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Research Article

Simulating Studies on Phosphate (PO_4^{3-}) Removal from Laundry Wastewater Using Biochar: Dudinin Approach

Eric York[1,*], James Tadio[2], Silas Owusu Antwi[3]

[1] Freelance Chemist (Freelancer.com), Level 37 Grosvenor Place, 225 George Street, Sydney, NSW 2000, Australia
[2] Centre for Environmental Sustainability and Remediation, RMIT University, Melbourne, VIC 3001, Australia
[3] Laundry and Textiles Services, Asokwa, Kumasi 00233, Ghana
E-mail: yorkeric90@gmail.com

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Abstract: Wastewater from the Laundry wash processes contain a diverse range of chemical pollutants that can have detrimental effects on human health and the environment. In this study, simulation studies by Spyder Python software v3.2 to assess the efficacy of biochar in removing PO_4^{3-} from wastewater were conducted. Through modelling and simulation, the mechanisms involved in the adsorption process of phosphate by biochar were studied by altering variables that are specific to the phosphate from common laundry detergents. These included aqueous solubility, initial concentration, and temperature using Dudinin and Astakhov (DA). Results showed that concentration equilibrates near the highest concentrations for CaO-rich biochar-120 mg L^{-1}, Pine sawdust biochar-57 mg L^{-1} while Peanut, *Eucalyptus polybractea* and Crawfish biochar equilibrated at near concentration. CO_2-activated Thalia, Sewage sludge, *Broussonetia papyrifera* Leaves biochar equilibrated just at the lower concentration. Soyer bean Stover biochar exhibited a sharp rise and fall peak in mid-concentration at 130 mg L^{-1} Volume. The modelling results were consistent with experimental findings from literature ensuring the accuracy, repeatability, and reliability of the simulation study. The simulation study provided insights into adsorption for PO_4^{3-} from wastewater by biochar using concentration per volume that can be ideally adsorbed under the given conditions. Studies showed that applying the principle experimentally in real wastewater with all its complexity is warranted and not far-fetched.

Keywords: phosphate adsorption; biochar; simulation; aqueous solution

1. Introduction

Conventional methods for treating wastewater struggle to efficiently eliminate the diverse array of contaminants found in laundry wastewater. Phosphate, a common byproduct of laundry wastewater, poses a significant threat to environmental health. It serves as a primary contributor to eutrophication, which poses various risks to the flora and fauna within ecosystems [1]. In recent years, phosphate has been detected in wastewater from various sources. However, the two main sources of concern are: (i) the presence of phosphate in sewage and residual traces in treated sewage effluent (TSE), and (ii) the runoff from agricultural lands due to the leaching and dissolution of phosphate fertilizers by rainwater, resulting in the release of phosphate into rivers and other surface and groundwater bodies [2]. Phosphate from runoff from fertilizers has been linked to excessive algae growth and the production of microcystins (MCs) in surface waters [3]. Addressing this issue, there's a user-friendly technology that offers a relatively simple design and allows for the renewal of adsorbents

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while generating minimal by-products[4,5]. Various adsorbents have been employed to removal of phosphates from aqueous solutions, including zeolites, polymeric adsorbents, porous silica, activated carbon, and clay minerals[6–8]. Among these, activated carbon has been extensively used for phosphate removal due to its porous structure, stability, and large surface area. However, many activated carbons contain hydrophobic or weakly charged groups on their surface, limiting their phosphate adsorption capacity. To overcome this limitation, activated carbons have been modified or impregnated with metal ions to enhance their phosphate adsorption capabilities[9]. Nonetheless, the pursuit of more cost-effective adsorbents with greater phosphate capacity remains an ongoing endeavor. Biochar, a carbon-rich material produced through the pyrolysis of biomass, exhibits promising adsorption properties for both organic and inorganic compounds such as phosphate, owing to its high surface area and porous structure. Since Chen et al.[10] initiated the removal of phosphate using biochar (BC), scientific interest in utilizing BC and its composites for phosphate remediation has been steadily increasing. This trend is driven by factors like its cost-effectiveness, wide availability of diverse feedstocks, and ease of modification. Various feedstocks including plant biomass, agricultural and animal wastes, as well as solid wastes, have been employed for BC production[11]. With a current estimated cost ranging from 350 to 1200 USD/ton, biochar presents a more economically feasible alternative compared to activated carbon (which costs USD 1100–1700 per ton). Krasucka et al. (2021)[12] utilized biochar filters in laundry facilities, showcasing their potential for wastewater treatment in this context. Numerous laboratory experiments have underscored the efficacy of biochar in mitigating pollutants in wastewater. Recently, York, Tadio, and Darko[13] employed biochar derived from giant reed to successfully remove lead from aqueous solutions, while Duwiejuah et al.[14] the removal of various metals, including Pb, Cd, and Hg, using biochar sourced from shea and peanut shells. However, these investigations have primarily been confined to laboratory settings, and applying the same methodologies to real wastewater scenarios remains a challenge[15]. Despite the complexity of elucidating the mechanisms underlying adsorption in such matrices, the wastewater from laundry operations shares similarities with that from mining, petroleum refining, and battery manufacturing processes[16]. Our study focuses on targeting one of the primary pollutants in laundry wastewater, namely phosphates. Yet only a limited number of studies have evaluated the efficacy of biochars for phosphate removal from actual wastewater streams. Phosphate removal from wastewater streams is influenced by the presence of organic and inorganic species, bacterial components, and various other contaminants[17]. It's worth noting that numerous studies have demonstrated that phosphate removal from wastewater is a complex process, surpassing simple tests conducted in synthetic waters[17]. This complexity often arises from the competition between phosphate and other contaminants for available adsorption sites, the interaction between phosphate and organic matter present in real streams, and the potential blockage of adsorbent pores by biological and organic substances[18]. In our pursuit of future trials involving biochar for remediating real wastewater, we believe that simulated studies can provide insights into practical approaches for managing phosphate-polluted laundry wastewater using biochar within a complex aqueous matrix, particularly considering the limitations of time in remediation. To the best of our knowledge, no research has yet presented a simulation study on phosphate removal in laundry wastewater using biochar. Recent studies have developed models to predict the adsorption of non-polar, low molecular weight organic compounds onto activated carbons in aqueous phases[19]. These models integrate the physical properties of activated carbons and those of the target contaminants, specifically organic compounds. However, similar tests have yet to be conducted for biochar. Using the concept of Dudinin and Astakhov (DA) equation, the model needs three input factors: the limiting pore volume Wo, a molecular descriptor for the target chemicals (N), and a term that uses the state of adsorption, whether homogeneous or heterogeneous, on the surface (n) of the standard activated carbon. The first parameter, Wo, is associated with the porosity (PSD) of the adsorbent. The second factor, which is the molecular descriptor is delineated by the pairs of the molecular connectivity index (MCI) correlations, and the state (nature) of adsorption was determined to be 1 after statistical analysis (Equation (1)[20]):

$$W = Wo \exp\left[-\left(\frac{\varepsilon}{100N}\right)^{n}\right] \quad (1)$$

In Equation (1), W = the volume of chemical adsorbed (mL g^{-1})
Wo = the limiting adsorption volume (mL g^{-1})
n = the exponential constant (-) = 1.1 from[21]
ε= RT I n (Cs/C) in aqueous phase (4.184 J moL^{-1})

