Adsorption Kinetics Project

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1. Introduction

Welcome to the Adsorption Kinetics project! This project aims to solve and visualize the kinetics of adsorption using two different models: PVSDM (Pore Volume-Surface Diffusion Model) and QPVSDM (Quadratic Pore Volume-Surface Diffusion Model). These models help analyze how adsorbates are taken up by adsorbents over time. This README provides a detailed overview of the project, input parameters, usage instructions, and more.

2. Project Overview

The primary objective of this project is to simulate and compare the PVSDM and QPVSDM models with experimental data. The project requires users to input various parameters and experimental data to perform the simulations. After the calculations, the app generates plots to visualize the results and compare the models with the experimental data.

3. Input Parameters

To run the simulation successfully, you need to provide the following input parameters:

- Bulk tab:

    1. **Omega (ω):** The dimensionless adsorbent dosage.
    2. **Biot Number (Bi):** A dimensionless number used to characterize the relative importance of external mass transfer to internal mass transfer.

- Solid/solute tab:

    1. **Mean Radius of Adsorbent (R):** The mean radius of the adsorbent in centimeters.
    2. **Pore/Surface Diffusivity Ratio (D_{sp}):** The ratio of pore diffusivity to surface diffusivity.
    3. **Pore Diffusivity (D_p):** Pore diffusivity in square centimeters per second.
    4. **Adsorbent Porosity (ε):** The porosity of the adsorbent material.

- Equilibrium tab

    1. **Langmuir Parameters (a and b):** The dimensionless Langmuir parameters.
    2. **Final Time (t_f):** The total time for the simulation in minutes.

- Data tab:

    - Follow the instructions in the app.

4. Usage

To use the app, follow these steps:

1. **Input Parameters:** Enter the required input parameters as specified above.

2. **Experimental Data:** Provide the experimental adsorption data in a suitable format. This typically includes data points of adsorption at various time intervals.

3. **Run the Simulation:** Execute the simulation to calculate adsorption kinetics using both PVSDM and QPVSDM models.

4. **Plot Results:** The app will generate plots comparing the simulation results of both models with the provided experimental data.

Steps 2-4 will run automatically after uploading the experimental data.

5. Results

The app produces visual results that include:

- A plot comparing the PVSDM and QPVSDM model predictions with the experimental data.

These results help you evaluate how well the chosen adsorption models fit your experimental data.

6. Getting Started

To get started with this project, follow these steps:

1. Clone this repository to your local machine. Alternatively, you can download the full project.

2. Follow the usage instructions mentioned above to run the app with your specific input data.

7. Contributing

Please cite our article: Rodrigues et al. (2023). "Development of a phenomenological model including porous and surface diffusion for batch adsorption". If you would like to contribute to this project or report issues, just click on the "Need help?" button and e-mail me. Feel free to reach out if you have any questions or need further assistance with this Adsorption Kinetics project. Happy simulating and analyzing!

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