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Hydrogen storage: predicting at room temperature in a series of activated carbons

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Fuel cell vehicles hold significant promise for decreasing both energy consumption and carbon dioxide emissions. Hydrogen storage is the key technology towards the hydrogen society [1]. Vehicular hydrogen has been stored in special tanks at very high pressures (700 bar) with obvious disadvantages in the energy cost of compression and safety. The use of adsorbed H2 instead of compressed H2 can be a solution to enable safer and more economical storage. Conducting experimental studies of H2 adsorption at high pressures may present operational difficulties and risks. In this study we propose the prediction of H2 adsorption up to 700 bar using the Monte Carlo algorithm in the grand canonical ensemble and the representative pores method that we applied previously in the prediction of isotherms of C1 to C4 [2], H2S [3,4]. Based in that methodology, we predict the adsorption capacity of H2 at 298K between 0.8 to 700 bar on different commercial carbons using textural information of N2 at 77K and CO2 at 273K. At pressures up to 100bar we obtained a good agreement with the experimental data available.

The samples ACC10 and WKL20 have considerable volumes of pores concentrated in the region of well-defined micropores and show a maximum adsorption at 240 bar. The samples ACC15 and ACC20, which have pore volumes in the mesopore region, reach maximum adsorption at pressure of 190. The ACC20 sample presents the highest adsorption amount of 3.15 mmol/g. Among the simulated isotherms of figures 5 and 6, we highlight the carbon Maxsorb, the best result after that presented by carbon ACC20, with 2.96 mmol/g at 130 bar. The Maxsorb sample has simultaneously high volumes in the micro and mesopore regions. This means that an activated carbon that has well-developed regions of microporosity and mesoporosity will have considerable adsorption capacity at relatively small pressures. It was possible to determine the maximum pressure where the highest adsorption of H2 occurs at 298 K with emphasis on Maxsorb that reached 6.14 wt % at 700 bar, near the US Department of Energy (DOE) target value of 6.5 wt.% .

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