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Please fill in your manuscript title.	Machine Learning-Enhanced Multiscale Modelling and Nanopore Characterisation for Improved Hydrocarbon Recovery from Tight Formations

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Abstract

Objectives/Scope:

Shale rock and bitumen-saturated carbonate deposits hold substantial amounts of hydrocarbons but remain largely inaccessible, with current recovery in the single-digit percent performance. Enhancing oil and gas recovery from these challenging deposits requires improved reservoir characterization and description of the hydrocarbon-mineral interactions in sub-micron and nanoscale pores. The project objective is to develop a machine learning (ML)-enabled predictive engineering model that would help enhance hydrocarbon recovery from tight rock formations by optimizing the recovery conditions. The model would couple the nanopore characterization using field emission scanning electron microscopy (FE-SEM) imaging with molecular modeling of the hydrocarbon distribution and flow through nanopores, both enhanced by ML.

Methods, Procedures, Process:

Hydrocarbon-bearing rock SEM images are analyzed using a modified and extended convolutional neural network (CNN) approach that requires fewer training images to yield a precise segmentation. In this ML approach, a U-network architecture for image segmentation is employed to enhance feature and reduce spatial information. The molecular-level modeling of representative rock nanopores containing hydrocarbons of different composition is conducted using molecular dynamics (MD) simulations and the one-/three-dimensional reference interaction site model (1D/3D-RISM) theory of solvation at 20-120°C and 1-300 bar, conditions representative of industrial recovery.

Results, Observations, Conclusions:

Tight rock characterization results contain nanopore distributions from FE-SEM and CNN as well as rock and hydrocarbon compositions. The physicochemical models—built based on the characterization results—provide a molecular-level description of the hydrocarbon-rock interactions using MD and 1D/3D-RISM. The MD trajectories provide insights into the interactions in bulk hydrocarbons and with pore walls. The density profiles within the nanopores are generated to show the temperature and pressure effects on hydrocarbon organization near the pore surface at the nanoscale. The 3D-RISM results represent the system state corresponding to very long MD simulations and are particularly effective in reproducing the effects of additives, such as water, salts and polar molecules in oil. The hydrocarbon-rock interactions parameters calculated for a few thermodynamic conditions and hydrocarbon compositions are interpolated using ML to address the entire temperature, pressure and compositional ranges. In the engineering model, these parameters are employed to develop solutions to the non-Darcy flow equation,

taking into account the fluid-wall interactions that become dominant in the nanopore flow regime. In conclusion, the ML approaches CNN and interpolation are employed to characterize the FE-SEM images of hydrocarbon-bearing tight formations and calculate oil-rock interaction parameters in the entire range of recovery conditions.

Novel/Additive Information:
These characterization and modeling results would be incorporated into an artificial intelligence-based decision-making tool for oil and gas recovery from tight formations that accounts not only for engineering modeling but also for life cycle and economic analyses.