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# Discovery Science of Hydraulic Fracturing and Shale Fundamentals

Mohamed Mehana\*<sup>1</sup>, Javier E. Santos<sup>1,2</sup>, Chelsea Neil<sup>1</sup>, Matthew R. Sweeney<sup>1</sup>, Jeffery Hyman<sup>1</sup>, Satish Karra<sup>1</sup>, Hongwu Xu<sup>1</sup>, Qinjun Kang<sup>1</sup>, James William Carey<sup>1</sup>, George Guthrie<sup>1</sup> and Hari Viswanathan<sup>1</sup>, 1. Los Alamos National Lab, 2. University of Texas at Austin.

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### **Abstract**

Hydrocarbon production from shale reservoirs is inherently inefficient and challenging since these are low permeability plays. In addition, there is a limited understanding of the fundamentals and the controlling mechanisms, further complicating how to optimize these plays. Herein, we summarize our past and current efforts to reveal the shale fundamentals and devise development strategies to enhance extraction efficiency with a minimal environmental footprint. Integrating these fundamentals with machine learning, we outline a pathway to improve the predictive power of our models, enhancing the forecast quality of production, thereby improving the economics of operations in unconventional reservoirs. For instance, we have developed science-informed workflows and platforms for optimizing pressure-drawdown at a site, which allow operators to make reservoir-management decisions that optimize recovery in consideration of future production. Recently, our work relies on the hybridization of physics-based prediction and machine learning, whereby accurate synthetic data (combined with available site data) can enable the application of machine learning methods for rapid forecasting and optimization. Consequently, the workflow and platform are readily extendable to operations at other sites, plays, and basins.

### Introduction

Shale reservoirs have redefined the energy landscape of the world (Melikoglu, 2014). Shale reservoirs currently contribute to 70% of U.S. natural gas production and 60% of U.S. oil production (Perrin & Geary, 2019). However, these reservoirs possess unique characteristics that entail custom-designed development plans (Mehana & El-monier, 2016). Currently, we recover less than 10% of the hydrocarbons in place from these low permeability plays with the most efficient development plan (Alharthy et al., 2015). This low efficiency is also due to the limited understanding of shale characteristics' effects on the fluid properties and transport through porous media. Therefore, a fundamental understanding and quantification of these effects are required for devising better development plans to improve the current recovery factors (Middleton et al., 2017).

Shale reservoirs are governed by physical processes that differ from those that dominate conventional reservoirs (Sondergeld et al., 2010). Whereas the porous flow dominates the latter described adequately by Darcy's law, the former is dominated by flow in fractures and tight matrix (Hyman et al., 2015). Consequently, the strategies and tools honed over decades for conventional reservoirs do not readily transfer to unconventional reservoirs, inhibiting the ability to optimize reservoir management and, hence, to

maximize recovery (Mehana et al., 2021a; Mehana et al., 2021b). Consequently, it is commonly accepted that shale reservoirs have poor recovery efficiencies (Seales et al., 2017).

The unique characteristics of shale include the abundance of the nanopores and the heterogeneous mineralogy (Clarkson et al., 2013; Ross & Bustin, 2009). Nanoconfinement of fluids brings a multitude of unconventional physicochemical processes (Chen et al., 2015b; O'Malley et al., 2016; Riewchotisakul & Akkutlu, 2015). For instance, confined fluids' phase behavior and properties significantly deviate from the bulk behavior (Liu & Zhang, 2019). In addition, adsorption is the primary storage mechanism for hydrocarbons, unlike conventional reservoirs (Ambrose et al., 2010). Notably, shale matrix, especially organic pores, also experience a certain degree of deformation, affecting their productivity (Neil et al., 2020b).

