2° Simposio sobre Adsorción Adsorbentes y sus Aplicaciones

# PORE SIZE CHARACTERIZATION STRATEGIES USING ISOTHERMS OF DIFFERENT PROBE-GAS

***P. Silvino, D. Gonçalves, R. Gonçalves, S. Lucena*, D. Azevedo***

Grupo de Pesquisa em Separações por Adsorção – GPSA, Dept. de Eng. Química, Centro de Tecnologia, Universidade Federal do Ceará, BRASIL

*lucena@ufc.br

**ABSTRACT**

*Pore size distribution (PSD) is an essential textural data of an activated carbon (AC) sample, it is a characteristic combination of different pore sizes which can represent the molecular framework of sample. Surface area, total volume of pores and adsorptive capacity can be estimated by PSD. To obtain the PSD for an AC is necessary to compare its experimental isotherm with a local isotherm database (Kernel), obtained for different size pores via molecular simulation. This distribution must be unique for a given sample, independent of the probe-gas used, however a PSD obtained for a gas do not always reproduce the adsorptive behavior of that sample with other gases. Adsorption isotherms of WV-1050 AC, with nitrogen at 77 K, carbon dioxide at 298 K and methane at 303 K where analyzed, yielding its respective PSD based on Kernels generated via grand canonical Monte Carlo (GCMC) simulations. The PSDs obtained for nitrogen and carbon dioxide was used, individually, to reproduce the three experimental isotherms, yielding significant deviations. Trough volume normalization, the isotherm fitting was significantly enhanced.*

**Keywords**: Molecular Simulation, Adsorption, Pore Size Distribution.