223b Water Adsorption Isotherms in Molecularly Reconstructed Models of Activated and Un-Activated Carbons Obtained from Saccharose

Alberto Striolo, Surendra K. Jain, Jorge P. Pikunic, Roland J.-M. Pellenq, Ariel Chialvo, Keith E. Gubbins, and Peter T. Cummings

We present recent developments aimed at improving our understanding of water adsorption in carbons. To investigate the effect of pore morphology on the features of adsorption isotherms, we previously simulated the adsorption of water in carbon-slit pores [1], single-walled carbon nanotubes [2,3], and connected carbon-slit pores [4]. We consider now the adsorption of water in realistic representations of carbon adsorbents. Two carbon samples are considered: a semi-coke, named CS1000, and an activated form of this carbon, CS1000a. Experimentally, the CS1000 sample was obtained by pyrolysis of pure saccharose at 1000„aC under nitrogen flow. The CS1000a sample was obtained by heating the CS1000 sample in a CO2 atmosphere for 20 hours. We used a constrained Reverse Monte Carlo method to build carbon molecular models that match the experimental structure factors of both CS1000 and CS1000a. The Reverse Monte Carlo method was combined with appropriate constraints for bond angle and coordination number to describe three-body correlations [5,6]. Using the grand canonical Monte Carlo algorithm, we compute adsorption isotherms and isosteric heats of adsorption for water in CS1000 and CS1000a at 298 and 498 K. We discuss our results with comparison to the adsorption of water in independent carbon-slit pores and with experimental results. Our results provide evidence that suggests the need for a molecularly precise representation of the adsorbent material for the accurate prediction of water adsorption in both activated and un-activated carbons.

Key words: SPC/E water, isosteric heat of adsorption, adsorption/desorption hysteresis

References 1. A. Striolo, A.A. Chialvo, P.T. Cummings, and K.E. Gubbins, Water Adsorption in Carbon-Slit Nanopores, Langmuir, 19 (2003) 8583-8591. 2. A. Striolo, K.E. Gubbins, A.A. Chialvo, and P.T. Cummings, Simulated Water Adsorption Isotherms in Carbon Nanopores, Molecular Physics, 102 (2004) 243. 3. A. Striolo, A.A. Chialvo, K.E. Gubbins, and P.T. Cummings, Water in Carbon Nanotubes: Adsorption Isotherms and Thermodynamic Properties from Molecular Simulation, Journal of Chemical Physics, (2005) in press. 4. A. Striolo, K.E. Gubbins, A.A. Chialvo, and P.T. Cummings, Effect of Pore Connectivity on Water Adsorption Isotherms in Non-Activated Graphitic Nanopores, Adsorption, (2005) in press. 5. J. Pikunic, C. Clinard, N. Cohaut, K.E. Gubbins, J.-M. Guet, R.J.-M. Pellenq, I. Rannou, J.-M. Rouzand, "Structural Modeling of Porous Carbons: Constrained Reverse Monte Carlo Method", Langmuir 19 (2003) 8565-8582. 6. S.K. Jain, J.-P. Pikunic, R.J.-M. Pellenq, K.E. Gubbins, "Effects of Activation on the Structure and Adsorption Properties of a Nanoporous Carbon Using Molecular Simulation", Adsorption (2005) in press.