Shale is a fine-grained clastic sedimentary rock composed of a mixture of quartz, clay, and carbonate minerals (Rickman et al., 2008). However, the percentages of these minerals differ among shale plays. For instance, Eagle Ford is a carbonate-rich shale, while Barnett is a quartz-rich play (Chermak & Schreiber, 2014). Apart from the heterogeneous mineral composition, the total organic content (TOC) of shale formations adds one degree of complexity to these reservoirs' characterization (Curtis et al., 2012). Historically, this content is the hydrocarbon source for conventional reservoirs. Contrary to other minerals, organic matter does not have a definite chemical structure. However, the organic matter's maturity critically determines the organic pores' main characteristics and fluids therein.

The heterogeneous mineral composition and the thermal maturity of shale pores explain the mixed wettability nature of shale. Besides being a critical property for transport, wettability also affects the fluid distribution in the pores. Uniquely, shale formations usually have a complex natural fracture system that plays a significant role in hydraulic fracture operations' success.

Shale reservoirs have become a significant energy resource. Nevertheless, they are challenging to develop efficiently because of our current limited understanding of their controlling mechanisms. In this article, we summarize our main projects and contributions to further our knowledge of shale reservoirs. **Figure 1** categorizes our projects into fundamental projects targeting the matrix, fractures, and simulations of their phenomena and machine-learning projects relying on the physics derived from the fundamental ones.

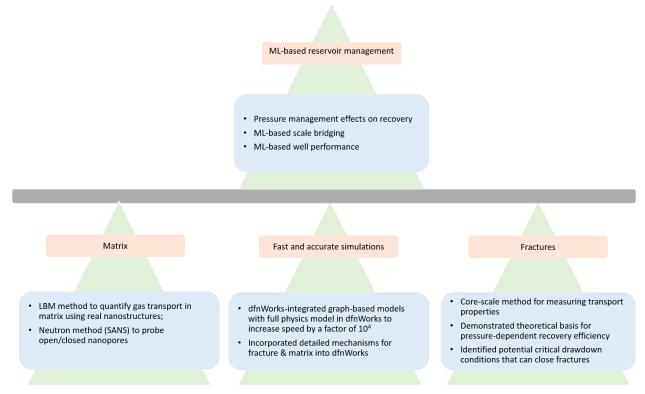


Figure 1. Schematic diagram showing R&D pieces needed to develop the science base and toolsets for science-informed machine learning to support a fractured shale's hydrocarbon recovery operation.

Shale formations have redefined the world's energy landscape and provide possible geological storage for carbon dioxide. Herein, we summarize our main contributions to reveal the fundamentals of shale formations and develop efficient numerical models to better control and optimize them. We organized the rest of this article as follows: the matrix processes section discusses the main nanopores processes, the hydraulic fracturing section discusses the experimental and modeling results about fracture propagation, the science-informed machine learning section summarizes our work to accelerate high-fidelity simulation and scale-bridging, and finally, the shale enhanced oil recovery and CO<sub>2</sub> sequestration briefly discusses our modeling and experimental results in this regard.

### **Matrix Processes**

Traditionally, shale formations are considered either a source rock or a reservoir seal, mostly because of their ultralow (nanoDarcy) permeability and the abundance of nanopores. Developing these formations as reservoirs would necessitate a fundamental understanding of the anomalous phenomena controlling the fluid behavior in the matrix pores. In essence, fluids confined in these pores usually behave differently than larger conventional pores, as the fluid/solid interactions dominate the fluid behavior in those nanopores. Under these conditions, the continuum assumption of the fluid phase is usually violated. As a result, simulating fluid flow through shales with a conventional reservoir simulator may lead to inaccurate results leading to predictions of key quantities of interest such as permeability that can be incorrect by several orders of magnitude (Chen et al., 2015a). Consequently, the standard thermodynamic principles are not applicable at these conditions, which requires various studies to reveal the physics of confined fluids.

