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«ҚАЗАҚСТАН РЕСПУБЛИКАСЫ
ҰЛТТЫҚ ҒЫЛЫМ АКАДЕМИЯСЫ» РҚБ

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OPTIMIZATION OF CO_2 HUFF-N-PUFF PARAMETERS FOR ENHANCED GAS RECOVERY IN SHALE RESERVOIRS: A COMPOSITIONAL SIMULATION STUDY

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Abstract. With the growing importance of unconventional reservoirs in meeting global energy demands, improving gas recovery from shale formations has become a critical challenge. Primary recovery from such ultra-tight formations typically remains below 10%, necessitating the use of Enhanced Gas Recovery (EGR) techniques. This study investigates the potential of carbon dioxide Huff-n-Puff (CO_2-HnP) as an EGR method specifically tailored for shale gas reservoirs. The main objective is to optimize key operational parameters — injection pressure, injection rate, and soaking time — to maximize gas recovery in low-permeability environments. *Methods. To* evaluate the effectiveness of CO_2-HnP, a commercial compositional reservoir simulator was used to model key operational parameters:

injection pressure, injection rate, and soaking time. Sensitivity analyses were conducted to determine the optimal set of parameters for maximizing gas recovery. *Results.* The results support the hypothesis that including adsorption and diffusion significantly enhances recovery. Specifically, a configuration of 800 MSCF/day injection rate, 5500 psi injection pressure, and zero soaking time yielded the highest gas recovery. Gas adsorption improved cumulative recovery by 9%, while the addition of molecular diffusion, modeled using the Sigmund correlation, contributed an additional 19% over a 40-year period. *Practical value.* These findings underscore the importance of mass transfer in gas displacement and demonstrate the practical applicability of CO_2-HnP for field-scale implementation. The study offers a robust framework for designing efficient and sustainable strategies to optimize gas production from shale formations.

Key words. CO2 injection, Huff-n-Puff, EOR, unconventional reservoirs, shale gas.

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CO_2 HUFF-N-PUFF ПАРАМЕТРЛЕРІН ОҢТАЙЛАНДЫРУ АРҚЫЛЫ ТАҚТАТАС КЕН ОРЫНДАРЫНДА ГАЗ ӨНДІРУДІ АРТТЫРУ: ҚҰРАМДЫҚ МОДЕЛЬДЕУ ЗЕРТТЕУІ

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Аннотация. Сланецті коллекторлардан көмірсутек өндіру – бүгінгі таңда энергетикалық қауіпсіздік пен тұрақты даму үшін ерекше маңызды бағыттардың бірі болып отыр. Дегенмен, дәстүрлі емес коллекторлардан бастапқы газ өндіру деңгейі әлі де 10%-дан төмен, бұл өндірудің тиімді әдістерін іздеуді қажет етеді. Осы ғылыми жұмыста көмірқышқыл газы негізінде Huff-n-Puff (HnP) әдісін қолдана отырып, сланецті газ кен орындарында газ өндіруді арттырудың (EGR) технологиялық мүмкіндіктері қарастырылады. Зерттеу мақсаты – өте төмен өткізгіштігі бар коллекторларда газ өндіру тиімділігін арттыру үшін негізгі технологиялық параметрлерді оңтайландыру. *Әдістер.* CO_2-HnP әдісінің тиімділігін бағалау үшін негізгі технологиялық параметрлер – айдау қысымы, айдау жылдамдығы және ұстап тұру уақыты – өзгертіле отырып, коммерциялық құрамдас резервуар симуляторы қолданылды. Қабат флюидтерінің қозғалысын нақтырақ көрсету үшін модельге газдың адсорбциясы мен молекулалық диффузия сияқты маңызды масса алмасу механизмдері енгізілді. Газ өндіруді барынша арттыру мақсатында сезімталдық (сезімтал параметрлер) талдауы жүргізілді. *Нәтежиелер.* Сезімталдықты талдау нәтижелері бойынша газ өндірудің ең жоғары көрсеткіштері 800 MSCF/тәулік айдау жылдамдығы, 5500 psi қысым және сіңдіру уақытының болмауы жағдайында байқалды. Сонымен қатар, модель масса алмасудың негізгі процестерін – газ адсорбциясы мен молекулалық диффузияны — ескереді. Газ адсорбциясы жиынтық өндіруді 9%-ға арттырса, молекулалық диффузияны (Сигмунд корреляциясы негізінде) қосу газ өндіруді 40 жыл ішінде шамамен 19%-ға арттыратыны анықталды. *Практикалық құндылық.* Бұл зерттеу газды ығыстыру механизмдеріндегі масса алмасу процестерінің маңыздылығын көрсетіп, CO_2-HnP әдісінің өндірістік ауқымда қолдануға болатындығын дәлелдейді. Зерттеу нәтижелері сланц коллекторларынан газ өндіруді тиімді әрі тұрақты арттыру стратегияларын жасау үшін пайдалы негіз бола алады.

Түйін сөздер. CO_2 айдау, Huff-n-Puff әдісі, мұнай алуды арттыру (EOR), дәстүрлі емес коллекторлар, тақтатас газы.

