



Understanding model crude oil component interactions on kaolinite silicate and aluminol surfaces: towards improved understanding of shale oil recovery

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Shale oil is currently of interest for unconventional resource exploration and development. Understanding the mechanism of interaction between the complex mixture of organic compounds in shale oil and minerals making up the reservoir rock-oil interface will assist recovery. In this study, molecular dynamics simulation is used to study the adsorption characteristics of a model oil mixture within nanoscale intra-particle pores of kaolinite minerals, which form pore filling structures in shale rock. To better understand the effects of oil composition, temperature and pressure on the adsorption properties of the model oil mixture, a range of temperatures (298 K, 323 K, 348 K and 373 K) and pressures (1 bar, 50 bar, 100 bar and 200 bar) representing up to reservoir conditions were used. This study shows that adsorption and arrangement of oil molecules is dependent on surface of kaolinite and the distance away from it. The simulations show polar compounds are likely to be adsorbed on aluminol kaolinite basal surfaces, while alkanes preferentially to be adsorbed on silicate surfaces. In addition, the number of oil molecule bound layers, and total adsorption amount on the silicate surface is greater than the aluminol surface. The density of adsorbed oil is reduced with increase in temperature, while the effect of pressure is not as significant. On the basis of performed molecular simulations, we show the adsorption rate of shale oil on the surfaces of kaolinite sheets and assess the removable capacity of the model oil.