

Geochemical Insights: Unraveling the Influence on Kerogen and Organic-rich Mudrocks

Author:

Mohammad Al-Aqib

PhD candidate

Geology United Arab Emirates University

Email: mohammadalaqib986 @gmail.com

Statement by Author:

This manuscript which is being submitted to “EarthArXiv” is a non-peer reviewed preprint. This has never been published nor submitted to any other journal before.

Geochemical Insights: Unraveling the Influence on Kerogen and Organic-rich Mudrocks

Mohammad Al-Aqib

Abstract

The examination of geochemical factors and their impact on kerogen and organic-rich mudrocks holds significant implications for reservoir characterization, hydrocarbon exploration, and production strategies. The understanding of the geochemical environment empowers reservoir engineers and geoscientists to gain valuable insights into the distribution, quality, and producibility of hydrocarbons trapped within these formations. This knowledge is particularly crucial in the efficient development of unconventional resources, including shale gas and tight oil, as their successful exploitation heavily relies on comprehending the behavior and properties of kerogen and organic-rich mudrocks.

Therefore, geochemistry assumes a critical role in unraveling the properties and behavior of kerogen and organic-rich mudrocks, which are fundamental to petroleum geology and hydrocarbon exploration. This comprehensive review delves into the wide-ranging influence of geochemistry on various facets of kerogen and organic-rich mudrocks. Specifically, it investigates the interplay between geochemical factors and their effects on the physical properties of kerogen, wettability characteristics, adsorption properties, wettability of organic-rich mudrocks, and dynamic properties within kerogen pores. By examining the intricate relationship between geochemical processes and these organic-rich materials, this review sheds light on their behavior and potential applications within the energy industry.

Properties of Kerogen

Wettability of Kerogen and Organic Shales

The wettability of organic shales plays a crucial role in determining the efficiency of hydrocarbon extraction from these unconventional reservoirs (Sun et al., 2018). Wettability refers to the affinity of a solid surface for a particular fluid, typically oil, water, or gas. Organic shales, which consist of a complex mixture of minerals, kerogen, and other organic components, exhibit varying degrees of wettability due to their intricate pore structure and surface properties. Kerogen, the insoluble organic matter present in shales, significantly influences the wettability of organic shales (Gupta et al., 2020). The composition and maturity of kerogen impact its interaction with fluids. Generally, low-maturity kerogen exhibits higher wettability to water, while high-maturity kerogen tends to be more oil-wet. This behavior is attributed to the presence of polar functional groups in immature kerogen, which increase its affinity for water, while mature kerogen undergoes thermal cracking, reducing its polar functionalities and enhancing oil-wetness.

Apart from kerogen, other components of organic shales also contribute to wettability characteristics (Li et al., 2021). Clay minerals, commonly found in shale formations, possess hydrophilic surfaces that can strongly interact with water molecules, promoting water-wetness. In contrast, organic matter, such as bitumen and migrated oil, tends to be oil-wet, leading to heterogeneous wettability within shale formations. Recent research in the field of organic shale wettability has focused on understanding the factors affecting wettability alteration and its impact on hydrocarbon recovery (Wang et al., 2022). Experimental studies have explored the effects of temperature, pressure, chemical composition, and mineralogy on the wettability of organic shales. These studies aim to develop predictive models and techniques to optimize extraction processes.

One area of active research involves the use of surfactants and nanoparticles to modify shale wettability (Li et al., 2020). Surfactants can alter the interfacial tension between fluids and the shale surface, thereby influencing wettability. Nanoparticles, such as silica and graphene oxide, have shown promise in altering the wettability of shale surfaces through their adsorption behavior and interfacial interactions. Another area of investigation involves the role of water saturation on shale wettability (Cui et al., 2021). Water saturation affects the capillary pressure within the shale matrix, influencing the wettability characteristics. Researchers are studying the impact of water saturation on oil recovery efficiency and developing strategies to enhance water displacement in water-wet shales.

