

EOR SIMULATION STUDY IN A SHALE OIL RESERVOIR: Supercritical CO₂ Injection Considering Molecular Diffusion, Capillary Pressure and Geomechanical Effects in Vaca Muerta

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Resumen

El progresivo declive a nivel mundial en la cantidad y el tamaño de descubrimientos de tipo convencional ha derivado en una reciente reevaluación de activos ya conocidos, inicialmente considerados como recursos menos atractivos. Dentro de este grupo, yacimientos de tipo no convencional tales como los reservorios de *shale oil* resultan particularmente interesantes en base al significativo volumen de hidrocarburos que puede esperarse en este tipo de *plays* usualmente de extensión regional. Sin embargo, a pesar del uso de tecnologías innovadoras y de estrategias de perforación y terminación de pozos con un fuerte foco en la optimización continua, el factor de recuperación en pozos no convencionales es aun relativamente bajo, con estimaciones oscilando entre 2% y 15% para yacimientos en US donde se concentra la gran mayoría de los reservorios no convencionales desarrollados hasta el momento. El presente estudio tiene como objetivo evaluar los resultados del uso de CO₂ EOR como una opción para maximizar la recuperación en un pozo horizontal de *shale oil* en la formación Vaca Muerta, un *play* ubicado en Argentina que presenta una de las oportunidades más atractivas a nivel mundial en el área no convencional con más de 310 trillones de pies cúbicos de gas y 16 billones de bbl de petróleo *in place*. Un modelo numérico fue desarrollado para representar un pozo horizontal con múltiples fracturas hidráulicas produciendo desde un reservorio de *shale oil* en la formación Vaca Muerta, que fue finalmente ajustado en base a la producción histórica del pozo. Una detallada revisión de la bibliografía disponible fue necesaria, combinando los trabajos más recientes sobre modelado de inyección de CO₂ en yacimientos de *shale oil* en US con la experiencia desarrollada en modelado y simulación numérica en yacimientos de Vaca Muerta. Como resultado, distintos aspectos que afectan el flujo de los hidrocarburos en tales pozos han sido considerados: difusión molecular en la fase petróleo, presiones capilares y efectos geomecánicos sobre porosidad y permeabilidad en base a la presión poral.

El estudio sugiere que un esquema de inyección cíclica de CO₂ permitiría incrementar el factor de recuperación en un pozo de *shale oil* horizontal alrededor de un 16% con respecto a la producción original, luego de 10 años de tratamiento. Si se incluyen consideraciones económicas en el proceso de optimización, el Valor Presente Neto incremental podría alcanzar los 0,78MM\$, con un incremento en el FR de un 11,1%. Adicionalmente, el estudio sugiere que la inyección de gas rico produce resultados comparables, mientras que la inyección de gas seco puede afectar negativamente la producción. Distintas conclusiones sobre las condiciones de operación se extrajeron del proceso de optimización y la relevancia del mecanismo de difusión molecular fue analizado. Aun cuando los procesos físicos controlando el flujo de hidrocarburos a nivel de poro en reservorios *shale* es todavía materia de discusión, se hace evidente que cualquier alternativa con potencial para incrementar la recuperación en este tipo de reservorios de gran potencial productivo merece debida atención.

Abstract

The decline in the amount and size of conventional oilfield discoveries worldwide led to a reassessment of previous oil and gas assets, initially seen as less attractive resources. Within this category, unconventional fields such as shale oil reservoirs became particularly attractive considering the significant volume of hydrocarbons expected to be present in this type of regionally-extended play. However, despite the application of innovative technological solutions and rigorously optimized drilling and completion approaches, the recovery factor from this type of asset is still known to be very low, with estimations ranging between 2% and 15% for fields in the US where most of the unconventional assets have been developed so far (Balasubramanian et al., 2018; Shen et al., 2016).

The present work aims to evaluate the performance of CO₂ EOR (Enhanced Oil Recovery) as an option to maximize recovery from a horizontal shale oil well located in the Vaca Muerta formation, a recently developed play in Argentina presenting one of the highest potentials for unconventional resources worldwide, with more than 310 TCF of gas and 16 billion bbl of oil in place (EIA, 2013). A conceptual simulation model was created and history matched to represent a real multi-fractured horizontal well producing from a shale oil reservoir in Vaca Muerta. A thorough review of related bibliography has been carried out, combining the latest standards of CO₂ injection modeling in US shale oil fields with the expertise developed in simulation models at Vaca Muerta. As a result, various effects assumed to influence hydrocarbon behavior have been included, namely: intra-phase molecular diffusion, capillary pressures and pressure-dependent geomechanical effects which influence the permeability and porosity of fractures and matrix as reservoir pressure decreases.

This study suggests that CO₂ cyclic injection could produce up to 16% increase in RF (Recovery Factor) from original production for multi-fractured horizontal shale oil wells in Vaca Muerta after 10 years of treatment. When including economic considerations in the optimization analysis, a maximum incremental NPV (Net Present Value) of 0,78MM\$ with a RF increase of 11,1% from the expected production can be achieved. Furthermore, the evaluation suggests that wet gas also provides a comparable production increase. Various conclusions regarding operational conditions have been extracted from the optimization process and the relevance of molecular diffusion mechanism has been analyzed. Even though physical processes affecting hydrocarbon production at the pore scale in the extremely tight shale matrix are still a matter of discussion, it becomes clear that any alternative with the potential to increase the recovery from these massive hydrocarbon accumulations deserves proper attention. Furthermore, in view of an increasing concern regarding the greenhouse effect motivating a shift in economies towards a low-carbon approach, re-utilization of anthropogenic CO₂ emissions in EOR could present a further positive environmental impact, either reducing the current carbon footprint or providing the basis for future CCS (Carbon Capture & Storage) projects in the area.

Introduction

The Vaca Muerta formation, a black and dark grey rich marine shale originally defined by Weaver (1931), is located at the Neuquén Basin, in Central-West Argentina, extending over approximately 30.000 km². Forming a depositional system with overlain Quintuco, VM fm (Vaca Muerta formation) was deposited during a transgressive period between the Late Jurassic and the Early Cretaceous (Sagasti, Ortiz et al., 2014). Shales and marls deposition occurring in anoxic conditions permitted the development of organic-rich sediments, with TOC values between 1% and 8%, peaking to 12% in the richer, deeper section at the base. The significant areal extension leads to a considerable variation in the quality and characteristics of the reservoir. Matrix porosity ranges from 4% to 13%, averaging 9%, while the extremely low matrix permeability spans “from hundreds of nanodarcies to tens of microdarcies” (Fernandez & Berrios, 2012). Additionally, hydrocarbon maturation window indicates dry gas, wet gas and condensate and oil prone areas approximately from West to East (Figure 1).

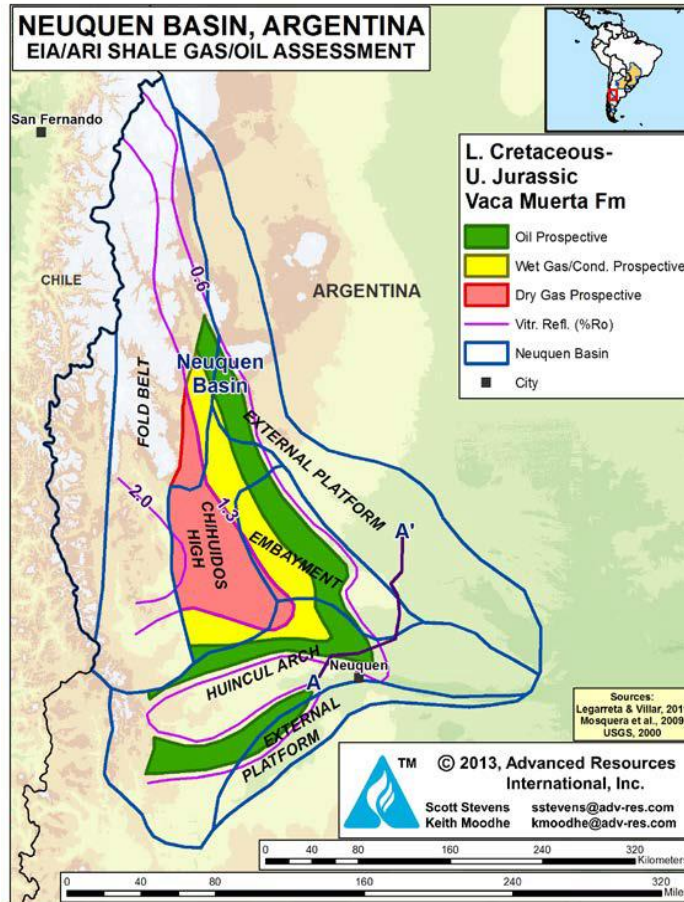


Fig. 1 – Prospective areas in VM. From EIA (2013).

At the time of the study, EOR research in Vaca Muerta was strictly limited to the work published by Tuero and Crotti (2017), in which they explored the theoretical basis and included lab and field experiments with water injection in the oil window of the VM fm. Regarding EOR expertise in unconventional shale and tight oil reservoirs involving gas injection, available information is mostly focused on US and Canadian/Chinese fields, particularly at the Bakken fm (Sheng, 2017). A bibliographic summary is classified in experimental, simulation and field studies and succinctly described below:

- Laboratory studies using CO₂ in cores extracted from liquid-rich shale oil Bakken intervals suggested that, unlike conventional reservoirs, molecular diffusion plays a significant role in hydrocarbon extraction from the tight matrix, either dominating oil transport (Sorensen et al., 2014) or complementing pressure-driven advective “Darcy” flow (Alharthy et al., 2015). It is assumed that gas injected in shales at miscible conditions will act as a solvent, mobilizing the CO₂-oil mixture developing in a narrow region near the matrix-fracture interface, and therefore extracting oil in a counter-current flow from the matrix to the fractures. Additional beneficial mechanisms include “re-pressurization, viscosity and interfacial tension reduction through oil swelling, wettability alteration and relative permeability hysteresis”.
- Regarding numerical simulation studies, the most widely applied modeling approach involves the use of compositional fluid models, either adopting dual porosity (Kurtoglu,

2013; Sahni et al., 2018) or dual permeability (Alfarge et al., 2017; Phi et al., 2017; Kim et al., 2017; Jia et al., 2017) grids to represent the interaction between shale matrix and natural/induced fractures system. The preferred production method that has been modeled in papers is the Huff n' puff process. A single well is required for this technique, where an initial high-pressure, gas injection period typically in the order of days or months, is followed by a soaking period where the well is shut in. During the injection and soaking stages, miscibility of oil and injected gas is expected to develop with the mentioned beneficial effects. Finally, the well is put back in production during a third stage for a limited time, where an increase in oil production is expected. These three stages conform a cycle, which is periodically repeated. Other modeled techniques include gas flooding -from injection to producing wells- and WAG -where gas injection is alternated with water-.

