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Characterization and Modeling of Silica Nanoparticles Transport Flow for Enhanced Oil Recovery

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Abstract – We present a combined experimental and modeling study of Silica nanoparticles transport flow through permeable media under oil reservoir conditions (temperature, pressure and salinity). We have used Fourier transform infrared (FTIR) spectroscopy, ultraviolet-visible (UV-Vis) spectrophotometer, zeta potential analyzer and dynamic light scattering to characterize the stability of silica nanoparticle dispersions. Complementary, Molecular Dynamics has been used to model and characterize the structural, vibrational and dynamic properties of SiO_2 nanoparticles under H_2O with different concentration of NaCl. A good agreement between the MD simulations and experiments has been observed for the spectroscopic properties (FIG.1).

Nanotechnology opens several opportunities on applications in the Oil & Gas industry. Particulary, subsurface applications of nanotechnology seem to be promising in modify and monitoring reservoir properties, such as wettability and interfacial tension between rock and fluids. In this work, we present a combined experimental and modeling study of Silica nanoparticles transport flow through permeable media under oil reservoir conditions (temperature, pressure and salinity). From the experimental side, we have used Fourier transform infrared (FTIR) spectroscopy, ultraviolet-visible (UV-Vis) spectrophotometer, zeta potential analyzer and dynamic light scattering to characterize the stability of silica nanoparticle dispersions. The surface charge of silica nanoparticle is found to be negative for measured samples having pH greater than 5. The isoelectric point is calculated to be around pH 3.44 by using zeta potential data. The effect of pH and salts such as NaCl, $CaCl_2$ and $MgCl_2$ on dispersion stability are evaluated using these methods. The change in peak position of Si-O bond and its peak intensity are observed as the pH of the nanoparticle dispersion is changed from basic (pH 9) towards acidic (pH 3). The concentration of nanoparticle in the dispersion is kept constant throughout for all experiments. The shift of the peak position towards lower energy may be due to a change in bond order of Si-O as pH decreases. The increase in absorbance of Si-O peak could be a result of a change in molar extinction coefficient (absorbance coefficient). This result indicates a structural change in nanoparticle dispersion as pH decreases and salt concentration increases. To better understand these effects at molecular level, we have applied Classical Molecular Dynamics to model and characterize the structural, vibrational and dynamic properties of SiO_2 nanoparticles under H_2O with different concentration of NaCl in reservoir conditions of Pressure and Temperature. A model of SiO_2 nanoparticles has been build using Monte Carlo techniques. The spectroscopic properties such as Raman and Infra-Red was obtained through Molecular Dynamic calculations using a interatomic potential that mimics an ab-initio data [1] and compared with the experimental ones (Fig. 1). A good agreement between the MD simulations and experiments has been observed. The ionic radial distribution function and H_2O orientation molecules in the MD simulations reveals the molecular mechanisms observed experimentally.

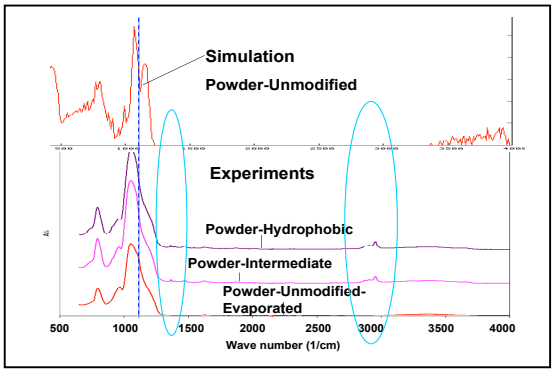

Figure 1: Infra-red spectra comparison between Molecular Dynamic simulations (upper) and FTIR experiments spectra (bottom) for functionalized and unmodified SiO_2 nanoparticles dispersion.

References

[1] A .Pedone et al, Chem.Mater., **20**, 2522, 2008