Slippage and adsorption are critical surface phenomena whose effects are magnified under confinement. Wang et al. (2016) used the Lattice Boltzmann method (LBM) to simulate a homogenous shale matrix considering both the slippage and adsorption effects on the fluid transport. They observed that the slippage effect is more substantial than the adsorption effect at the lower pressures, leading to higher apparent permeability than intrinsic permeability. On the other hand, the slippage effect is weaker than adsorption at

higher pressures, resulting in apparent permeability lower than intrinsic permeability at higher pressures. In addition, they highlighted the impact of surface and Knudsen diffusion on the apparent permeability, as shown in **Figure 2**. Both surface and Knudsen diffusion contributions to the fluid transport are magnified at low pressures where the apparent permeability is two orders of magnitude higher. Conversely, these contributions are reduced at higher pressures. In addition, they found that surface diffusion is highly promoted for pores less than 20 nm.

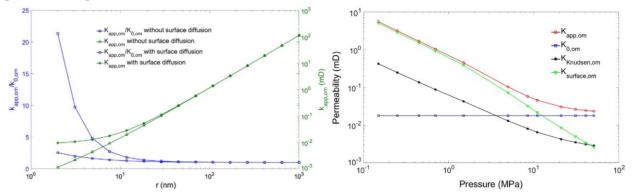


Figure 2. The contribution of surface and Knudsen diffusion to the apparent permeability for different pore radiuses (the left,  $P_{in} = 22$  MPa and  $P_{out} = 20$  MPa) and pressures (the right, The average pore radius, r = 2 nm, and standard deviation = 0.25 nm.) (Wang et al., 2016).

Observation of fluid behavior within the matrix using experimental methods is challenging due to the small size of shale nanopores. Experimental techniques, such as optical microscopy and X-ray/neutron micro-tomographic imaging, lack the necessary resolution to infer structures and properties of nanopores (Yang et al., 2019). Furthermore, although electron microscopic methods can resolve nanoscale features (Yoon & Dewers, 2013), they are challenging to combine with in situ environmental cells containing fluids. Recently, a research team at Los Alamos National Lab (LANL) has made significant inroads to address this problem using small-angle neutron scattering (SANS) combined with an *in situ* pressure cell to provide experimental data over relevant length scales and environmental conditions (Hielm et al., 2018; Neil et al., 2020a; Neil et al., 2020b). SANS provides in situ measurements of the relevant structures and properties of geomaterials, including the unique capability to probe both open and closed pores and pores smaller than the typical probing molecules used for mercury intrusion or gas absorption (Xu, 2020). Employing SANS, the team revealed key new insights into the behavior of pressurized fluid within shale nanopores, including water accessibility differences between clay- and carbonate-rich shale nanopores (Neil et al., 2020a) and trapping of methane gas in shale nanopores due to kerogen deformation (Neil et al., 2020b).

Matrix processes are complex, which necessitates integrating multiple techniques to reveal the main controlling mechanisms. One example was integrating experiments and molecular simulation to quantify the confinement effects on the methane transport in shale pores (Neil et al., 2020b). Neil et al. (2020b) highlighted the significance of pressure management to optimize hydrocarbon recovery. Basically, they found that producing aggressively with large pressure gradients can close off matrix pores, entrapping hydrocarbons and reducing production as shown in **Figure 3**. In addition, they reported a reduction of the diffusion coefficients under confinement.

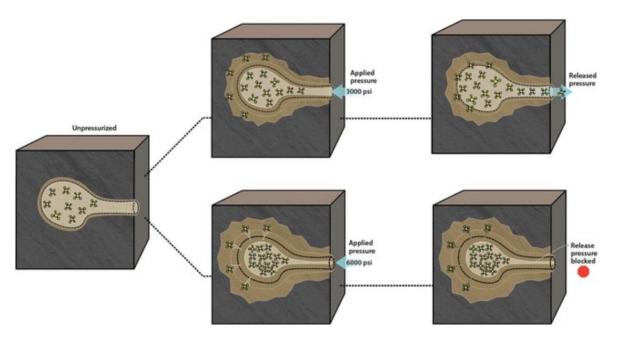


Figure 3. The schematic depicts the pressure cycling on the matrix deformation and fluid retention (Neil et al., 2020a). First, the methane is injected into the shale samples at a pressure of 3000 psi for the upper branch, and then the fluid is produced at ambient conditions. On the other hand, the fluid is injected at 6000 psi in the lower branch. More retention is observed for the higher pressure cycles, mostly because of the organic pores' collapse.