- (c) In relation to EOR pilot projects employing gas in liquid rich unconventional reservoirs, information is limited and restricted to five Huff n' puff cases in the US and four flooding cases reported in China, the US and Canada (Sheng, 2017; IHS, 2016; Rassenfoss, 2017). Results are in general not conclusive regarding the effects of the implemented techniques, although wide variability between the field characteristics and operational parameters restricts the comparison between different cases. The most successful pilot has been reported by EOG at Eagle Ford, where between 30% and 70% increase in reserves has been declared. However, no further details have been provided. Independent analysis relying on public data suggests a Huff n' puff process using gas sourced at the reservoir, possibly enriched with heavier components (IHS, 2016).

The objectives of this study can be better understood by asking the following open questions:

- Is miscible CO₂ injection a suitable EOR method to increase oil recovery in shale oil wells in a resource play like Vaca Muerta?
- What is the optimal cyclic injection scheme?
- What is the impact of injection gas composition?
- What is the impact of molecular diffusion?

Methods and Procedures

The present study is based on diverse information, which tries to resemble a typical horizontal well drilled across the VM fm, with the landing point located around 3.000 m. The horizontal section extends over 1.500 m and has 15 hydraulic fractures evenly spaced every 100 m. Available data includes completion design, a set of composite logs (dataset not included), flowback and a production test data (including rates, pressures, temperatures, etc.) for approximately the first year of production. Compositional and PVT experimental data, as well as oil-water and oil-gas relative permeability and capillary pressure curves were assumed for imbibition and drainage scenarios. Additionally, log and core-derived poroperm data in a nearby vertical well was available to be used as to check the validity of such assumptions.

Preliminary Analysis & Well Characterization

Initial production data analysis was carried out in Excel spreadsheets, applying Rate Transient Analysis and Flowing Material Balance techniques to characterize the well prior to the definition of the simulation model, as proposed by Fernandez & Berrios (2012) and later Suarez et al. (2013) for Vaca Muerta wells. At first, proper identification of flow regimes in a log-log normalized flowrate vs. material balance time plot is required. Then, the linear plot considering equations for a horizontal oil well and the flowing material balance plot were used to estimate the effective permeability at the stimulated volume K_{SRV} , hydraulic fracture half-length X_{mf} , and stimulated hydrocarbon pore volume -SRV- (Figure 2). Effective porosity and water saturation profiles for the shale matrix have been estimated from the aforementioned log dataset, applying the simplified workflow proposed by Cuervo et al. (2016) for petrophysical analysis of Vaca Muerta wells. Core data, including porosity, air permeability and water saturation data was used to validate the log-derived calculations and to generate a poro-perm relationship that was required to define a synthetic permeability profile which was later applied to populate the grid. In absence of a second well to interpolate data, a homogeneous distribution has been assumed to distribute permeability and porosity of the shale matrix.

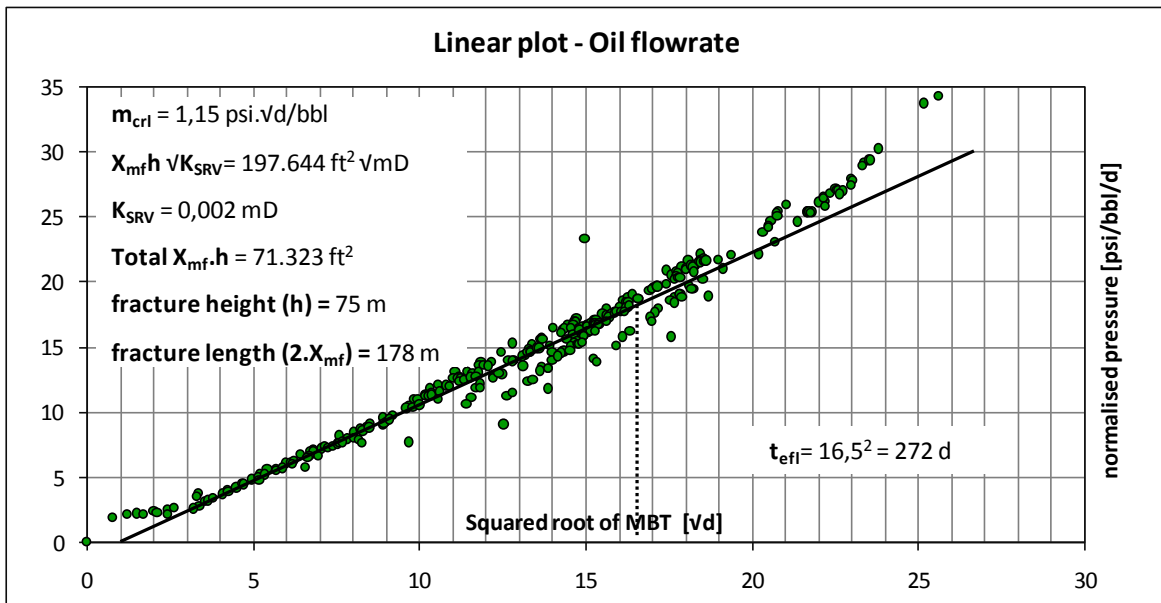


Fig. 2 – Linear plot of normalised pressure versus square root of Material Balance Time.

Grid Definition

Given that compositional fluid behaviour and molecular diffusion effects will be included in the simulation and also limitations on computational capacity, a single porosity model was built to represent the well drainage volume using integrated reservoir modelling and simulation software. 15 equally spaced hydraulic fractures were included in the horizontal section, for modelling purposes assumed to be planar and orthogonal to the wellbore. An SRV (stimulated rock volume) region with enhanced permeability was defined surrounding the explicit hydraulic fractures, which in turn is located within a third region representing the un-stimulated shale matrix characterized by the log derived petrophysical properties. The dimensions of the well model are 400m x 1.700m x 75m in X, Y and Z directions respectively, with a total of 237.375 cells. A Cartesian type grid with a cell size of 80m for Δx and 100m for Δy was adopted for the parent cells. A Δz value equal to 3m was required

to reasonably capture the layered characteristics of the shale, coinciding with the typical vertical correlation length in marine environments. The horizontal well penetrates in the Y direction, and logarithmically spaced LGR (local grid refinement) was applied in X and Y directions to model the pressure drop developing towards the fracture plane in the adjacent SRV. LGR was also applied on the un-stimulated matrix cells immediately surrounding the well to minimize the size contrast between refined cells in the SRV and parent cells in the matrix. No logarithmic spacing was applied in this case, resulting in cell size of 26,66m for Δx and 33,33m for Δy (Figure 3 and Table 1).

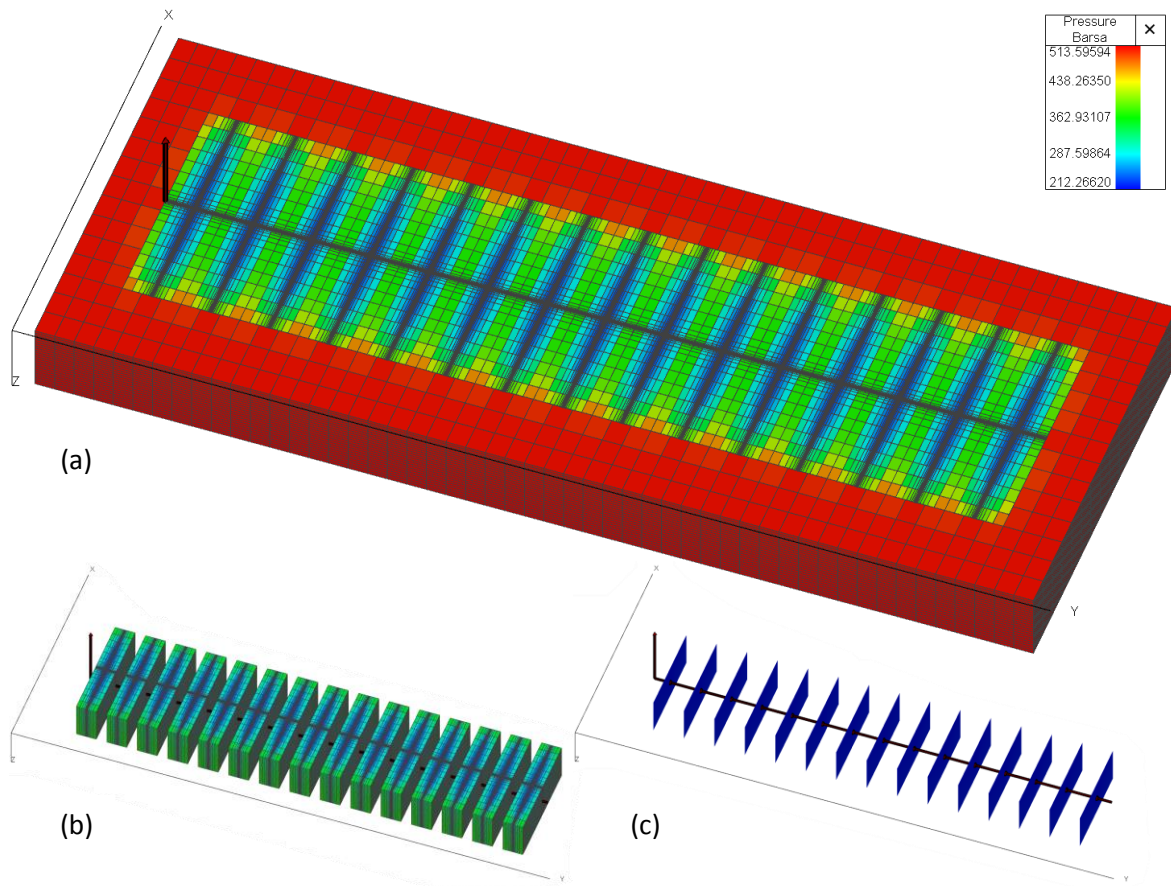


Fig. 3 – Full well model (a), SRV (b) & HF (c) detail – Base case pressure after 10 years depletion.

