML-VL-DL-IL-PL-TL cases. The red rectangle designates the boundaries of the stimulated zone. The lateral is omitted for clarity.

285

286 The elevated pressure areas corresponding to CO₂ propagation are well within the reservoir
 287 boundaries for the case with high porosity (Fig. 3a), while the case with low porosity shows
 288 pressure propagation reaching the boundaries (Fig. 3b). This suggests that flow in the reservoir
 289 with low porosity experience a boundary effect resulting in a pseudo-steady flow regime with
 290 almost constant injection rates. Fig. 4a and Fig. 4b present the results of RTA for the four limiting
 291 cases depicted in Fig. 2a and Fig. 2b.

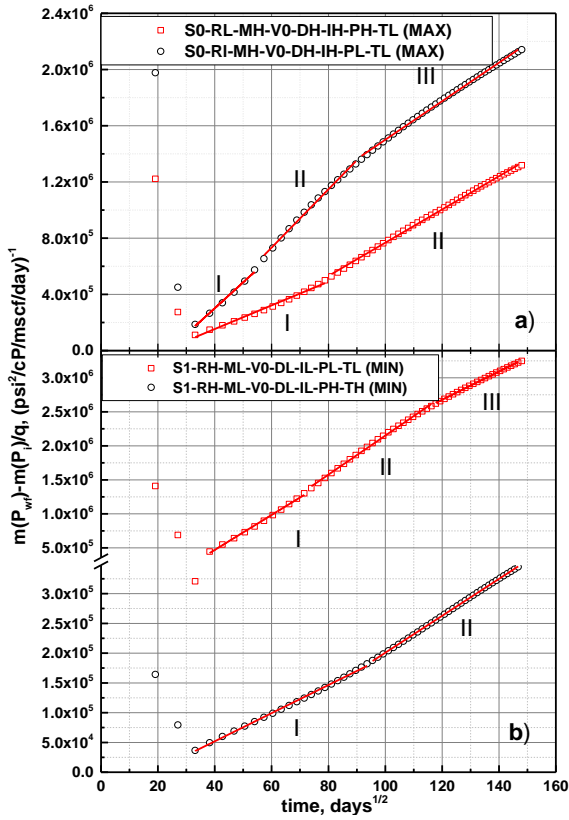


Fig. 4. The performance characteristic plot of pressure-normalized injection rates as a function of time at different flow regimes for **a)** the S0-RL-MH-V0-DH-IH-PH-TL and S0-RL-MH-V0-DH-IH-PL-TL cases and **b)** the S1-RH-ML-V0-DL-IL-PH-TH and S1-RH-ML-V0-DL-IL-PL-TL cases providing maximum and minimum efficiency factors, respectively.

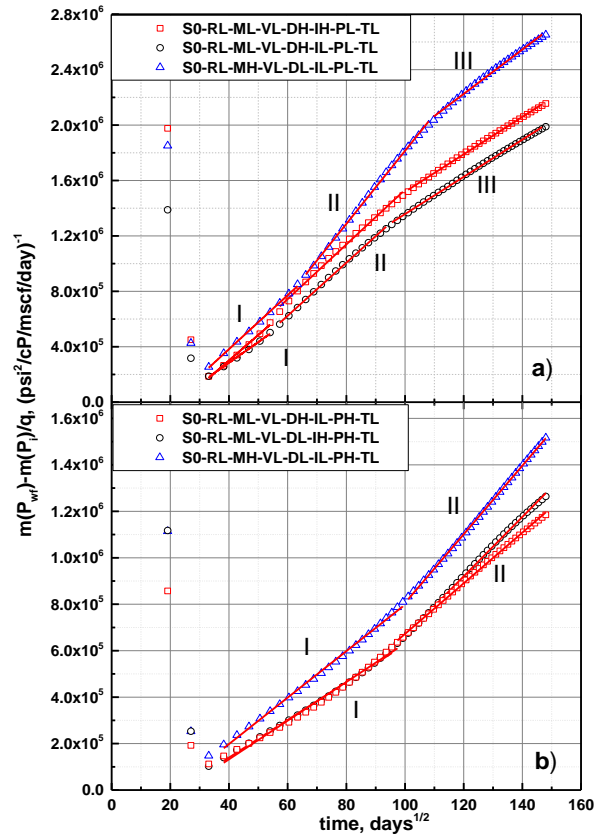


Fig. 5. The performance characteristic plot of pressure-normalized injection rates as a function of time at different flow regimes for **a)** the S0-RL-ML-VL-DH-IH-PL-TL, S0-RL-ML-VL-DH-IL-PL-TL, and S0-RL-MH-VL-DL-IL-PL-TL cases and **b)** for the S0-RL-ML-VL-DH-IL-PH-TL, S0-RL-ML-VL-DL-IH-PH-TL, and S0-RL-MH-VL-DL-IL-PH-TL cases demonstrating Regimes I-III and I-II, respectively.