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ОПТИМИЗАЦИЯ ПАРАМЕТРОВ CO_2 HUFF-N-PUFF ДЛЯ ПОВЫШЕНИЯ ИЗВЛЕЧЕНИЯ ГАЗА ИЗ СЛАНЦЕВЫХ ПЛАСТОВ: КОМПОЗИЦИОННОЕ МОДЕЛИРОВАНИЕ

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Аннотация. В условиях растущего значения трудноизвлекаемых коллекторов в обеспечении глобального спроса на углеводороды, крайне актуальной становится задача повышения эффективности добычи газа из сланцевых формаций. Первичная газоотдача из таких пластов, как правило, не превышает 10%, что требует применения методов увеличения нефте- и газоотдачи. В данном исследовании рассматривается использование технологии CO_2 Huff-n-Puff (HnP) в качестве способа повышения газоотдачи (EGR) для сланцевых газовых месторождений. Целью работы является оптимизация ключевых технологических параметров — давления закачки, скорости закачки и времени выдержки — для увеличения извлекаемости газа из низкопроницаемых коллекторов. *Методы.* Для оценки эффективности метода CO_2-HnP использовался коммерческий композиционный симулятор пластов, в котором варьировались ключевые технологические параметры: давление закачки, скорость закачки и время выдержки. В модель были включены важнейшие механизмы массообмена — адсорбция газа и молекулярная диффузия — что позволило более точно отразить поведение флюидов в недрах. Путем проведения чувствительного анализа были определены оптимальные параметры для максимизации извлечения газа. *Результаты.* Полученные результаты подтвердили гипотезу о том, что учёт адсорбции и диффузии существенно увеличивает газоотдачу. Наилучшие показатели достигаются при давлении 5500 psi, скорости закачки 800 MSCF/сутки и отсутствии времени выдержки. Учет адсорбции обеспечивает прирост извлечения газа на 9%, а включение молекулярной диффузии на основе корреляции Сигмунда увеличивает совокупную добычу на 19% за 40 лет. *Практическая ценность.* Таким образом, работа подчеркивает ключевую роль массообменных процессов в механизмах вытеснения газа и демонстрирует высокий практический потенциал применения CO_2-HnP в промышленных условиях. Результаты могут быть использованы для разработки эффективных и устойчивых стратегий увеличения газодобычи из сланцевых коллекторов.

Ключевые слова: закачка CO_2, метод Huff-n-Puff, увеличение нефтеотдачи (EOR), нетрадиционные коллекторы, сланцевый газ.

Introduction. In the dynamic landscape of global energy, unconventional oil and gas reservoirs have emerged as pivotal players, reshaping the traditional paradigms of hydrocarbon exploration and extraction. Unlike conventional enhanced oil recovery (CO_2-EOR), which has been widely applied in mature oil fields, CO_2-EGR presents a promising alternative for boosting hydrocarbon recovery from tight gas-bearing formations. This approach not only improves gas recovery but also enables the permanent geological storage of CO_2, addressing both energy security and environmental concerns. The dual-purpose nature of CO_2-EGR—enhancing production from difficult-to-develop resources while contributing to long-term carbon sequestration—aligns closely with global climate mitigation goals(IPCC, 2023, Ding, et al., 2019; Wang, et al., 2020).

In 2022, the U.S. Energy Information Administration (EIA) approximates that the production of dry natural gas from shale formations in the United States amounted to around 28.6 trillion cubic feet (Tcf), constituting approximately 79% of the total U.S. dry natural gas production for that year (EIA, 2021). Despite the significant oil and gas reserves in the unconventional reservoirs and current advancement of technologies, the oil and gas recovery factor from the primary depletion is limited to a low recovery factor (<10%)(Alfarge, Wei, et al., 2017). This means that more than 90% of the original oil and gas in place is left unrecovered in shale reservoirs. One EGR method that has become frequently used in tight reservoirs is cyclic gas injection (i.e., Huff-n-Puff, or HNP). One HNP cycle consists of three stages (Figure 1). First, gas is injected into a well at a high pressure (huff), followed by a period of shut-in to achieve miscibility (soaking), and lastly bringing the well back to production (puff). One advantage of this technique is that it does not involve drilling extra wells, since gas is injected into the same producing well. Even though the performance is tied to the properties of injected gas, delivering gas supplies to the field can be costly or impractical. This technique, though, allows produced gas to be recycled back into the formation, and hence becomes particularly attractive if there is adequate availability of produced gas on site.

H&P in unconventional reservoirs has been tested in numerous field pilots and scaled up, particularly in the Eagle Ford, over the last decade (Atan, et al., 2018; Eltahan, et al., 2021; Ganjdanesh, et al., 2019; Zhao, et al., 2020).

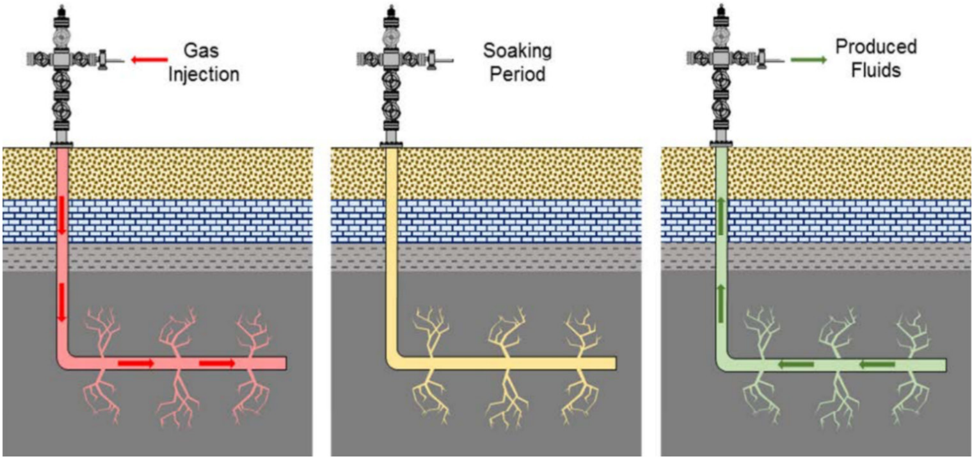


Figure 1 ─ Schematic showing stages of a Huff-n-Puff EOR cycle (from GeoMark Research 2018).