Fluid Model

A compositional model is strictly required both to represent the multi-contact miscibility process developing between supercritical CO₂ and oil at the reservoir conditions and to incorporate the molecular diffusion mechanism. Therefore, the original fluid composition was reduced to 7 pseudo-components: CO₂, N₂, C₁, C₂, C₃, C₄-C₆ and C₇+ to minimize simulation time. The EOS was tuned using a PVT module available within the same software. The reference for calibrating the parameters for the Peng-Robinson adopted EOS -including Solution GOR, B_o, B_g, and oil and gas viscosity– was representative of available data from typical PVT experiments on fluid samples collected at the field object of this study. Additional experiments describing the interaction between reservoir oil and CO₂ such as swelling, RBA or VIFT tests are also recommended for tuning the EOS. Since the experiments were not available, for this conceptual simulation study an estimation of the minimum miscibility pressure (MMP) was carried out applying Emera & Sarma correlation (Emera et al., 2005). The

Bubble Pressure for the oil is 161,5 Bars (2.342 psia), while GOR and B_o values at Bubble Pressure are 150,1 sm^3/sm^3 and 1,603 rm^3/sm^3 . The phase diagram for the adopted pseudo-components composition is presented in Figure 4. The MMP for CO_2 and reservoir oil is found to be 288,9 Bars (4.191 psi). Other features considered in the model are described in the following sections.

Table 1 - Model parameters	
Dimensions (x,y,z)	400m x 1.700m x 75m
Number of cells	237.375
Average porosity	6,6 %
Average matrix K	0,00019 mD
K_{SRV}	0,002 mD
Average S_w	0,35
HF conductivity	85 mD-ft
HF height	75 m
HF length	178 m
Amount of HF	15
Reservoir Pressure	500 Bar @ 3.010 m
Reservoir Temperature	134° C @ 3.190 m
Landing depth	3.190 m
Length of horizontal section	1.500 m

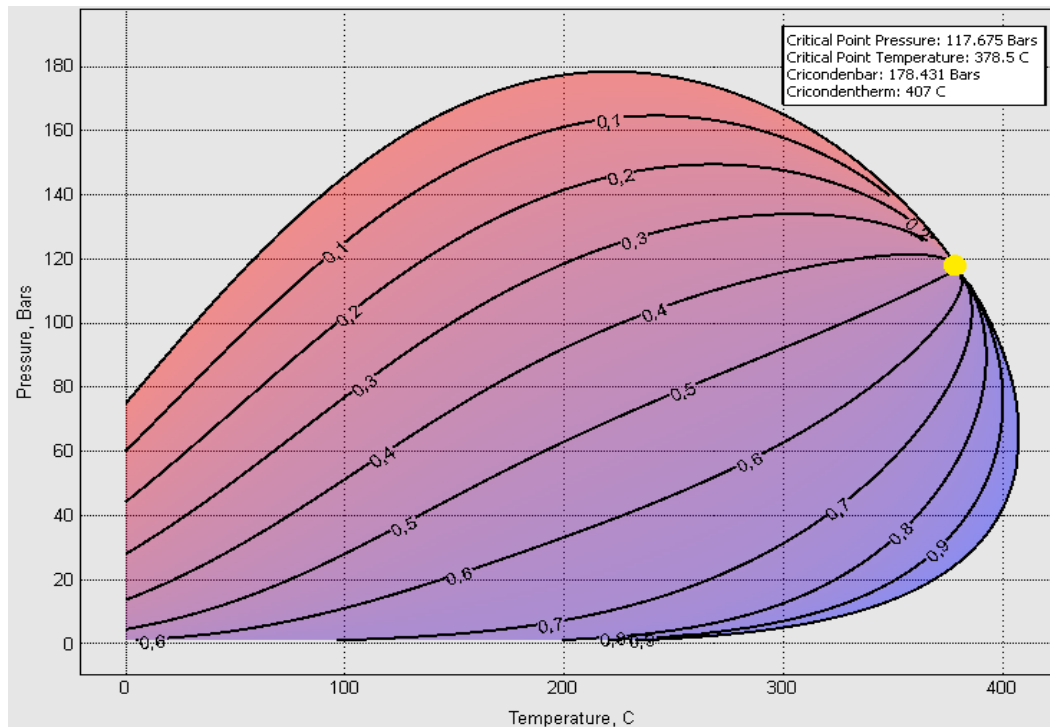


Fig. 4 – Phase diagram for the fluid in the reservoir.

Molecular Diffusion

As mentioned, molecular diffusion effect is assumed to play a major role in CO₂ EOR processes developing in shale oil reservoirs. The process is represented in reservoir simulators applying Fick's law, where molecular diffusion of a particular component is solely driven by the concentration gradient and multiplied by a constant diffusion coefficient representative of that component in the mixture. For the present study, only intra-phase molecular diffusion has been considered, since experimental data or correlations required to estimate cross-phase molecular diffusion is still limited. The Sigmund correlation (Sigmund, 1976) was used to calculate the effective diffusion coefficient D_{ik} (Equation 1) for each component i in the hydrocarbon multicomponent system k from binary diffusion coefficients D_{ij} . The full procedure for calculation is included in the appendix section.

$$D_{ik} = \frac{1 - y_{ik}}{\sum_{j \neq i} y_{ik} D_{ij}^{-1}} \quad [1]$$

Geomechanical Effects

As suggested by Suarez et al. (2013), geomechanical effects play a significant role on production in VM wells, observing a reduction of the effective permeability as the average reservoir pressure declines. Pressure dependent transmissibility multipliers were considered in the model to represent both permeability and pore volume reduction at the hydraulic fracture, the SRV and the un-stimulated matrix regions (Figure 5). For a dual-porosity model in VM, Manestar et al. (2017) employed an exponential function to model the change in pore volume, and then coupled permeability variation to pore volume using a potential function. For the present study, the effect of pressure in permeability and pore volume was modelled using independent exponential functions, as presented in Equation 2 for the case of permeability.

$$\frac{k}{k_i} = e^{-\gamma(p_i - p)} \quad [2]$$

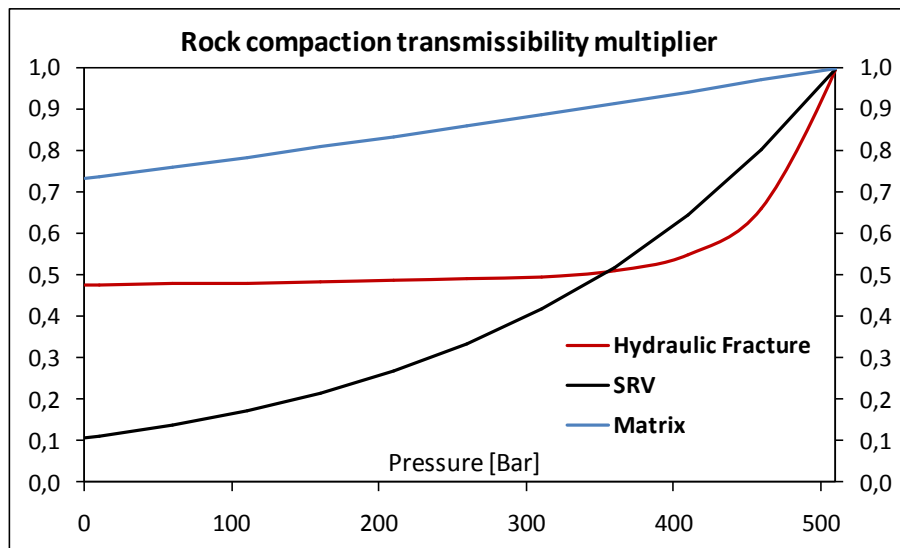


Fig. 5 – Transmissibility multipliers after Assisted History Matching.

Capillary Pressure

An additional effect in shale reservoirs, specifically described by Tuero and Crotti (2017) for the VM fm, resides in the significant incidence of capillary pressures in these extremely tight formations. In their work, the importance of capillary pressures associated to the micro- and macro-pores in the shale matrix is stressed in order to properly represent the flowback and negligible water production experienced in some multi-fractured horizontal wells in certain regions in VM shale reservoirs. Oil-water capillary pressures for the hydraulic fracture, SRV and matrix were therefore considered in the model, for drainage and imbibition cases (Figure 6). Capillary pressure curves were assumed along with relative permeability curves, designed to represent the flowback dynamics. Maximum P_c was considered as a matching variable at the history matching due to the impact of this variable to match flowback water retention effects and early production. Capillary pressure curves were modelled using the model proposed by Bentsen and Anli.

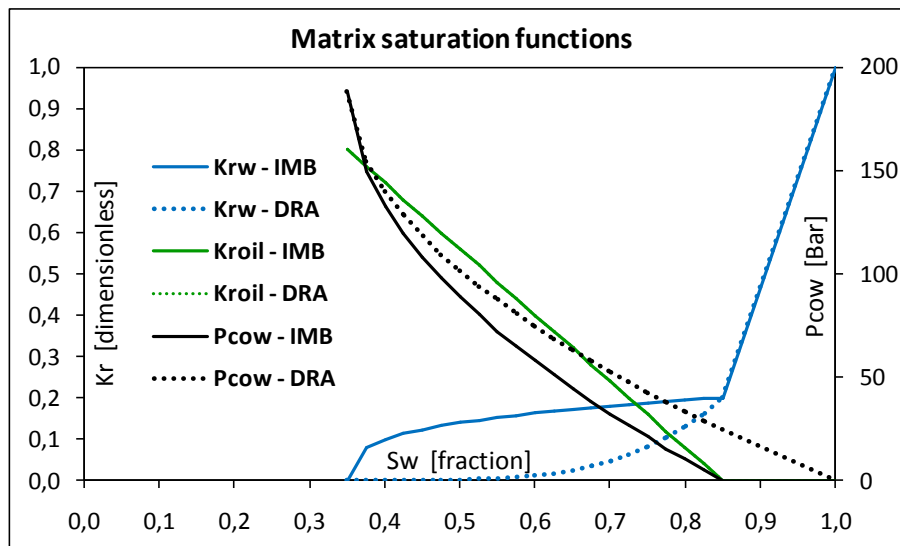


Fig. 6 – Matrix saturation functions after Assisted History Matching.

Assisted History Matching

Historical data considered for the model include the fracturing period, the first shut-in period after the fracturing treatment, the flowback, the second shut-in period after the flowback, and finally the production period lasting approximately one year. The effective permeability of the hydraulic fracture, $P_{c_{max}}$ and shape coefficient at the capillary pressure curves and pressure-dependent permeability and pore volume multipliers were considered as matching variables. A differential evolutionary algorithm was applied for the optimization of an objective function, minimizing the total error between simulated and measured points. The parameters considered in the objective function were: oil flowrate, water flowrate, total water injected and flowing bottomhole pressure. After 400 runs an optimal model was selected for the evaluation of the EOR strategies. Results of matching can be seen in Figure 7, where time is presented in days since start.

