Geophysical Research Abstracts,
Vol. 11, EGU2009-4350, 2009
EGU General Assembly 2009

The influence of modification of pore walls by organic molecules on adsorption, solvation forces and fluid transport in slit-like pores

M. Borowko (1), A. Patrykiejew (1), S. Sokolowski (1), and Z. Sokolowska (2)

(1) MCS University, Department for the Modeling of Physico-Chemical Processes, Lublin, Poland (borowko@hektor.umcs.lublin.pl), (2) Department of Physical Chemistry of Porous Materials, Institute of Agrophysics, Polish Academy of Sciences, Lublin, Poland

Soil organic matter and clay particles can form together the so-called clay-organic complexes. In the case of layered clays, like montmorillonite, that exhibit slit-like porous structure, the organic chains can be bonded to both pore walls. Consequently, instead of channels with bare surfaces, we are dealing with pores possessing modified surfaces, covered with organic particles. In extreme cases the organic molecules can form "bridges" fixing the pore width.

The presence of chemically bonded particles covering pore walls causes that the adsorption, possibility of swelling (or shrinking), transport of gases and water, as well as ions changes, compared with non-modified pores.

In this work we use density functional theory to study behavior of fluids in slit-like pores with walls modified by tethered chain molecules. We investigate how the confinement and chemical modification of pore walls affect adsorption and solvation force. Two models of the pore walls are considered. According to the first model, the chain molecules are chemically bonded by their end segments to opposite walls of the pore, forming flexible pillars. In the other the chains build up a brush at each wall due to bonding of the first segment at one wall. The non-bonded terminating segment of a molecule is strongly attracted via a short-range potential to any wall of the pore. Then a pillar-like or loop-like structure of chains can be formed. In the first model the solvation force at the wall-to-wall is repulsive for narrow pores and strongly attractive for wider pores of the order of the nominal chain length. Oscillations of the solvation force are induced by adsorbed fluid structure and by ordered structure of segments on the fragment of entirely attractive force curve. In the second model, however, the solvation force decays to zero as the pore width increases. Attractive force can be induced at intermediate separation between walls due to modification of the pore walls.

Moreover, we also discuss the application of computer simulations to study the formation of liquid meniscus in the pore with modified walls and its transport through the pore under external pressure applied.