MONSAIC
Monte Carlo Simulation for Adsorption in Nanoporous Materials and Integrated Characterization

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User Manual
Platform MONSAIC

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Introduction

Objective of the Platform

The "MONSAIC" platform, developed in Python, offers an accessible and user-friendly platform for visualizing and analyzing adsorption data related to nanoporous materials. MONSAC utilizes libraries or kernels of simulated adsorption isotherms that incorporate details about the geometry and functional groups of nanoporous materials. Its main goal is to enable users to characterize nanoporous materials, both texturally and energetically, through the fitting of experimental adsorption isotherms in a simple and intuitive manner.
By allowing the use of kernels developed from detailed models, including the influence of functional groups and specific geometries, MONSAIC maximizes the accuracy of characterization and its applicability in various scientific and technological fields.

Requirements and Installation

The porous materials characterization platform is a Python-based application designed to provide a simple and accessible user experience. One of its main advantages is its ease of installation, as it does not require prior installation of Python or any other specific software.

Installation Steps

1. Download the platform: Visit the official website (https://monsaic.unsl.edu.ar/) and download the compressed installation file in `.rar` format.

2. Install on PC: After downloading, extract the file into a folder (MONSAIC). Then, run the installation file located within the folder (`MONSAIC.exe`). The installation process is intuitive and requires only following the on-screen instructions.

3. Complete the Installation: Once the installation finishes, the platform is ready for immediate use. This process may take a few moments. No additional configuration or supplementary installations are required.

System Requirements

While the platform does not require the prior installation of Python or other specific programs, it is important to ensure that your computer meets the minimum system requirements for optimal

performance. These requirements are generally moderate and may vary depending on the software version and operating system used.

User Interface

The platform interface has been designed intuitively to facilitate the characterization of porous materials. This section describes how to interact with the different areas of the interface.

The interface is divided into four main parts: Fit Data, Kernel Parameters, Options, and Fit, in addition to the visualization of the selected experimental isotherm. The following outlines the process for performing a fit of an experimental isotherm using MONSAIC:

1. Fit Data

- In this section, the experimental isotherm to be fitted is loaded using the file selection box.
- By clicking the "Open" button, a window opens allowing the user to choose the experimental isotherm file. MONSAIC can read files in .dat or .txt format containing two columns: relative pressure (p/p_0) and adsorbed amount
- Once the file is selected, the program will ask the user to specify the units in which the isotherm is expressed (cm^3/g STP or mmol/g). Since MONSAIC operates internally with *mmol/g* and *relative pressure (p/p_0)*, it is essential to check that the experimental isotherm is expressed in compatible units before proceeding.
- After this confirmation, the experimental isotherm is plotted in the corresponding area of the interface, along with the table of loaded values

2. Kernel Parameters

- In this section, the kernel of simulated isotherms to be used in the fit is selected The list displayed in this section contains all the isotherm databases included and accessible in the current version of the application (*Figure 1*).
- When a kernel is chosen, information regarding the molecular models and parameters used in its construction is displayed in the lower panels, including: adsorbate type, temperature, pore model, and percentage of heterogeneity.

3. Options

- In this section, the characterization techniques to be applied should be selected (Specific Surface Area, BET Area, Regularized PSD, Enthalpy Prediction, etc.).
- "Obtain Regularized PSD" option: By selecting this option, the user enables the construction of the L-curve and the possibility to manually choose the regularization parameter. It is important to note that this calculation may take several minutes to complete.

- Regarding the PSD provided by the platform: In all cases, the pore size distribution (PSD) is obtained through a regularization procedure.