C = the concentrations of aqueous solution (mg L^{-1})
Cs = Solubility (mg L^{-1})
R = Gas constant (8.314 J K^{-1} moL^{-1})
T = Absolute temperature (K)
N = Normalizing factor, and 100 is a scale factor.
The Wo was calculated from the PSD values following the approach described in Equation (2)[22]

$$Wo = V3.2 + 0 : 055 \text{ mL g}^{-1} \quad (2)$$

The granular activated carbon (GAC), V3.2 shows the micropore volume for pores with diameters less than 3.2 nm. The study presented robust model simulations and predictions, that were solely tested for single aromatic compounds, and non-polar aliphatic compounds, with no examination conducted on phosphate. Previous endeavours aimed to incorporate various organic compound groups into the correlation equation for the descriptors N, yet the inclusion of multiple compound groups resulted in significantly reduced fitness. Organic compounds with carbon numbers less than nine are recognized as a prevalent contaminant group in water[23]. Given the substantial influence of chemical properties such as the sizes of compounds and their functional groups, it is anticipated that the model parameters established for non-polar compounds may not apply to polar compounds. Consequently, choosing these models to accommodate polar inorganic species like phosphate could introduce a new scale of dimensions, leveraging combinations of ionic descriptors, linear solvation energy (LSER), solute hydrophobicity, polarizability, and equilibrium aqueous concentrations, as explored elsewhere[21]. In this study, we utilize simulation studies, employing the Dudinin and Astakhov (DA) equation, to assess the adsorption behaviour of biochar and explore its potential for removing PO_4^{3-} from laundry wastewater.

2. Method

2.1 *Physico-Chemical Properties of Adsorbates and Isotherm Data*

The adsorption isotherms data for the removal of phosphate in aqueous medium sourced from relevant literature are used in this study[11]. These datasets were utilized to construct models, with specific details provided in Table S1 in the supplementary Material S1. However, due to discrepancies observed in some results post-simulation, only a subset of the reported isotherms could be included. All the figures in this paper contain the remaining simulation results. For the examined chemicals (anion), the aqueous solubility and density data values were obtained from various sources including Chemical Book, IPCS InCHEM, Australian EPA, ChemSpider, Phisit, Alpes Chemicals, National Toxicology Program's Chemical Solubility Compendium, and online databases. Open-source software packages such as Spyder Python in Anaconda, and ALOGPS from the Laboratory for Ionic Bonds, Connectivity, Virtual Computational Chemistry Laboratory, ACD, and Coordinates were utilized for data analysis. The MCI (Molecular Connectivity Index) parameters for the tested phosphate ion compounds were acquired using PaDEl-Descriptor. Advanced Chemistry and EPI Suite V.4 were employed, as molecular weight, and water solubility, to estimate chemical density for the study of phosphate.

2.2 *Modelling Approach*

A simulation model utilizing Spyder Python v3.2 was developed based on the Dudinin and Astakhov (DA) equation to show the adsorption process of PO_4^{3-} onto biochar surfaces. This program offers a user-friendly interface to facilitate inputting data for graphical analysis. The simulation incorporated various parameters including adsorption volume, initial pollutant concentration, and biochar characteristics. Adsorption isotherms were generated to depict the equilibrium relationship between the adsorbent and the adsorbate. The model's validity was assessed using experimental data from relevant literature sources[11]. Furthermore, the impact of different biochar properties such as surface area and pore size distribution on pollutant removal were investigated.

2.2.1 *Standard User Interface Code for Single Phosphate Concentration*

Please refer to Supplementary Material S2 for computational details and visit ericjamessimulator.info to access the simulation tool.

2.2.2 *Error Estimation*

The normalizing parameter, N, depends on the adsorbate under investigation, which is calculated from the regression of Molecular Connectivity Indices. In the analysis, error estimation and marginalization are approached using a regression method as outlined by[21]. The correlation equations yielding the best fit and corresponding plots were employed for the laundry phosphate compounds examined. Within the regression process, Molecular Connectivity Index (MCI) was correlated with the adsorption data. Additionally, Crittenden et al.[24] assessed the errors in the experimental data and fitted models using the following formula:

$$\%\mathrm{SDEV} = \sqrt{\frac{\Sigma\left(\frac{\mathrm{Wcorrelation}-\mathrm{Wdata}}{\mathrm{Wdata}}\right)^2}{\mathrm{Wdata}-1}} \times 100 \tag{3}$$

Herein, Wcorrelation and Wdata represent the volume as determined from the correlation and the experimental data for the aqueous-phase concentrations, respectively, and Ndata is the number of data points. The results illustrated that biochar effectively adsorbs PO_4^{3-} present in laundry wastewater.

Adsorption isotherms were generated to depict this phenomenon. The data suggested that increasing the surface area and optimizing the pore size distribution of biochar improved its capacity to adsorb phosphate in wastewater. Furthermore, the modeling outcomes aligned with experimental observations from the literature, validating the accuracy, repeatability, and reliability of the simulation study. Through the simulation, a deeper understanding of the mechanisms underlying biochar adsorption for PO_4^{3-} removal from laundry wastewater was obtained, utilizing concentration per volume that can ideally be adsorbed under the given standard curve. These simulation results were consistent with fundamental principles of adsorption, including Langmuir and Freundlich isotherm models, as demonstrated below in Figure 1:

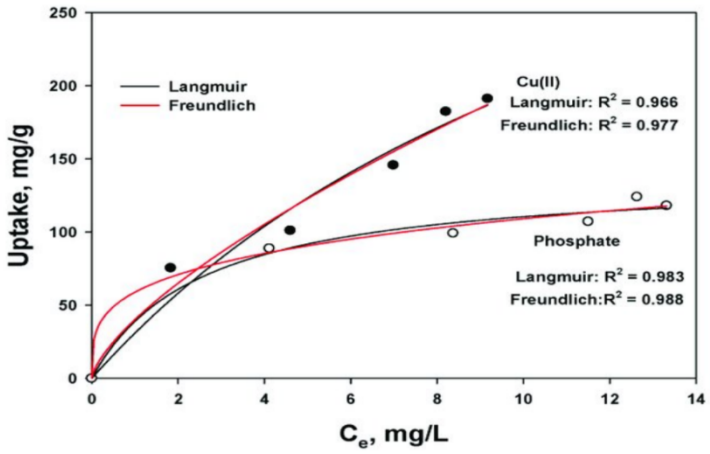

Figure 1. Shows Langmuir and Freundlich model adopted from[25] subject to copyright.

