Contribution ID: **224**   Type: **Oral 20 Minutes**

Non-uniform density of gas confined in nanopores.

Tuesday, 15 May 2018 11:17 (15 minutes)

Unlike macroscopic objects, any system of nanometric size shows characteristics that strongly depend on its size and geometric form. It is the consequence of the fact that the major part of atoms (or molecules) of nano-object is located at its surface, their cohesive energy is smaller than for the atoms in the bulk.

Here we show that when a fluid is confined in nano-volume, delimited by non-interacting pore walls, its density is heterogeneous, decreases close to the pore wall, and, on average, is smaller than the density of bulk fluid. The heterogeneity of distribution of fluid density, resulting from the nano-confinement, progressively weakens when the pore size increases, and totally disappears for pores larger than 5 nm. On the other side, in the limit of very small pores, the fluid density approaches the ideal gas value. This effect should be distinguished from the well know heterogeneity of density of fluids adsorbed in nanopores, driven by the difference between the strength of fluid-fluid and fluid-pore wall interactions, that varies with the distance from the pore wall.

The reported observation has non-trivial influence on evaluation of excess/total adsorption in nanopores, as these two quantities are calculated assuming the known –and homogeneous –bulk density of gas in the pore. Additionally, the gas density in the pores depends on the definition of the pore volume which is neither straightforward nor unique. The right estimation of both: pore volume and gas density is essential for quantitative interpretation of experimental adsorption isotherms: evaluation of pore size distribution and of the amount of adsorbed gas. We analyze this problem on an example of five gases: H_2, CH_4, the two intensively studied energy vectors, and N_2, Ar, and Kr, commonly used for characterization of porous structures. For H_2, the distributions of densities of gas confined in adsorbing and not adsorbing pores are compared and commented.

References

Acceptance of Terms and Conditions

Click here to agree

Primary author: FIRLEJ, Lucyna (University of Montpellier, France)

Co-author: Prof. KUCHTA, Bogdan (Madirel, University Aix-Marseille, France)

Presenter: FIRLEJ, Lucyna (University of Montpellier, France)

Session Classification: Parallel 4-E

Track Classification: MS 1.12: Fluids in Nanoporous Media