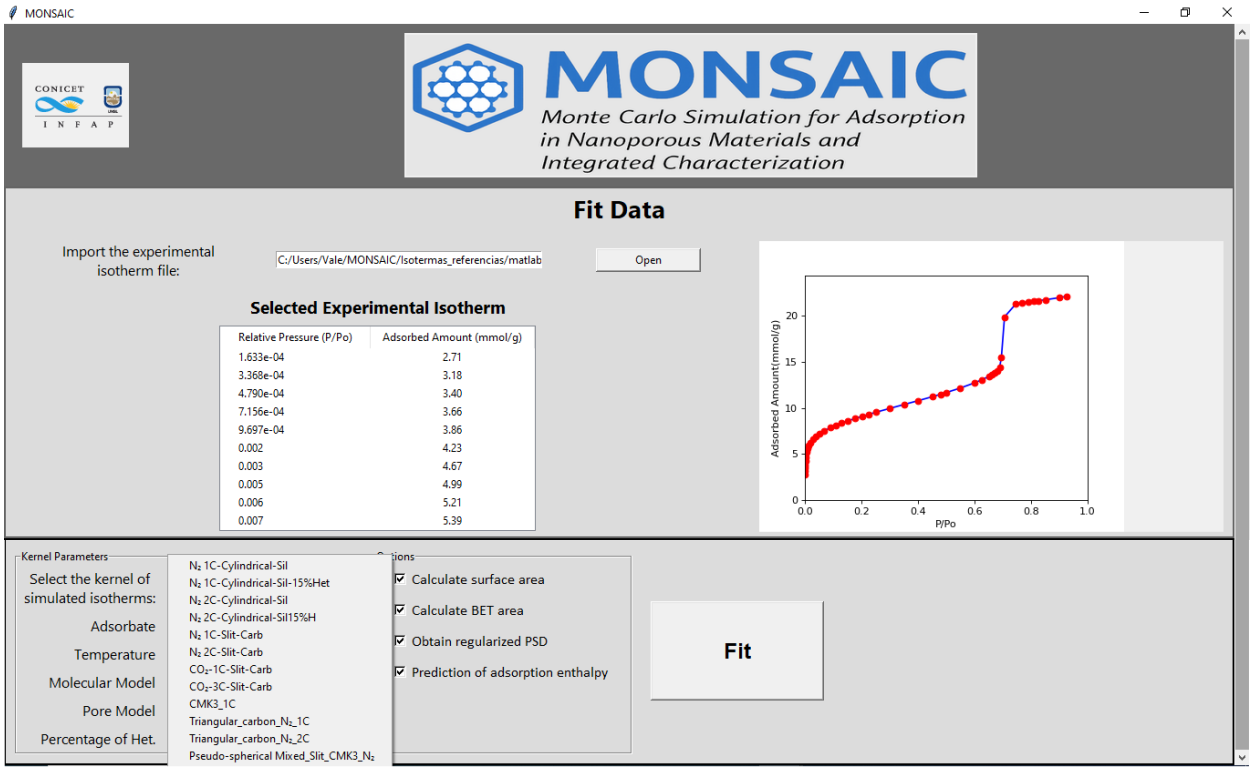

Figura 1: Main MONSAIC Interface.

— If the "Regularized PSD" option is not selected, the platform automatically applies the optimal regularization parameter estimated via machine learning.

— If the option is selected, the user can explore the L-curve and manually adjust the parameter value.

Note: The final report will not be generated until all selected options have been executed.

4. Fit

- Once the parameters are configured, click the "Fit" button to execute the fit of the experimental isotherm.
- The results are displayed in a new window, showing the fit graphs, the pore size distribution (PSD), the associated error, and all previously selected options (for example, enthalpy estimation, L-curve generation, or BET surface area calculation).
- All results, including graphs and numerical values, can be exported in various formats: PDF (detailed report with tables and graphs) and a spreadsheet file (.xlsx format) for further data analysis.

5.Visualization of Results and Interpretation

The visualization of the fitting results provides a detailed understanding of the characteristics of nanoporous materials. Below, the main elements of the visualization are described, including clarifications regarding the magnitudes of the data:

5.1 Fitting Graphs

- Two fitting graphs are presented: one in linear scale and the other in logarithmic scale. These graphs display the experimental and fitted isotherms, allowing for a direct comparison of the data.

5.2 Pore Size Distribution (PSD)

The pore size distribution is calculated from the fit performed using the regularization parameter obtained through *machine learning* (λ_{ml}) techniques, representing the different pore sizes present in the analyzed porous material. This distribution can be visualized either using bar plots for a more detailed representation or as a continuous line, the default option. In the case of mixed-geometry models, both representations display the contribution of each pore geometry along with its percentage of the total distribution. Additionally, users can enable or disable the display of individual contributions, or the total distribution, by clicking on the corresponding item in the plot legend (*Figure 2*).