The influence of crucial parameters pH and temperature on the adsorption capacity of biochar were examined, revealing their effect on the efficiency of phosphate removal. The Dudinin and Astakhov (DA) equation offers a comprehensive framework for understanding the adsorption behavior of phosphate onto various biochar materials, as detailed in Table S1 of the Supplementary Materials. This equation incorporates key parameters that govern the adsorption process, facilitating a thorough examination of the interaction between biochar surfaces and phosphate ions. By analyzing the data in the table and incorporating it into the simulation model, the parameter Wo, which represents the limiting adsorption volume of

phosphate, is correlated with the pore size distribution (PSD) of the biochar. The calculated Wo values play a crucial role in determining the phosphate adsorption capacity for each biochar material investigated. However, only a subset of the studies mentioned earlier have been reported in this context, as previously mentioned. The remaining simulation results are available in Supplementary Materials S1. The presence of micropores with diameters less than 3.2 μm, as reflected in Python V3.2, significantly contributes to the adsorption process. The molecular descriptor N, derived from phosphate ion connectivity index (PCI) correlations, characterizes the chemical properties of the targeted phosphate ions, consistent with findings reported elsewhere. This descriptor captures the structural features that influence the interactions between phosphate ions and biochar surfaces. The value of n (1) indicates the nature of adsorption, with higher values suggesting a more rapid decrease in adsorption with increasing energy. This parameter offers insights into the degree of surface heterogeneity and its impact on the adsorption process. Modeling results utilizing different biochar variants in the study reveal valuable insights into the adsorption process. Through the application of the DA equation in each scenario, a deeper comprehension of adsorption dynamics, influencing factors, and optimal pH conditions is achieved. The determination of parameters Wo, N, and n aids in predicting the adsorption efficacy of these biochar materials under diverse circumstances. Employing the DA equation for each biochar type allows for the estimation of parameters Wo, N, and n, offering an enhanced understanding of adsorption behaviors and mechanisms. This equation facilitates the anticipation of adsorption patterns under varying conditions and aids in evaluating factors affecting the adsorption process. The utilization of various kinetic and isotherm models, alongside the identification of optimum pH conditions, further enriches our understanding of the interplay between biochar materials and phosphate ions. The current modeling approach provides valuable insights into the adsorption behavior of target chemicals in deionized water, streamlining the process of obtaining model parameters for predicting adsorption capacities in natural water systems.

Results indicate that the concentration nears equilibrium at the highest concentrations for CaO-rich (120 mg L^{-1}) and Pine sawdust (57 mg L^{-1}) biochar, while Peanut, Eucalyptus polybractea, and Crawfish biochars approach equilibrium at intermediate concentrations. CO_2-activated Thalia, sewage sludge biochar, and Broussonetia Papyrifera Leaves biochar equilibrate at lower concentrations. Only Soybean Stover biochar exhibits a sharp rise and fall peak at a mid-concentration of 2 mg L^{-1}. Peanut Shell Biochar reaches equilibrium at a near concentration following simulation.

Figures 2–10 depict the model simulations of phosphate adsorption capacities onto eight different biochars. The experimental data were obtained from eight reports, encompassing adsorption data for phosphate obtained from Peanut Shell Biochar, Crawfish Biochar, CaO-rich Biochar, Pine Biochar, Broussonetia Papyrifera Leaves Biochar, Sewage Sludge Biochar, Soybean Stover Biochar, Eucalyptus Polybractea and CO_2-Activated Thalia Biochar[26,27]. The fitting equations for N with the Molecular Connectivity Index (MCI) are provided in Supplementary Material S2. It is noted that the discrepancies between the N values obtained from isotherms and those calculated using the fitting equation are reported, with an average error of 1% and 95% of the adsorption curve having an error of less than 0.5%. Figures 2, 3 and 9 illustrate that the models reasonably align with the experimental data, with an average Standard Deviation (SDEV) of 43%. The good simulation results, derived from the regression of phosphate adsorption onto eight different biochars explain the model approach can effectively involve both the biochars and properties of phosphate examined in this study. Analyzing the simulated results, it is observed that the data from three reports (Figures 2, 3 and 9) exhibit good fits, whereas the remaining data show high discrepancies from the models, with an average Standard deviation exceeding 50%. Like the cases shown in Figures 4–7, the bigger disparities in the models and the data may be from the complexity of the ionic structure interactions with biochar. These intricate interactions make the simulation of Molecular Connectivity Indices (MCIs) somewhat challenging. Moreover, the limited availability of only eight biochar in this study restricts the capacity to provide comprehensive descriptions for all phosphate interactions with other untested biochar samples.

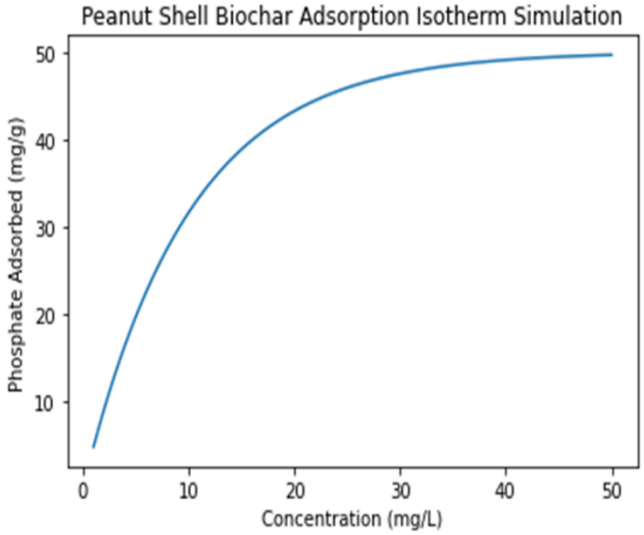

Figure 2. Peanut Shell Biochar Adsorption Isotherm Simulation.

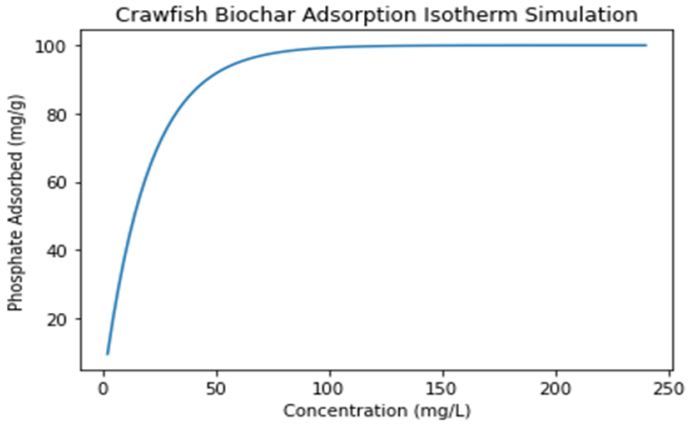

Figure 3. Crawfish Biochar Adsorption Isotherm Simulation.

