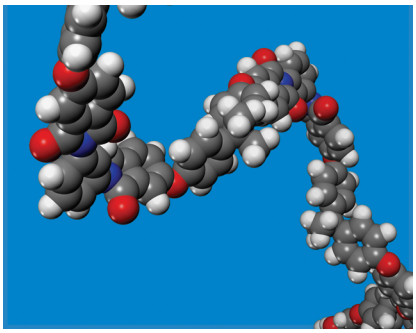
CASE STUDY

REMOVING ORGANIC CONTAMINANTS FROM DRINKING WATER—UNDERSTANDING ZEOLITE WATER ADSORPTION



"We use this type of computational work to develop an understanding of why certain organic molecules have an affinity for certain adsorbents"

Dr R. Thompson
Department of Chemical Engineering
Worcester Polytechnic Institute

Modules used

- COMPASS
- Sorption

Industry Sectors

- Environmental Chemistry
- Chemicals

Organizations

- Worcester Polytechnic Institute, MA

Researchers at the Worcester Polytechnic Institute in Worcester, MA, have used the COMPASS force field and the Sorption module from Accelrys Inc. to predict water adsorption isotherms in silicalite and in dealuminated zeolite Y (DAY)[1].

The affinity that adsorbents have for water can influence their effectiveness in removing organic contaminants from drinking water. The results show that the simulations using the COMPASS force field can correctly predict the shape of water adsorption isotherms and adsorption levels. This paves the way to use Sorption simulations for studying these important systems.

RESULTS

Simulations on water adsorption in zeolite can reveal insight into the competitive adsorption of water with other organic components[2]. Moreover, water can be used as a probe of zeolite properties such as the acid strength[3] product quality, and micropore volume[4]. For these reasons, it is important to investigate the specific properties of water in confined media such as zeolites.

Fig. 1 shows the simulated adsorption isotherms for water in silicalite at five temperatures and over 2 pressure ranges.

The results show that the simulations predict the isotherm shapes for silicalite and DAY (not shown in Fig. 1) at all pressures in agreement with experimental measurements. However, it was observed that at low pressures the amount of adsorbed water was under-predicted in the all-silica zeolites. This was subsequently traced to the intrinsic properties of real zeolites which can contain impurities and defects. These observations can be used to give insights on the possible

structures of the real zeolites. By investigating the influence of various defects on the computed adsorption isotherms, it should be possible to determine the defect types qualitatively.

The study thus provides validation for using Sorption to predict isotherms for these systems, as well as a method for probing the influence of defects on zeolite performance.

Dr R. Thompson, Department of Chemical Engineering, Worcester Polytechnic Institute, said "We use this type of computational work to develop an understanding of why certain organic molecules have an affinity for certain adsorbents, to learn how molecules move through nanoporous materials, and to design new adsorbents that have an enhanced affinity for organic compounds." Dr Thompson continued, "The computations were used to evaluate how water molecules interact with adsorbent pores, potentially interfering with adsorption of organic compounds in water remediation processes."

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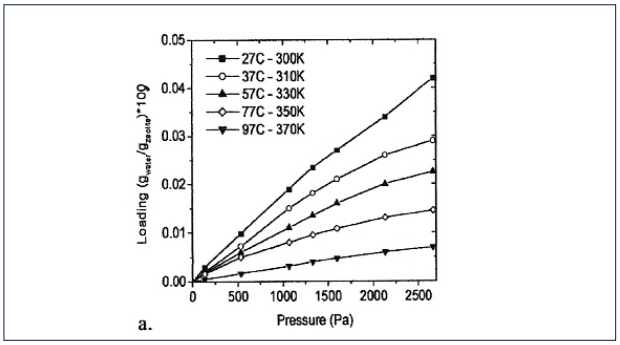

Figure 1. ***a.*** *Water adsorption isotherms in defect-free silicalite from 300 to 370K at low pressures*

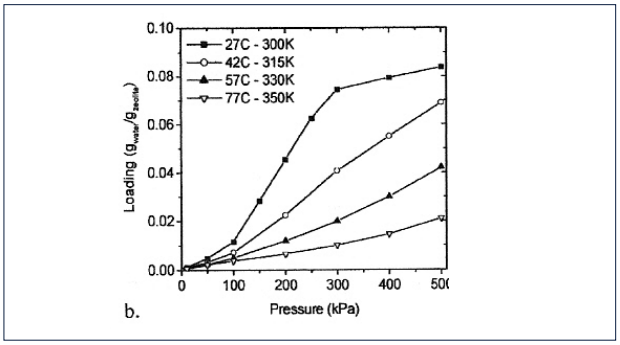

Figure 1. ***b.*** *Water adsorption isotherms in defect-free silicalite from 300 to 350 K at high pressures*

REFERENCES

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2. Khalid, M.; Joly, G.; Renaud, A.; Magnoux, P. Ind. Eng. Chem. Res. **2004**, 43, 5275.
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