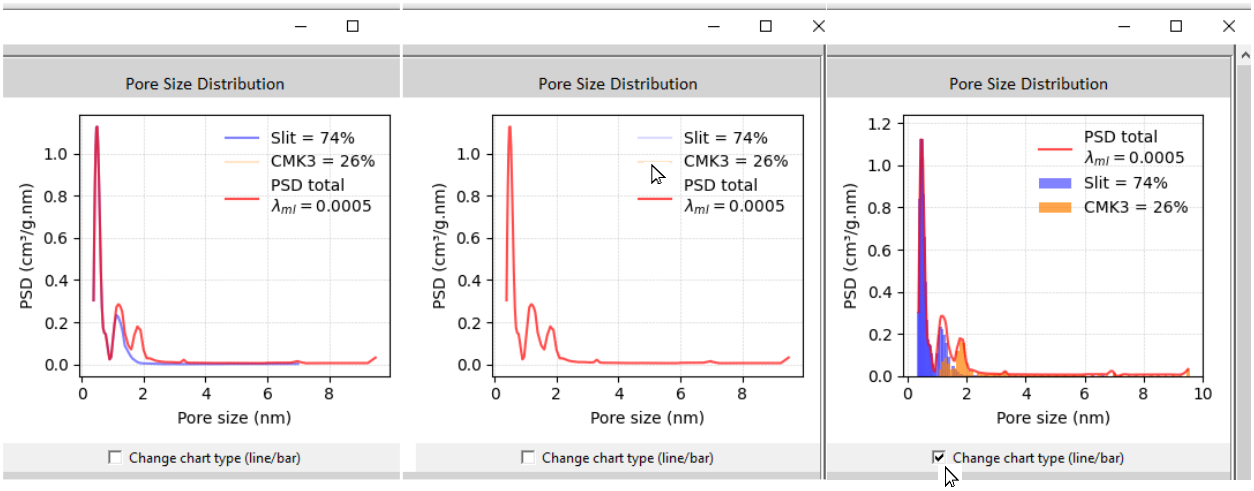

Figure 2: Visualization of contributions in models with mixed geometries.

Definition of H: The pore width (H) is defined as the distance between planes tangent to the first layer of atoms on the pore wall. This is essential for consistent comparisons across characterization methods[1,2].

- Cylindrical geometries: H is the distance between planes tangent to the wall atoms[9].
- Triangular geometries: H is the diameter of the inscribed circle within the triangular cross-section[2,4].

- CMK-3 geometries: H corresponds to the diameter of a circle circumscribed by three carbon rods[3].

5.3 Fitting Error, Pore Volume, and Surface Area

Information on the fitting error, total pore volume and the surface area calculated from the pore size distribution is provided. These data are useful for evaluating the quality of the fit and the effectiveness of the model used [1,2].

The following figure shows an example of the visualization of the obtained results, including the fitting plots and the pore size distribution. In this case, an experimental nitrogen adsorption isotherm at 77 K, corresponding to an activated carbon sample, was fitted using a database of single-pore nitrogen adsorption isotherms at 77 K in slit-shaped pores, based on the pseudo-spherical potential model for the adsorbate. The results include two fitting plots (one in linear scale and one in logarithmic scale) and the corresponding pore size distribution, which is displayed as a continuous line but can also be visualized as a bar chart (*Figure 2*). Additionally, the fitting error, total pore volume, and surface area calculated from the PSD are reported.

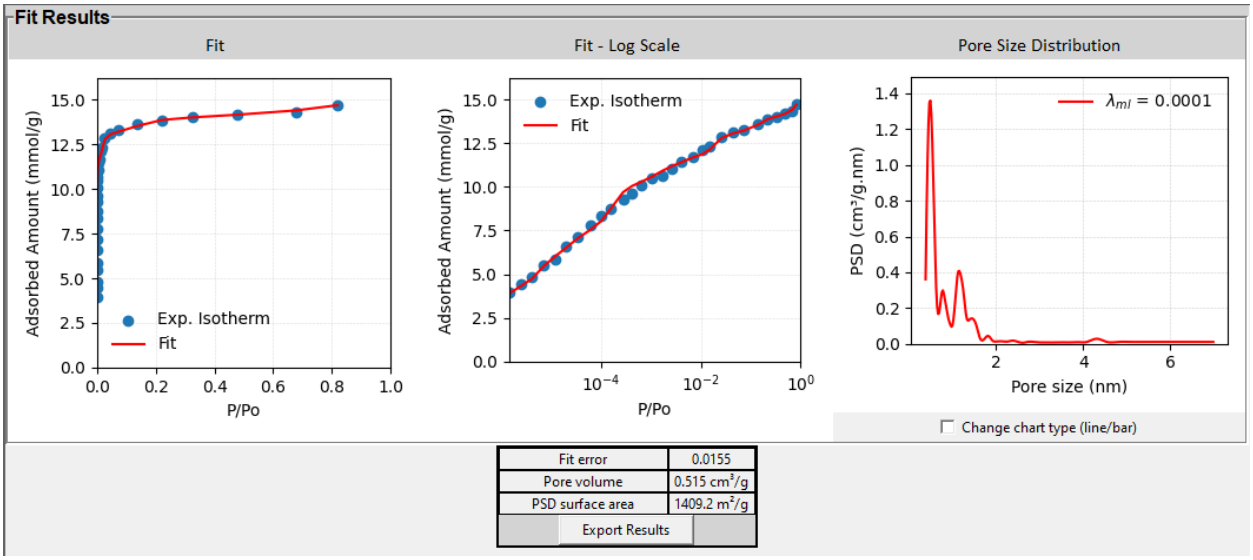

Figure 3: Visualization of Results.

5.4 BET Surface Area Calculation

The Brunauer-Emmett-Teller (BET) method remains one of the most widely used procedures for evaluating the surface area of nanoporous materials [2,5].

The application of the BET method involves two stages:

First stage: MONSAIC transforms the adsorption isotherm into a BET plot, from which it obtains the value of the BET monolayer capacity, n_m.