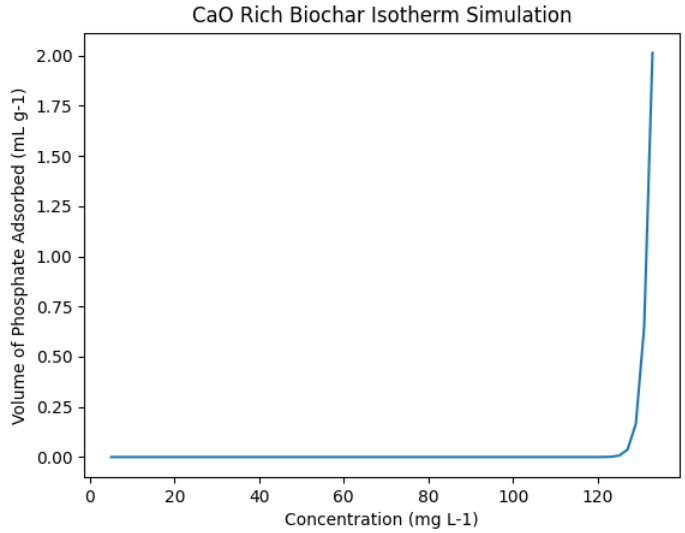

Figure 4. CaO Rich showed Biochar Adsorption Isotherm Simulation.

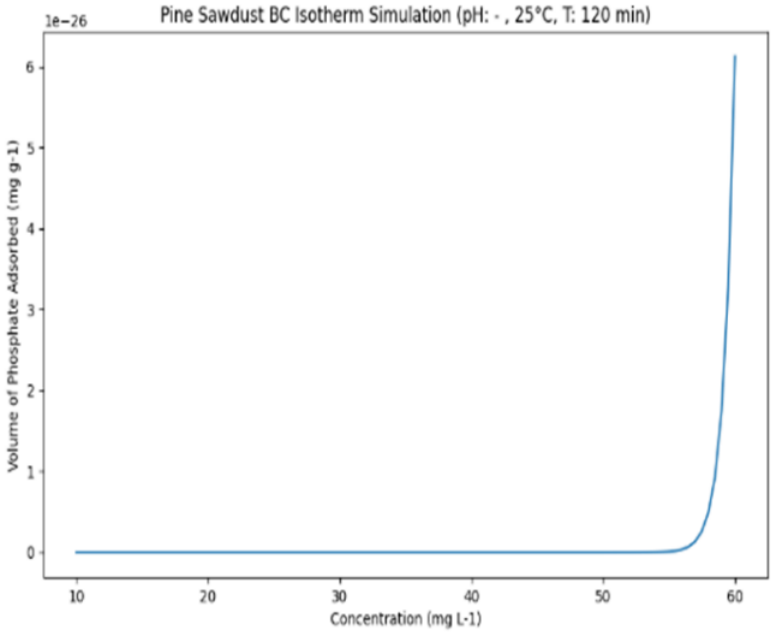

Figure 5. Pine Biochar Adsorption Isotherm Simulation.

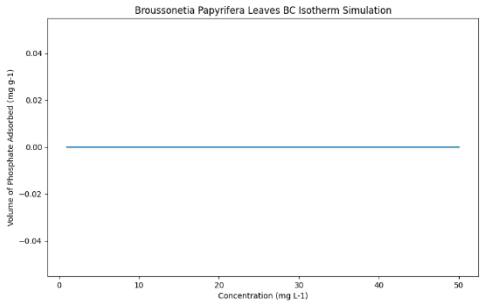

Figure 6. Broussonetia Papyrifera leaves BC isotherm Simulation.

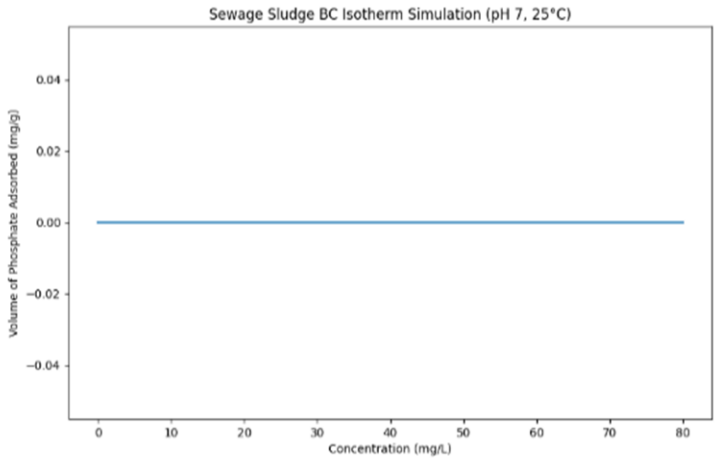

Figure 7. Sewage sludge BC isotherm Simulation.

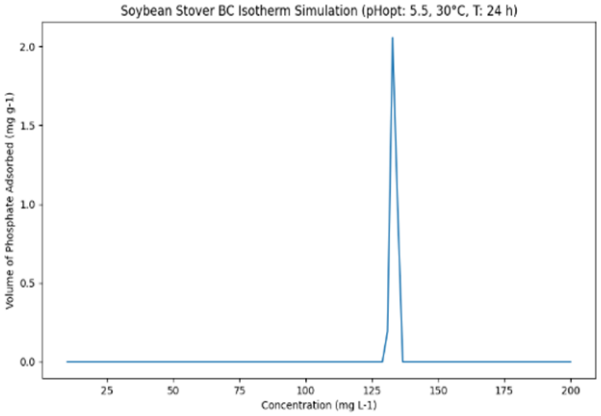

Figure 8. Soya bean Stover BC isotherm Simulation.

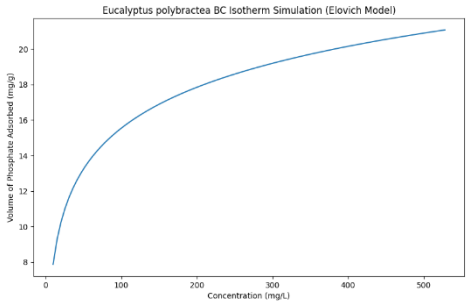

Figure 9. Eucalyptus Polybractea BC isotherm Simulation (Elovich Model).

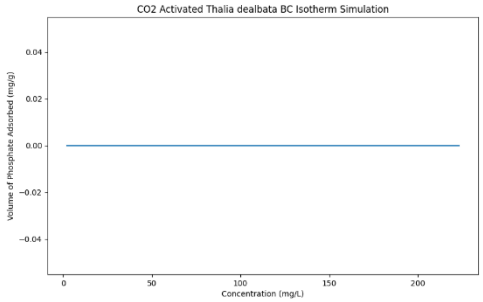

Figure 10. CO_2 Activated Thalia dealbata BC isotherm Simulation.