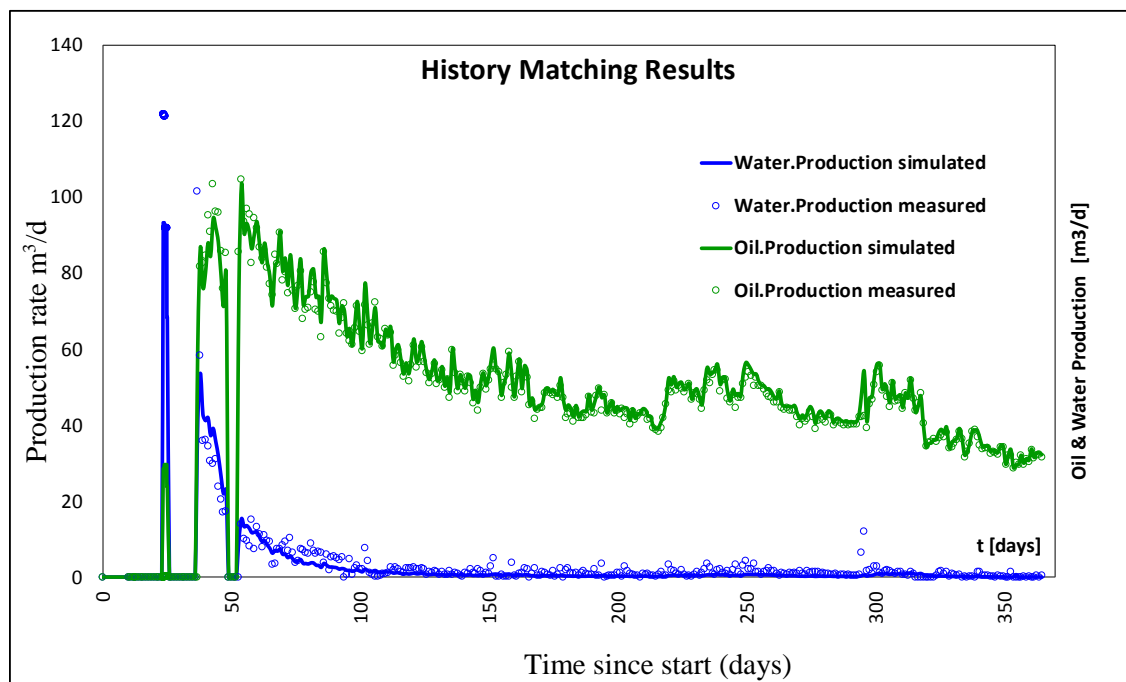


Fig. 7 – Oil and water flowrates after Assisted History Matching.

Huff n' puff Cycle Optimization

Consideration of molecular diffusion effect in the model significantly increases the simulation time, even compared to the base compositional model. Due to limited computational resources at the time of the study, a fast approximation was preferred rather than a precise but slower result. Therefore, a simplification was adopted to carry out the optimization, following described. The full well model was run to simulate a “do nothing” base case, consisting of 10 years of production controlled by a constant bottomhole pressure. A simplified model consisting of a single fracture and the related SRV was run for the same conditions, and cumulative production after 10 years multiplied by the total number of fractures was compared with the full well model results. The error in cumulative oil production after 10 years was 1,3%. It is known that completion design optimization in multi-fractured horizontal wells aims to minimize or delay the interference effect between fractures. Keeping in mind that the objective of the present project is to provide a conceptual assessment of gas injection in the shale reservoir and since resources were limited, the interference effect within the considered timeframe was assumed negligible, and a simplified single-fracture version of the model was used for the investigation of optimal injection parameters.

With regards to the considered injection strategies, the high uncertainty related to the distribution of reservoir properties -and how this may impact the inter-well connectivity- is a major limitation for evaluation of a gas flooding case. Therefore, only a Huff n' puff injection case has been evaluated. Three main scenarios were initially defined for the investigation of the optimal Huff n' Puff cycle: in the scenario (a1) a single cycle lasting 365 days is completed each year; in the scenario (a2) a total of 2 cycles lasting 183 and 182 days are completed per year, while in scenario (a3) 3 cycles of 122, 122 and 121 days are completed per year. For all scenarios the bottomhole injection pressure is set at 680 Bars, allowing a safety margin below the fracturing pressure and ensuring miscibility conditions by exceeding the MMP in more than 300 Bars. The injection flowrate and the amount of injection and

soaking days were selected as the optimization variables. The amount of production days per cycle is indirectly optimized as the total cycle days minus injection and soaking days. In this case a custom objective function has been used, defined by the incremental NPV value obtained from incremental oil revenue minus associated taxes, incremental Opex and CO₂ cost. As a result, the ratio of incremental oil vs. total injected CO₂ is maximized. The following values have been assumed for incremental NPV calculations:

- Oil price of 70 \$/bbl, based on last 12-month average Brent price (US EIA, 2018)
- Opex for Vaca Muerta shale oil wells of 7 \$/bbl (YPF, 2018)
- CO₂ purchasing price of \$12,8 /metric tonne (Global CCS Institute, 2018) and no recycling considered
- 12% taxation on gross revenue
- 10% annual discount rate

The injection flowrate was initially set at 150.000 m³ of CO₂ per day. For all three cases, the total number of injection days per year is initially set as 50 days, and the total amount of soaking days as 7. These quantities are evenly distributed depending on the amount of huff n' puff cycles per year. For all evaluated scenarios, the gas injection starts right after the end of historical data, i.e. after 328 days of production, and huff n' puff injection scheme is repeated for ten years. Initially, a stochastic optimization approach was applied, using an evolutionary algorithm in a similar way to the AHM. However, after incorporation of molecular diffusion the increase in simulation time motivated a "step by step" optimization procedure to restrict the scope to a limited number of scenarios. The best case for each evaluated scenario is selected based on the resulting incremental NPV (Δ NPV) compared to the "do nothing" base case. Although a simplified single-fracture model was used for the optimization as mentioned before, all figures, plots and conclusions are presented for a full well case.

Results

Primary Production

A base case was run to estimate the well recovery factor, extending well production during 10 years after the end historical data. The well is controlled by a constant bottomhole pressure of aprox. 200 Bar, equal to the last historical value. The EUR (Expected Ultimate Recovery) for the "do nothing" base case scenario is 56.450 m³ (\approx 356.000 bbl) of oil, leading to a base recovery factor of 7,28%. The steep decline in well flowrate during the first 2 to 3 years implies that 70% of the EUR is produced within the first 5 years. This is consistent with flow behavior in shale or tight reservoirs, where high initial production rapidly declines as pressure disturbance travels within the SRV, and then stabilizes in a lower but relatively constant flowrate once boundaries of the SRV have been reached and a "leaky" boundary is assumed to be established with the un-stimulated matrix.

Cycle Duration

All three scenarios that were evaluated produced an improvement in the well recovery factor, although there is a clear increase in recovery as the cycle becomes shorter. The increase in the EUR after 10 years of treatment for the 1-cycle per year, 2-cycles per year and 3-cycles per year cases is 12,%,

13,5% and 14,2% respectively. The CO₂ utilization ratio per incremental oil bbl confirms a more efficient use of injected gas in the shorter cycles, ranging from 57,9 Mscf/bbl for the 1-cycle per year case to 50,6 Mscf/bbl for the 3-cycles per year case, for the same total amount of injected CO₂ (75 MMm³). In addition to an increase in recovery, the use of shorter stimulation cycles provides a further beneficial effect accelerating well production. This is evidenced in the ΔNPV going from 0,23\$MM in the 1-cycle year case to 0,51MM\$ and 0,63MM\$ for shorter scenarios (figure 8 & table 2). It should be mentioned that all scenarios are considering no-recycling of CO₂, which could improve ΔNPV.

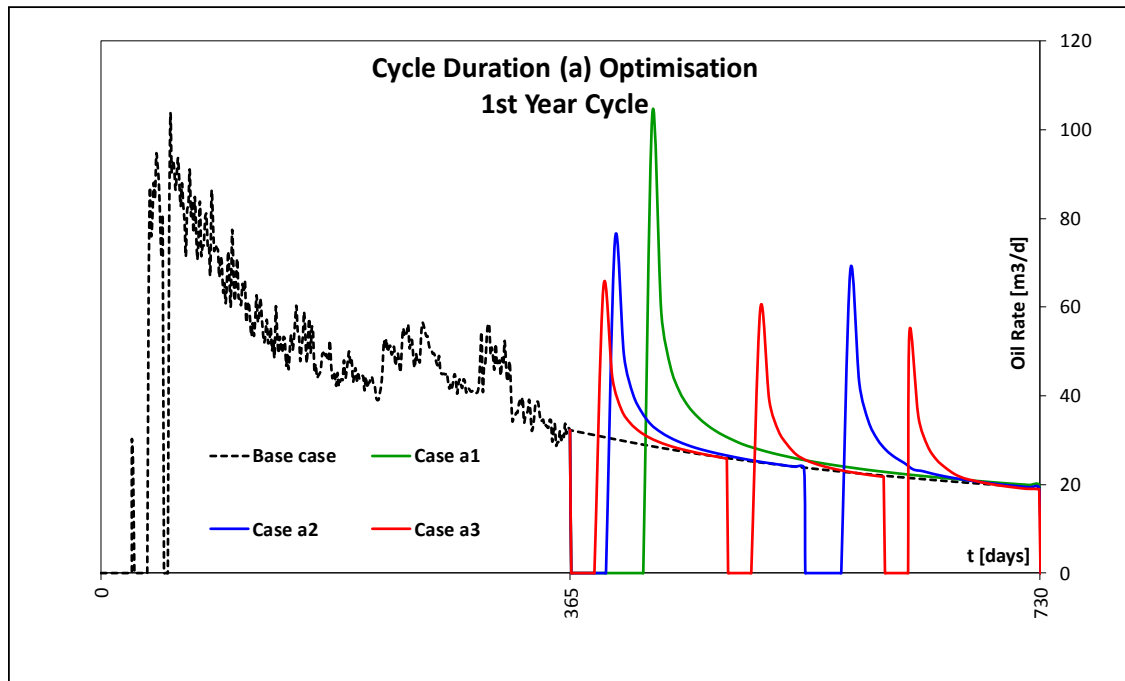


Fig. 8 – Oil rate for cycle duration optimisation case.

Injection Rate

Considering the 3-cycles per year injection scheme with the initial definitions, optimal injection rate was evaluated. An increase of 30% in the injection rate to 195.000 m³/d leads to a further increase in RF, being EUR 15,8% higher than the base case. However, a CO₂ utilization ratio of 59,1 Mscf/bbl indicates a less efficient use of injected gas, confirmed by a reduction of the ΔNPV to 0,49MM\$. On the contrary, a 30% reduction of injection rate to 105.000 m³/d leads to a lower incremental recovery of 12,4% but a more efficient use of CO₂ about 40,6 Mscf/bbl produces an incremental NPV of 0,73MM\$, which is higher than the base injection rate case of 150.000 m³/d. An additional case reducing the flowrate to 75.000m³/d leads to a CO₂ utilization ratio of 33,3 Mscf/bbl, nevertheless the incremental oil recovery drops to 10,8% reducing ΔNPV to 0,72MM\$. Hence, optimal injection rate is found to be 105.000 m³/d (Table 2).