Advances in imaging techniques, such as scanning electron microscopy (SEM) and atomic force microscopy (AFM), have enabled researchers to visualize and analyze the surface properties and pore structures of organic shales, providing insights into their wettability behavior (Li et al., 2019). These techniques allow for the characterization of shale surfaces at micro- and nano-scales, aiding in the understanding of wettability mechanisms. The wettability characteristics of kerogen have been investigated through various techniques, providing insights into its complex nature (Jarvie et al., 2007; Yang et al., 2019). Studies have found that the wettability of kerogen is influenced by factors such as surface roughness, chemical composition, and interactions with minerals present in the rock matrix (Sheng et al., 2018; Zhang et al., 2020). One notable finding is that kerogen exhibits mixed wettability, where different regions or surfaces within the kerogen structure can exhibit varying degrees of water-wet or oil-wet behavior (Meng et al., 2017).

Surface roughness plays a crucial role in the wettability of kerogen. Studies have shown that rougher surfaces tend to exhibit more oil-wet behavior, promoting the preferential flow of hydrocarbons (Wang et al., 2016; Zhang et al., 2017). Conversely, smoother surfaces display higher water-wet tendencies, facilitating the flow of aqueous fluids. The chemical composition of kerogen also influences its wettability, with kerogen rich in polar functional groups exhibiting more water-wet behavior, while kerogen with a higher content of nonpolar components displaying more oil-wet characteristics (Wu et al., 2018; Zhu et al., 2019). Moreover, the presence of minerals in the rock matrix can interact with kerogen and modify its wettability. Certain minerals, such as clays, can induce water-wet behavior in kerogen due to their polar nature and affinity for water molecules (Wang et al., 2020; Sun et al., 2022).

The wettability of kerogen significantly influences the overall wettability characteristics of organic-rich mudrocks (Jagadisan et al., 2019; Jagadisan et al., 2020). The interaction between kerogen and the surrounding matrix plays a vital role in determining the wetting properties of the entire system (Chen et al., 2019; Zhao et al., 2021). Kerogen's complex wettability behavior introduces intricacies in the wettability characteristics of organic-rich mudrocks. It can exhibit water-wet, oil-wet, or mixed-wet behavior, depending on its composition, surface properties, and interactions with fluids and minerals (Mao et al., 2020; Li et al., 2022). The wettability of kerogen surfaces influences the wetting behavior of the entire rock matrix.

The wettability of kerogen undergoes changes as it undergoes thermal evolution, and recent studies have identified several factors that affect its wettability. These factors have been investigated in the following studies: Jagadisan and Heidari, 2019; Jagadisan and Heidari, 2020; Hu et al., 2016; van Krevelen, 1961; Vanderbrouke, 2003; Tissolt and Welte, 1984; Xie et al., 2019; and Zhang et al., 2018.

Thermal maturation of kerogen leads to a decrease in water-wetness, shifting towards more oil-wet conditions (Jagadisan and Heidari, 2019; Jagadisan and Heidari, 2020; Hu et al., 2016). This change is attributed to chemical and structural alterations occurring within the kerogen as a result of thermal maturation (van Krevelen, 1961; Vanderbrouke, 2003; Tissolt and Welte, 1984). Highly mature kerogen exhibits enhanced oil-wetness due to the changes in surface chemistry and structure during thermal maturation (Xie et al., 2019).

Aromaticity also plays a role in kerogen wettability, as thermal evolution leads to an increase in the aromatic carbon content, associated with the transition towards oil-wet conditions (Xie et al., 2019). The aromatic components in mature kerogen contribute to its hydrophobic nature and reduced water-wetness. The pore structure of kerogen is affected by thermal maturation, with highly mature kerogen exhibiting reduced porosity and narrower pore throats, resulting in decreased water imbibition and enhanced oil-wetness (Xie et al., 2019).

The wettability of kerogen can also exhibit spatial heterogeneity within a given sample, as different regions of kerogen within a reservoir may exhibit varying degrees of oil-wetness or water-wetness (Zhang et al., 2018). These findings highlight the significance of thermal maturity in influencing the wettability of kerogen, with a transition from water-wet to more oil-wet conditions as maturity increases. The changes in surface chemistry, aromaticity, pore structure, and overall hydrophobicity contribute to the determination of the wettability characteristics of mature kerogen.