3. Adsorption Mechanism

The removal of phosphate from aqueous solutions is governed by the physical and chemical interactions between phosphate and biochar. Understanding the adsorption mechanism is crucial as it directly relates to adsorption isotherms, kinetics, capacity, and adsorption thermodynamics. In this context, Dudinin parameters play a significant role. For ease of reference, the mechanisms of phosphate adsorption with biochar, as reported in the literature, are summarized in Table 1 and Supplementary Material S1. These mechanisms may vary and include electrostatic interactions, Lewis's acid-base interactions, ion exchange, ligand exchange, precipitation, crystallization, inner-sphere complexation, outer-sphere complexation, and hydrogen bonding are illustrated in Figure 5. However, the simulation studies utilize this mechanism under basic conditions, where the parameter Wo, representing the limiting adsorption volume of phosphate, is associated with the pore size distribution (PSD) of the biochar. Simulation figures demonstrate that the model should closely match

the experimental data, depicting Langmuir, Elovich models, and Freundlich [28,29]. Nonetheless, anomalies were observed in the simulation of other biochars. This is likely due to insufficient conditions and adsorption data for the biochar, resulting in improper simulation outputs. The correlation of N with the Molecular Connectivity Index is not as strong as for the adsorbents reported in the successful simulated plots in the study. Therefore, higher errors between the adsorption data and the generated models are expected in some cases. For the approximately 28 biochars modeled, the error of our model simulation was 56% SDEV, which is generally lower. The model only employs three or four simple physicochemical parameters, such as aqueous solubility and temperature, to describe the properties of phosphate compounds in common laundry detergents. The results of the model can effectively incorporate the properties of biochar, comparable to activated carbon in this context. The discrepancy between the models could be attributed to the relationship between the biochar condition and the phosphate ions. In this study, only phosphate, an anion, was involved, limiting the capability to provide good fits and descriptions for other pollutants such as cations and other inorganics.

4. Potential Application of the Model

The Dudinin model developed in this study has been tested in simulations of the adsorption capacities of biochar obtained from approximately 8 successful reports for phosphate onto biochar. Since the modeling requires N, which can easily be obtained from the nature of the anion (phosphate) simulated with MCI, and the key biochar property, it is very easy to extrapolate the results to other biochars provided there is a prior relationship with the targeted pollutant, such as phosphate. In a previous study, a model was developed to predict the adsorption of LMWNPOCs onto ACs, using a similar approach to that applied in this current study [23]. In this work, the models were restricting the scope to only phosphate in laundry wastewater, a single correlation equation for N values suffices to characterize phosphate properties, allowing modification of the model approach to suit potential phosphate adsorption conditions. Phosphate adsorption onto biochar in natural water is known to be influenced by various factors such as co-existing ions. It would be highly beneficial if the current model approach to be adapted for simulating adsorption in natural water systems. To predict adsorption in natural streams of water accurately, information on adsorption in DI water and the interaction of phosphate with other ions, such as sodium adsorption characteristics, is essential.

5. Conclusions

Simulation studies using the Dudinin equation for the first time demonstrate biochar's potential for phosphate removal from laundry wastewater. DA models were successfully built and tested for the adsorption of phosphate onto biochar. Similar to studies elsewhere, aqueous solubility and key parameters N can be derived based on phosphate simulated with experimental measurements and MCI. Using the results of the current study and those from Bunmahotama et al. [21] model gives a clear means to predict phosphate adsorption onto biochar in water, based on the chemical structures of the targeted adsorbate. Moreover, it can be extended and coupled with other pollutants or co-existing ions for predicting adsorption in natural water, albeit requiring additional experimental efforts to get the parameters of the model. This research underscores the effectiveness of biochar adsorption and emphasizes the importance of optimizing biochar properties to enhance PO_4^{3-} adsorption capacity in laundry wastewater. The findings from these simulation studies can aid researchers and industries in predicting the effectiveness of biochar derived from similar precursors for wastewater treatment, thereby facilitating informed decision-making in setting up remediation strategies for environmental sustainability. Overall, the findings support biochar as a sustainable and efficient alternative for wastewater treatment, with future endeavors focusing on experimental validation of the simulation results and optimization of operating conditions for practical applications.

Supplementary Material

Supplementary Material S1: Summary of some reports and adsorption isotherms of anions (phosphate) used in this study.

Table S1. Summary of the reported studies on phosphate removal with unmodified BC from aqueous solutions.