Second stage: The platform calculates the BET surface area, a(BET), from n_m by adopting an appropriate value for the molecular cross-sectional area, σ, depending on the adsorbate used.

If the "*Calculate BET area*" option was selected in *"Options" (Figure 1)*, a section dedicated to this characterization technique will appear in the Fit Results window. In this section, a table will be displayed containing the data for the selected isotherm.

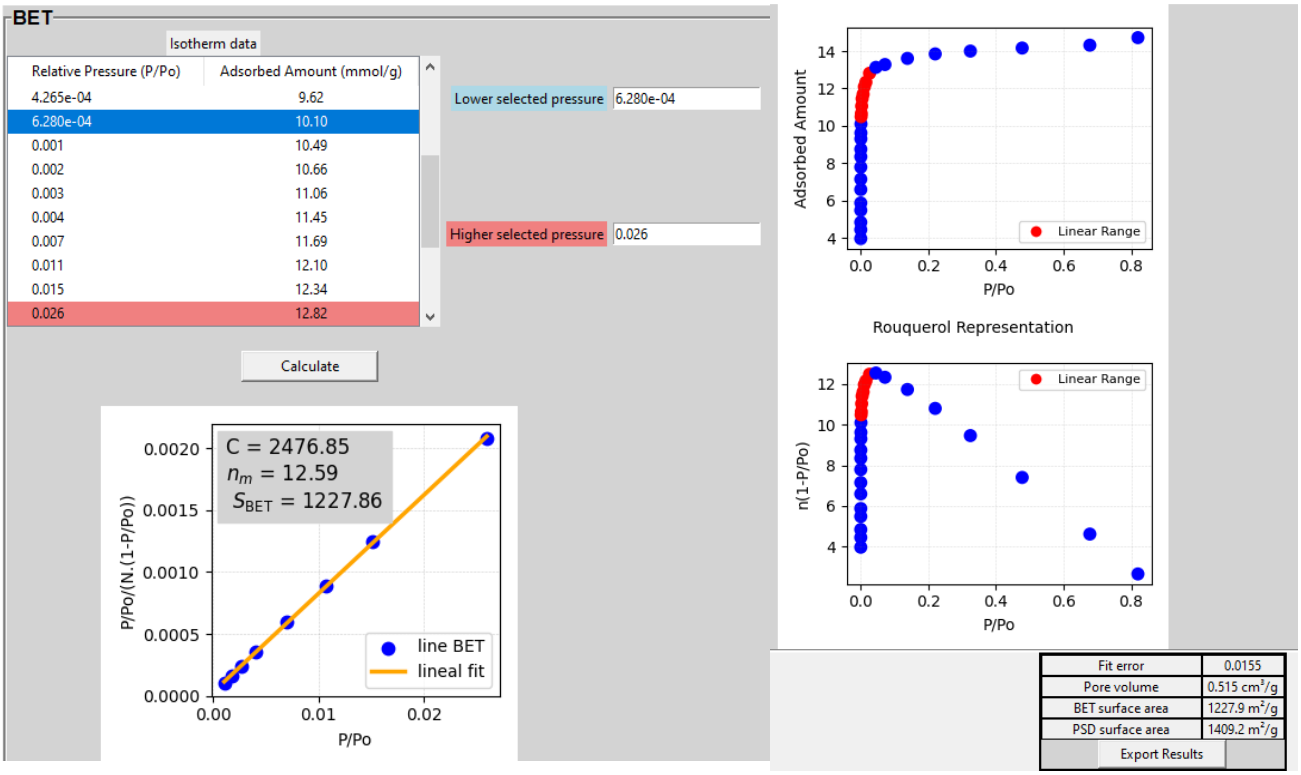

Figura 4: Example of BET surface area determination. The graph on the right shows the BET plot used to calculate the surface area, while the graph on the left displays the original isotherm with the selected pressure interval highlighted. Additionally, the plot of the Rouquerol function $n(1-p/p_0)$ vs. p/p_0 is included to support the appropriate selection of the BET fitting range.

To begin with the calculation:

1. **Pressure Range Selection:**

Specify to the MONSAIC the pressure range you wish to use for the analysis. This is done by clicking directly on the data table:

- The first click selects the lower limit of the range, which will be stored in the "Lower selected pressure" field.
- The second click selects the upper limit, which will be stored in the "Higher selected pressure" field.
- Finally, press the "Calculate" button to obtain the results.

2. **Display of Results:**

Once the calculation is completed, the application displays three graphs:

- **BET graph**: Represents the linear relationship between $\frac{p/p_o}{n(1-p/p_o)}$ and p/p_o. This graph shows the calculated values of C, n_m, and the BET area.
- **Isotherm graph**: Shows the original adsorption curve with the selected pressure interval highlighted.
- $\boldsymbol{n(1-p/p_o)}$ **vs.** $\boldsymbol{p/p_o}$ **plot:** Displays $n(1-p/p_o)$ vs. p/p_o, with the selected pressure interval highlighted for BET application.