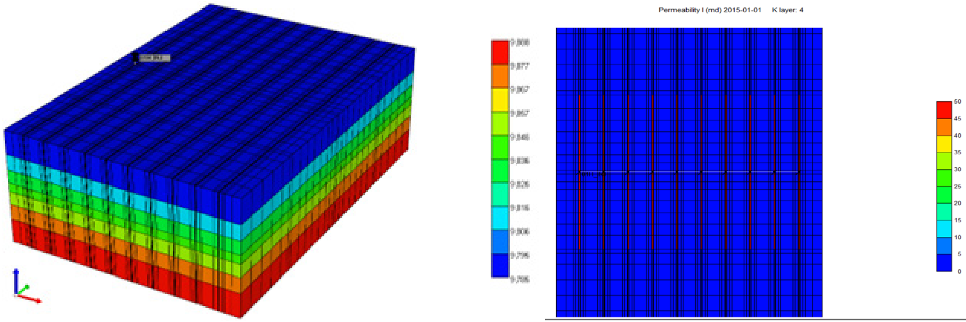
The efficiency of the CO_2 injection process depends on various factors, which can be categorized into controlled and measured parameters. Measured parameters, such as reservoir rock and fluid characteristics, are beyond our control. On the other hand, controlled parameters, including injection pressure, injection rate, and soaking time, are within our influence. Li et al. (2023) investigated effects of various injection rates, injection days, production days, shut-in time, and circulation cycles on the final methane recovery rate through orthogonal experiments. Jing et al. (2023) suggested that CO_2 may be favorable compared to produced gas as an EOR agent. They highlighted that increasing the injection rate can enhance the Recovery Factor (RF) but up to certain limits, which is influenced by oil price or economic conditions. As hydrocarbons are not being produced during the soaking time, certain authors argue that this period is deemed irrelevant, (Mukherjee, et al., 2020; Yu, et al., 2014). Consequently, initiating production immediately after the injection phase is considered by some. While soaking time does increase overall downtime, potentially causing production losses, certain researchers choose to incorporate it into their models. Higher injection rates often lead to increased pressure in the reservoir, promoting better displacement of the native gas and improving the sweep efficiency. This, in turn, enhances the recovery of gas, especially methane, from the reservoir. The choice of an optimal injection rate is crucial for maximizing gas recovery while ensuring the economic feasibility of the operation. However, it's essential to strike a balance, as excessively high injection rates may result in issues such as premature breakthrough and channeling, diminishing the overall effectiveness of the CO_2 injection process. Understanding the nuanced relationship between injection rates and gas recovery is key to designing and implementing successful CO_2 injection strategies for enhanced gas recovery in reservoirs. Some study highlighted the significance of molecular diffusion as a transport mechanism in unconventional fractured reservoirs, a factor often overlooked in conventional, non-fractured multi-component petroleum upstream simulations dominated by convection (Cronin, et al., 2021). In ultra-tight formations, where convection is slow, and thin blocks surrounded by fractures increase contact area, molecular diffusion becomes crucial for hydrocarbon production. In the shale matrix, molecular diffusion is expected to dominate mass transfer, while convection viscous flow prevails in natural fractures. Authors emphasized the significance of molecular diffusion as a crucial flow mechanism in shale oil reservoirs characterized by low matrix permeability and a densely fractured network (Jia et al., 2019). Investigations into diffusion coefficients between gas and oil under high pressure, considering the effect of low-permeability porous media, are limited. The validity of empirical correlations widely used in the oil and gas industry, developed several decades ago, might be questionable. Their work provided a brief review of methods for measuring diffusion coefficients in liquid-saturated porous media. The authors suggested that future research should focus on obtaining in-situ molecular diffusion coefficients in tight porous media to enhance the understanding of this phenomenon. This is crucial for modeling diffusion more accurately during composition and pressure changes in the matrix/fracture system where gas injection and production occur.

This study investigates the application of EGR in unconventional reservoirs, emphasizing to shale reservoirs, utilizing a commercial compositional reservoir simulator. The primary objective is to analyze the mechanisms involved in gas recovery during CO_2 Huff-n-Puff. The study thoroughly investigates the influence of operational parameters namely injection pressure, injection rate, and soaking time, on the processes of CO_2- EGR, identifying the most critical factors controlling these processes. Additionally, special consideration was given to processes such as adsorption and molecular diffusion.

Materials and methods.

To analyze the realistic effects of CO_2 injection in an unconventional gas reservoir, we have constructed a numerical model of shale reservoir. We have collected daily pressure and gas production data of a shale gas formation in the Eagle Ford, that is published from the literature. We addressed the uncertain or missing parameters by assigning arbitrary values within reasonable ranges associated with shale gas reservoirs.

