ADSORPTION OF HYDROGEN AND METHANE MIXTURES IN CARBONACEOUS CAVITIES

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Hydrogen clean production is a requested technology when considering hydrogen fuel cells for energetic applications. A considered alternative to obtain hydrogen without producing CO/CO_2 as byproducts is methane catalytic decomposition. Several carbon-based catalysts materials have been proved in this reaction including activated carbon, carbon black carbon fiber and carbon nanotubes. On the other hand, behaviour of hydrogen and methane mixtures confined in carbonaceous cavities has been studied to consider carbon-based membranes(1) for gas separation, as a necessary purification stage that follows hydrogen production.Dependence on operational pressure and selectivity for methane and hydrogen separation has been shown in several works(2), exhibiting a methane selectivity that decreases as pressure is increased. When using molecular simulation in the context of studying mixed gas adsorption, focused either in gas storage or gas separation, there are several characteristics that are accessible. Some of these characteristics are component density profile or mass distribution within the cavity volume, and single pore size adsorption capacity and selectivity, which allow a microscopic description of phenomena. These results leads, in some extension, the material design, focusing desirable characteristics and performance.
In this presentation, we use Grand Canonical Monte Carlo simulation of pure hydrogen and methane and their binary mixtures confined in cylindrical carbon cavities. Besides adsorption isotherms and equilibrium selectivity, density profiles and adsorption energy distribution functions were obtained. Adsorption energy distributions can be considered as a useful tool to study energetic heterogeneity of adsorption phenomena (3). Extension and characteristic of hydrogen physisorption are established. For carbon mesopores hydrogen density profile shows two regions that corresponds to an adsorbed phase and a compressed fluid in the middle of pore width. Tendency in the variation of methane selectivity with pressure is explained considering adsorption energy of both compounds. Energy distribution functions for mixture adsorption reveal an enhacement in hydrogen adsorption when comparing these results to pure compound adsorption. In addition, these results indicate that a selective desorption could be obtained in several pore sizes

[1] M. B. Rao, S. Sicar. J. Membr. Sci. **110**, 109 (1996).

[2] A. M. Vieira- Linhares, N. A. Seaton. Chem. Eng. Sci **58**, 4129 (2003).
[3] G. Calleja et al. Appl. Surf. Sci. **252**, 4345 (2006).