Injection Days

Total injected gas is proportional both to injection rate and injection days per cycle. In agreement with injection rate analysis, an increase from 50 to 65 injection days per year yields a 13,6% increase in RF, however Δ NPV is 0,67MM\$. By reducing the injection days to 35 days per year incremental RF drops to 10,9% but the NPV can be incremented to 0,76MM\$. Further attempt reducing injection days to 30 days produces a lower Δ NPV, and total injection time is set as 35 days per year.

Soaking Days

A reduction in total soaking days from 7 to 5 is detrimental in all aspects: incremental oil falls from 6.391 m³ to 6.346 m³ while Δ NPV is also reduced to 0,75MM\$ whit an increasing ratio of 32,5 Mscf/bbl. On the contrary when extending soaking to 12 days the RF increases by 11,1% and Δ NPV also increases to 0,78MM\$ even though total production time is reduced. CO₂ utilization ratio of 31,9 Mscf/bbl indicates a more efficient process. It is evident that oil-CO₂ dynamics are critical for the definition of optimal soaking time.

Optimal Huff n' Puff Scheme

The optimal scheme (Table 2) has 3 cycles per year with an injection flowrate of 105.000 m³/d, requiring a total of 35 injection days and 12 soaking days per year.

Table 2 - Summary of Huff n' Puff Optimisation Process								
Optimisation Stage	Scenario	Case	Incremental oil [m ³]	RF [%]	RF Increase [%]	Total Gas [MMm ³]	Gas utilisation [Mscf/bbl]	Δ NPV [MM\$]
-	-	Base case	0	7.28%	-	-	-	-
Cycle duration	1 cycle/y	Case a1	7,276	8.19%	12.4%	75	57.9	0.23
	2 cycles/y	Case a2	7,913	8.27%	13.5%	75	53.2	0.51
	3 cycles/y	Case a3	8,314	8.32%	14.2%	75	50.6	0.63
Injection rate	195 Mm ³ /d	Case b1	9,259	8.43%	15.8%	97	59.1	0.49
	172 Mm ³ /d	Case b2	8,854	8.38%	15.1%	86	54.7	0.57
	105 Mm³/d	Case b3	7,260	8.19%	12.4%	52	40.6	0.73
Injection days	75 Mm ³ /d	Case b4	6,316	8.07%	10.8%	37	33.3	0.72
	65 days/y	Case c1	7,939	8.27%	13.6%	68	48.3	0.62
	35 days/y	Case c2	6,391	8.08%	10.9%	37	32.3	0.76
Soaking days	30 days/y	Case c3	5,970	8.03%	10.2%	31	29.6	0.74
	9 days/y	Case d1	6,432	8.08%	11.0%	37	32.1	0.77
	5 days/y	Case d2	6,346	8.07%	10.9%	37	32.5	0.75
	12 days/y	Case d3	6,475	8.09%	11.1%	37	31.9	0.78
	15 days/y	Case d4	6,497	8.09%	11.1%	37	31.8	0.78

Sensitivity to CO₂ Purchasing Price

It can be seen from Figure 9 that there is a direct relationship between total amount of injected CO₂ and RF increase. However, the trend is reverted when considering Incremental NPV. Sensitivity analysis indicates that 10% variation in CO₂ purchasing price will produce in average a 40% variation in incremental NPV. Furthermore, if CO₂ purchasing price is reduced by 25% to 9,6 \$/metric tonne then NPV becomes almost insensitive to total injected CO₂ and options with higher recovery factor become viable (Figure 9).

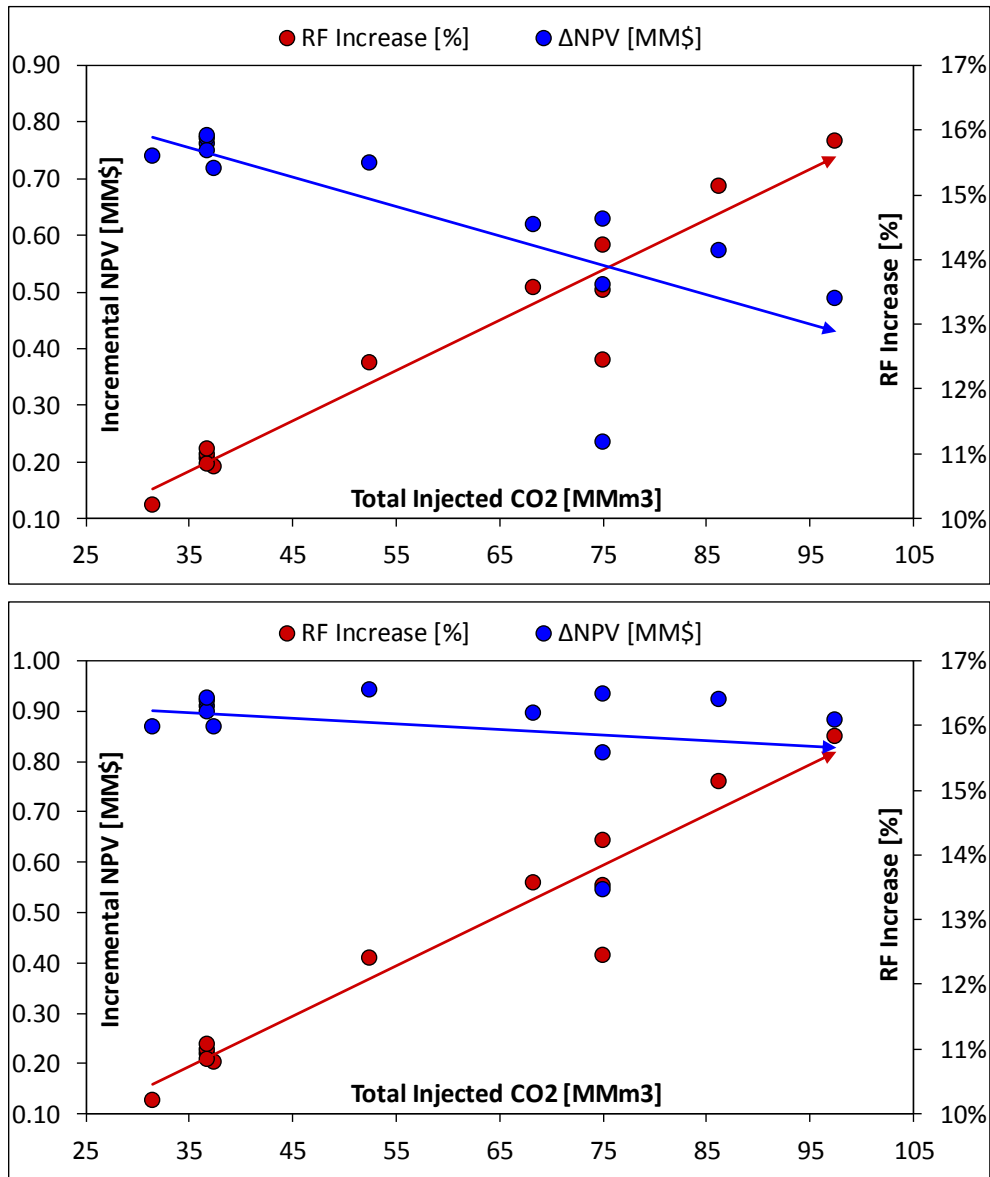


Fig. 9 – RF increase and Incremental NPV vs. Total Injected CO₂ – base CO₂ price (above) and 25% price-reduction (below).

Sensitivity to Gas Composition

Considering the optimal huff n’ puff scheme, pure CO₂ injection gas was replaced by 100% molar C₁, representing DRY GAS case, and by an enriched mixture of light hydrocarbons defined as 70% C₁, 15% C₂, 15% C₃, representing the WET GAS case. Evaluation was limited to a technical approach comparing the increase in RF after 10 years of treatment and ΔNPV was omitted (Figure 10). For the WET GAS case it is interesting to point out that in the medium term the performance surpasses the CO₂ case. Cumulative oil recovery is higher for the WET GAS during the first 68 months of treatment, i.e. the first 17 injection cycles. After that point there is a crossover of the cumulative production curves and the increase in RF for the WET GAS at the end of 10 years.

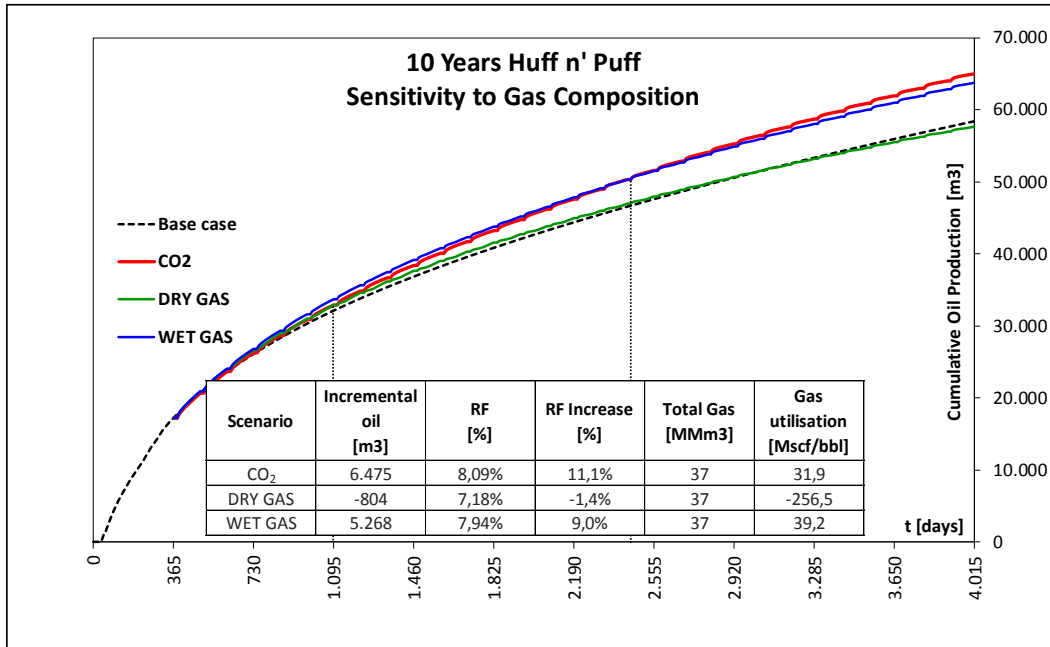


Fig. 10 – Sensitivity Analysis to Injected Gas Composition.