For numerical modeling, the compositional simulator CMG-GEM (CMG, 2022) was used by setting up 3D reservoir model with dimensions of 545 ft × 800ft × 130 ft, which corresponds to length, width, and thickness, respectively (Figure 2).



(a) 3D Grid Top view (b) 2D Permeability I view

Figure 2 - Shale gas reservoir model.

Table 1 - Parameters used in basic reservoir model.

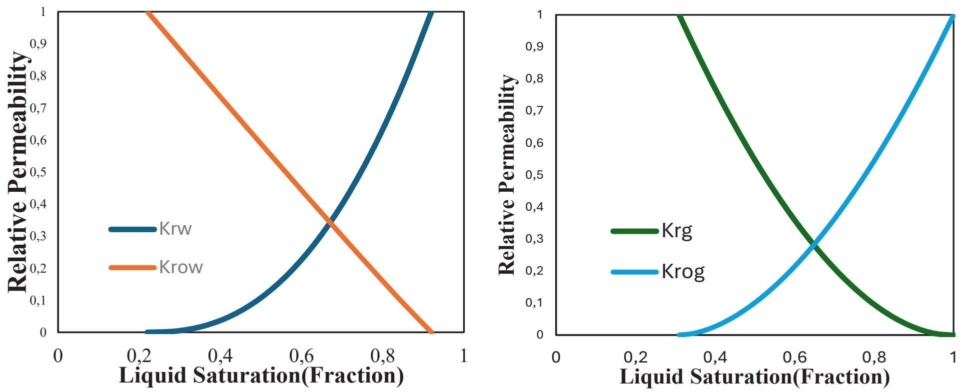
Parameter	Value	Unit
Number of grid blocks (x*y*z)	83x27x7	-
Model dimensions	545x800x130	ft
Depth to top layer	9785	ft
Matrix permeability	500	nd
Average water saturation	0.30	fraction
Reservoir temperature	256	^{0}F
Total compressibility	2E-06	psi^{-1}
Initial reservoir pressure	4700	psi
Reservoir porosity	5	%

We acknowledge that the field gas composition in a typical gas reservoir consists of multiple hydrocarbon components. However, for our study, we focus solely on methane, the predominant component, and assume the reservoir fluid to be 100% methane. Table 2 lists the critical properties of these pseudo components which were used for phase behavior calculation. The gas properties were determined for this well using the Peng-Robinson equation of state using CMG-WinProp.

Table 2 - Compositional data for the Peng-Robinson equation of state.

Component	Pc, atm	Tc, K	Acentric Factor	Molecular Weight	Volume Shift	Vc for viscosity	Parachor
CO_2	72.8	304.2	0.225	44.01	-0.111	0.094	78.0
CH4	45.4	190.6	0.0080	16.0	-0.175	0.099	77.3

Relative permeability strongly depends on the wettability of the shales. Figure 2 shows the relative permeability curves for matrix.



(a) Water/oil relative permeability curve (b) Liquid/gas relative permeability curve
Figure 3 - Relative permeability curves for matrix: (a) water/oil (b) liquid/gas

The local grid refinement (LGR) technique was used to represent the fractures by assigning their properties to the innermost block of a refined block (see Figure 2). The reservoir model is designed for a 452 ft section of a horizontal well and includes 10 fracture clusters, each of which is represented by a planar fracture (Figure 3). The cluster spacing and fracture half-length are set at 52 ft and 200 ft, respectively. Table 2 shows the other parameters of the fractures. Also, Figure 3.7 shows the fracture relative permeability curves used in this study.

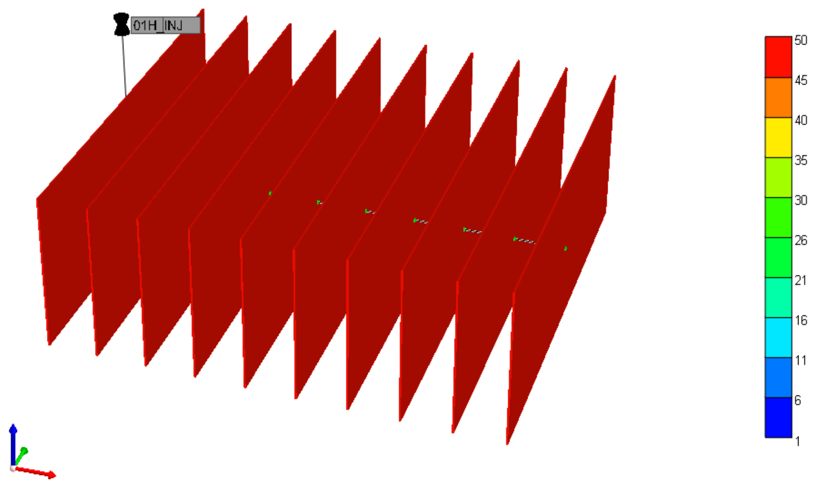


Figure 4 - Hydraulic fractures along the considered section of a horizontal well.