5.4.1 Selection of the Appropriate Pressure Range (IUPAC Criteria [5])

To reliably determine the BET area, it is essential to correctly select the pressure range in which the BET equation will be applied. According to IUPAC criteria, the following is recommended:

- **Recommended Range:**

For type II and type IVa isotherms, it is suggested to work within the approximate range of $p/p_o \approx 0.05$ a 0.30, as this range shows the necessary linearity in the BET graph.

- **Validation Criteria:**

a) Behavior of $\frac{p/p_o}{n(1-p/p_o)}$:

Within the selected range, the term $\frac{p/p_o}{n(1-p/p_o)}$ must increase continuously as p/p_o. increases. If any discontinuity or decrease is observed, it could indicate a transition to multilayer adsorption or micropore filling, suggesting that the range is not appropriate.

b) Positive Intercept in the Linear Fit:

When constructing the BET graph (where $\frac{p/p_o}{n(1-p/p_o)}$ is plotted as a function of as p/p_o), the linear fit should yield a positive intercept (the y-intercept), since it is equal to $1/(C\,n_m)$. A negative intercept indicates that data from pressures outside the valid region for BET analysis have been included.

c) Inclusion of the Monolayer Capacity (n_m):

Once n_m is calculated and shown in the graph, verify that the p/p_o value corresponding to n_m is within the selected range. This confirms that the range correctly covers the transition toward monolayer adsorption.

d) Review of the Isotherm Graph:

Examine the adsorption isotherm, in which the selected pressure range is highlighted. This range should cover the region where the monolayer is formed, generally identified by the **"knee point"** of the isotherm, where adsorption increases sharply before transitioning to multilayer formation.

e) Plot of $n(1 - p/p_o)$ vs. p/p_o

This curve displays on the vertical axis the product of the adsorbed amount and the pressure differential, $n(1 - p/p_o)$, plotted against p/p_o. The valid BET range corresponds to the region where this function increases strictly monotonically. Any interval in which $n(1 - p/p_o)$ stops rising (inflections or declines) should be excluded, as it indicates the onset of multilayer adsorption or micropore filling and leads to unreliable monolayer content estimates.

Note that the BET area value will appear in the data report.

5.5 Regularization and Smoothing

MONSAIC applies Tikhonov regularization to smooth the pore size distribution (PSD), ensuring a stable and physically meaningful solution. This technique mitigates the effects of noise and ill-posedness in the inversion of the adsorption integral equation.

Regularization Process

The regularization workflow includes the following steps:

- Selection of λ values: Users can manually input a list of regularization parameters (λ) or use a preloaded default set.
- User-guided λ selection: The L-curve is displayed to the user as a practical and intuitive tool for selecting the regularization parameter (λ), especially when visual inspection is preferred.
- Final PSD calculation: Once the optimal λ (also referred to as α) is selected, MONSAIC uses it to compute the regularized PSD.

5.5.1 Machine Learning-Assisted Prediction

In addition to the manual input, MONSAIC incorporates a machine learning (ML) module that automatically predicts an optimal regularization parameter (λ). This prediction is based on descriptors extracted from the uploaded isotherm and the selected adsorption kernel.

The ML model, trained on a diverse dataset of simulated and experimental isotherms, uses a *Random Forest algorithm* to estimate λ, reducing subjectivity and accelerating the analysis. This predicted parameter is used to compute the initial regularized PSD, which is automatically displayed as the first result, allowing users to compare it with alternative regularization options.

The initial PSD is automatically regularized using the machine learning–predicted λ, which is displayed on screen as $\boldsymbol{\lambda}_{\mathrm{ml}}$. It is important to note that this predicted value may not always be the optimal choice for regularization; depending on the model and the experimental isotherm, it could underestimate or overestimate λ. In such cases, users are encouraged to explore other values using the L-curve to select the most appropriate regularization parameter. To try a different value, users can view the L-curve, select a new λ directly from the graph, and press "Obtain regularized PSD" to update the distribution with the chosen parameter.

5.5.2 Regularization Technique

The regularization technique aims to "smooth" the PSD obtained from the fit. To enforce this smoothness, the equation is used [2,6]:

$$R_{REG} \equiv \sum_{i=1}^{n}\left[N_{exp}(P_i,T) - N_{mod}(P_i,T)\right]^2 + \lambda \sum_{j=1}^{m}\left(f_j^{*(2)}\right)^2 \delta H_j$$

where the second term on the right accounts for the roughness of the PSD.

