

GUIDELINES FOR THE REPORTING OF DATA ON ADSORPTION AND DIFFUSION IN POROUS MATERIALS

The following describes requirements necessary for manuscripts reporting data on adsorption and diffusion in porous materials to be published in the *Journal of Chemical and Engineering Data (JCED)*. These guidelines are given as a supplement to the general *Author Guidelines* for JCED:

http://pubsapp.acs.org/paragonplus/submission/jceaax/jceaax_authguide.pdf

- **In scope adsorption and diffusion data**

- Equilibrium adsorption data from measurements controlling temperature, pressure, and/or composition (or, more generally, the chemical potential) of the adsorbate(s) or batch measurements controlling adsorbent dosage and initial adsorbate concentration.
- Single- and multicomponent adsorption from gas, vapor, liquid, and supercritical fluid phases (solid-liquid, solid-vapor, solid-gas, and solid-supercritical fluid).
- Single- and multicomponent diffusion in porous materials under equilibrium conditions (i.e., without chemical potential gradient and solely controlled by the molecules' self-diffusivity).
- Thermodynamics of adsorption (e.g., Henry's coefficient, isosteric heat of adsorption, free energy of adsorption).

- **Out of scope**

- Adsorbent materials with unknown or hardly reproducible properties (i.e., chemical composition, structure, pore size distribution, defects), such as natural product materials, when these are not sourced from large batch suppliers and materials data sheets are not available.
- Work that mainly focuses on adsorbent synthesis and characterization.
- Adsorption kinetics (i.e., transient uptake measurements); batch and/or dynamic column adsorption experiments, when these are not used to measure equilibrium properties.

- **Article title and Abstract**

- The presence of new experimental and/or computational data should be made clear in the title, which must include the name of the adsorbent(s) and adsorbate(s). Abbreviations should not be used.
- The abstract must include all of the following: (i) chemical systems; (ii) experimental/computational methods; (iii) measured properties, including experimental/simulation conditions; and (iv) macroscopic modeling approaches (if applicable).

- **Chemical substances**

- Their description must be included in a chemical sample table that conforms with the general *Author Guidelines* cited above.
- The table should also include molecular weights, purities, sources, and either CAS registry numbers or 2D/3D chemical structures of adsorbates and adsorbents.
- The mode of sample pre-treatment and outgassing, and the composition of the adsorbents must be specified, and their surface chemistry and area, as well as, pore size distribution must be characterized or, for crystalline materials, their atomic structure must be provided.

- **Experimental and/or computational methods**

- *Description*: the experimental and/or computational method must be fully described, including the approach used to quantify the method's uncertainties. Methods used to attain and confirm the establishment of equilibrium conditions must be described.
- *Validation*: the experimental and/or computational method must be validated by measurements for, at least, one system for which multiple consistent data are available in the literature. The results from the validation measurement(s) must be presented in tabular form, and deviation from literature values must

be given in numerical or graphical form. If exactly the same apparatus or computer algorithm/software was used for a prior publication, description of this prior work can substitute for new validation measurements. For computational approaches setting the chemical potential (μ) of the adsorbates, a description preferably with validation must be provided for the conversion of μ to pressure or concentration from lowest to highest value.

- *Reproducibility*: the measurement of one adsorption isotherm or diffusivity should be repeated for two (or more) separate aliquots from the same batch and activated individually, resulting in two (or more) independent data sets. The results from these measurements must be presented in either tabular or graphical form.
- **Experimental and/or computational data**
 - All measured experimental and/or computational equilibrium adsorption and diffusion data must be reported in stand-alone tables, as described in the general *Author Guidelines* cited above. The standard uncertainty or the relative standard uncertainty must be included for all quantities.
 - For the studied systems, a graphical comparison must be provided for all available literature data, as described in the *Author Guidelines*; the studied systems should be compared to related systems in the literature (e.g., with same adsorbate or same adsorbent).
- **Adsorption data**
 - The amount of measured adsorption equilibrium data presented must be substantial. Specifically, at least 4 different experimentally measured adsorption isotherms (e.g., at different temperatures or with different adsorbates) should be presented with a minimum of 40 data points (combination of adsorbent, adsorbate, temperature, and pressure/solution concentration). Measuring adsorption and desorption branches and using two or more cycles is highly recommended.
 - For all adsorption data sets, the equilibrium conditions must be completely described. For multicomponent adsorption, this must include a description of both the adsorbed (in the porous material) and adsorptive (reservoir) phases in a manner that satisfies the Gibbs phase rule *after equilibrium between the phases has been achieved*.
 - All measured adsorption data should also be presented graphically with the amount adsorbed plotted against the equilibrium partial pressure or concentration (linear or logarithmic) in scatter charts including error bars.
 - For adsorption measurements made at high pressure, the isotherms should be presented in terms of the surface excess amount of adsorbed substance and plotted against gas fugacity (or density) in scatter charts including error bars. The skeletal volume of the solid and its uncertainty should be reported, too.
 - For adsorption from a solution phase, a clear description with supporting evidence must be provided as to how the amount of solvent adsorbed is determined. For adsorption of ionic species, a clear description with supporting evidence must be provided on the extent of counter-ion adsorption or ion exchange.
 - Fitting measured adsorption isotherm data to macroscopic adsorption isotherm functions is encouraged. Model fittings (e.g., Langmuir isotherm) may be shown alongside the experimental data in figures. However, model fittings are not primary data, and their detailed description and the resulting parameters should be presented in the Supporting Information.
 - If thermodynamic data are deduced from adsorption isotherms, then the temperature interval for adsorption isotherm measurements should be appropriate for the absolute temperature of interest (e.g., 30 K near room temperature).
 - The reporting of isosteric heats of adsorption estimated from the experimental isotherm data is strongly encouraged; to this end, the description of the procedure for computing the isosteric heat of adsorption must include statement of all mathematical and thermodynamic simplifications and the equation of state (if used).

- Calculation of standard Gibbs energy, enthalpy, and entropy of adsorption must be based on data in the Henry's law region and the activity/fugacity model for the adsorbate reservoir must be described.
- For molecular modelling and simulation, the thermodynamics of transfer processes can be described via standard state convention (using molar concentration as standard state) or via relation to excess chemical potential (using the ideal gas as reference state).
- **Diffusion data**
 - The amount of measured equilibrium data presented must be substantial. At least 10 different experimentally measured diffusivities should be presented (e.g., at different temperatures, loadings, total concentrations or with different adsorbate/adsorbent pairs).
 - A clear description with supporting evidence must be provided to support that the measurement pertains to diffusion within a homogeneous material and under equilibrium.
 - All measured diffusion data should also be presented graphically with the diffusivities plotted against, e.g., the inverse of temperature, loading or total concentration, in scatter charts including error bars.