Table 3 - Parameters of the Hydraulic Fractures

Parameter	Value	Unit
Fracture permeability	50	md
SRV permeability	0.0325	md
Fracture width	0.6	ft

Fracture half-length	200	ft
Fracture height	146.5	ft
Fracture spacing	200	ft

We investigate the impact of CO_2 H&P on our reservoir model presented in Chapter 3 with single porosity system without considering mechanisms such as adsorption and diffusion. In the simulation of CO_2 H&P scenario, we assume a development plan that starts with initial production for three years, and then the H&P cycles begin with CO_2 injection. Each H&P cycle consists of one year of CO_2 injection, followed by one year of production and this process is repeated until the completion of the 40-year period. Figure 4 illustrates the average pressure and initial production of the reservoir for the base case without CO_2 H&P scenario with initial reservoir pressure at 4700 psi for 16 0000 days (43 years).

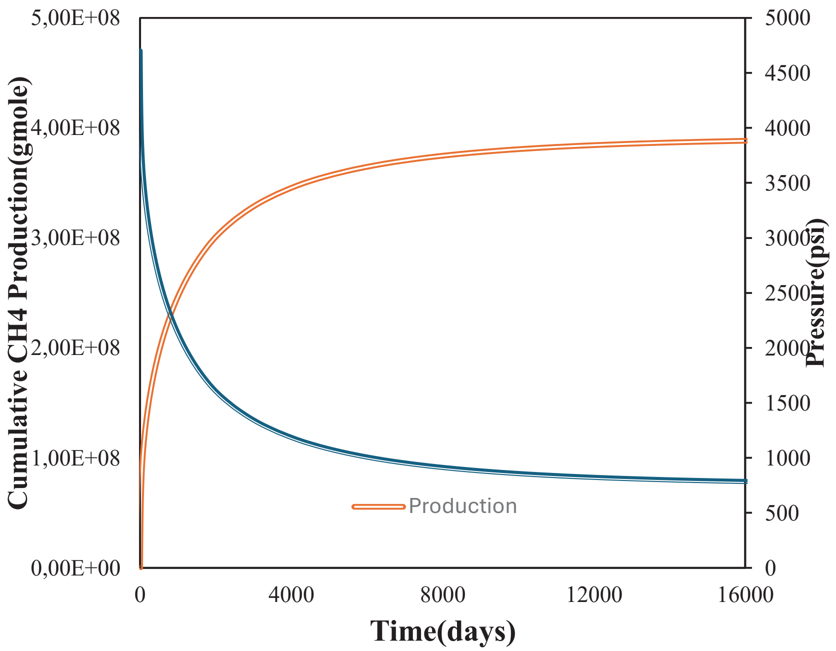


Figure 5 - Base case: reservoir average pressure and cumulative CH4 production.

Results

1. Sensitivity analysis of operational parameters

Injection Pressure

Three injection pressures—4500 psi, 5000 psi, and 5500 psi—were tested to assess their impact on cumulative methane production over a 40-year period. The simulations indicated that varying injection pressure had no significant effect on methane recovery, suggesting that within the tested range, injection pressure is not a critical factor for Enhanced Gas Recovery (Figure 5).

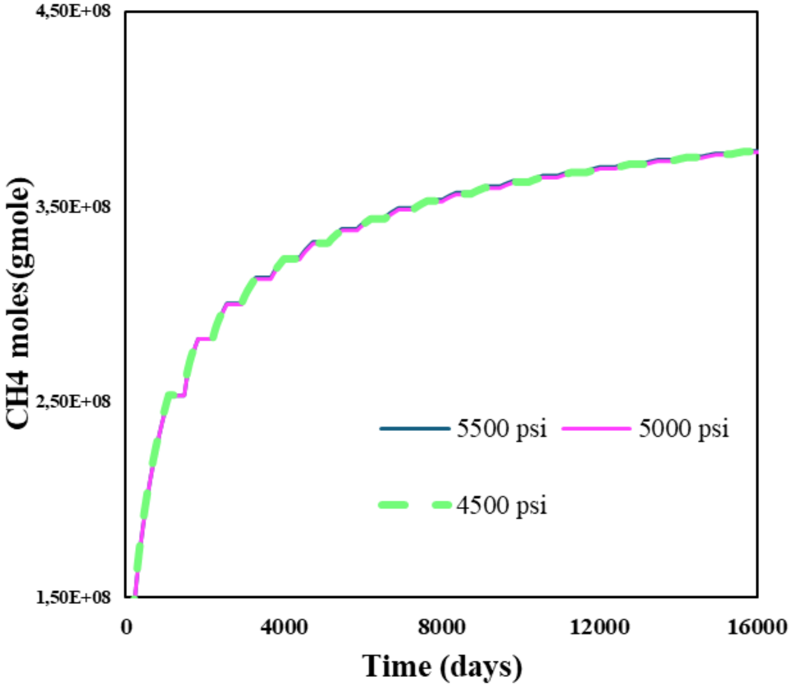


Figure 6 - Cumulative CH4 production under varying injection pressure.

Soaking Time

Three scenarios were evaluated to determine the effect of soaking time on methane production:

- **Case 1**: 12 months injection, 12 months production, no soaking
- **Case 2**: 12 months injection, 6 months soaking, 12 months production
- **Case 3**: 12 months injection, 3 months soaking, 12 months production

The results demonstrated that the scenario without a soaking period yielded the highest methane recovery, while longer soaking times resulted in decreased production (Figure 6).

