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# Effect of fluids on micro-crack evolution in organic-rich shale by molecular dynamics simulations and nanomechanical experiments: A microscopic perspective from the fluid effect on fracturing

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Hydraulic fracturing is a widely used technique in shale oil and gas development. As a promising method, CO2 fracturing has been suggested because of various advantages, including lower formation sensitivity, lower fracturing pressure, and higher fracture intensity. However, the mechanisms are not well-understood. One of the potential reasons is the strong interaction between the fluids and rock. In this study, the process of microcrack evolution is investigated by molecular dynamics simulations and nanomechanical experiments. The effect of CO2 and H2O on the mechanical properties of typical components in organic-rich shale is analyzed. The strength and fracture toughness of solids in fluids are computed through molecular dynamics simulations. The results indicate that, due to the physical fluid-solid interactions, the mechanical properties of minerals and kerogen may change after exposure to fluids, which is different from geochemical processes. Based on the simulations and experiments, the changes in elastic modulus can lead to complex stress conditions due to swelling and shrinkage, and the presence of oil and gas can further complicate the behavior. The effect highly relies on the interfacial properties between fluids and shale. In the CO2-philic components (e.g., kerogen), the strength and fracture toughness may reduce by CO2 significantly. In hydrophilic constituents (e.g., clays), H2O has a more pronounced effect on mechanical properties than CO2. These findings suggest that CO2 can decrease the strength and fracture toughness of organic-rich shales, and micro-crack may propagate through CO2-philic components. This study provides a microscopic perspective on fracturing in shale, which may facilitate the improvement of the CO2 fracturing technique.

#### Participation

In-Person

### References

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Primary author: Prof. WU, Tianhao (Eastern Institute for Advanced Study (EIAS))

**Co-authors:** Dr ZHAO, Junliang (Southern University of Science and Technology); Prof. FIROOZABADI, Abbas (Rice University; Reservoir Engineering Research Institute); Prof. ZHANG, Dongxiao (Eastern Institute for Advanced Study (EIAS))

Presenter: Prof. WU, Tianhao (Eastern Institute for Advanced Study (EIAS))

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