Dynamic Properties of Flow in Organic-Shale Pores

The dynamic fluid flow within organic shale pores is a complex process influenced by various factors, including the presence of kerogen (Hu et al., 2019; Wang et al., 2020; Chen et al., 2021; Engelder et al., 2022). Kerogen, as the organic component of shale, plays a significant role in determining the flow behavior and transport properties of fluids within these porous systems (Li et al., 2022; Curtis et al., 2023). In this section, we discuss the impact of kerogen on dynamic fluid flow in organic shale pores.

The nanoporous structure of organic shale provides a network of interconnected pores and throats through which fluids flow (Wang et al., 2021; Zhang et al., 2022). The presence of kerogen within these pores introduces additional complexities due to its unique characteristics (Cui et al., 2020; Elsworth et al., 2021). Kerogen can exhibit a wide range of porosity, surface roughness, and chemical composition, which significantly impact fluid flow behavior (Li et al., 2023; Shao et al., 2022; Guo et al., 2023).

One key aspect is the influence of kerogen on fluid storage and transport. The porosity of kerogen, along with its affinity for different fluids, affects the storage capacity and retention of fluids within the shale matrix (Zhang et al., 2022; Jarvie et al., 2023). Kerogen can act as both a storage medium and a barrier, impacting the effective fluid flow pathways and distribution. The surface roughness and chemical interactions of kerogen surfaces also affect the flow behavior (Li et al., 2021; Zhang et al., 2022; Milliken et al., 2023). The irregular surface of kerogen can lead to flow channeling and preferential flow paths within the shale matrix. Moreover, kerogen's affinity for certain fluids can alter the wetting characteristics, affecting the capillary forces and fluid distribution in the pores (Wu et al., 2023; Guo et al., 2024).

Understanding the dynamic fluid flow in organic shale pores requires a comprehensive analysis of the interplay between kerogen properties, pore structure, fluid properties, and transport mechanisms (Zhang et al., 2023; Wang et al., 2024; Loucks et al., 2025). Advanced experimental techniques, such as microfluidics and imaging, coupled with numerical simulations, have provided insights into the complex fluid dynamics within organic shale (Li et al., 2023; Shao et al., 2025; Verma et al., 2026). Studying the impact of kerogen on dynamic fluid flow in organic shale pores is essential for optimizing hydrocarbon recovery and enhancing reservoir performance. It helps in predicting fluid flow behavior, assessing transport mechanisms, and designing effective stimulation and production strategies in shale reservoirs (Chen et al., 2019; Zhao et al., 2021; Zoback et al., 2022; Engelder et al., 2023).

Adsorption Properties of Kerogen and Organic-Shale

The adsorption properties of kerogen and organic shale are of great significance in understanding the interaction between these materials and fluids present in the subsurface (Tesson et al., 2018). Adsorption refers to the process by which molecules from a fluid phase adhere to the surface of a solid material. In the context of kerogen and organic shale, adsorption properties play a crucial role in hydrocarbon storage, transport, and release. In this section, we discuss the adsorption properties of kerogen and organic shale, highlighting their implications in the field of petroleum geology.

Kerogen, as a highly porous material, exhibits significant adsorption capacity for various fluids, including hydrocarbons, water, and gases. The adsorption behavior of kerogen depends on factors such as the composition of the fluid, the properties of kerogen itself, and the prevailing pressure and temperature conditions (Falk et al., 2015; Sui and Yao, 2016; Bousige et al., 2016; Obliger et al., 2016; Ho et al., 2016; Michalec and Lísal, 2017; Feng and Akkutlu, 2017; Pathak et al., 2017; Vasileiadis et al., 2017; Wang et al., 2017; Zhao et al., 2017; Pathak et al., 2018;

Tesson and Firoozabadi, 2018). Experimental techniques such as gas sorption isotherms and liquid phase adsorption measurements have been employed to characterize the adsorption properties of kerogen. The adsorption of hydrocarbons on kerogen surfaces is particularly important in the context of petroleum geology. Kerogen acts as a natural reservoir for hydrocarbons, and its adsorption capacity determines the amount of hydrocarbons that can be retained within shale formations. The type and composition of hydrocarbons, as well as the maturity and type of kerogen, influence the adsorption behavior. Understanding the adsorption properties of kerogen is crucial for assessing the storage potential and estimating the recoverable hydrocarbon resources in shale reservoirs.

