Nanoparticles have already contributed to the technological advances in a variety of industries, such as medicine, electronics, biomaterials and renewable energy production, etc., over the last decade. Recently, a new interest springs up with the application of nanoparticle-based technology in the upstream petroleum industry. Large-scale molecular dynamics simulations could provide fundamental understanding of the role of smart nanoparticles on the upstream oil production, such as enhancing oil transport in micro/nano-sized channel and the prevention of pressure-induced crack of cement sheath behind the casing.

INTRODUCTION

Energy is the number one in the humanity’s top ten problems for the next 50 years. Currently, the main source of energy comes from the easily accessible energy such as oil, gas, and coal. And the oil and gas resource will still dominate the energy mix in near future, although renewable energy such as solar, wind power, biomass, fuel, and geothermal energy, will experience fast growth. With the passing of the era of easy oil and the increasing difficulty of finding new economic resources, much attention of the traditional oil and gas industry has been directed to extract more resources from existing mature oilfields, and from the fields exposed to extremely harsh environments by exploring new technologies and solutions.

Nanoparticles defined between 1 and 100 nanometers in size hold unexpected properties that differ remarkably from those observed in bulk materials primarily originating from the large surface-area-to-volume ratio. Structurally, the decreasing of particle size can directly result in changes in spacing between atoms. This effect is related to the compressive strains induced by the compression of surface atoms, as a result of reduction of surface energy. Small nanoparticles therefore adopt a different crystal structure than their bulky counterpart. Once the compressive strain becomes critical, phase transformation spontaneously occurs. From the chemical point of view, size reduction changes the chemical reaction ability due to the increase in surface area to volume ratio. For example, the utilization of nanocatalysts in catalytic processes significantly enhances the rate, selectivity and efficiency of chemical reactions, and simultaneously result in reduction of waste and pollution. Moreover, a substance can dissolve easily at nanoscale although may not be soluble in water at micro/nano-sized scale due to a significant effect of the fluid, wettability alternation, dispersion and flow behavior of nanoparticles and its link to the atomistic structures. A fundamental understanding of the role of nanoscale on the oil-water binary mixture in a confined nanochannel was studied by using MD simulations based on CLAY force-field. A set of computational experiments in which hydrophilic silica nanoparticles mixed with an oil-water system confined in kaolinite clay nanochannels were performed by MD simulations.

We first examine the effect of nanoparticle on a clay-oil-water system without a driving pressure. Figure 1 presents initial and equilibrium configuration snapshots of a clay-oil-water-nanoparticle multiphase system. Nanoparticles and especially enhanced oil recovery. This paper presents some insights on the effect of nanoparticle on oil/water binary mixture transport through a nanosized channel by MD simulation [1]. In addition, we also discuss the study of nanoparticle-based smart cement for oil and gas production by using large scale computational resources.

NANOPARTICLES FOR ENHANCED-OIL-RECOVERY

Up to now, oil recovery has experienced its primary and secondary stages, some bottlenecks are met in the conventional methods. One of the most promising potentials is to utilize the nanoparticles to increase the recovery efficiency of oil in the reservoirs. It mainly reflects in these aspects: changing the properties of the fluid, wettability alternation of rocks, advanced drag reduction, strengthening sand consolidation, reducing the interfacial tension and increasing the mobility of the capillary-trapped oil. MD simulation is a powerful tool to understand the deformation and flow behavior of nanoparticles and its link to the atomistic structures. A fundamental understanding of the role of nanoscale on the oil-water binary mixture in a confined nanochannel was studied by using MD simulations based on CLAY force-field. A set of computational experiments in which hydrophilic silica nanoparticles mixed with an oil-water system confined in kaolinite clay nanochannels were performed by MD simulations.

To reveal the effect of nanoparticles on the oil-water flow through the nanochannel, three cases of one, two and four nanoparticles placed in water phase of left reservoir were investigated, respectively. Figure 2 displays a typical flow-time snapshot of oil/water fluid with four nanoparticles in a clay nanochannel. It is observed that the flow pressure of oil-water mixture with nanoparticle through the confined nanochannel is found to be strongly channel size dependent. The presence of nanoparticles not only alters the dynamical and structural properties of oil-water-clay systems, but also enhances the oil-water flow through the nanochannel at a small nanoparticle concentration, which implies that nanoparticles can be potentially utilized for enhanced oil recovery. While the nanoparticle-free oil-water flow behaves in a laminar flow manner, with the increase concentration of nanoparticle the flow tends to change from laminar to turbulent type. The nanoparticles first slide along the clay wall in a local low velocity with the process of breaking and forming hydrogen bonds, whereas it goes closer to the aqueous environment, and escapes from the attractive clay wall ultimately to enter into the nanochannel.
Why the integrity problem of cement sheath occurs so often? The answer should trace back to the cement hydration process. The reaction between the water and cement is associated with a loss in volume because the reaction product (solid matter) occupies a less volume than the reactants (cement + water). This volume loss favors pores in the binder phase and can be considered an integral part of the gel and capillary pore structure of solid product [4]. On the further hydration, the pore water is consumed and the pore structure is gradually emptied, resulting in the pressure reduction. This pore structure in the cement sheath could grow with the time, the volume shrinkage on the cement interface, which leads to the potential pathway for the gas migration.

NANOPARTICLE ENABLED CEMENT FOR OIL AND GAS PRODUCTION

Nanoparticle-based cement to avoid the abovementioned problem. Smart nanoparticles have been developed to design a qualified candidate of nanoparticles from the molecular structure with the aid of MD simulations. Next, MD simulations under the NOTUR platforms will be conducted to study the behavior of nanoparticles in cement in the hydration process, to predict the physical and chemical interaction between smart nanoparticles and cement, as well as to better understand the mechanism of cement shrinkage counteraction by nanoparticle. Lastly, in order to link the relationship between the cement mechanical strength and introduced nanoparticles, mechanical loading tests of MD simulations are carried out to investigate the mechanical strength and failure scale. The laboratory work consists of nanoparticle selection, property control and the effect of nanoparticles in cement is ultimately guided by the outcome from MD calculations.

Acknowledgement

This work is funded by the Research Council of Norway via NANOD21/PETROMAKS2 project WINPA (project no. 234624/070) and PETROMAKS2 project SustainCEM (project no. 228971/F30). The computational resources are provided by NITUR - the Norwegian meta-center for computational science. The authors would like to thank Professor Zhiliang Zhang, PhD candidates Mao Wang and Yi Dong for contributing part of the text and proof-reading the manuscript.