292 The I, II, and III numbers on the plots identify Regimes I, II, and III, respectively. Indeed, the cases
 293 with low porosity values demonstrate three flow regimes, while high porosity of the shale reservoir
 294 leads to only two regimes. To further explore the effect of porosity on the flow regimes, RTA was
 295 performed for other cases. The results given in Fig. 5 have confirmed the above trend. The
 296 examples of pressure distributions are given in Fig. 6 showing that flow is localized with SRV for
 297 Regime I, continues within the reservoir boundaries through natural fractures and matrix pore for
 298 Regime II, and experiences the presence of reservoir's boundaries for Regime III. Obviously, the
 299 increase of the reservoir size would eliminate the prevailing Regime III at the end of injection
 300 period for cases with low porosity.

301 [Table 2](#) collects bulk permeabilities, time periods, and efficiency factors for flow regimes
 302 in selected cases. This effective (bulk) formation permeabilities, k , are calculated using Equations

303 5-7 with contributions to the completion parameter estimated for each flow regime as described in
 304 the last paragraph of Section III. The changes in flow regimes are associated with change in
 305 reservoir permeability for CO₂ flow that includes “contributions” from induced and natural
 306 fractures and matrix pores. The resulted permeabilities are computed to be on the orders of 10⁻²,
 307 10⁻³, and 10⁻⁵ md for Regimes I, II, and III, respectively (Table 2). Interestingly, the comparison
 308 of the efficiency factors for the cases comprising only Regime II and cases comprising Regimes II
 309 and III demonstrates that a transition from II to III does not lead to noticeable change in the value
 310 of the efficiency factor.

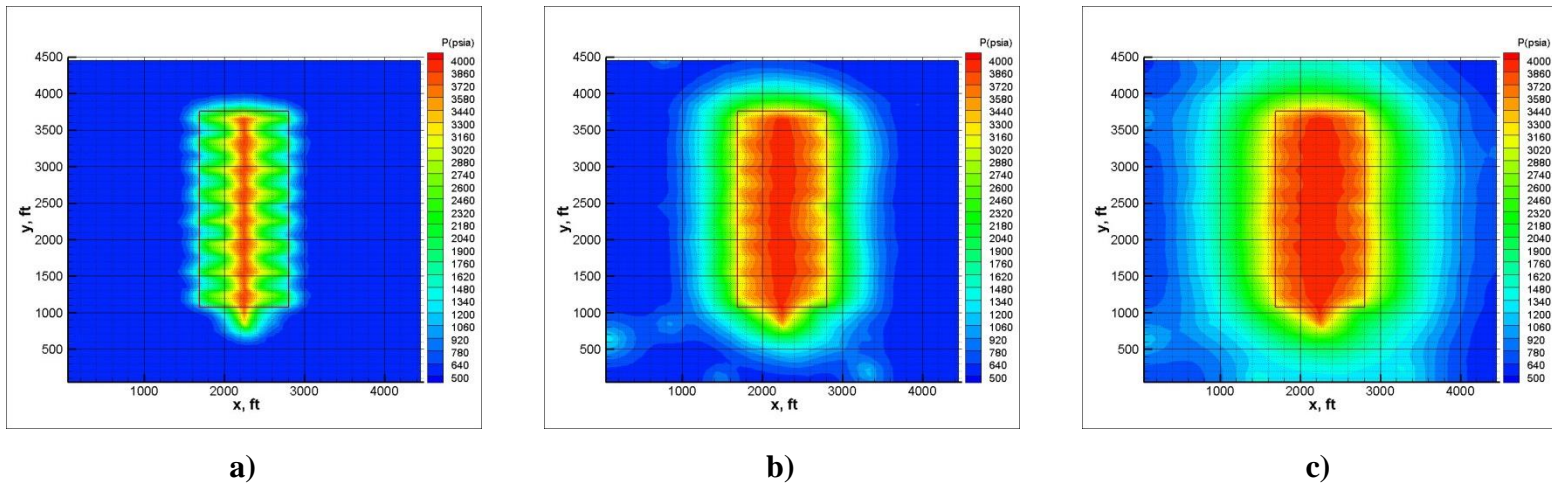


Fig. 6. Pressure distributions in the middle horizontal plane of the shale reservoir after **a)** Regime I; 10 years (case S0-RL-MH-VL-DH-IH-PH-TL); **b)** Regime II; 60 years (case S0-RL-MH-VL-DH-IH-PH-TL) and **c)** Regime III; 60 years (case S0-RL-MH-VL-DH-IH-PL-TL) of CO₂ injection. The red rectangle designates the boundaries of the stimulated zone. The lateral and hydraulic fracture locations are omitted for clarity.