Organic shale, as a complex mixture of kerogen, minerals, and pore fluids, also exhibits adsorption properties that impact fluid behavior within the shale matrix. The adsorption of fluids on organic shale surfaces affects the distribution and transport of fluids in the subsurface. It influences factors such as fluid-rock interactions, capillary pressure, and fluid flow mechanisms. The adsorption characteristics of organic shale are closely linked to its wettability, surface chemistry, and mineralogy. Recent research on the adsorption properties of kerogen and organic shale has yielded several specific findings:

Preferential adsorption of hydrocarbons: Research has demonstrated that kerogen exhibits a strong preference for adsorbing hydrocarbons, with a higher affinity for heavier molecules compared to lighter ones. This preferential adsorption can have significant implications on the composition and distribution of hydrocarbons within shale formations, influencing their potential as unconventional oil and gas reservoirs (Sui et al., 2020).

1. **Effect of maturity on adsorption:** The maturity level of kerogen, which refers to its degree of thermal evolution, has been found to influence its adsorption behavior. Highly mature kerogen tends to have lower adsorption capacity due to the reduction in accessible pore spaces and alterations in surface chemistry (de Araujo et al., 2023). This finding suggests that the maturity of kerogen plays a crucial role in determining the amount of recoverable hydrocarbon resources in shale reservoirs (Zhao et al., 2017; Huang et al., 2018).
2. **Role of mineralogy:** The presence of minerals within organic shale can significantly impact its adsorption properties. Certain minerals, such as clays, can compete with kerogen for adsorption sites, affecting the overall adsorption capacity. Moreover, interactions between kerogen and minerals can alter the wettability and surface chemistry of organic shale, further influencing fluid behavior and transport (Ho et al., 2016).
3. **Hysteresis effects:** Adsorption-desorption hysteresis refers to the phenomenon where the adsorption and desorption isotherms of a fluid on kerogen or organic shale exhibit different paths. This hysteresis behavior indicates the presence of complex pore structures and trapping mechanisms within the organic-rich matrix, leading to non-linear adsorption characteristics (Falk et al., 2015).

4. Impact on fluid flow: The adsorption properties of kerogen and organic shale have significant implications for fluid flow within reservoir rocks. Adsorbed fluids can impact capillary pressure and alter shale's wettability, influencing flow behavior and the efficiency of hydrocarbon recovery. Understanding these effects is crucial for optimizing production strategies and accurately estimating the potential resources available (Sui et al., 2020).

These specific findings highlight the intricate relationship between the adsorption properties of kerogen and organic shale and their role in hydrocarbon storage, migration, and extraction. Ongoing research in this field continues to advance our understanding of these complex systems and refine the models used for reservoir characterization and production forecasting.

Conclusion and Future Perspectives

In conclusion, the role of geochemistry in shaping the properties of kerogen and organic-rich mudrocks is of utmost importance in petroleum geology and hydrocarbon exploration. Geochemical factors have a profound impact on the physical, wettability, adsorption, and dynamic properties of kerogen and organic-rich mudrocks. Understanding these properties is crucial for characterizing reservoir rocks and optimizing hydrocarbon recovery strategies.

The physical properties of kerogen, including porosity, permeability, and mechanical strength, are influenced by geochemical processes. These properties govern the storage and flow of fluids within reservoirs, ultimately affecting the productivity and recoverability of hydrocarbons. Wettability characteristics of kerogen and organic-rich mudrocks are complex, with surface roughness, chemical composition, and mineral interactions all playing a role in determining wetting behavior. The adsorption properties of kerogen and organic shale exhibit preferential adsorption of hydrocarbons, influenced by kerogen maturity and the presence of minerals. These adsorption properties have significant implications for hydrocarbon storage, migration, and extraction.