This expression can also be written in compact form as:

$$R_{REG}\left(f_j^*,\lambda\right) \equiv R_{ERROR}\left(f_j^*\right) + \lambda F_{RUG}\left(f_j^*\right)$$

These terms are labeled as R_{ERROR}, F_{RUG}, and R_{REG} in the result files generated by MONSAIC for transparency and reproducibility.

The goal of the regularization method is to smooth the PSD by searching for a specific value of λ, called the λ_critical.

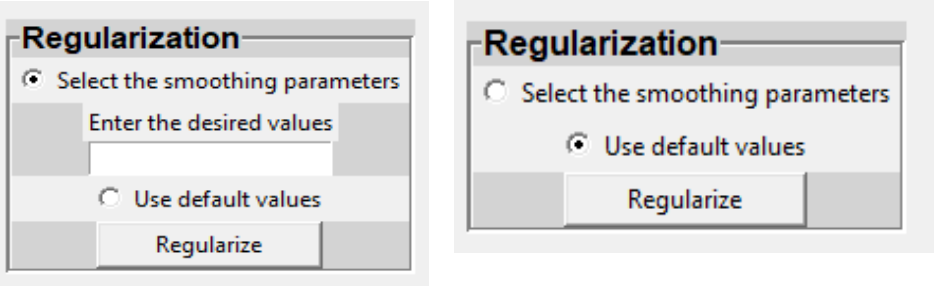

Figure 5: Display of the section for regularized PSD calculation (left). Pop-up window for manual input of the regularization parameter values (left).

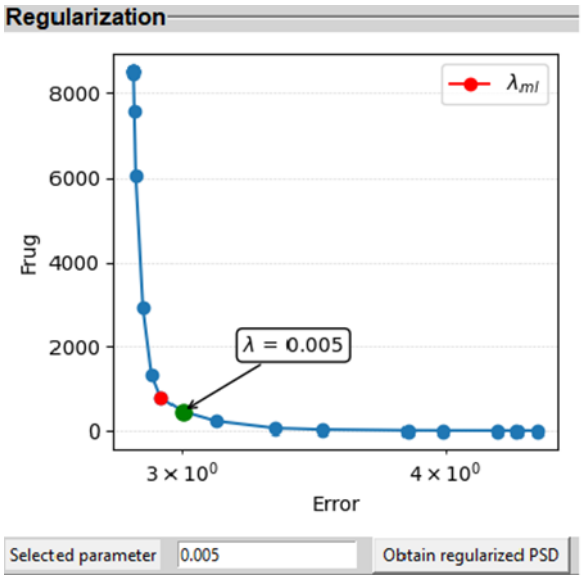

Figure 6: L-curve generated by MONSAIC. The user can click any point on the curve to interactively select the corresponding regularization parameter (λ), which will be used to compute the PSD.

The implementation of this technique in MONSAIC is simple: initially, the option "*Regularized PSD*" must be selected in *"Options" (Figure 1)*. This action enables a new section within the Fitting Results window. In this section, the user can choose to manually enter a list of regularization parameter values or use a predefined set provided by the platform. These values are then used by MONSAIC to compute the curves associated with the regularization process. The platform generates the L-curve, which is displayed on screen and allows the user to interactively select the regularization parameter (λ) to be applied for smoothing the PSD. The numerical data used to construct the curve are also included in the output report for further analysis.

To manually enter the λ values, the option "Select values" must be checked *(Figure 5)*, hich will display a box where the required parameters should be entered. The number of data entries is not limited, although entering a larger number of parameters significantly increases the program's calculation time. If this option is not selected and the "Use default values" box is checked,

MONSAIC will use a pre-loaded list of values in the application. These parameters are**:**1e-8, 5e-8, 1e-7, 5e-7, 1e-6, 5e-6, 1e-5, 5e-5, 1e-4, 5e-4, 1e-3, 5e-3, 1e-2, 5e-2, 1e-1, 5e-1, 1, 5, 7, 10.

Users must press the "**Regularize**" button for MONSAIC to compute and display the L-curve, which illustrates the trade-off between fitting accuracy and smoothness [6]. The curve is shown on screen, and users can interactively explore different regularization levels, with the corresponding λ value displayed when selecting or pointing to a specific point on the curve (*Figure 6*). This functionality allows informed selection of the smoothing parameter used to compute the regularized PSD. The selected value will then appear in the "Selected parameter" box. Alternatively, users can manually input a λ value either in decimal format (using a dot as separator, e.g., 0.25) or in scientific notation (e.g., 1e-6).

