

S3.2.1 ADSORPTION MECHANISMS OF VOC ONTO ACTIVATED CARBON USING 1H NMR AS A USEFUL TOOL

Pierre Le Cloirec, Guirec Le Bozec, Sylvain Giraudet, Laurent Le Polles
Ecole Nationale Supérieure de Chimie de Rennes

Volatile organic compounds (VOC): benzene, cyclohexane, dichloromethane, were adsorbed onto an activated carbon fiber cloth. ^1H (magic angle spinning, MAS, and pulse field gradient, PFG) nuclear magnetic resonance (NMR) techniques were carried out. The peak surface areas and shifts of the signals were analysed the MAS NMR was shown to be very useful to quantify the amount (0.2 to 4 mol.kg⁻¹) of adsorbed molecules (VOC and/or water) in the porosity of the adsorbent. The mechanisms of interactions between adsorbed organic molecules and the carbon walls were proposed. The positions of the adsorbed molecules inside the pore volume are given. The proton-wall distance was less than 0.15 nm. This observation was obtained from the chemical shift in NMR spectra and was confirmed by the pore size distribution of the adsorbent.

PFG NMR was used to assess the diffusivities of VOC inside the porous structure. The surface diffusion coefficients (DS) were estimated at approximately $4 \cdot 10^{-12}$ m².s⁻¹ for cyclohexane, $1 \cdot 10^{-11}$ m².s⁻¹ for benzene and $4 \cdot 10^{-11}$ m².s⁻¹ for dichloromethane. These values have to be confirmed but they could be used in kinetic models or breakthrough curve modelling.