311

312 **Table 2**

313 Bulk formation permeabilities (k_{bulk}) estimated using RTA for different flow regimes and corresponding efficiency factors for cases of interest.

case	Regime I			Regime II			Regime III		
	Range, years	k_{bulk} , md	Efficiency factors	Range, years	k_{bulk} , md	Efficiency factors	Range, years	k_{bulk} , md	Efficiency factors
S0-RL-MH-VL-DH-IH-PH-TL (MAX)	3-19	0.047	0.43-0.60	20-60	0.010	0.60-0.55	-	-	-
S0-RL-MH-VL-DH-IH-PL-TL (MAX)	3-9	0.026	0.56-0.59	10-23	0.009	0.59-0.56	24-60	1.826E-5	0.56-0.51
S1-RH-ML-VL-DL-IL-PH-TH (MIN)	3-30	0.012	0.17-0.29	31-60	0.004	0.29-0.27	-	-	-
S1-RH-ML-VL-DL-IL-PL-TL (MIN)	3-17	0.007	0.23-0.30	18-38	0.003	0.30-0.28	39-60	4.274E-6	0.28-0.26
S0-RL-ML-VL-DH-IL-PH-TL	3-25	0.019	0.33-0.47	26-60	0.008	0.48-0.45	-	-	-
S0-RL-ML-VL-DL-IH-PH-TL	3-25	0.037	0.33-0.54	26-60	0.009	0.55-0.54	-	-	-
S0-RL-MH-VL-DL-IL-PH-TL	3-27	0.032	0.26-0.44	28-60	0.006	0.46-0.44	-	-	-
S0-RL-ML-VL-DH-IL-PL-TL	3-9	0.014	0.41-0.47	10-28	0.005	0.47-0.45	29-60	1.011E-5	0.45-0.42
S0-RL-ML-VL-DH-IH-PL-TL	3-9	0.039	0.53-0.59	10-25	0.010	0.59-0.53	26-60	1.803E-5	0.53-0.51
S0-RL-MH-VL-DL-IL-PL-TL	3-12	0.023	0.37-0.46	13-33	0.006	0.46-0.46	34-60	1.339E-5	0.46-0.41

314

315

316

317 The behavior is in contrast with the transition from Regime I to II that leads to a clear change in
318 the efficiency factors. In other words, continuous active transport of CO₂ as a free phase from the
319 wellbore into SRV results in increasing the efficiency factors, which starts to decrease once CO₂
320 transitions occur into unstimulated zones through natural fracture network. The comparison of the
321 permeability values and corresponding efficiency factors reveals that a high efficiency factor does
322 not always translate to high bulk formation permeability and vice versa. In other words, the ability
323 of a reservoir with high permeability to faster transmit fluids would not necessarily translate into
324 a better storage potential of the fractured shale because their physical meaning signify potential
325 ease of CO₂ injectivity and efficient utilization of storage volume, respectively.

326 **Contribution of Adsorption to Storage**

327 Among various parameters used to design simulation cases that account for variability in their
328 magnitude per their values in the literature, adsorption of CO₂ is one of those parameters. [Fig. 7a](#)
329 shows the amount of CO₂ stored for three limiting cases, which are storage without adsorption,
330 storage with low adsorption, and storage with high adsorption ([Table S1](#)). The clay minerals and
331 organic matter content in shale rock lead to high (e.g. large clay and organic content) or low (e.g.
332 large inorganic content) adsorption, respectively. In the simulations performed in this work the
333 difference in shale total organic content (TOC) and clay content is captured through low and high
334 values of Langmuir constants ([Table S1](#)). The rocks favorable for adsorption can store ~44% more
335 CO₂ than the rocks where there is no adsorption (% change from 23.2 to 33.4 bscf of stored CO₂
336 after 60 years of injection, [Fig. 7b](#)), or they can store 33% more CO₂ compared to rocks with
337 relatively low adsorption (% change from 25.1 to 33.4 bscf, [Fig. 7b](#)). One can reasonably expect
338 that mineralogy and organic matter of most shale reservoirs would facilitate adsorption that lies
339 somewhere between those two limiting cases of low and high adsorption. Following that, the
340 amount of CO₂ that can be stored on average by means of adsorption is ~26% of the CO₂ stored as
341 free phase (the arithmetic average of % changes from 23.2 to 33.4 and 23.2 to 25.1 bscf, [Fig. 7b](#)).