Sensitivity to Molecular Diffusion Coefficients

The incidence of molecular diffusion mechanism in oil recovery has been evaluated varying the diffusion coefficients calculated from Sigmund’s method. For the maximum case where all coefficients are increased by 30%, there is a 26% increase in RF respect to the base coefficients case. Furthermore, the Δ NPV increases by 48% to 1,15MM\$. On the other hand, when coefficients are reduced by 30%, the RF is 29% lower than the case with the base coefficients and there is a 53% reduction in the Δ NPV falling to 0,36MM\$ (Figure 11 and table 3). Molecular diffusion rates represented by the coefficients are clearly very important for the process and inaccurate estimation may lead to gross errors in the calculated recovery.

In a further evaluation omitting molecular diffusion mechanism in the simulation model (Figure 12) it can be seen that cyclic gas injection in the reservoir will result detrimental for oil recovery, regardless the gas being injected. Even though the overall behavior is similar to the previous case where CO₂ yields the highest RF and DRY GAS the lowest, final RF for all three cases is below the base case where no gas is injected. It is clear that in these extremely tight reservoirs where injectivity is restricted by the ultra-low permeability, molecular diffusion providing an additional mass-transport mechanism is critical. This confirms molecular diffusion as a key aspect that should not be omitted when modelling cyclic gas injection in VM oil wells.

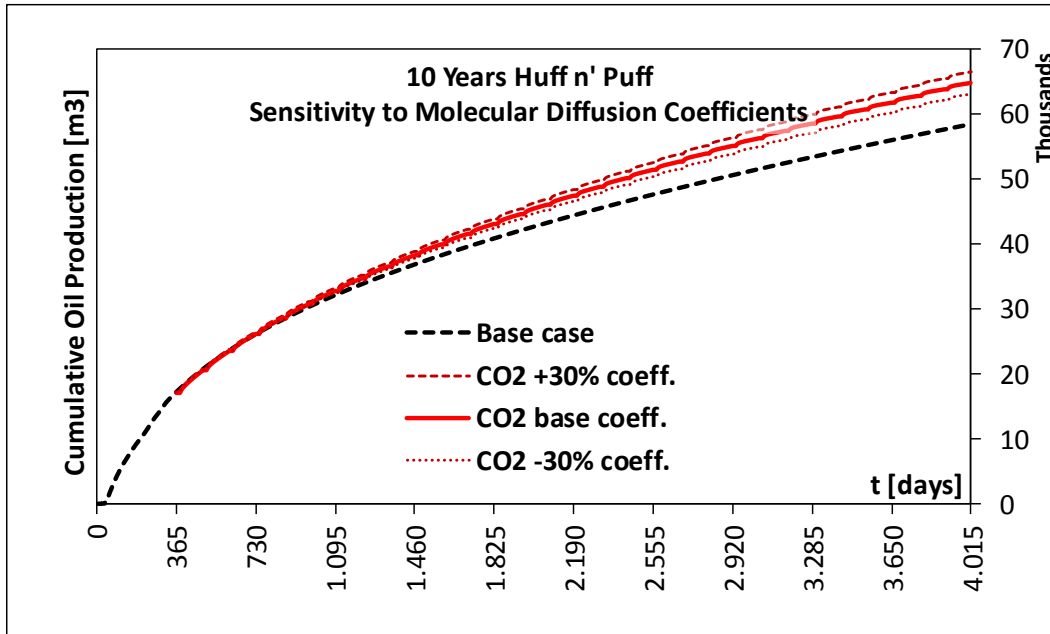


Fig. 11 – Cumulative Oil for CO₂ Assuming Different Molecular Diffusion Coefficients.

Table 3 – Sensitivity Analysis Assuming Different Molecular Diffusion Coefficients				
Scenario	RF Increase [%]	Total Gas [MMm3]	Gas utilisation [Mscf/bbl]	ΔNPV [MM\$]
CO ₂ base coeff.	11.1%	37	31.8	0.78
CO ₂ +30% coeff.	14.0%	37	25.3	1.15
CO ₂ -30% coeff.	7.9%	37	44.4	0.36

CO₂ Effect in Production

Injection of CO₂ at defined operational conditions-i.e. 134° C and around 680 Bars- turns the CO₂, originally in gaseous state, into a supercritical fluid being physically similar to, but not strictly, liquid or gas. As the super critical fluid – for simulation purposes considered to be a gas - is injected into the reservoir at a pressure higher than the MMP, a multiple-contact miscibility process develops between the injected gas phase and the in-situ oil phase. Khabibullin et al. (2017) provided a detailed description of developing mechanisms, which is summarized here. Two elementary physical processes provide the fundamental basis for the phase interaction: the vaporization process, where there is a transition of elements from the liquid phase to the vapor phase, and the condensation process, being the opposite where elements from the vapor phase condense into the liquid phase. These physical processes simultaneously occurring lead to the actual driving mechanisms developing at reservoir: vaporizing gas drive and condensing gas drive. Khabibullin et al. (2017), also mention a third mechanism, the vaporizing/condensing gas drive. Forward and backward contacts between interacting phases will develop either in vaporizing and condensing drives, but producing different

effects: while forward contacts in vaporising drive will develop a miscibility front, the same contacts in a condensing drive will derive in the creation of a dry gas bank; on the other hand, backward contacts in a vaporising drive case will control the residual oil saturation, while in a condensing case the miscibility zone will develop at the trail of the contact between oil and gas phases.

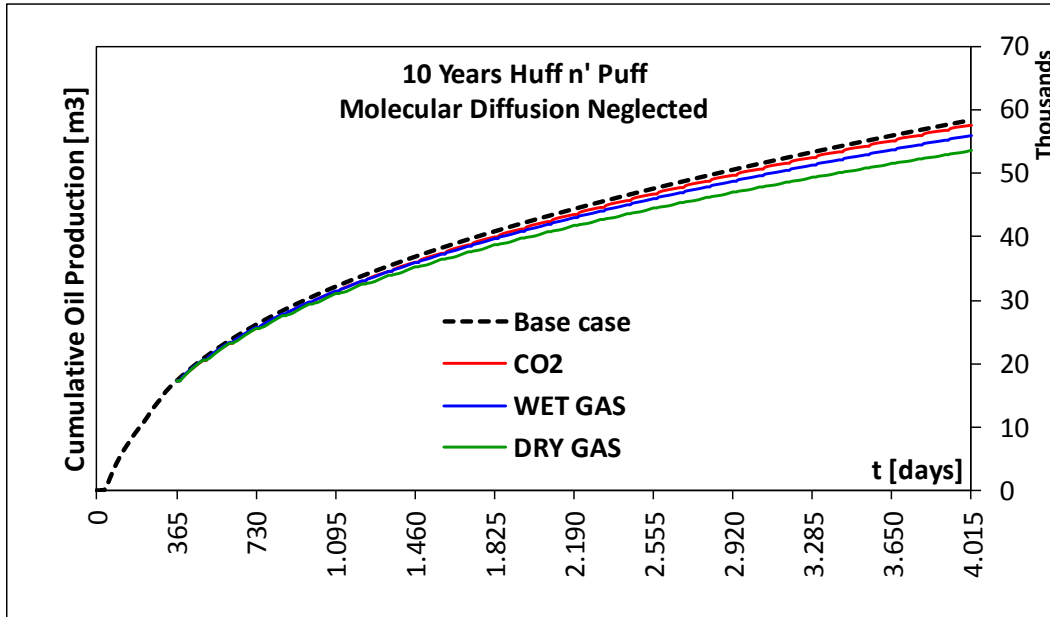


Fig. 12 – Cumulative Oil for CO₂, WET GAS & DRY GAS Cases Neglecting Molecular Diffusion.

For a CO₂ miscible case, vaporizing drive is assumed to dominate the process, developing a miscible area where the CO₂ molar fraction in oil phase increases. As a result of the increase in CO₂ molar fraction, a concentration gradient will develop within the oil phase, “triggering” the molecular diffusion mechanism. That mechanism will transport the CO₂ from an area of higher concentration – the miscible zone within the fractures, or at the fracture/SRV interface- to an area of lower concentration – the “original” oil, deep into the SRV-. An increase in CO₂ molar fraction in the oil phase will derive in further effects affecting oil recovery:

- As oil composition gradually becomes richer in CO₂, there is a sustained **reduction in the viscosity of the oil phase**. The difference with the base case is presented in Figure 13, being the effect more noticeable approaching the miscible zone, near the hydraulic fractures. Even considering that viscosity of VM oil is relatively low, a further reduction will lead to an increase in the mobility of the oil phase $M_o = K \cdot K_{roi} / \mu_{oil}$, leading in turn to a higher flowrate per volume of rock for the same pressure drop.
- A secondary effect caused by increasing CO₂ molar fraction in the oil phase is given by an increase in the volume occupied by the same mass of oil, an effect known as “**oil swelling**”. As a result of this expansion process, oil droplets trapped in very small pores may result expelled towards larger pores being then able to flow towards the fractures and the wellbore, therefore increasing recovery.

