Diminished Fluid Transport through Carbon Nanochannels Induced by COOH Functionalization: Implications for Nanofiltration and Oil Recovery

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Natural rocks, present in shale reservoirs, exhibit a nanoscale porous structure. In particular, the shale gas can be occluded in an organic nanoporous material called kerogen. In the oil industry, kerogen is characterized by its maturity, which is measured by its O / C ratio. In this line, we model kerogen material as carbon nanochannels (CN) with carboxylic groups (COOH) anchored on their inner surfaces. As discussed in the scientific literature, extraordinarily high flow rates have been obtained in CNs that cannot be predicted with standard macroscopic theories. In this work, we determine the effects of COOH of the inner surfaces of CN on fluid transport. We consider water and methane as representative cases of polar / non-polar fluids and also mixtures of them. We found a significant reduction in flow rates for all fluids due to geometric distortion associated with COOH functionalization. In particular for water, we observed not only a dramatic reduction in flow rates, but also structural changes in which the COOH groups act as nucleation centers for water droplets. Consequently, we determine that the flow rates depend on the CN O / C ratio, or in other words, on the maturity of the kerogen. We determined that the presence of a small amount of dispersed COOH groups helps to distribute the water molecules along the walls of the nanochannel, opening a path for the hydrocarbons to flow. Therefore, the relationship between rock permeability and maturity can provide a way to identify high conductivity zones for hydrocarbon recovery. Another application is the possible use of chemical additives to improve the flow of hydrocarbons in kerogen-rich rocks.

Speaker Biography

Verónica M Sánchez has completed her PhD at the age of 28 years from University of Buenos Aires, Argentina. She has been a postdoctoral fellow at the Nanochemistry Group at CNEA (National Entity of Atomic Energy), Argentina. She completed also a postdoctoral fellowship at the Nanopetro Research Group at Federal University of ABC, SP, Brazil. She is currently an associate researcher at Institute of Physical Chemistry, Environment and Energy (INQUIMAE) - CONICET (National Scientific and Technological Council). She is leading a research line on Computational Simulation of Physical Chemistry Processes of interest in Energy and Catalysis. She is a professor at School of Science and Technology at University of San Martin, Buenos Aires, Argentina. She has 17 publications that have been cited over 450 times, and her publication H-index is 12.

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