342

343

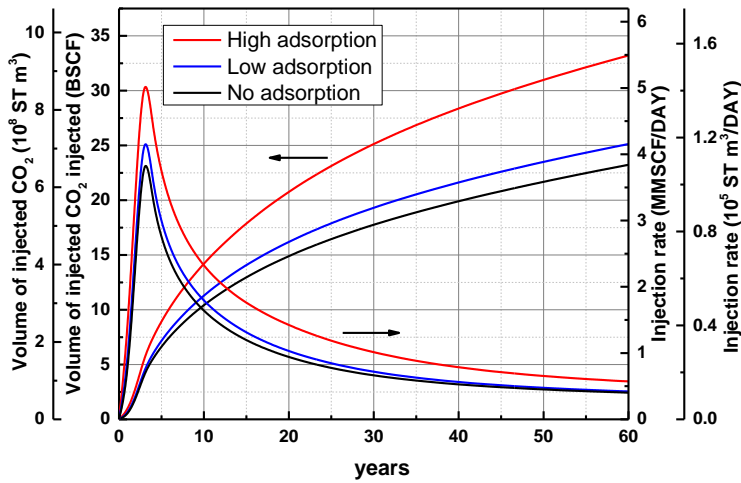


Fig. 7a. Total volumes of carbon dioxide injected and injection rates as a function of time for S0-RL-ML-VH-DH-IL-PH-TL (high adsorption), S0-RL-ML-VL-DH-IL-PH-TL (low adsorption), and S0-RL-ML-DH-IL-PH-TL (without adsorption) cases.

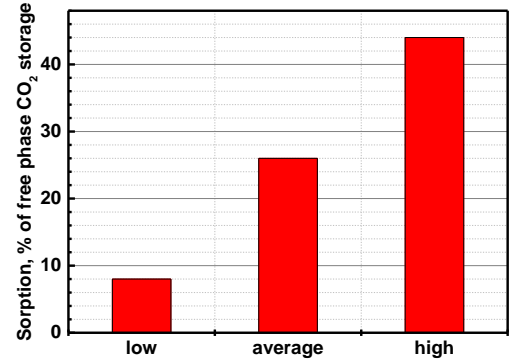


Fig. 7b. Adsorbed amounts of CO₂ relative to the amounts stored as a free phase (after 60 years of injection) based on the cases shown in Fig. 7a.

344

345 Several mechanisms of fluid transport exist in shale rocks at local scales that have been
 346 studied by researchers specifically to understand i) the uptake of fracturing fluid by shale [2,40-
 347 43], and ii) the non-Darcy flux of gas in organic matter or pores of the order of nanometers [44-
 348 47]. Although these local-scale mechanisms, which are often coupled together, have been studied
 349 by various researchers to some extent, there is lack of a simple mathematical model for these
 350 mechanisms in comparison to viscous flow and adsorption that were accounted by well-known
 351 Darcy's law and Langmuir isotherm, respectively, in this study. Therefore, these mechanisms are
 352 rarely accounted in numerical simulators, so it is difficult to assess their impact on flow regimes
 353 of CO₂ in shale reservoirs.

354 V. Conclusions

355 Numerical simulations of CO₂ injection into depleted fractured shale reservoirs were used to
 356 estimate volume of CO₂ stored for a range of reservoir parameters and injection scenarios, where
 357 the selected range is expected to cover parameter variability in gas-dominant organic-rich shale
 358 reservoirs at the national and regional scale. Numerical simulations were performed by considering
 359 free-phase and adsorbed phase as two mechanisms of CO₂ storage in shales. RTA was performed
 360 to identify flow regimes of CO₂ in depleted shale during the injection period. It was found that the

361 maximum efficiency factors occur within 15-30 years of injection for the studied cases and their
362 maximum value is accompanied with a transition from the dominant transient flow regime within
363 SRV (Regime I) to flow within unstimulated zones (Regime II). A practical implication of this
364 result suggests that closely-spaced configuration of multiple horizontal wells would favor better
365 storage efficiency because such a configuration would lead to better areal sweep of the reservoir,
366 and hence efficient CO₂ storage. Unlike a closely-spaced configuration, multi-well configuration
367 with large spacing would allow the CO₂ to move quickly through preferential pathways (e.g. a
368 fractures), thus leading to inefficient reservoir sweep [1].

369 The bulk formation permeabilities estimated for different flow regimes using RTA show
370 that high values of bulk permeability does not always translate to high efficiency factors; this is
371 because, although, both high permeability and high efficiency factors are favorable for storage of
372 CO₂ in depleted shale, their physical meaning signify potential ease of CO₂ injectivity and efficient
373 utilization of storage volume, respectively.

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