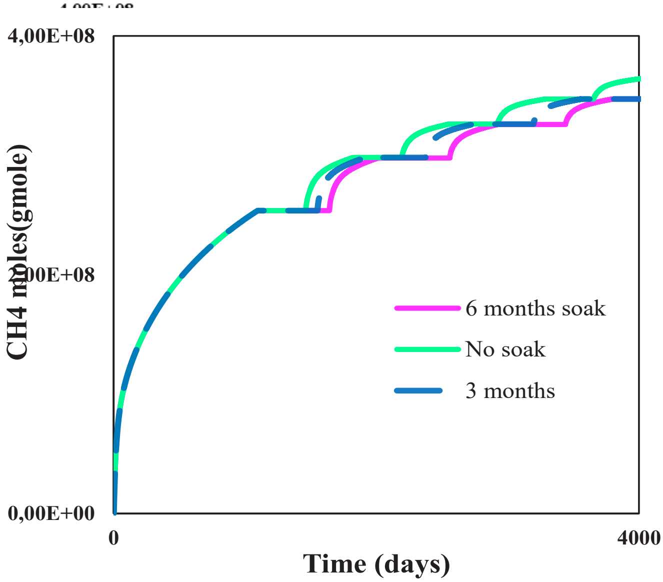


Figure 7 - Cumulative CH4 production under varying soaking time plans.

Injection Rate

Injection rates of 200, 400, and 800 MSCF/day were tested at a constant injection pressure of 5500 psi and no soaking time. The cumulative methane production increased with higher injection rates, with the optimal rate identified as 800 MSCF/day. CO_2 storage also increased proportionally with injection rate (Figure 7).

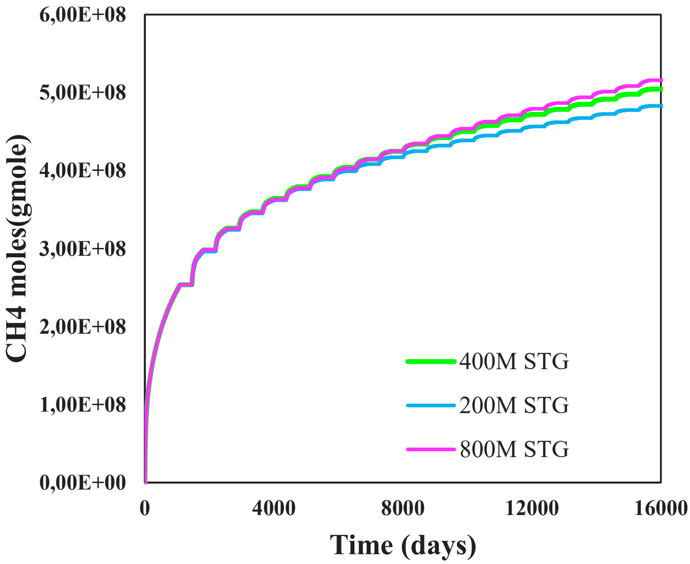


Figure 8 - Cumulative CH4 Production under varying injection rate.

Based on the sensitivity analysis, the optimal parameters for further study were determined to be an injection pressure of 5500 psi, an injection rate of 800 MSCF/day, and no soaking period. Under these conditions, the CO_2 Huff-n-Puff (H&P) scenario resulted in a 2.5% decrease in methane recovery compared to the case without CO_2 injection.

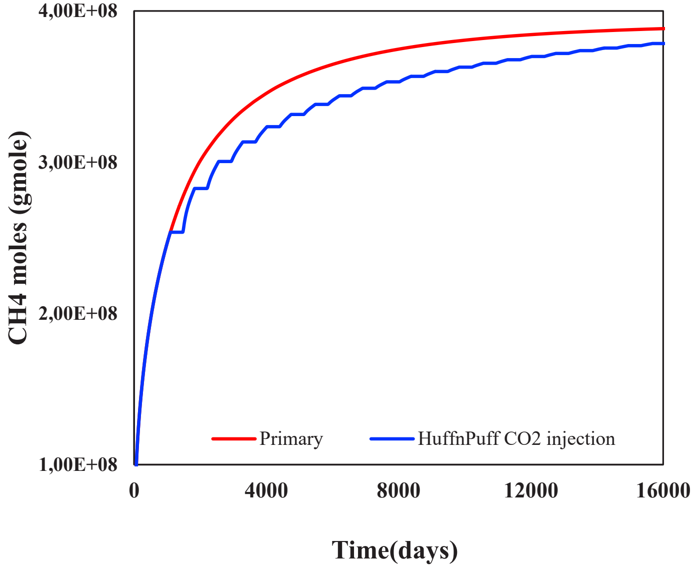


Figure 9 - Cumulative CH4 production without and with CO_2 H&P.