Adsorbent/Feedstock	Pyrolysis Conditions (Temperature and Time)	Studied Phosphate Concentration (mg/L)	N2 Surface Area (m^2/g)	PZC	Elemental Composition of	*Qm* (mg/g)	Kinetic Model	Isotherm	Adsorbent dose D (g/L), Optimum pHopt Equilibrium time (T)	Mechanism of Adsorption	Ref
Undigested sugar beet tailings BC	600 °C, 2 h	15–640 (PO_4^{3-})	336	–	Mg: 9.79 wt% Ca: 9.78 wt% Fe: 0.75 wt% Al: 0.24 wt% Zn: 0.03 wt% K: 1.97 wt%	133.09 (PO_4^{3-}) at pH 7, 22 °C	Nth order, n = 1.14	F, L-F	D: 2 pH_{opt}: 5.2 T: 24 h	Electrostatic interactions	30
Peanut shell BC	700 °C, 3 h	1–50 (PO_4^{3-})	328.96	–		7.57 (PO_4^{3-}) at pH 7, 30 °C	PSO, Intra particle diffusion	L	D: 2 pH_{opt}: 12 T: >20 h	Chemisorption	27
Crawfish BC	800 °C	2–240 (PO_4^{3-})	–	–	Mg: 0.51 wt% Ca: 7.00 wt% Fe: 0.25 wt% Al: 1.39 wt% K: 0.11 wt%	70.9 (PO_4^{3-}) at pH 6, 25 °C	PSO	L, F	D: 2 pH_{opt}: 2–10 T: 15 min	Ion exchange, precipitation	26
CaO rich Eggshell and rice straw BC composite	800 °C, 2 h	5–200 (P)	25.8	5.36	Mg: 0.64 wt% Ca: 41.2 wt% Fe: 909 mg/kg Al: 932 mg/kg K: 1.04 wt% Si:2908 mg/kg	231 (P) at Ph 7, 25 °C	PSO	L	D: 0.25 pH_{opt}: 5–11 T: 6 h	Precipitation	31
Broussonetia papyrifera leaves BC	500 °C, 2 h	–	9.53	–	Mn: 0.14% Mg: 1.35 wt%	35.63 at pH 7, 25 °C 32.58	PSO, Intra particle diffusion	L at 30 °C	D: 5 pH_{opt}: 4–11 T: 120 min	Surface precipitation	32
Undaria pinnatifida roots BC	400 °C, 2 h	1 – 200 (PO_4^{3-})	70.29	8.11	Ca: 1.73 wt%	(PO_4^{3-}) at pH 7,	–	F at 25 °C	D: 1 pH_{opt}: - T:	Endothermic adsorption.	33
Laminaria japonica powder BC	600 °C, 1 h	5 – 1000 (PO_4^{3-})	79.95	–	K: 0.69 wt% Mg: 2.61 wt% Ca: 6.15 wt% K: 28.29 wt%	30 °C 160.7 (PO_4^{3-}) at pH 6, 30 °C	PSO	L L-F	D: 1 pH_{opt}: T: 24 h	–	34
Ca-alginate granular beads Laminaria japonica BC	600 °C, 1 h		242.34	8.42	–	157.68 (PO_4^{3-}) at pH 6, 30 °C			D: 1 pH_{opt}: 6 T: 24 h		35
Sewage sludge BC	600 °C, 3 h	–	31.35	11.2	Mg: 1.99 wt% Ca: 19.38 wt% Fe: 3.16 wt% Al: 6.49 wt% Si: 8.33 wt% K: 0.82 wt%	303.49 (PO_4^{3-}) at 25 °C	PSO	L-F	D: 2 pH_{opt}: 4 T: 5 h	Electrostatic interactions, ligand exchange	35
Soybean stover BC	700 °C, 3 h	10 – 200 (P)	420.33	–	–	90.9 (P) at pH 5.5, 40 °C	PSO	L, F	D: 4 pH_{opt}: 5.5 T: 24 h	Surface precipitation	36
Pine sawdust BC	750 °C, 15 min	10–60 (PO_4^{3-})	219	–	–	15.11 (PO_4^{3-}) at 25 °C	PSO	F	D: 1 pH_{opt}: - T: 120 min	–	37
Maize straw BC	350–550 °C	100 – 2000 (P)	4.05	–	–	9.47 (P) at RT 12.52 (P) at RT	–	L	D: 100 pH_{opt}: - T: 24 h	–	38
Rice hull BC			8.2								
Pine BC			97.2			14.48 (P) at RT					
Sesame straw BC	600 °C, 2 h	0–400 (P)	319.4	–	Mg:4861 mg/kg Ca: 0.54 wt% Fe:14.98 mg/kg K: 9.4 mg/kg	15.46 (P) at 25 °C	–	F	D: 2 pH_{opt}: - T: -	Electrostatic interactions and metal-ion complex formation.	39
Sesame straw BC	700 °C	5–500 (P)	413	–	Mg: 0.75 wt% Ca: 3.7 wt% Al: 0.05 wt%	116.58 (PO_4^{3-}) at 25 °C	PSO	L-F	D: 2 pH_{opt}: - T: 12 h	–	22
Sugar cane bagasse BC	700 °C, 60 min	25–400 (P)	131	–	–	13.21 (P) at pH 7, 20 °C	–	L	D: 2 pH_{opt}: 3 – 4 T: -	Ion exchange	40
Miscanthus giganteus BC			244			16.1 (P) at pH 7, 20 °C					
Wood BC	600 °C, 10 h	25–150 ppm (P)	147	–	–	11.98 (P) at pH 7, 25 °C	PSO	L, F, Timken	D: 1.25 pH_{opt}: - T: 10 h	Electrostatic interactions, ligand exchange	41
Corncobs BC			123			11.4 (P) at pH 7, 25 °C					
Rice husks BC			11			8.09 (P) at pH 7, 25 °C					
Sawdust BC			7			10.07 (P) at pH 7, 25 °C					
Sewage sludge BC	650 °C, 30 min	5–80 (PO_4^{3-})	149.47	3.27	Ca: 0.52 atomic% Fe: 3.35 atomic%	15.15 (PO_4^{3-}) at 25 °C	–	L	D: 4 pH_{opt}: 7 T: -	Ligand exchange, columbic interaction, Lewis acid base interaction, surface precipitation	38
CO_2 activated Thalia dealbata BC	700 °C, 2 h	–	223.1, N_2 228.3, CO_2	–	Mg: 4.42 g/kg Ca: 19.66 g/kg Fe: 0.64 g/kg Al: 0.44 g/kg	4.96 (P) pH 7, RT	–	L	D: 4 pH_{opt}: - T: -	Surface precipitation	22
Eucalyptus polybractea BC	720 °C, 20 min	10–528 (P)	233	–	Mg: 0.2 atomic% Ca: 1.3 atomic% K: 0.3 atomic%	3.66 (P) at RT	Elovich	F	D: 3.33 pH_{opt}: - T: 1	–	23

Supplementary Material S2: Standards User Interface Code for Single Phosphate Concentration
Enter the initial phosphate concentration (mg L^{-1}): 10
Enter the aqueous solubility (mg L^{-1}): 14 (for common phosphate detergents)
Enter the micropore volume for pores smaller than 3.2 nm (mL g^{-1}): 3.19
Enter the temperature (K): 353.15 (as used in sinners' cycle)

```
import NumPy as np
import matplotlib.pyplot as plt

# Constants
n = 1.1
N = 1 # Normalizing factor (can be adjusted as needed)
R = 8.314 # J K^(-1) mol^(-1)

# Input parameters
Cp_initial = float(input('Enter the initial phosphate concentration (mg L^(-1)): '))
Cs = float(input('Enter the aqueous solubility (mg L^(-1)): '))
V3_2 = float(input('Enter the micropore volume for pores smaller than 3.2 nm (mL g^(-1)): '))
T = float(input('Enter the temperature (K): '))

# Calculate Wo using Equation 2
def calculate_Wo(V3_2):
return 0.055 + V3_2

# Calculate epsilon using Equation 1
def calculate_epsilon(Cs, Cp, T):
return R * T * np.log(Cs / Cp)

# Calculate W using Equation 1
def calculate_W(Wo, epsilon):
return Wo * np.exp(-(epsilon / (100 * N)) ** n)

# Generate a range of phosphate concentrations
Cp_min = 0.01 # mg L^(-1)
Cp_max = 10 # mg L^(-1)
Cp_num = 1000
Cp_range = np.linspace(Cp_min, Cp_max, Cp_num)

# Calculate the corresponding values of W for each Cp value
Wo = calculate_Wo(V3_2)
epsilon_range = calculate_epsilon(Cs, Cp_range, T)
W_range = calculate_W(Wo, epsilon_range)

# Convert volume of chemical adsorbed to adsorption capacity
adsorption_capacity_range = W_range * (Cp_initial - Cp_range)/1000

# Plot the isotherm
plt.plot(Cp_range, adsorption_capacity_range)
plt.xlabel('Phosphate concentration (mg L^(-1))')
```

```
plt.ylabel('Adsorption capacity (mg g^(-1))')
plt.title('Isotherm of adsorption of phosphate')
plt.show()
```