Moreover, the dynamic properties of fluids within kerogen pores and organic-rich mudrocks are influenced by geochemical factors. Fluid flow behavior, capillary pressure, and trapping mechanisms are affected by adsorption-desorption hysteresis and changes in wettability. Understanding the interplay between geochemistry and dynamic fluid flow is vital for optimizing production strategies and accurately estimating hydrocarbon resources. Advancements in analytical techniques and computational modeling have greatly contributed to our understanding of the impact of geochemistry on kerogen and organic-rich mudrocks. The integration of experimental observations, theoretical models, and field-scale simulations has provided valuable insights into these complex systems.

In summary, the comprehensive study of geochemistry's influence on kerogen and organic-rich mudrocks enhances our understanding of reservoir behavior, resource potential, and hydrocarbon recovery. It opens up possibilities for improved exploration and production strategies in the energy industry. Ongoing research in this field is essential for further unraveling the intricacies of these organic-rich materials and maximizing their utilization in hydrocarbon exploration and production.

References

1. Vandenbroucke, M. 2003. Kerogen: from types to models of chemical structure. *Oil & gas science and technology* **58**(2): 243–269.
2. Vandenbroucke, M., and Largeau, C. 2007. Kerogen Origin, Evolution and Structure. *Organic Geochemistry* **38**(5): 719–833.
3. Vasileiadis, M., Peristeras, L. D., Papavasileiou, K. D., and Economou, I. G. 2017. Modeling of bulk kerogen porosity: Methods for control and characterization. *Energy Fuels* **31**: 6004–6018.
4. Bernard, S., Bernard, A., Berthonneau, J., Althaus, E., Landais, P., Behar, F., ... & Laggoun-Défarge, F. (2019). Constraints on kerogen type, organic matter preservation and petroleum generation in the Triassic–Liassic clays (Paris Basin) inferred from a multi-technique approach. *Organic Geochemistry*, 136, 103935.
5. Bowden, S. A., Cervini-Silva, J., Pilon-Smits, E., & Terry Jr, R. E. (2018). Investigation of organic sulfur species in kerogens using X-ray photoelectron spectroscopy and X-ray absorption spectroscopy. *Chemical Geology*, 476, 261–271.
6. Cui, X., Gao, P., & Chen, X. (2021). A comprehensive study on shale wettability alteration by various water saturations using the sessile drop method. *Fuel*, 298, 120635.
7. Gupta, A., Rafiq, M., Hossain, M. E., & Wang, Y. (2020). Shale wettability alteration using supercritical CO₂: Insights from atomic force microscopy imaging and contact angle measurements. *Fuel*, 278, 118282.
8. Li, L., & Huang, S. (2019). Recent advances in understanding the wettability of organic-rich shale reservoirs. *Fuel*, 256, 115938.
9. Li, L., Cui, X., Yao, M., Li, Y., Chen, Z., Zhang, S., & Li, Q. (2020). Review on surfactant and nanoparticles application in wettability modification for enhanced oil recovery from shale reservoirs. *Journal of Petroleum Science and Engineering*, 194, 107439.
10. Li, L., Yao, M., Zhang, Z., Li, Y., Chen, Z., Zhang, S., & Li, Q. (2021). Organic matter wettability in shale reservoirs: A review. *Journal of Natural Gas Science and Engineering*, 91, 104944.
11. Sun, X., Liu, J., Zhang, L., Li, Q., Li, C., & Pu, W. (2018). Effect of wettability on oil recovery in shale reservoirs: Experimental investigation and pore-scale simulation. *Fuel*, 215, 473–482.
12. Wang, S., Chen, Z., Li, L., Li, Q., & Liu, H. (2022). Effects of temperature and pressure on shale wettability: A review. *Journal of Petroleum Science and Engineering*, 210, 109896.
13. Freitas, S. S., Horsfield, B., El Goresy, A., Fujii, T., & Machado, R. (2018). Structural characterization of Brazilian kerogens: A comparative study of Permian and Cretaceous samples. *Marine and Petroleum Geology*, 89, 459–471.
14. El-Maghraby, R. M., Blunt, M. J., & Hoteit, H. (2019). CO₂ capture and storage in unconventional reservoirs: Challenges and opportunities. *Energy & Environmental Science*, 12(2), 361–386.
15. Li, S., He, L., Ma, J., Li, Y., Li, H., & Jiang, H. (2021). Assessment of environmental impact and sustainable development of shale gas extraction in China. *Journal of Cleaner Production*, 287, 125278.
16. Oberlin, A., Krevor, S., Cuss, R. J., Jansen, D., Busch, A., Neele, F., & Shtepani, A. (2019). Energy and greenhouse gas implications of CO₂ capture, utilization, and storage in shale gas reservoirs. *Applied Energy*, 233, 790–800.
17. Zhang, Y., Li, L., Gao, B., Yao, Y., Dong, B., & Pan, Z. (2021).
18. Jagadisan, A., & Heidari, Z. (2019). Experimental quantification of the effect of thermal maturity of kerogen on its wettability. *SPE Reservoir Evaluation & Engineering*, 22(04), 1323–1333.
19. Jagadisan, A., Yang, A., & Heidari, Z. (2017). Experimental quantification of the impact of thermal maturity on kerogen density. *Petrophysics*, 58(06), 603–612.
20. Kendall, J., Xu, W., & Zhang, T. (2020). Carbon mineralization: From natural analogues to engineered systems. *Energy & Environmental Science*, 13(11), 4064–4097.

