Challenges of computational simulations addressed for an industrial application of nanomaterials/nanoscience

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Nanotechnology is an emerging field that has been attracting broad interest, especially from the scientific community. The interest of the scientific community is to study new phenomena that come from the effects of scale (usually surface to volume ratio). The exploration of these new phenomena may lead to many new materials and devices with a vast range of applications, such as in nanomedicine, nanoelectronics, biomaterials, energy production, and consumer products

One particular area of industrial interest of nanotechnology application is in the energy sector, more specifically in the Oil & Gas Industry. As oilfields are becoming older and the production is depleting in conjunction with the decline of oil prices which affected the profit margin, oil producers are concentrating more on enhanced oil recovery from existing oil fields than investing in new ones.

Enhanced Oil Recovery (EOR) is a set of techniques employed after water and/or gas flooding, to extract more oil from a reservoir. Among these techniques are CO2 injection, thermal injection (in situ combustion or steam injection) and chemical EOR. Chemical EOR employs materials dissolved in water, such as alkalines, polymers, surfactants and more recently nanoparticles and graphene oxide nano sheets. The use of these nanomaterials together with polymers, alkalines and surfactants, shows some advantages such as increased effectiveness of oil recovery and at the same time a decrease in the amount of material needed.

In this talk I will address the challenge to model effects such as wettability at the nanoscale, transport of fluid in nanochannels, and the behavior of these materials in a complex fluid, in a multi-scale approach.