Failure envelope and fracture toughness of kerogen by molecular dynamics simulations: Connecting molecular-scale to micro-continuum scale in fracture mechanics

TIANHAO WU[1] AND ABBAS FIROOZABADI[1,2]*

[1]Reservoir Engineering Research Institute, Palo Alto, California 94301, USA (tianhaowu@rerinst.org)
[2]Chemical and Biomolecular Engineering Department, Rice University, Houston, Texas 77005, USA
(*correspondence: af@rerinst.org)

Hydrocarbon in organic-rich shale is one of the most important unconventional resources. Hydraulic fracturing is the common stimulation method to create fractures in shale formations for oil and gas production. The failure mechanism of fracturing and mechanical properties of shale media are often investigated by the triaxial compression tests and Brazilian tensile tests with shale core samples. In consideration of the difficulties in the experiments of rock failure, molecular dynamics simulations have been given much attention to obtain the properties at the micro-continuum scale and gain insights into the mechanisms. In this study, we provide a practical method by molecular dynamics simulations to acquire the failure envelope and fracture toughness of kerogen from organic-rich shale, which can be used as the rock failure criteria in macroscopic simulations. The results show that Mohr–Coulomb failure criterion and tensile strength criterion can describe the failure envelop of the kerogen very well. The kerogen matrices have lower fracture toughness than typical minerals. Our work reveals that kerogen is a potential weak component in shale, and the fractures may initiate and propagate around kerogen aggregates. The effects of different fracturing fluids, including H_2O, CO_2, and N_2, are also examined. This work sets the stage for investigating the complex mechanisms of hydraulic fracturing in shale at pore-scale.