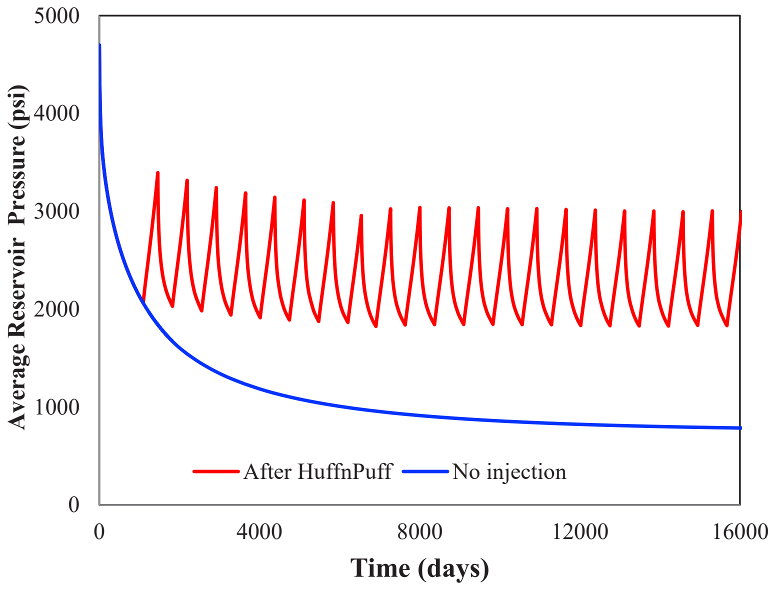


Figure 10 - Average reservoir pressure with and without CO_2 injection over time.

2. Effect of Adsorption

To explore the impact of adsorption on methane recovery Langmuir isotherm adsorption curve is chosen to describe the adsorption of the two components (Figure 10). The adsorption equation is used to describe the adsorption behavior of CH4 and CO_2. The Langmuir isotherm equation with two fitting parameters is as follows (Langmuir, 1918):

$$V(P) = \frac{V_L P}{P+P_L} \tag{1}$$

where V(P) is the gas volume of adsorption at pressure P, V_L is the Langmuir volume, referred to the maximum adsorbed gas volume at the infinite pressure, and P_L is the Langmuir pressure which represents the pressure corresponding to a one-half Langmuir volume. In the model, an extended Langmuir isotherm is implemented to model the competitive multicomponent adsorption and desorption process:

$$w_i = \frac{w_{i,max} B_i y_{ig} P}{1+\sum B_j y_{jg}} \tag{2}$$

where w_i is the moles of adsorbed component *i* per unit mass or rock, $w_{i,max}$ is the maximum moles of adsorbed component *i* per unit mass or rock, B_i is the parameter for Langmuir isotherm relation, P is the pressure, and y_{jg} is the molar fraction of adsorbed component *i* in the gas phase. The Langmuir isotherm is often determined in laboratory using core samples. The data on adsorption provided in this study is drawn from existing literature on the Eagle Ford shale formation. (Yu, et al., 2013)

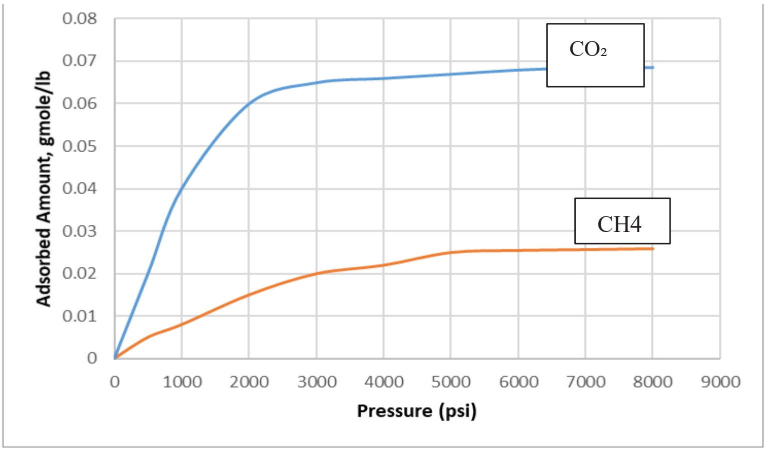


Figure 11 - CH4 and CO_2 Langmuir isotherms.

When adsorption was considered in the simulations, methane production increased by 9.2% by the end of the production period. This enhancement is attributed to CO_2's higher adsorption affinity, which enables it to displace CH_4 from the surface of organic matter, thereby improving gas recovery (Figure 11).

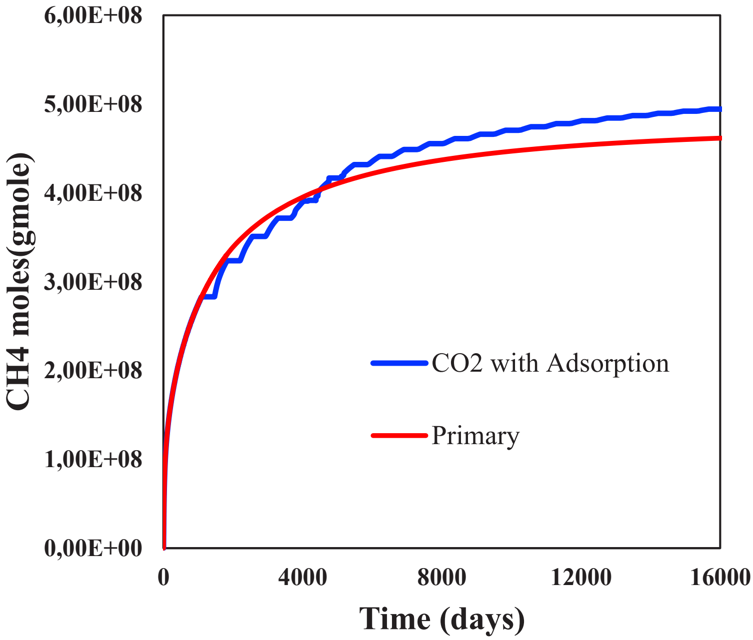


Figure 12 - CH4 production before and after CO_2 Huff Puff with adsorption process being activated.