# **Hydraulic Fracturing**

Hydraulic fracturing is a stimulating technique that has been used since the 1950s to bypass the near-wellbore damage or accelerate the hydrocarbon recovery from conventional formations. However, in shale, hydraulic fracturing is a completion technique needed to create the fracture network artificially. In essence, the fracturing operation entails pumping the fracturing fluid at a pressure higher than the minimum horizontal stress. Conceptually, the procedure does not differ from conventional or unconventional formations. However, the propagation of the fracture significantly varies depending on the formation type.

Given the shale characteristics, the fracture topography patterns differ from the conventional formations and depend on the failure mode and the bedding layers' orientation. Carey et al. (2015) observed that when the shear loading is parallel to the shale beddings, it leads to a better peak permeability of 900 md, 30 times higher than what was achieved with the load perpendicular to the beddings as shown in **Figure 4**. In addition, they identified the activation of natural fractures as the primary source of permeability enhancement. They extended their scope to account for the impact of stress cycling on permeability (Carey et al., 2017). Naturally, hydrocarbon reservoirs' development entails several stressing cycles during the fracturing, stimulating, or enhanced oil recovery stages. They found 5-15 times enhancement in the permeability due to stress cycling.

# Hydraulic Fracture Experiment Direct Shear Experiment

Figure 4. Fracture topography patterns in Utica shale from hydraulic fracture and direct shear experiments.

Bažant et al. (2014) attributed the fracturing success to creating a dense fracture system (theoretically, 0.1 m spacing is required, however fractures are typically spaced 10 m). They advised against using high injection rates to create the fracture network. Interestingly, they devalued the natural fractures' existence for creating dense fracture networks, mainly because these fractures are prone to localizations. Rahimi-Aghdam et al. (2019) numerically demonstrated that the weak layers in the shale formations are responsible for the hydraulic fracture branching, as shown in **Figure 5**. This branching might reconcile between the theoretical fracture density needed to provide the current recovery rates and the typical fracture density adopted during the fracturing operations.

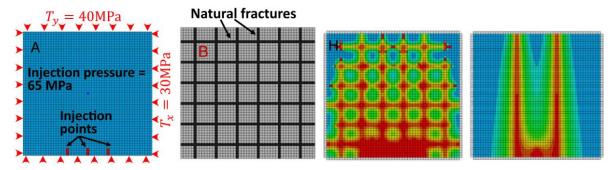


Figure 5. The impact of natural fractures and weak layers on fracture propagation (Rahimi-Aghdam et al., 2019): A) the initial conditions, B) the natural fractures and weak layers distribution, C) the fracture propagation with the presence of weak layers D) the fracture propagation without the weak layers

The fate of the fracturing fluid is still elusive. Although the fracturing operations require a large volume of fracturing fluid, less than half of these fluids flow back. O'Malley et al. (2016) found that most fracturing fluid could only be stored in the matrix. However, shale's ultra-low permeability nature makes it challenging to explain how these fluids could be transported and trapped in the matrix. Mehana and El-Monier (2015) studied osmosis as fracturing fluid transport mechanisms into the matrix. The salinity contrast between the fracturing fluid and the formation brine would induce a pressure gradient. They found that the osmotic pressure might be responsible for up to 50% of the fracturing fluid into the matrix. Notably, the capillary suction is another mechanism for the fracturing fluid transport into the matrix. Shale gas reservoirs are naturally in a water under-saturated state.

The entrapment of these fracturing fluids could affect both the well performance and life. Firstly, these fluids affect the hydrocarbon mobility near the wellbore, reducing the ultimate recovery of the well. Secondly, the fluid/rock interactions affect the petrophysical properties and strength of the rock. Mehana et

al. (2018) related the impact of the trapped fluids on the formation strength to the formation mineralogy. Unlike the common belief, the formation strength is enhanced if it has more than 8% siderite and anhydrite content. However, the bottom line is the impact of these trapped fluids is adverse to hydrocarbon recovery. Therefore, LANL has pioneered the search for alternative environmentally-friendly fracturing fluids.