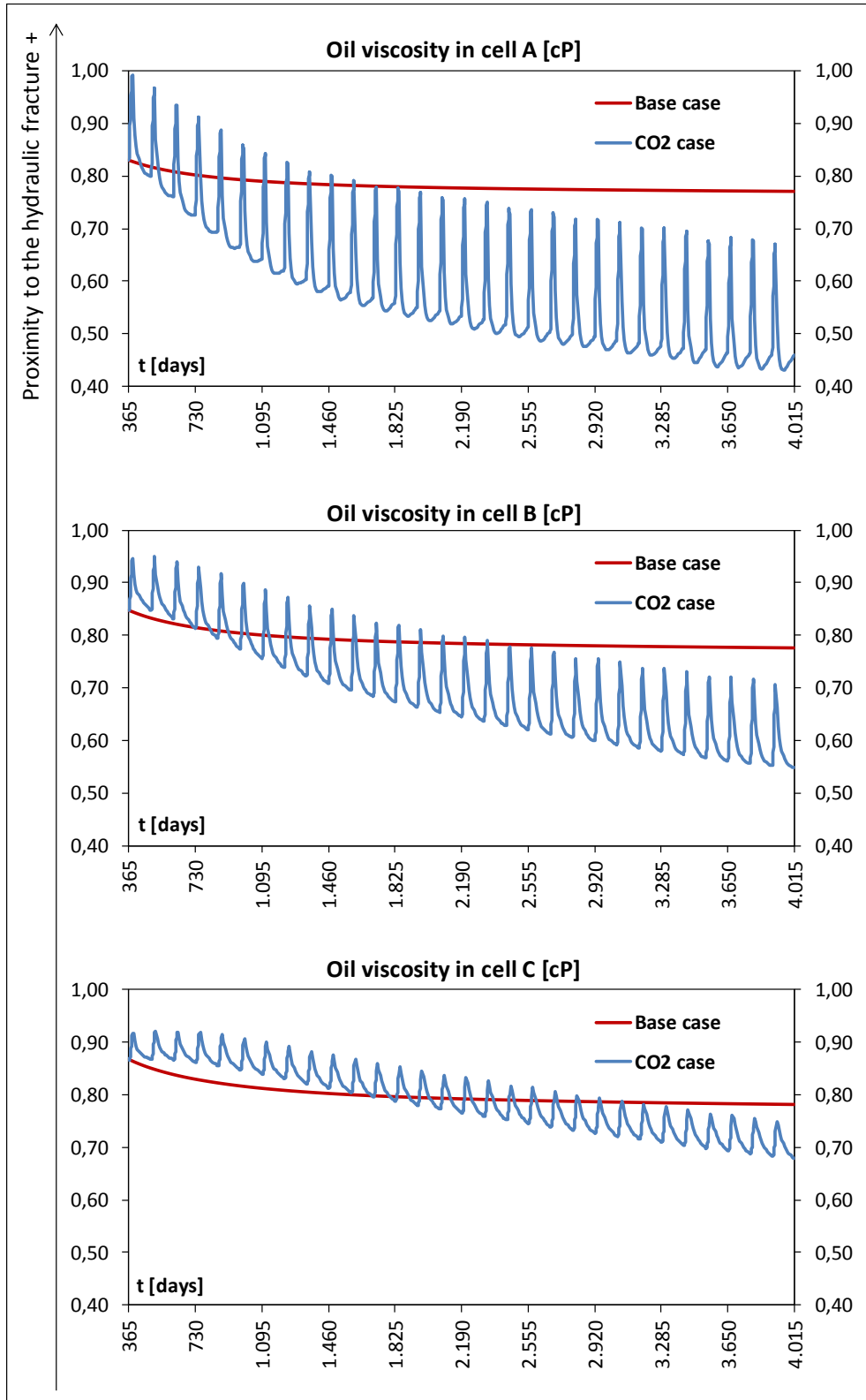


Fig. 13 – Oil viscosity vs. time for base case and cyclic CO₂ injection case for cells A, B and C, being A the closest to the miscible zone.

An additional consequence of gas injection into the reservoir comes with the consequent *re-pressurization* of the SRV surrounding the hydraulic fractures. It is well known that rock compaction developing as pore pressure decreases will negatively affect the effective permeability of the formation and the fractured zone in shale reservoirs. An increase in pressure will counteract the effect, “expanding” at least temporarily, the matrix pores and small fractures providing the flow path in the SRV and the hydraulic fracture in a reversible process. Consequently, a further increase in oil phase mobility M_o should be expected, this time as a result of an increase in K . The effect, modelled using pressure-dependent rock compaction tables, can be seen in Figure 14, where transmissibility multipliers are presented for the same time step in the base case and huff n’ puff scenarios.

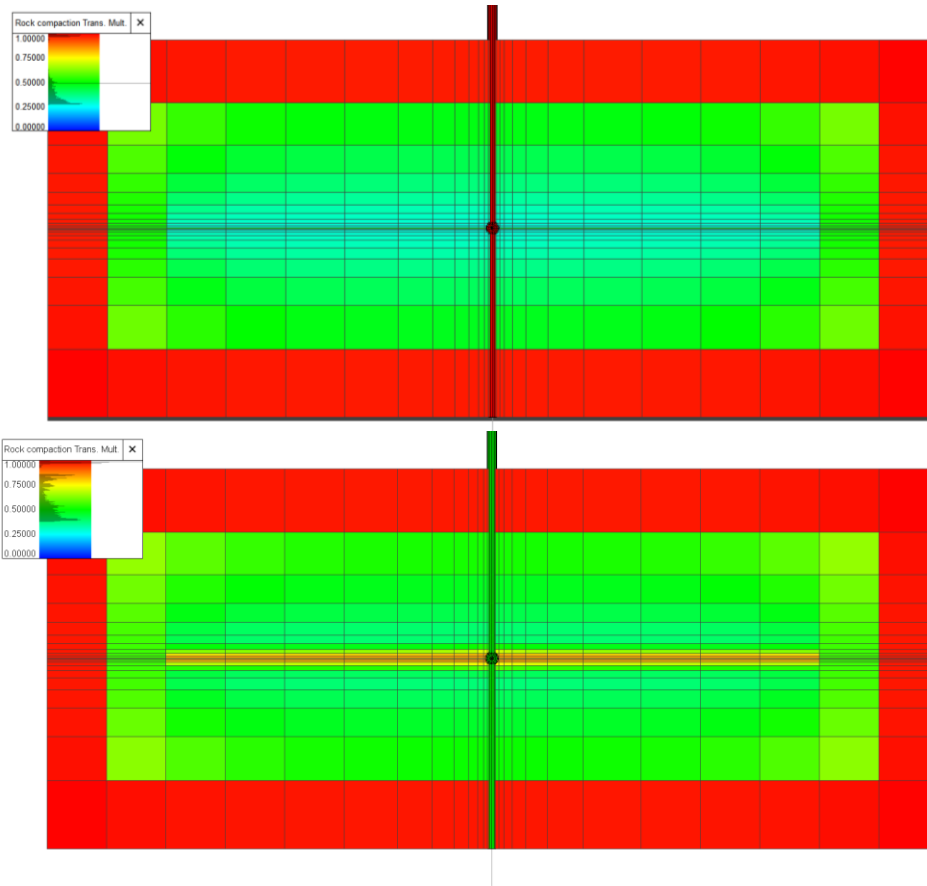


Fig. 13 – Transmissibility multipliers top view for the base case (above) and CO₂ huff n’ puff case (below), for the same time step.

Discussion

It can be concluded from this study that CO₂ cyclic injection can offer a potential alternative for increasing primary oil recovery in VM horizontal wells. For a situation with the characteristics considered in the present model, this study suggests that up to 16% increase in RF could be technically possible after 10 years of treatment. When including economic considerations in the optimization analysis, a maximum incremental NPV of 0,78MM\$ with an RF increase of 11,1% from the original

production can be achieved. Several conclusions regarding operational conditions can be extracted from the optimization process:

- Shorter huff n' puff schemes with 3 cycles per year are preferred, providing both higher final incremental recovery and acceleration of the production profile. It is worth emphasizing that the same amount of injected gas distributed in shorter periods produces better results. This seems to confirm a certain "capacity" of the reservoir fluid to assimilate the injected CO₂, which stresses the importance of accurate diffusion rates estimation.
- Increasing CO₂ injection rates lead to an increase in oil recovery. However, above approximately 100.000 m³/d the efficiency of the process represented by the CO₂ utilization ratio (Mscf of CO₂/incremental oil bbl) decreases and incremental NPV starts to decrease.
- As with injection rate, extending the injection period will lead to higher oil recoveries. However, the maximum number of days for optimizing ΔNPV at current conditions is 35 days per year.
- A reduction of soaking days may have detrimental effects in recovery and incremental NPV. On the contrary, it has been seen that an increase in soaking days at the expense of production days will increase recovery and ΔNPV. This is assumed to be related to the CO₂ diffusion, giving more time to the CO₂ to penetrate the SRV. The maximum number of soaking days before deferred production overcomes benefits from soaking time is 12 days per year.
- Cyclic injection of a "wet gas" mixture also produces positive results. In the mid-term the wet gas surpasses the performance of CO₂ injection but after approx. 6 years there is a crossover. Results are comparable in the long term, with an incremental RF of 9% for the wet gas from the base case. On the contrary, injection of pure C₁ maintaining the same injection scheme reduces RF in the long term (-1,4% from the base case).
- The rate at which the molecular diffusion mechanism develops in the reservoir has a significant impact in the results of the simulation. A 30% change in the diffusion coefficients will have similar impact in the RF, although the change in ΔNPV may be as high as 50%. Omission of molecular diffusion mechanism will produce negative results, regardless the injected gas composition. Therefore, both inclusion of molecular diffusion and accurate estimation of diffusion rates is critical for successful modeling of the huff n' puff process.

Suggestions for Future Work

- It has been reported that some areas in VM present a higher degree of natural fracturing (Licitra et al., 2015), which could allow deeper penetration of CO₂ into the matrix. It is recommended for further evaluations of CO₂ injection to select a candidate well where natural fractures are expected to be active and include this feature in the model.
- Cyclic gas injection has been evaluated in a relatively early stage of the well's lifecycle. It is recommended for future studies to investigate the effect of miscible gas injection in a depleted scenario, i.e. where a significant saturation of free gas is expected in the SRV as a result of prolonged production below saturation pressure. A volume of compressible free gas may allow a deeper penetration of CO₂ during the injection phase, and through molecular diffusion it could be possible to reach the oil at or near the un-stimulated matrix.

- CO₂ interaction with reservoir oil is a key aspect of the process. For further modeling efforts, it is highly recommended to carry out swelling test as well as Slim Tube, RBA or VIFT lab tests to properly calibrate EOS and provide more accurate values for the MMP.
- Molecular diffusion coefficients have a major impact in the success of this methodology and in optimization of the injection cycle. Laboratory tests providing empirical data regarding real diffusion rates for CO₂ and VM oil in shale samples is highly recommended before any pilot test in the field.
- As mentioned in the optimization section, a step by step approach was applied to select optimal operational parameters due to limited computational capacity. If possible, a stochastic optimization approach using an optimization algorithm is recommended to determine the best combination of operational parameters.
- A single porosity compositional model was used, aiming to balance the accuracy of the model and computational capacity available. As stated in introduction section, dual-porosity compositional models have been commonly applied for modeling CO₂ injection in shales. The approach proposed by Kurtoglu (2013), where both dual-porosity is used to model natural fractures/stimulated volume and discrete hydraulic fractures are included as the connection of the reservoir to the wellbore, is recommended to evaluate the process.
- The study evidences high NPV sensitivity to CO₂ purchasing price, currently relying on public data from projects in US/Canada. A feasibility/economic study to evaluate installation cost of an anthropogenic CO₂ capture plant at Loma Campana Thermal Power Station could shed some light on realistic cost estimation for local CO₂ supply. Furthermore, ensuring low-cost local supply may significantly increase project's NPV by making viable the options with higher technical recovery.