Enter the aqueous solubility (mg L^{-1}): 14 (for common Phosphate detergents)
Enter the micropore volume for pores smaller than 3.2 nm (mL g^{-1}): 3.19
Enter the temperature (K): 353.15 (temperature in sinners' cycle)
Enter initial phosphate concentration (mg L^{-1}): 10
The rest of Simulation of the actual biochar can be found in the supplementary materials
Sure! Here's the program rewritten to allow input for five concentrations:
"'python

```python
import numpy as np
import matplotlib.pyplot as plt

# Constants
n = 1.1
N = 1 # Normalizing factor (can be adjusted as needed)
R = 8.314 # J K^(-1) mol^(-1)

# Initialize a list to store the five initial phosphate concentrations
Cp_initial_list = []

# Get input for five initial phosphate concentrations
for i in range(5):
Cp_initial = float(input(f'Enter initial phosphate concentration {i+1} (mg L^(-1)): '))
Cp_initial_list.append(Cp_initial)

# Get input for other parameters
Cs = float(input('Enter the aqueous solubility (mg L^(-1)): '))
V3_2 = float(input('Enter the micropore volume for pores smaller than 3.2 nm (mL g^(-1)): '))
T = float(input('Enter the temperature (K): '))

# Calculate Wo using Equation 2
def calculate_Wo(V3_2):
return 0.055 + V3_2

# Calculate epsilon using Equation 1
def calculate_epsilon(Cs, Cp, T):
return R * T * np.log(Cs / Cp)

# Calculate W using Equation 1
def calculate_W(Wo, epsilon):
return Wo * np.exp(-(epsilon / (100 * N)) ** n)

# Generate a range of phosphate concentrations
Cp_min = 0.01 # mg L^(-1)
Cp_max = 10 # mg L^(-1)
```

```
Cp_num = 1000
Cp_range = np.linspace(Cp_min, Cp_max, Cp_num)

# Plot the isotherm for each initial concentration
for Cp_initial in Cp_initial_list:
# Calculate the corresponding values of W for each Cp value
Wo = calculate_Wo(V3_2)
epsilon_range = calculate_epsilon(Cs, Cp_range, T)
W_range = calculate_W(Wo, epsilon_range)

# Convert volume of chemical adsorbed to adsorption capacity
adsorption_capacity_range = W_range * (Cp_initial - Cp_range)/1000

# Plot the isotherm
plt.plot(Cp_range, adsorption_capacity_range, label=f'Initial concentration:
{Cp_initial} mg L^(-1)')
plt.xlabel('Phosphate concentration (mg L^(-1))')
plt.ylabel('Adsorption capacity (mg g^(-1))')
plt.title('Isotherm of adsorption of phosphate')
plt.legend()
plt.show()
```

This updated code will prompt you to enter five initial phosphate concentrations and then calculate and plot the adsorption isotherm for each concentration.