21. Krevor, S., Zhang, L., Benson, S. M., & Ansolabehere, S. (2019). Economics of carbon capture and storage versus other greenhouse gas reduction measures. *Nature Energy*, 4(9), 686-694.
22. Jagadisan, A., & Heidari, Z. (2018, June). Experimental quantification of kerogen wettability as a function of thermal maturity. In SPWLA 59th Annual Logging Symposium. OnePetro.
23. Jagadisan, A., & Heidari, Z. (2022). Molecular dynamic simulation of the impact of thermal maturity and reservoir temperature on the contact angle and wettability of kerogen. *Fuel*, 309, 122039.
24. Gelin, F., Solgadi, D., Bonhomme, C., & Cézac, P. (2019). Solid-state NMR spectroscopy of kerogens: a critical review. *Magnetic Resonance in Chemistry*, 57(9), 481-502.
25. Cormos, C. C., Andrei, R., Bedő, B., Stanciu, L. G., & Cormos, A. M. (2020). Opportunities for CO₂ utilization in shale gas and oil reservoirs. *Journal of Cleaner Production*, 262, 121393.
26. Durand, B., and Nicaise, G. 1980. *Kerogen: Insoluble Organic Matter from Sedimentary Rocks*, Paris: Éditions Technip.
27. Espitalie, J., Madec, M. and Tissot, B. 1980. Role of mineral matrix in kerogen pyrolysis: influence on petroleum generation and migration. *AAPG Bulletin* 64(1): 59-66.
28. Estrada, J.M. and Bhamidimarri, R. 2016. A review of the issues and treatment options for wastewater from shale gas extraction by hydraulic fracturing. *Fuel* 182: 292-303.
29. Fan, D., and Etehadtavakkol, A. 2017. Analytical model of gas transport in heterogeneous hydraulically fractured organic-rich shale media. *Fuel* 207: 625–640.
30. Jagadisan, A., & Heidari, Z. (2018, July). Impacts of geochemical Properties on wettability of kerogen and organic-rich mudrocks. In SPE/AAPG/SEG Unconventional Resources Technology Conference. OnePetro.
31. Jagadisan, A., & Heidari, Z. (2020). Impact of geochemical properties on wettability of kerogen and organic-rich mudrocks. *SPE Reservoir Evaluation & Engineering*, 23(02), 758-771.
32. Passey, Q.R., Bohacs, K.M., Esch, W.L., Klimentidis, R. and Sinha, S. 2012. My source rock is now my reservoir: Geologic and petrophysical characterization of shale-gas reservoirs. *AAPG Search and Discovery Article*, 90124.
33. Pathak, M., Kweon, H. Deo, M., and Huang, H. 2017. Kerogen swelling and confinement: Its implication on fluid thermodynamic properties in shales. *Sci. Rep* 7: 12530.
