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Inverse gas chromatography, a new technique for correlating surface energy porous media to saturation

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Multiphase flow and reactive transport in porous media play a key role in various applications needed for establishing hydrogen as an alternative energy carrier. To successfully establish hydrogen, the porous media facilitating the hydrogen flow in presence of another fluid, needs to be optimized in terms of reactivity and transport properties. Two important parameters controlling reactivity and multiphase flow transport in a porous medium are surface area and surface energies of porous media surface in relation to saturation. In this study, inverse gas chromatography (iGC) is proposed to simultaneously measure surface energy distribution and surface areas of porous media in correlation to saturation.

Inverse gas chromatography (iGC) is a powerful, sensitive, and relatively fast technique for characterizing the physicochemical properties of porous media such as BET surface area and surface energy distribution [1]. In this technique, a single gas, known as probe molecules, is injected into a column packed with the porous sample under investigation. The probe molecules pass through the column, interact with the porous material, and the retention time of the probe molecules is measured at the end of the column. Measuring the retention time for different probes, e.g. polar and non-polar, enables us to determine a wide range of physicochemical properties of the porous material. Recent advances in commercial IGC enable users to perform the iGC measurements at different controlled humidity. Due to the capillary condensation, different relative humidity can create wide range of saturation. By performing classical iGC experiments in these conditions, surface energy distribution and surface area of sample, for the first time, can be correlated to saturation under same experimental conditions. Depending on the degree of hydrophilicity of the sample, water follows different adsorption/saturation mechanisms as relative humidity of experiments increases. In the following paragraph, the expected results of iGC measurements on Teflon samples, representing hydrophobic situation, is discussed.

The water molecules' presence in the system initially adsorb on surface high-energy sites, i.e. polar functional group or cracks on the surface, and then as the relative humidity of experiments increases, based on the competition between cohesive and adhesive forces, water adsorption would continue on either the surface or the initial adsorbed molecules to form clusters [2,3]. In the case of the hydrophobic sample, the water saturation mechanism follows the latter scenario. In this stage, a decrease in polar component of the surface energy is expected (shown in Figure 2). The increase in size clusters as RH increases would result in a slow decrease in measured dispersive component and BET surface area. Clusters continue to grow until they reach to critical size when first stable nanodroplets can form on the surface. The formation of nanodroplets will cause an abrupt decrease in BET surface area and, conversely, increase in the polar component of surface energy due to the formation of stable water surface. As the RH of experiments increases, nanodroplets start to merge and slowly cover the surface, which results in a further decrease in surface area and a slow decrease in surface energy components.

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