Supercritical carbon dioxide has been proposed as a non-aqueous fracturing fluid, reducing the environmental footprint and enhancing hydrocarbon recovery (Middleton et al., 2014). Middleton et al. (2015) summarized the main merits of carbon dioxide, including superior adsorption, hydrocarbon mobility enhancement, and sequestration benefits. Recently, experimental investigations have quantified the benefits of using  $CO_2$  as a fracturing fluid. They observed a reduction in the fracturing pressure and increased the fracture network's complexity (Zhang et al., 2017). Natural gas is critical for enabling more renewable penetration onto the grid since it can load balancing the grid against renewables such as solar and wind that are intermittent. As the world prepares for future energy and climate scenarios, unconventionals with  $CO_2$  as a fracturing fluid and storage sink have the potential to play a large role in a new  $CO_2$  economy.

Despite the unprecedented success of hydraulic fracturing in developing shale reservoirs, significant environmental concerns have been raised. While it is unlikely for hydraulic fractures to create fractures that connect drinking water aquifers with shale formations, it is still possible to create fractures that connect with faults and natural fractures. However, the majority of the reported leaks are associated with wellbore integrity. Wellbore integrity is also a cause of fugitive methane leaks and could be one of the more straightforward ways to lower the carbon footprint of unconventional sites. On the other hand, induced seismicity is mainly associated with wastewater disposal, where the pore pressure increases, reducing the effective stress and reactivating the fault. In addition, hydraulic fractures could directly intersect with the fault zone. While disposal regulations have eased the severity of induced seismicity consequences, current research devises innovative fracturing fluids and addresses wellbore integrity problems.

Using dfnWorks, Hyman et al. (2015) simulated a shale's production profile's main characteristics where they observed an initial peak followed by a steep decline. They matched features enabling advective transport. They intentionally did not include the matrix diffusion, small scales processes, which might explain the observed mismatch during the later time of the well life. When matrix diffusion was considered, better results were reported for the production tail (Karra et al., 2015). They suggested that other matrix processes are responsible for the remaining mismatch during the late production.

In the same vein, Lovell et al. (2018) refuted the perceived notion of matrix diffusion effect on the production from shale reservoirs, as shown in **Figure 6**. Instead, they demonstrated that matrix diffusion in the region of the fractured zone significantly impacts production from the first year. Interestingly, they also found that the depth of the fractured region did not affect the production curves' shape. However, the total mass of the hydrocarbon produced increases with the depth.

Investigating another mysterious subsurface phenomenon, O'Malley et al. [26] integrated a DFN model with statistical analysis to reveal the fate of the fracturing fluids. With less than 30% of injected fracturing fluids reproduced, valid concerns have been raised about the impact of these trapped fluids on the well performance and formation strength. They showed that most of the missing water (about 90%) resides in the matrix with a lesser amount in the fractures (about 10%). They suggested that capillary forces are a significant driver for water imbibition into the ultra-tight shale matrix. This has implications for storing fluids such as  $CO_2$  at unconventional sites that could lower the environmental footprint while increasing ultimate recovery. In addition, it could be a driver for a  $CO_2$  economy in future climate-constrained scenarios.

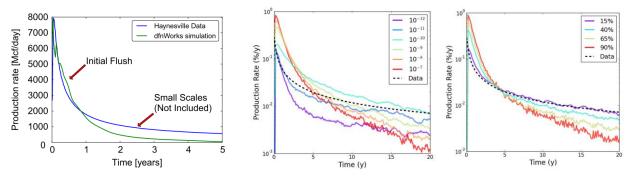


Figure 6. dfnWorks Monte Carlo predictions of well performance: A) highlighting the need to include the advective transport in the smaller fracture and the diffusion from the matrix to properly model the production tail (Hyman et al., 2015) b) highlighting the impact of diffusion coefficient on the production curve (Lovell et al., 2018) c) highlighting the effect of the percentage of free hydrocarbon outside the fractured zone on the production curve.

