Nanoscience meets the oil industry: Clues for problem solving from molecular scale insight

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The electronics revolution has given us analytical facilities that make it possible to see directly at the molecular level. Although designed for characterising nanoscale technological materials, these facilities can effectively be applied to natural systems, to provide insight about reactions that take place at the solid-fluid interface, to reveal the nanometer scale structure of solids, and to provide new ideas for solving problems through fundamental understanding of how nature works. There are many examples.

We have demonstrated that pore surface wettability is heterogeneous at the nanometre scale, using atomic force microscopy (AFM) with functionalised tips in chemical force mapping (CFM) mode. X-ray photoelectron spectroscopy (XPS) proves that *all* mineral surfaces have associated organ-ic compounds, even those that have never seen oil, and this material offers anchor points for hydrophobic compounds, regardless of the wetting properties of the underlying mineral. Results from CFM and XPS complement predictions from density functional theory (DFT) and molecular dynamics (MD), to show that sorption of organic molecules or ions can change surface tension dramatically. Only 10% substitution of Mg^{2+} and SO_4^{2-} in calcite for example, decreases the oil-water contact angle by 45 º or more, depending on its initial value. X-ray nanotomography (XNT) and focused ion beam scanning electron microscopy (FIB-SEM) yield 3D images with <40 nm voxel dimension, of the internal structure of rocks, allowing prediction of porosity, permeability and other petrophysical parameters from drill cuttings.

An exciting aspect of our partnership with oil companies is that our insight about solid-fluid interactions and our new methods and software for observing fluid flow can be applied across a range of disciplines, because the work is fun-damental, revealing basic chemical, physical and biological relationships. So new knowledge about how to change pore surface properties to release more oil can be used for remediating contaminated soil and groundwater. The effect of surfactants on pore surfaces provides insight into how organisms control their environment, to biomineralise shells, bones and teeth. The ability to predict fluid behaviour in core plugs is easily transferred to other porous media, such as catalysts, filtration membranes and biomineralised material.