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# The influence of surfactant flooding on oil displacement in Nano-Silica Pores

Wednesday, 2 June 2021 09:00 (1 hour)

Surfactant flooding has considered to be one of the most useful approach to recovery residual oil that trapped in pore space after waterflooding. From a macroscopic perspective, this is the surfactant molecules –that are adsorbed on the oil/water interface –would significantly reduce the interfacial tension (IFT) and thus result in the change of wettability in the oil-water reservoir system. However, the microscopic mechanism of surfactant structure (the hydrophilic headgroup and the hydrophobic hydrocarbon chain) effecting on IFT and contact angle is still lack of deep investigation.

In the present study, we performed a detailed molecular dynamics (MD) simulation (all the simulations are conducted with the open-source MD code - LAMMPS) study to understand the displacement and transportation of oil droplets in nanopores with surfactant solution interactions at the atomic levels. We first demonstrated the surfactant molecules forming micelle process in a water environment and then revealed the mechanism of two factors (interfacial thickness and interface formation energy) effecting on surfactant-IFT reduction as well as the temperature sensitivity with respect to IFT. Related results are consistent with previous simulation and experimental work (Palazzesi et al., 2011; Xu et al., 2013). The surfactant molecules have been further added into water/oil system to investigate the influence of surfactant flooding on oil droplet displacement and transportations. Liquids/silica pore surface wettability associated with the surfactant additions is evaluated by the contact angle of oil droplet at the three-phase contact line.

# **Time Block Preference**

Time Block A (09:00-12:00 CET)

#### References

Reference

Palazzesi, F., Calvaresi, M., Zerbetto, F., 2011. A molecular dynamics investigation of structure and dynamics of SDS and SDBS micelles. 7, 9148-9156.

Xu, J., Zhang, Y., Chen, H., Wang, P., Xie, Z., Yao, Y., Yan, Y., Zhang, J., 2013. Effect of surfactant headgroups on the oil/water interface: An interfacial tension measurement and simulation study. J. Mol. Struct. 1052, 50-56.

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Track Classification: (MS6-B) Interfacial phenomena in multiphase systems