### **Science-informed Machine Learning**

Recent developments in machine learning have transformed many processes' efficiency, but they have lagged in impacting subsurface operations, particularly for unconventional reservoirs. This delay is mainly attributed to the limitations of sufficient subsurface data on these systems. Machine learning techniques tend to require large amounts of data. Therefore, this effort focuses on devising physics-informed machine learning approaches that require less observational data. We also use standard machine learning efforts to analyze large databases of wells to determine trends and critical mechanisms. Fracture networks impart a higher degree of site-specificity in reservoir properties relative to conventional reservoirs, and the properties are often less well defined. **Figure 7** outlines the main LANL applications of machine learning to accelerate and improve current subsurface models.

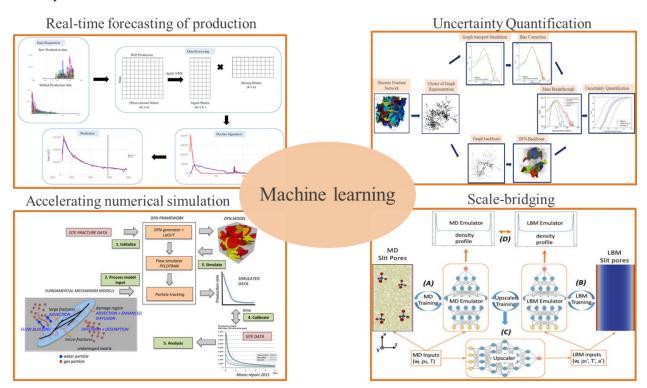


Figure 7. A summary of LANL's main applications of machine learning for subsurface modeling, including well performance predictions, uncertainty quantification, accelerating numerical simulations, and bridging the scales between molecular and pore scales.

Nano-confinement significantly affects fluid behavior, which substantially deviates from the bulk behavior. However, most continuum-scale simulators overlook nanoconfinement effects and assume bulk behavior.

URTeC 5406

This overlook results in misleading predictions about the original hydrocarbon in place and well performance. On the other hand, molecular simulations naturally capture and quantify the nanoconfinement effects on fluid behavior. However, the current computational resources only allow modeling systems of a few nanometers for a few nanoseconds.

A promising approach is to develop scale-bridging schemes to connect atomistic-scale simulations with pore- and reservoir-scale simulations. Lubbers et al. (2020) proposed one of these scale-bridging schemes, which relies on deep learning techniques to quantify the adsorption characteristics in silt pores and inform LBM simulations. Essentially, they trained neural network simulators to predict the density profiles of the fluid at different conditions using molecular- and pore-scale simulation. Then, they trained another network to perform the upscaling. Apart from the computational speedup, they demonstrated the indirect coupling's applicability to scale the adsorption characteristics.

In the same vein, Santos et al. (2020) adopted an active learning framework to accelerate neural network training. They devised an approach to sample the parameter space efficiently to model methane adsorption in complex pores using an active learning approach. They successfully reached the accuracy of conventional techniques using only 10% of the dataset. This work is the initial stage to develop a workflow to estimate the adsorption characteristics on the fly and inform LBM, enabling larger time and length scales. Wang et al. (2021) extended the work scope to model the transport properties using reinforcement learning. They used MD and LBM datasets to train physics-constrained neural networks.

The hydraulic fracturing success highly determines shale well performance since hydraulic fractures mechanically create conductive pathways connecting the natural fractures. Consequently, the production profile displays unique characteristics that differ from those observed in conventional reservoirs. The production rate quickly climbs to a peak, then gradually decreases with a long tail. Unlike the reservoir boundaries for conventional wells, the drainage area for a shale well usually corresponds to the mechanically stimulated reservoir volume. The hydrocarbon's initial flush corresponds to the hydrocarbon residing in the hydraulic and natural fractures, marking the production history's linear flow portion. Unlike the conventional wells, the boundary-dominated flow does not usually follow the linear flow. However, intermediate flow regimes corresponding to the complexity of the fracture network are observed. These intermediate flow regimes are named complex fracture depletion regimes. On the other hand, the long production tail usually accounts for the matrix phenomena such as desorption and diffusion.