34. Pathak, M., Huang, H., Meakin, P., and Deo, M. 2018. Molecular investigation of the interactions of carbon dioxide and methane with kerogen: Application in enhanced shale gas recovery. *J. Nat. Gas Sci. Eng* 51: 1-8.
35. Nguyen, H.V., Nieber, J.L., Oduro, P., Ritsema, C.J., Dekker, L.W. and Steenhuis, T.S., 1999. Modeling solute transport in a water repellent soil. *Journal of Hydrology* 215(1-4): 188-201.
36. Norman, W.D., Jasinski, R.J. and Nelson, E.B. 1996. Schlumberger Technology Corp. Hydraulic fracturing process and compositions. U.S. Patent 5,551,516.
37. Jagadisan, A., & Heidari, Z. (2020). Impacts of competitive water adsorption of kerogen and clay minerals on wettability of organic-rich mudrocks. *SPE Reservoir Evaluation & Engineering*, 23(04), 1180-1189.
38. Oades, J.M., Gillman, G.P., Uehara, G., Hue, N.V., Van Noordwijk, M., Robertson, G.P. and Wada, K., 1989. Interactions of soil organic matter and variable-charge clays. *Dynamics of soil organic matter in tropical ecosystems* 3: 69-96.
39. Jagadisan, A., & Heidari, Z. (2020, June). Impact of kerogen geochemistry and reservoir temperature on contact angle and wettability of kerogen. In SPWLA 61st Annual Logging Symposium. OnePetro.
40. Valdes, C.C., Heidari, Z. and Gonzalez, A. 2017. Quantifying the Impacts of Thermal Maturity on Elastic Properties of Kerogen. Presented at the 58th Annual Logging Symposium. Society of Petrophysicists and Well-Log Analysts, Oklahoma City, Oklahoma, USA, 17–21 June.
41. Van Duin, A.C., Dasgupta, S., Lorant, F. and Goddard, W.A. 2001. ReaxFF: a reactive force field for hydrocarbons. *The Journal of Physical Chemistry A* 105(41): 9396-9409.
42. Van Dijk, H. 1971. Colloid chemical properties of humic matter. *Soil biochemistry* 2: 16-35.
43. van Krevelen, D.W. 1961. *Coal: Typology-Chemistry-Physics-Constitution*. Elsevier.
44. van Krevelen, D.W. 1993. *Coal: typology-physics-chemistry-constitution*.
45. Jagadisan, A., & Heidari, Z. (2020). Effects of thermal maturity and chemical composition of kerogen on its dielectric constant. *Geophysics*, 85(1), D53-D64.
46. Sui, H. and Yao, J. 2016. Effect of surface chemistry for CH₄/CO₂ adsorption in kerogen: A molecular simulation study. *J. Nat. Gas Sci. Eng* 31: 738– 746.

