Contribution ID: **748** Type: **Poster Presentation**

Innovating porous materials characterization for hydrogen-storage applications

Thursday, 25 May 2023 15:30 (1h 30m)

Multiphase flow and reactive transport in porous media play a key role in various applications needed for establishing hydrogen as an alternative energy carrier. 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 in relation to saturation. In this study, inverse gas chromatography is used to correlate surface energy distribution and surface areas at different relative humidity conditions. Due to capillary condensation, the varying humidity conditions reflect a range of saturation. The retention time of probing molecules injected, and the dispersive component of surface energy derived from it, are expected to decrease as humidity increases. The trend for polar/acid-base component of surface energy is not necessarily clear as the interaction of polar probes with water can cause tag-along or displacement effects.

Methodology: Inverse Gas Chromatography
Inverse gas chromatography (iGC) has been reported as a powerful, sensitive, and relatively fast technique for characterizing the physicochemical properties of porous media such as BET surface area and energy distribution of the surface [1]. In this technique, a single gas, known as probe molecule, 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.

Discussion: Measurement in humid conditions
Recent advances in commercial IGC enable users to perform accurate experiments at different humidity. The water molecules' presence in the system initially adsorb on high-energy sites of the surface and gradually change the surface area of porous material exposed to other components in the system [2]. By measuring surface energy at different relative humidity, one can correlate the surface area to surface energy. In practice, the presence of water in the system would hinder the adsorption of probe molecules, depending on intermolecular forces between them, known as a tag-along effect [3], and/or competition in adsorption. In the case of using non-polar probes, e.g. n-alkanes, it is expected to see a decline in retention time, surface area, and the dispersive component of surface energy as humidity increases. This is due to the fact that water molecules will interact with high-energy sites on the surface, covering part of it (figure 1). In the case of polar probes, used for the determination of polar or acid/base components of surface energy, the trend is not clear. Interaction between water and polar probes is stronger than with non-polar and may cause the formation of a cluster or concentration-dependent displacement effects. In this study, we assess the effect of water in the determination of surface area and surface energy by IGC, parameters which control multiphase flow and reactive transport in porous media.

Participation

In-Person

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Session Classification: Poster

Track Classification: (MS10) Advances in imaging porous media: techniques, software and case studies