Combining the extended linear flow and the indefinite onset of the boundary-dominated flow pose a challenge to the traditional forecasting approaches. Mehana et al. (2020a) adopted a Monte Carlo approach to predict shale reservoirs' well performance where mature wells' production characteristics predict the newer wells' performance. In addition, they observed that 75% of the production history is required for the deterministic methods to provide reliable results. Mehana et al. (2021a) used non-negative matrix factorization to extract the decline signature of shale wells' production profiles. These decline signatures were used to predict the well performance afterward. In addition, their approach provides early identification of underperforming wells.

Machine learning has been adopted to accelerate high-fidelity simulations of shale reservoirs. Wu et al. (2019) used convolution neural networks to estimate effective diffusivity using the LBM dataset. Besides the computational efficiency of LBM, they achieved six orders of magnitude speedup. However, they observed poor performance for low-diffusivity pore structures and suggested augmenting their approach with either multiscale feature extraction or geometrical properties to overcome this limitation. Similarly, using the LBM dataset, Guiltinan et al. (2020) used a deep learning approach to predict the residual saturations during multiphase displacement in heterogeneous fractures. They quantified the impact of the wettability heterogeneity on the residual saturations. One limitation of commonly used ML architectures is that they cannot train with large domains (>100³). Recently, Santos (2021) presented the MS-Net, a model

that enables predictions up to 850<sup>3</sup> on a single GPU. They showcase their results by accurately predicting single-phase flow in single fractures and propped fractures.

Fluid transport in fractured reservoirs is a fundamental research challenge. While the full-physics models' predictivity has reached a reasonable degree of maturity, the computational cost is still a massive road blocker. Srinivasan et al. (2018a) proposed integrating graph theory and machine learning to accelerate the fractured media's high-fidelity simulations. They demonstrated that the graph representations require significantly lower degrees of freedom to model microstructures, leading to four orders of magnitude speedup. One of the challenging pieces of the puzzle for discrete fracture modeling is the computational expense. One promising technique to improve computational efficiency is system reduction, where machine-learning techniques are leveraged to identify the most significant fractures. LANL's researchers pioneered backbone, connected sub-network, as a unit for classification instead of single fractures (Srinivasan et al., 2018b). Srinivasan et al. (2019) assessed the efficiency of using the random forest as a classification technique to identify the backbones for system reduction. They reported up to 90% of computational savings. They also highlighted the need for an efficient approach to generate the database required for training. They also examined the performance of logistic regression, where the reduced network could yield similar breakthrough curves similar to full-network ones (Srinivasan et al., 2020). Figure 8 compares the computational intensity of dfnWorks and graph-based models for different fractured systems.

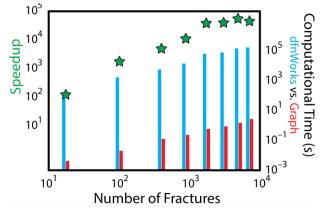


Figure 8. Comparison of computational speed for full-physics dfnWorks and the graph-based models trained from a suite of runs produced by dfnWorks. For large numbers of fractures, the graph-based models can be ~30,000 faster.

# Shale Enhanced Oil Recovery and CO<sub>2</sub> sequestration

While being an invaluable source of fossil energy and traditionally known as a seal rock for structurally storing CO<sub>2</sub> in geological formations, shale formations have become an avenue for utilizing CO<sub>2</sub> to enhance hydrocarbon recovery. CO<sub>2</sub> Enhanced Oil Recovery (CO<sub>2</sub>-EOR) techniques have been optimized and tested for various conventional reservoirs. These techniques provide pressure maintenance to avoid multiphase conditions, improve the sweep efficiency and tune the hydrocarbon phase properties to improve fluid mobility. However, shale characteristics significantly affect these techniques and require optimizing these techniques for shale reservoirs. For instance, waterflooding, which is the most common EOR technique in conventional reservoirs, is not practical for shale reservoirs, mostly because of the ultra-low permeability shale formation and the impracticality of the multi-well EOR operations. On the other hand, the gas injection, and CO<sub>2</sub> injection particularly, has become a promising EOR technique for shale reservoirs.