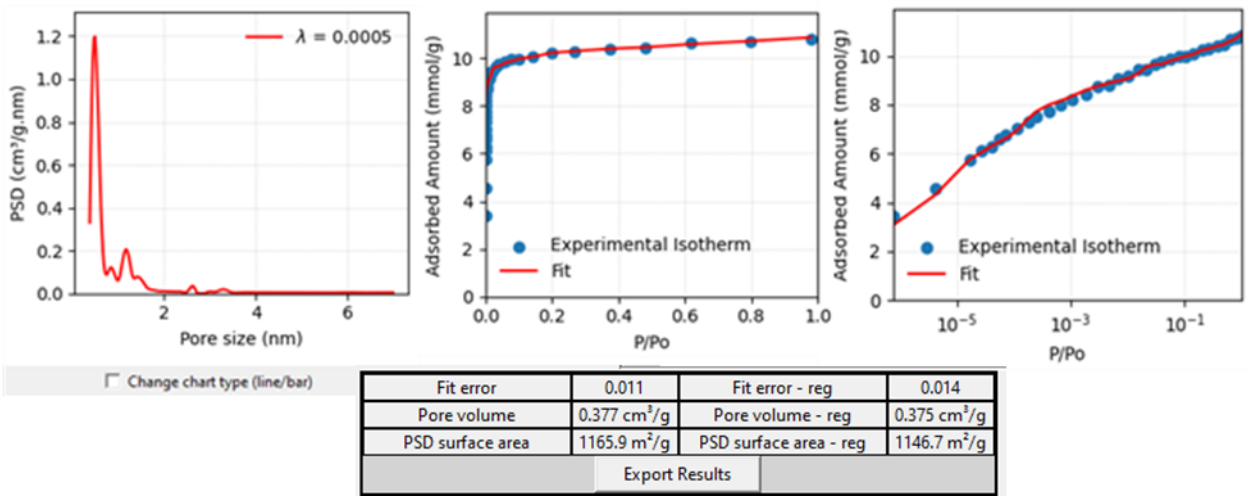

Figure 7: Visualization of the regularized PSD alongside the experimental isotherm fit.

Finally, the user must press the 'Obtain regularized PSD' button for MONSAIC to perform the regularization using the selected λ parameter. Once the calculation is completed, MONSAIC will display the regularized PSD together with the experimental adsorption isotherm fit and the user can try different values of the regularization parameter to explore their effect on the result.

Note: The construction of the L-curve may take several minutes, depending on the number of λ values and the complexity of the data.

Important: While MONSAIC is computing the L-curve, the user can continue working with other applications on their computer. Additionally, if the "Calculate BET area" option has been selected, these calculations can be performed in parallel without interrupting the L-curve processing.

5.6 Estimation of Adsorption Heat or Enthalpy

MONSAIC allows the estimation of adsorption enthalpies from the experimental adsorption isotherm and the PSD obtained from the fitting [7]. To do so, the option *"Prediction of adsorption enthalpy"* must be checked in the *Options* section *(Figure 1)*.

The adsorption enthalpy vs. amount adsorbed graph is included in the Fit Results window.

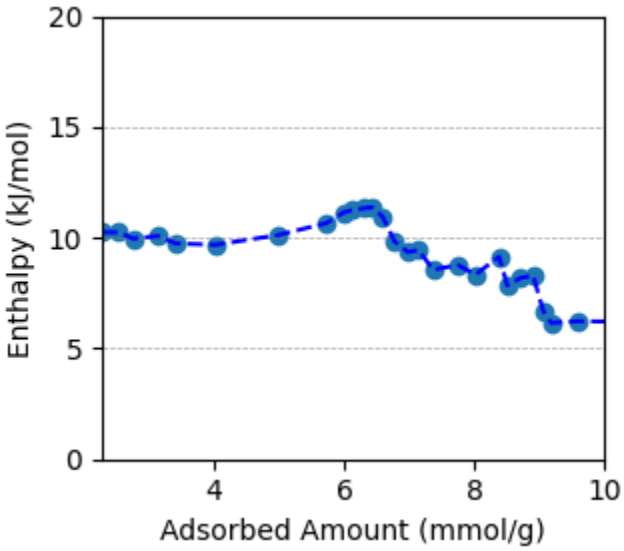

Figure 8: Visualization of the Adsorption Enthalpy vs. Adsorbed Amount graph.

List of Isotherm Kernels Available in the Application (Full Version)

This section details the available kernels, including relevant information about each one. [2,3,4,6,8,9].

Models	Nanoporous Materials
Nitrogen adsorption isotherms using pseudo-spherical models at 77 K in homogeneous cylindrical pores (MMO silica). *Pore Range: 0.31nm-11nm.*	Siliceous materials such as silica gels, porous glasses, MCM-41, SBA-15, MCM-48, etc.
Nitrogen adsorption isotherms using pseudo-spherical models at 77 K in heterogeneous cylindrical pores (MMO silica, 10% coverage). *Pore Range: 0.31nm-11nm.*	Siliceous materials with impurities or functional groups, such as silica gels, porous glasses, MCM-41, SBA-15, MCM-48, etc
Nitrogen adsorption isotherms using pseudo-spherical models at 77 K in heterogeneous cylindrical pores (MMO silica, 15% coverage). *Pore Range: 0.31nm-11nm.*	Siliceous materials with impurities or functional groups, such as silica gels, porous glasses, MCM-41, SBA-15, MCM-48, etc.
Nitrogen adsorption isotherms using multi-site models at 77 K in homogeneous cylindrical pores (MMO silica). *Pore Range: 0.31nm-11nm.*	Siliceous materials such as silica gels, porous glasses, MCM-41, SBA-15, MCM-48, etc.

