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# Computing the temperature dependence of adsorption selectivity in porous solids.

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**Abstract**

We describe a method that computes gas adsorption equilibria in porous solids, at arrays of temperature and mixture compositions. The method uses an initial dataset of single component adsorption isotherms, obtained either from experiment or grand canonical Monte Carlo simulations. It utilizes the Clausius Clapeyron equation to expand the number of the available isotherms for the adsorbate components at a specified sequence of temperatures. It employs the ideal adsorbed solution theory (IAST) on the expanded data for the complete range of mole fractions in the mixture. We show case the method considering experimental isotherms of $CO_2$ and $CH_4$ adsorption at near ambient temperatures, for an activated carbon cloth, an ordered mesoporous carbon and on the alpha phase of magnesium formate. In the same context, we produce a set of simulated adsorption isotherms for a zeolitic imidazolate framework, namely ZIF69. The adsorbate mixture capacities of $CO_2$ and $CH_4$ on ZIF69, predicted by the IAST method are validated with explicit mixture adsorption simulations performed at the same conditions of interest. The method is appropriate for fast screening the selectivity performance of porous solids aiming to minimize the effort regarding experiments for multicomponent physisorption.

*Keywords:* multicomponent adsorption, molecular simulation, Clausius Clapeyron, CO2 capture, zeolite, carbon, MOF

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