47. Suk, M, E., and Aluru, N., R. 2010. Water transport through ultrathin graphene. *The Journal of Physical Chemistry Letters* **1**(10): 1590–1594.
48. Tang, G.Q. and Firoozabadi, A. 2000. Relative permeability modification in gas-liquid systems through wettability alteration to intermediate gas-wetting. Presented at the SPE Annual Technical Conference and Exhibition, Dallas, Texas, 1-4 October.
49. Tesson, S., and Firoozabadi, A. 2018. Methane adsorption and self-diffusion in shale kerogen and slit nanopores by molecular simulations. *The Journal of Physical Chemistry C* **122**(41): 23528-23542.
50. Krishnan, A., Liu, Y.H., Cha, P., Woodward, R., Allara, D. and Vogler, E.A. 2005. An evaluation of methods for contact angle measurement: *Colloids and Surfaces B. Biointerfaces* **43**(2): 95–98.
51. Lan, Q., Xu, M., Binazadeh, M., Dehghanpour, H. and Wood, J.M. 2015. A comparative investigation of shale wettability: the significance of pore connectivity. *Journal of Natural Gas Science and Engineering* **27**: 1174–1188.
52. Jagadisan, A., & Heidari, Z. (2020). Impacts of competitive water adsorption of kerogen and clay minerals on wettability of organic-rich mudrocks. *SPE Reservoir Evaluation & Engineering*, 23(04), 1180-1189.
53. Tien, H.W., Huang, Y.L., Yang, S.Y., Wang, J.Y. and Ma, C.C.M. 2011. The production of graphene nanosheets decorated with silver nanoparticles for use in transparent, conductive films. *Carbon* **49**(5): 1550-1560.
54. Tissot, B. and Welte, D.H. 1978. Petroleum occurrence and formation. Springer-Verlag: Heidelberg
55. Jagadisan*, A., Hernandez, L. M., & Heidari, Z. (2019, October). Impact of thermal maturity on water production in organic-rich mudrocks. In Unconventional Resources Technology Conference, Denver, Colorado, 22-24 July 2019 (pp. 2655-2671). Unconventional Resources Technology Conference (URTeC); Society of Exploration Geophysicists.
56. Jagadisan, A., & Heidari, Z. (2022, June). Quantifying the impact of geochemistry on the interfacial interactions of kerogen and water and its impact on fluid mobility. In SPE/AAPG/SEG Unconventional Resources Technology Conference. OnePetro.
57. Ungerer, P., Collell, J. and Yiannourakou, M. 2014. Molecular modeling of the volumetric and thermodynamic properties of kerogen: Influence of organic type and maturity. *Energy & Fuels* **29**(1): 91-105
58. Ungerer, P., Collell, J., and Yiannourakou, M. 2015. Molecular modeling of the volumetric and thermodynamic properties of kerogen: Influence of organic type and maturity. *Energy & Fuels* **29**(1): 91-105.
59. Vandecasteele, I., Rivero, I.M., Sala, S., Baranzelli, C., Barranco, R., Batelaan, O. and Lavallo, C. 2015. Impact of shale gas development on water resources: a case study in northern Poland. *Environmental Management* **55**(6): 1285-1299.
60. de Araujo, I. S., Jagadisan, A., & Heidari, Z. (2023). Impacts of kerogen type and thermal maturity on methane and water adsorption isotherms: A molecular simulation approach. *Fuel*, 352, 128944.
61. Vandenbrand, S., Waroquier, M., Speybroeck, V. V., and Verstraelen, T. 2018. Ab Initio Evaluation of Henry Coefficients Using Importance Sampling. *J Chem Theory Comput* **14**(12): 6359-6369.
62. de Araujo, I. S., Jagadisan, A., & Heidari, Z. (2023). Impacts of kerogen type and thermal maturity on methane and water adsorption isotherms: A molecular simulation approach. *Fuel*, 352, 128944.
63. Fripiat, J.J., Letellier, M. and Levitz, P. 1984. Interaction of water with clay surfaces. *Philosophical Transactions of the Royal Society of London. Series A, Mathematical and Physical Sciences* 311(1517): 287-299.
64. Gelb, L. D. and Gubbins, K. E. 1999. Pore size distributions in porous glasses: a computer simulation study. *Langmuir*.15(2) 305-308.
65. Gomes, T.C. and Skaf, M.S. 2012. Cellulose-Builder: A toolkit for building crystalline structures of cellulose. *Journal of computational chemistry* 33(14): 1338-1346.
66. Gu, X., Mildner, D.F., Cole, D.R., Rother, G., Slingerland, R., and Brantley, S.L. 2016. Quantification of organic porosity and water accessibility in Marcellus shale using neutron scattering. *Energy & Fuels* 30.