Aknowledgements

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References

- Alfarge, D., Wei, M., & Bai, B. (2017, August). “*Feasibility of CO₂-EOR in Shale-Oil Reservoirs: Numerical Simulation Study and Pilot Tests*. *Carbon Management Technology Conference*.” <https://www.onepetro.org/conference-paper/CMTC-485111-MS>
- Alharthy, N., Teklu, T., Kazemi, H., Graves, R., Hawthorne, S., Braunberger, J., & Kurtoglu, B. (2015, September 28). “*Enhanced Oil Recovery in Liquid-Rich Shale Reservoirs: Laboratory to Field*.” Society of Petroleum Engineers. <https://www.onepetro.org/journal-paper/SPE-175034-PA>
- Balasubramanian, S., Chen, P., Bose, S., Alzahabi, A., & Thakur, G. C. (2018, April 30). “*Recent Advances in Enhanced Oil Recovery Technologies for Unconventional Oil Reservoirs*.” Offshore Technology Conference. <https://www.onepetro.org/conference-paper/OTC-28973-MS>
- Cuervo, S., Lombardo, E., Vallejo, D., Crousse, L., Hernandez, C., & Mosse, L. (2016, August 1). “*Towards a Simplified Petrophysical Model for the Vaca Muerta Formation*.” Unconventional Resources Technology Conference. <https://www.onepetro.org/conference-paper/URTEC-2437257-MS>
- EIA (June, 2013). “*Technically Recoverable Shale Oil and Shale Gas Resources: An Assessment of 137 Shale Formations in 41 Countries Outside the United States*”, Washington, DC: US Department of Energy. <https://www.eia.gov/analysis/studies/worldshalegas/pdf/overview.pdf>
- Emera, M. K., and Sarma, H. K. (2005). “*Use of genetic algorithm to estimate CO₂-oil minimum miscibility pressure—a key parameter in design of CO₂ miscible flood*.” *Journal of Petroleum Science and Engineering*, vol. 46, no. 1-2, pp. 37–52. <https://www.sciencedirect.com/science/article/pii/S0920410504001524>
- Fernandez Baessich, M., & Berrios, C. V. (2012, January 1). “*Integrated Dynamic Flow Analysis To Characterize an Unconventional Reservoir in Argentina: The Loma La Lata Case*”. Society of Petroleum Engineers. <https://www.onepetro.org/conference-paper/SPE-156163-MS>
- Global CCS Institute (2018, October). “*The CO₂ market*”. <https://hub.globalccsinstitute.com/publications/accelerating-uptake-ccs-industrial-use-captured-carbon-dioxide/2-co2-market>
- IHS Energy (June 2016). “*CO₂ EOR Potential in North Dakota—Challenges, policy solutions, and contribution to economy and environment report*”. <https://www.legis.nd.gov/files/committees/64-2014%20appendices/IHS%20Energy%20-%20Final%20Report.pdf>
- Jia, B., Tsau, J.-S., & Barati, R. (2017, June 12). “*Role of Molecular Diffusion in Heterogeneous Shale Reservoirs During CO₂ Huff-n-puff*.” Society of Petroleum Engineers. <https://www.onepetro.org.ezproxy1.hw.ac.uk/conference-paper/SPE-185797-MS>
- Khabibullin, R., Emadi, A., Abu Grin Z., Oskui R., Alkan H., Grivet M., Elgridi K., (2017) “*Investigation of CO₂ Application for Enhanced Oil Recovery in a North African Field - A New Approach to EOS Development*.” 19th European Symposium on Improved Oil Recovery – EAGE. https://www.researchgate.net/publication/316515853_Investigation_of_CO2_Application_for_Enhanced_Oil_Recovery_in_a_North_African_Field_A_New_Approach_to_EOS_Development
- Kim, T. H., Cho, J., & Lee, K. S. (2017, June 12). “*Modeling of CO₂ Flooding and Huff and Puff Considering Molecular Diffusion and Stress-Dependent Deformation in Tight Oil Reservoir*”. Society of Petroleum Engineers. <https://www.onepetro.org/conference-paper/SPE-185783-MS>
- Kurtoglu, B., (2013). “*Integrated Reservoir Characterization and Modeling in Support fo Enhanced Oil Recovery for Bakken*”, PhD thesis. Colorado School of Mines. USA.
- Licitra, D., Lovrincevich, E., Vittore, F., Quiroga, J., Oviedo, P., Montoya, V., Coleen S., Monti, L. (2015, July 20). “*Sweet Spots in Vaca Muerta: Integration of Subsurface and Production Data in*

Loma Campana Shale Development, Argentina". Unconventional Resources Technology Conference. <https://www.onepetro.org/conference-paper/URTEC-2153944-MS>

Manestar, G. J., & Thompson, A. (2017, May 17). "Dual Porosity Modeling for Shale Gas Wells in the Vaca Muerta Formation". Society of Petroleum Engineers. <https://www.onepetro.org/conference-paper/SPE-185548-MS>

Phi, T., & Schechter, D. (2017, February 15). "CO₂ EOR Simulation in Unconventional Liquid Reservoirs: An Eagle Ford Case Study". Society of Petroleum Engineers. <https://www.onepetro.org/conference-paper/SPE-185034-MS>

Rassenfoss, S. (October 2017). "Shale EOR Works, But Will It Make a Difference?" Journal of Petroleum Technology. <https://www.spe.org/en/jpt/jpt-article-detail/?art=3391>

Sagasti, G., Ortiz, A., Hryb, D., Foster, M., &Lazzari, V. (2014, August 25). "Understanding Geological Heterogeneity to Customize Field Development: An Example From the VacaMuerta Unconventional Play, Argentina". Unconventional Resources Technology Conference. <https://www.onepetro.org/conference-paper/URTEC-1923357-MS>

Sahni, V., & Liu, S. (2018, August 9). "Miscible EOR Process Assessment for Unconventional Reservoirs: Understanding Key Mechanisms for Optimal Field Test Design". Unconventional Resources Technology Conference. <https://www.onepetro.org.ezproxy1.hw.ac.uk/conference-paper/URTEC-2870010-MS>

Sheng, J. J. (2017). "Critical review of field EOR projects in shale and tight reservoirs", Journal of Petroleum Science and Engineering, Volume 159, Pages 654-665, ISSN 0920-4105. <https://www.sciencedirect.com/science/article/pii/S0920410517307283?via%3Dihub>

Shen, Z., & Sheng, J. J. (2016, April 11). "Experimental Study of Asphaltene Aggregation during CO₂ and CH₄ Injection in Shale Oil Reservoirs". Society of Petroleum Engineers. <https://www.onepetro.org/conference-paper/SPE-179675-MS>

Sigmund, P. M. (1976, July 1). "Prediction of Molecular Diffusion At Reservoir Conditions. Part II - Estimating the Effects Of Molecular Diffusion And Convective Mixing In Multicomponent Systems". Petroleum Society of Canada. <https://www.onepetro.org/journal-paper/PETSOC-76-03-07>

Sorensen J., Hawthorne S., Smith S., Braunberger J., Liu G., Klenner R., Botnen L., Steadman E., Harju J., Doll T., (2014, June). "SUBTASK 1.10 – CO₂ STORAGE AND ENHANCED BAKKEN RECOVERY RESEARCH PROGRAM, Final Report". National Energy Technology Laboratory. US Department of Energy. <https://www.undeerc.org/bakken/PDFs/JAS-Subtask%201.10%20Revised-Jun14.pdf>

Suarez, M., Vega Velasquez, L., Monti, L. J., & Thompson, A. R. (2013, April 10). "Modeling Vertical Multifractured Wells in Vaca Muerta Shale Oil Play, Argentina". Society of Petroleum Engineers. <https://www.onepetro.org/conference-paper/SPE-164537-MS>

Tuero, F., Crotti M, M., & Labayen, I. (2017, May 17). "Water Imbibition EOR Proposal for Shale Oil Scenarios". Society of Petroleum Engineers. <https://www.onepetro.org/conference-paper/SPE-185560-MS>

U.S. Energy Information Administration. "Brent Spot Price FOB (\$/bbl) report to 09/2018". <https://www.eia.gov/dnav/pet/hist/LeafHandler.ashx?n=pet&s=rbrte&f=w>

Weaver, C.E., (1931). "Paleontology of the Jurassic and Cretaceous of West Central Argentina". Memoir University of Washington 1, 469 p., Seattle.

YPF (2018, October). "1ST Quarter 2018, Earnings Webcast". <https://www.ypf.com/inversoresaccionistas/Documents/YPF-Q1-2018-Earnings-Webcast-Presentation.pdf>

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APPENDIX N° 1: Calculation of Molecular Diffusion Coefficients

Binary diffusion coefficients have been used to calculate effective diffusion coefficients D_{ik} for each component i in the hydrocarbon multicomponent system k :

$$D_{ik} = \frac{1 - y_{ik}}{\sum_{j \neq i} y_{ik} D_{ij}^{-1}}$$

Where y_{ik} is the molar fraction of each component in the multicomponent system and D_{ij} is the binary diffusion coefficient, obtained from Sigmund correlation (Sigmund, 1976):

$$D_{ij} = \frac{\rho_k^0 D_{ij}^0}{\rho_k} (0.99589 + 0.096016 \rho_{kr} - 0.22035 \rho_{kr}^2 + 0.032874 \rho_{kr}^3)$$

Being ρ_k the mixture density, ρ_{kr} the reduced molar mixture density and $\rho_k^0 D_{ij}^0$ the 0-pressure density diffusion product, respectively obtained from:

$$\rho_{kr} = \rho_k \left(\frac{\sum_{i=1}^n y_{ik} v_{ci}^{5/3}}{\sum_{i=1}^n y_{ik} v_{ci}^{2/3}} \right)$$

$$\rho_k^0 D_{ij}^0 = \frac{0.000022648 \left(\frac{1}{M_i} + \frac{1}{M_j} \right)^{0.5}}{\sigma_{ij}^2 \Omega_{ij}} T^{0.5}$$

Where M is the molar fraction, T is temperature and v_{ci} is the critical component molar volume. Furthermore, characteristic length σ_{ij}^2 can be obtained from:

$$\sigma_{ij} = \frac{(\sigma_i + \sigma_j)}{2}$$

$$\sigma_i = (2.3551 - 0.087 \omega_i) \left(\frac{T_{ci}}{P_{ci}} \right)^{1/3}$$

and the probability of binary molecular interaction can be obtained from Lennard-Jones model:

$$\Omega_{ij} = \frac{1.06036}{T_{ij}^{0.1561}} + \frac{0.193}{\exp(0.47635 T_{ij})} + \frac{1.03587}{\exp(1.52996 T_{ij})} + \frac{1.76474}{\exp(3.89411 T_{ij})}$$

Being

$$T_{ij} = \frac{K_B}{\varepsilon_{ij}}$$

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j}$$

$$\varepsilon_i = K_B (0.7915 + 0.1963 \omega_i) T_{ci}$$

Where T_{ci} & P_{ci} are critical temperature & pressure, K_B is Boltzmann constant and ω_i is acentric factor.