1-BUTANOL ABSORPTION IN P(S-DVB) ION EXCHANGE RESINS

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A highly crosslinked poly(styrene-divinylbenzene) resin, P(S-DVB), was modeled by a stochastic algorithm developed to that end. The generated polymer networks presented a complex topology characterized by a very heterogeneous distribution of crosslinks and length of polymer chains and by the existence of internal loops (closed polymer chains) of different size. These topological characteristics were found to be essential to reproduce satisfactorily, once the structures were relaxed (using MD), the experimental values of apparent density, porosity and pore volume.

Structures with a particular topology (selected based on its good agreement with experimental results) were used to study the effect of a polar solvent (1-butanol) on the resin structure by means of MD simulation. It is a well-known fact that P(S-DVB) resins swell in polar media.[1] Figure 1 represents the variation of the calculated volume increase (ΔV) against the concentration of absorbed alcohol (X_{OH}). For X_{OH} < 20% the resin matrix experiences a contraction, less pronounced as the X_{OH} increases. For X_{OH} > 20% the volume increases with the concentration of absorbed alcohol. Dotted lines represent the experimentally determined values of X_{OH} (vertical) and ΔV (horizontal) corresponding to the swollen resin. Thus, the swelling predicted by the model is in good agreement with the experimental results. Furthermore, preliminary calculations of the energy change between the dried and the swollen systems indicate that the maximum amount of 1-butanol that the resin can absorb is closed to 30%, enforcing the reliability of the obtained results.

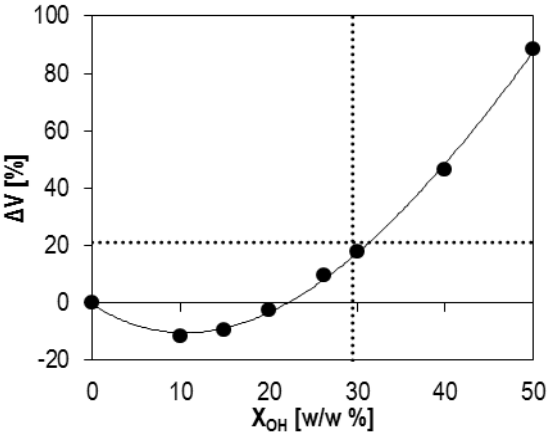

Figure 1. Variation of volume increasse (ΔV) against the concentration of absorbed 1-butanol.

A deeper study of the polymer matrix indicates that 1-butanol absorption entails important changes on the porosity and apparent density of the resin. For the lowest X_{OH} (10%) porosity is significantly reduced with respect to that of the dried resin. However, as the amount of absorbed

alcohol increases, the polymer matrix recovers some porosity and tend to be less dense (the volumetric fraction of the resin with low polymeric chain density increases whereas zones with very high density tend to disappear). All that indicates that the presence of 1-butanol causes the separation of the polymeric chains enhancing the accessibility to the inner part of the polymer network.

1) B. Corain, M. Zecca, K. Jerabek, *J. Mol. Catal*. A **2001**, *177*, 3–20.