3. Effect of Molecular Diffusion

The impact of molecular diffusion was assessed by simulating scenarios with CO_2 diffusion coefficients of 10^{-4} cm²/s, 10^{-3} cm²/s, and using the Sigmund correlation. CO_2 diffusion was modeled using CMG-GEM (CMG, 2022) compositional reservoir simulator built-in capability to handle molecular diffusion. Effects of adsorption are not considered for this case.

The results indicated that higher diffusion coefficients led to substantial increases in methane recovery, with improvements of approximately 6% and 19% for the 10^{-3} cm²/s and Sigmund correlation cases, respectively, compared to the scenario without diffusion.

Figure 12 shows the effects of different CO_2 diffusion coefficients on cumulative methane production.

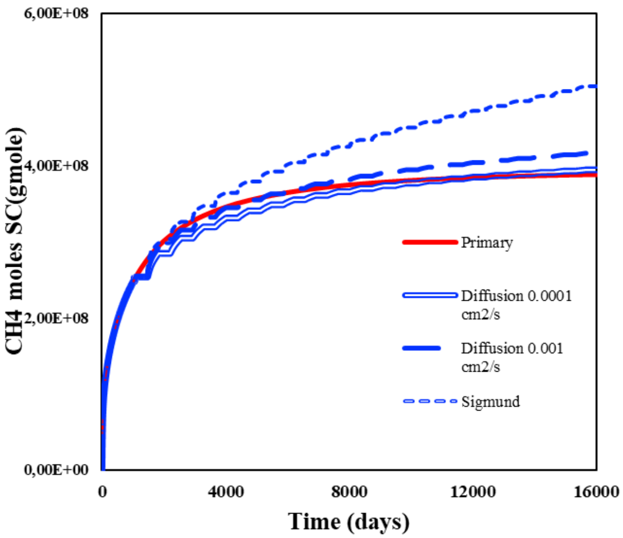


Figure 13 - CH4 production before and after CO_2 H&P with different molecular diffusion coefficients.

Discussion.

1. Interpretation of Injection Parameters

The sensitivity analysis conducted in this study revealed that injection rate significantly influences methane production and CO_2 storage, with higher rates leading to increased recovery. This aligns with the findings of Liu et al. (2021), who emphasized the importance of optimizing injection parameters to enhance gas recovery in shale reservoirs. In contrast, variations in injection pressure and soaking time showed minimal impact within the tested ranges, suggesting that, under certain reservoir conditions, these parameters may be of lesser priority for optimization.

2. Adsorption Effects

The incorporation of adsorption effects into the simulation models demonstrated a significant enhancement in methane recovery. This outcome corroborates findings from other researchers who have highlighted the role of CO_2's higher adsorption affinity in displacing CH_4 from adsorption sites. Figure 11 illustrates methane production comparing scenarios of H&P injection to no injection while activating adsorption during the simulation. Taking adsorption into account results in a 9.2% increase in methane production by the end of the production period. It is evident that methane production has declined during the first five years after injection compared to the case without injection. This suggests that there is a time delay for gas molecules to adsorb into the rocks until they reach a level at which they become influential to the results.

3. Molecular Diffusion Implications

The study's assessment of molecular diffusion effects underscores the importance of considering diffusion mechanisms in modeling CO_2 injection processes. The significant improvements in methane recovery associated with higher diffusion coefficients suggest that diffusion facilitates deeper CO_2 penetration into the reservoir, enhancing CH_4 displacement. These findings are consistent with literature emphasizing the role of molecular diffusion in gas transport within low-permeability formations (Alfarge, Wei, et al., 2017; Cronin, et al., 2021).

4. Limitations and Future Work

This study provides valuable insights into the effects of operational parameters, adsorption, and molecular diffusion on enhanced gas recovery. However, it is limited by the specific reservoir characteristics and simulation conditions used. To improve the generalizability of the findings, future work should investigate a broader range of reservoir types and operational scenarios.

Incorporating field data and conducting pilot-scale tests would strengthen the practical relevance of the results. Further research is also recommended on CO_2 Huff'n'Puff and flooding methods in larger reservoirs and longer horizontal wells with complex fracture networks. Natural fractures, which play a critical role in tight formations, should be included in future models to better reflect real reservoir behavior.

For greater accuracy, combining key mechanisms—such as diffusion and adsorption—is advised. Their interaction significantly influences methane recovery and CO_2 storage, and integrating them can enhance the predictive power of simulation models.

Conclusions.

- Injection rate of 800 MSCF/day an injection pressure of 5500 psi, no soaking period are chosen as the optimum parameters for CO_2 injection as a result of a sensitivity analysis.
- CO_2 Huff-n-Puff for EGR could be a viable choice, especially when taking into account mechanisms such as diffusion, adsorption.
- CO_2 huff-n-puff scenario is not suitable for CO_2 storage even considering diffusion, adsorption, and the presence of natural fractures because more than 80% of the injected CO_2 is reproduced quickly back to the surface.
- Gas adsorption leads to roughly 9% increase in gas recovery during 40 years of gas production.
- Molecular diffusion of CO_2 significantly contributes to the improvement of gas recovery in shale gas reservoirs. The utilization of the Sigmund correlation results in an approximate 19% increase in gas recovery.

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