

pyMono: Library for estimating the parameters of single-component isotherms

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ABSTRACT

This work presents the development of a Python library "pyMono" for the estimation of parameters of adsorption isothermal models. Adsorption, which began to be studied in the eighteenth century, is crucial for various industrial and environmental applications. In the hierarchical construction of a mathematical model to represent the adsorption process, the first step is the definition of an adsorption isotherm model. Theoretical models such as Langmuir isotherms, Sips, Toth, BET and GAB, are fundamental to understand and predict the adsorption equilibrium at the gas-solid and liquid-solid interfaces. The pyMono library allows the creation and analysis of experimental isotherms in a simple, fast and free way, supporting several theoretical models. It is designed to be used in any Python 3.0 environment, requiring additional libraries such as numpy, scipy, matplotlib, and csv. The software makes it possible to create isotherms directly from pressure/concentration and adsorbed quantity lists or by importing .xlsx or .csv files. In addition, it offers functions for parameter estimation, error calculation, and visual comparison between experimental and simulated data. To validate the tool, adsorption data from materials from recent studies were used, covering different adsorbents and experimental conditions. The validation included the analysis of 40 isotherms of articles published between 2022 and 2023, using different theoretical models to determine the accuracy of the estimated parameters, for which the mean absolute error was less than 10% were obtained by at least one model. pyMono proved to be effective in obtaining adsorption parameters, contributing to the advancement of studies in this area. The work highlights the importance of adsorption in purification and separation processes in industry, and the developed library represents a valuable tool for researchers working with adsorption.

Keywords: pyMono, Adsorption, Isotherms, Parameter estimation.

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