To gain more insights, Nguyen et al. (2018) experimentally evaluated carbon dioxide and nitrogen's potential to improve hydrocarbon recovery through huff and puff operations. They observed that carbon

URTeC 5406

dioxide yields higher recovery than nitrogen for both connected and dead-end fractures and that connected fractures usually have a better recovery than dead-end ones for both gases as shown in **Figure 9**. They attributed this behavior to the superior miscibility characteristics of carbon dioxide.

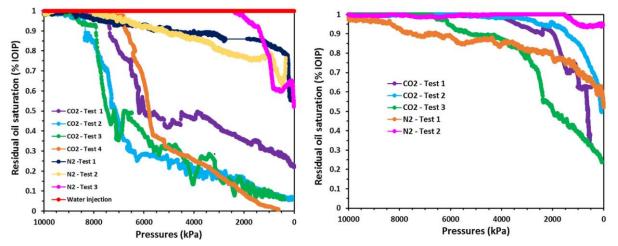


Figure 9. Residual oil saturation after huff and buff microfluidic experiment using carbon dioxide and nitrogen: connected fractures (right) and dead-end fractures (right). The experiments have been repeated up to four times to ensure the conclusions' reliability (Nguyen et al., 2018).

In addition, Mehana et al. (2020b) used molecular simulation to study carbon dioxide, nitrogen, and methane's performance to extract hydrocarbons from rough organic pores. They observed that confinement enhances hydrocarbons' adsorption to the pore surface, hindering the hydrocarbons' mobility. Besides, they observed recovery factors up to 90% for the concurrent displacements and recovery factors less than 20% for the counter-current displacements. Notably, they found that the limited diffusion and miscibility of nitrogen in hydrocarbons led to faster recovery. In addition, methane yielded better recovery for counter-current displacement. However, carbon dioxide provides the best candidate as long as miscibility is achieved, as shown in **Figure 10**.

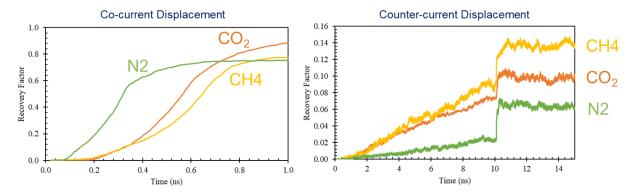


Figure 10. Molecular simulations' predictions of the efficiency of carbon dioxide, methane, and nitrogen to extract hydrocarbons from organic pores. Co-current displacement involves injecting the gas to displace the hydrocarbons to be produced from the other end of the pore. On the other hand, counter-current displacement, similar to huff and puff operations, involves injecting the gas and producing the hydrocarbons from the same pore's entry (adapted from Mehana et al. (2020b)).

### **Conclusions**

Energy security and independence are a top priority for any nation's existence. Technology advancements allowed the economic development of shale reservoirs as an energy resource. These reservoirs' unique characteristics and challenging nature require an in-depth understanding of their phenomena to devise better

URTeC 5406

strategies to improve these reservoirs' recovery factors with minimal environmental footprints. We, LANL scientists, have been working and collaborating on projects to optimize the matrix processes, improve fracturing operations, develop full-physics models, and design machine-learning frameworks. We plan to continue advancing our fundamental understandings of these reservoirs and devising innovative machine-learning frameworks to accelerate our high-fidelity simulation, bridge the scales, and reveal the hidden features in our data. We plan to extend and further our projects to advance carbon dioxide utilization and sequestration in shale reservoirs in preparation for future energy and climate scenarios.

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