Nitrogen adsorption isotherms using multi-site models at 77 K in heterogeneous cylindrical pores (MMO silica, 10% coverage). *Pore Range:0.31nm-11nm.*	Siliceous materials with impurities or functional groups, such as silica gels, porous glasses, MCM-41, SBA-15, MCM-48, etc..
Nitrogen adsorption isotherms using multi-site models at 77 K in heterogeneous cylindrical pores (MMO silica, 15% coverage). *Pore Range: 0.31nm-11nm.*	Siliceous materials with impurities or functional groups, such as silica gels, porous glasses, MCM-41, SBA-15, MCM-48, etc..
Nitrogen adsorption isotherms using multi-site models at 77 K in heterogeneous cylindrical pores (MMO silica, 25% coverage). *Pore Range: 0.31nm-11nm.*	Siliceous materials with impurities or functional groups, such as silica gels, porous glasses, MCM-41, SBA-15, MCM-48, etc.
Nitrogen adsorption isotherms using pseudo-spherical models at 77 K in slit pores (AC). *Pore Range: 0.31nm-11nm.*	Activated carbons, activated carbon fibers, novel micro/mesoporous carbons such as CMK-1, etc.
Nitrogen adsorption isotherms using multi-site models at 77 K in slit pores (AC). *Pore Range: 0.31nm-11nm.*	Activated carbons, activated carbon fibers, novel micro/mesoporous carbons such as CMK-1, etc.
Nitrogen adsorption isotherms using pseudo-spherical models at 77 K in triangular pores (AC). *Pore Range: 0.31nm-6nm.*	Activated carbons, activated carbon fibers, novel micro/mesoporous carbons such as CMK-1, etc.
Nitrogen adsorption isotherms using multi-site models at 77 K in triangular pores (AC).*Pore Range: 0.31nm-6nm.*	Activated Carbons, activated carbon fibers, novel micro/mesoporous carbons such as CMK-1, etc.
Argon adsorption isotherms using pseudo-spherical models at 87 K in slit pores (AC). *Pore Range: 0.31nm-6nm.*	Activated carbons, activated carbon fibers, novel micro/mesoporous carbons such as CMK-1, etc.
Argon adsorption isotherms using pseudo-spherical models at 87 K in cylindrical pores (MMO silica). *Pore Range: 0.31nm-6nm.*	Siliceous materials such as silica gels, porous glasses, MCM-41, SBA-15, MCM-48, etc.
Nitrogen adsorption isotherms using multi-site models at 77 K in cylindrical pores (AC). *Pore Range: 0.76nm-10nm.*	Activated carbons, activated carbon fibers, novel micro/mesoporous carbons such as CMK-3, etc.
CO_2 adsorption isotherms using pseudo-spherical models at 273 K in slit pores (AC). *Pore Range: 0.31nm-5nm.*	Ultramicroporous activated carbons, activated carbon fibers.

CO_2 adsorption isotherms using multi-site models at 273 K in slit pores (AC). *Pore Range: 0.31nm-5nm.*	Ultramicroporous activated carbons, activated carbon fibers.
Nitrogen adsorption isotherms using pseudo-spherical models at 77 K in CMK-3 nanostructured pores (AC). *Pore Range: 1.1nm-6.6nm.*	Nanostructured activated carbons with CMK-3 geometry.
Methane adsorption isotherms using pseudo-spherical models at 298 K in CMK-3 nanostructured pores (AC). *Pore Range: 1.1nm-6nm*	Nanostructured activated carbons with CMK-3 geometry.
Nitrogen adsorption isotherms using pseudo-spherical models at 77 K in mixed geometry pores (slit and triangular, AC) *Pore Range: 0.31nm-11nm*	Activated Carbons, activated carbon fibers, novel micro/mesoporous carbons such as CMK-1, etc.
Multisite nitrogen adsorption isotherm model at 77K in mixed geometry pores (slit and triangular, AC). *Pore Range: 0.31nm-11nm*	Activated Carbons, activated carbon fibers, novel micro/mesoporous carbons such as CMK-1, etc.
Nitrogen adsorption isotherms using pseudo-spherical models at 77 K in mixed geometry pores (slit and CMK-3, AC) *Pore Range: 0.31-11nm (CMK-3).*	Nanostructured activated carbons with CMK-3 or CMK-5 geometry.

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