Modelling Codes for Biochar in the study:

```
import numpy as np
import matplotlib.pyplot as plt

# Define the DA equation
def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 298 # K
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

# Define the Wo_from_PSD function
def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Undigested Sugar Beet biochar
C_range = np.linspace(15, 640, 100) # Concentrations (mg/L)
Cs = 133.09 # Aqueous solubility of phosphate (mg/L)
V3_2 = 2 # Micropore volume for pores with diameter < 3.2 nm (mL/g)
N = 0.336 # Molecular descriptor for phosphate (PO3-)
n = 1.14 # Exponential constant for the biochar surface

# Calculate Wo
```

```
Wo = Wo_from_PSD(V3_2)

# Simulate phosphate adsorption
W = DA_equation(C_range, Cs, Wo, N, n)

# Plotting the simulation results
plt.figure(figsize=(10, 6))
plt.plot(C_range, W)
plt.xlabel('Phosphate Concentration (mg/L)')
plt.ylabel('Phosphate Adsorption Capacity (mg/g)')
plt.title('Phosphate Adsorption by Undigested Sugar Beet Biochar')
plt.grid(False)

plt.show()

import numpy as np
import matplotlib.pyplot as plt

import numpy as np
import matplotlib.pyplot as plt

# Define the modeling equation
def simulate_crawfish_biochar(C, Qm, Kd):
W = Qm * (1 - np.exp(-Kd * C))
return W

# Parameters for Crawfish Biochar
C_range = np.linspace(2, 240, 100) # Concentrations (mg/L)
Qm = 100 # Adjust this value based on your data (maximum adsorption capacity, mg/g)
Kd = 0.05 # Adjust this value based on your data (adsorption rate constant, L/mg)

# Simulate isotherm
W = simulate_crawfish_biochar(C_range, Qm, Kd)

# Plotting
plt.plot(C_range, W)
plt.xlabel('Concentration (mg/L)')
plt.ylabel('Phosphate Adsorbed (mg/g)')
plt.title('Crawfish Biochar Adsorption Isotherm Simulation')
plt.grid(False)
plt.show()

import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 303.15 # K (30 °C)
```

```
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Laminaria Japonica Powder BC
C = np.linspace(1, 1000, 100) # Concentrations (mg L^(-1) ) - Adjusted the upper limit
Cs = 133.09 # Aqueous solubility (mg L^(-1))
V3_2 = 2 # Micropore volume for pores with diameter < 3.2 nm (mL g^(-1))
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 1 # Exponential constant for the biochar surface (adjusted as specified)

# Calculate Wo
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms for Laminaria Japonica Powder BC
W = DA_equation(C, Cs, Wo, N, n)

# Plotting for Laminaria Japonica Powder BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg L^(-1))')
plt.ylabel('Volume of Phosphate Adsorbed (mg g^(-1))')
plt.title('Laminaria Japonica Powder BC Isotherm Simulation')
plt.grid(False)
plt.show()

import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 298.15 # K (25 °C)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Sesame Straw BC
C = np.linspace(5, 500, 100) # Concentrations (mg L^(-1))
Cs = 133.09 # Aqueous solubility (mg L^(-1))
V3_2 = 2 # Micropore volume for pores with diameter < 3.2 nm (mL g^(-1))
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 1 # Exponential constant for the biochar surface (adjusted as specified)
```

```
# Calculate Wo
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms for Sesame Straw BC
W = DA_equation(C, Cs, Wo, N, n)

# Plotting for Sesame Straw BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg L^(-1))')
plt.ylabel('Volume of Phosphate Adsorbed (mg g^(-1))')
plt.title('Sesame Straw BC Isotherm Simulation (pH: -, 25°C, T: 12 h)')
plt.grid(False)
plt.show()

import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 293.15 # K (20 °C in Kelvin)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Miscanthus Giganteus BC
C = np.linspace(0, 244, 100) # Concentrations (mg L^(-1))
Cs = 133.09 # Aqueous solubility (mg L^(-1))
V3_2 = 16.1 # Micropore volume for pores with diameter < 3.2 nm (mL g^(-1))
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 1 # Exponential constant for the biochar surface (adjusted as specified)

# Calculate Wo
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms for Miscanthus Giganteus BC
W = DA_equation(C, Cs, Wo, N, n)

# Plotting for Miscanthus Giganteus BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg L^(-1))')
plt.ylabel('Volume of Phosphate Adsorbed (mg g^(-1))')
plt.title('Miscanthus Giganteus BC Isotherm Simulation (pH 7, 20 °C)')
```

```
plt.grid(False)
plt.show()

import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 298.15 # K (25 °C in Kelvin)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Corncobs BC
C = np.linspace(0, 123, 100) # Concentrations (mg/L)
Cs = 133.09 # Aqueous solubility (mg/L)
V3_2 = 11.4 # Micropore volume for pores with diameter < 3.2 nm (mL/g)
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 1 # Exponential constant for the biochar surface

# Calculate Wo
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms for Corncobs BC
W = DA_equation(C, Cs, Wo, N, n)

# Plotting for Corncobs BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg/L)')
plt.ylabel('Volume of Phosphate Adsorbed (mg/g)')
plt.title('Corncobs BC Isotherm Simulation (pH 7, 25 °C)')
plt.grid(False)
plt.show()

import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 303.15 # K (30 °C)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W
```

```
def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Laminaria Japonica BC
C = np.linspace(1, 1000, 100) # Concentrations (mg L^(-1)) - Adjusted the upper limit
Cs = 133.09 # Aqueous solubility (mg L^(-1))
V3_2 = 2 # Micropore volume for pores with diameter < 3.2 nm (mL g^(-1))
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 1 # Exponential constant for the biochar surface (adjusted as specified)

# Calculate Wo
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms for Laminaria Japonica BC
W = DA_equation(C, Cs, Wo, N, n)

# Plotting for Laminaria Japonica BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg L^(-1))')
plt.ylabel('Volume of Phosphate Adsorbed (mg g^(-1))')
plt.title('Laminaria Japonica BC Isotherm Simulation (pH 6, 30 °C, T: 24 h)')
plt.grid(False)
plt.show()


import numpy as np
import matplotlib.pyplot as plt

# Define the modeling equation
def simulate_pine_biochar(C, Qm, Kd):
W = Qm * (1-np.exp(-Kd * C))
return W

# Parameters for Pine Biochar
C_range = np.linspace(10, 60, 100) # Concentrations (mg/L)
Qm = 14.48 # Maximum adsorption capacity (mg/g)
Kd = 0.1 # Adsorption rate constant (L/mg)

# Simulate isotherm
W = simulate_pine_biochar(C_range, Qm, Kd)

# Plotting
plt.plot(C_range, W)
plt.xlabel('Concentration (mg/L)')
plt.ylabel('Phosphate Adsorbed (mg/g)')
plt.title('Pine Biochar Adsorption Isotherm Simulation')
plt.grid(False)
```

```
plt.show()

import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 298.15 # K (25 °C in Kelvin)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Rice Husks BC
C = np.linspace(0, 11, 100) # Concentrations (mg/L)
Cs = 133.09 # Aqueous solubility (mg/L)
V3_2 = 8.09 # Micropore volume for pores with diameter < 3.2 nm (mL/g)
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 1 # Exponential constant for the biochar surface

# Calculate Wo
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms for Rice Husks BC
W = DA_equation(C, Cs, Wo, N, n)

# Plotting for Rice Husks BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg/L)')
plt.ylabel('Volume of Phosphate Adsorbed (mg/g)')
plt.title('Rice Husks BC Isotherm Simulation (pH 7, 25°C)')
plt.grid(False)
plt.show()

import numpy as np
import matplotlib.pyplot as plt

import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 298.15 # K (25 °C in Kelvin)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
```

```
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Sawdust BC
C = np.linspace(0, 7, 100) # Concentrations (mg/L)
Cs = 133.09 # Aqueous solubility (mg/L)
V3_2 = 10.07 # Micropore volume for pores with diameter < 3.2 nm (mL/g)
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 1 # Exponential constant for the biochar surface

# Calculate Wo
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms for Sawdust BC
W = DA_equation(C, Cs, Wo, N, n)
# Plotting for Sawdust BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg/L)')
plt.ylabel('Volume of Phosphate Adsorbed (mg/g)')
plt.title('Sawdust BC Isotherm Simulation (pH 7, 25°C)')
plt.grid(False)
plt.show()

import numpy as np
import matplotlib.pyplot as plt

def Elovich_equation(C, alpha, beta):
W = alpha + beta * np.log(C)
return W

# Parameters for Eucalyptus polybractea BC
C = np.linspace(10, 528, 100) # Concentrations (mg/L)
alpha = 0.2 # Alpha parameter for Elovich equation
beta = 3.33 # Beta parameter for Elovich equation

# Simulate isotherms for Eucalyptus polybractea BC using Elovich equation
W = Elovich_equation(C, alpha, beta)

# Plotting for Eucalyptus polybractea BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg/L)')
plt.ylabel('Volume of Phosphate Adsorbed (mg/g)')
plt.title('Eucalyptus polybractea BC Isotherm Simulation (Elovich Model)')
plt.grid(False)
```

```
plt.show()

import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 303.15 # K (30 °C)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Soybean Stover BC
C = np.linspace(10, 200, 100) # Concentrations (mg L^(-1) )
Cs = 133.09 # Aqueous solubility (mg L^(-1) )
V3_2 = 2 # Micropore volume for pores with diameter < 3.2 nm (mL g^(-1) )
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 4 # Exponential constant for the biochar surface (adjusted as specified)

# Calculate Wo
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms for Soybean Stover BC
W = DA_equation(C, Cs, Wo, N, n)

# Plotting for Soybean Stover BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg L^(-1))')
plt.ylabel('Volume of Phosphate Adsorbed (mg g^(-1))')
plt.title('Soybean Stover BC Isotherm Simulation (pHopt: 5.5, 30°C, T: 24 h)')
plt.grid(False)
plt.show()

import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 298 # K (25 °C)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
```

```
return 0.055 + V3_2

# Parameters for CaO Rich Biochar
C = np.linspace(5, 200, 100) # Concentrations (mg L^(-1))
Cs = 133.09 # Aqueous solubility (mg L^(-1))
V3_2 = 2 # Micropore volume for pores with diameter < 3.2 nm (mL g^(-1))
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 1.14 # Exponential constant for the biochar surface

# Calculate Wo
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms
W = DA_equation(C, Cs, Wo, N, n)

# Plotting
plt.plot(C, W)
plt.xlabel('Concentration (mg L^(-1))')
plt.ylabel('Volume of Phosphate Adsorbed (mL g^(-1))')
plt.title('CaO Rich Biochar Isotherm Simulation')
plt.grid(False)
plt.show()

import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 298.15 # K (25 °C in Kelvin)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Sewage Sludge BC
C = np.linspace(0, 80, 100) # Concentrations (mg/L)
Cs = 133.09 # Aqueous solubility (mg/L)
V3_2 = 3.27 # Micropore volume for pores with diameter < 3.2 nm (mL/g)
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 4 # Exponential constant for the biochar surface

# Calculate Wo
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms for Sewage Sludge BC
W = DA_equation(C, Cs, Wo, N, n)
```

```
import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 303.15 # K (30 °C)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Sewage Sludge BC
C = np.linspace(1, 31.35, 100) # Concentrations (mg L^(-1)) - Adjusted the upper limit
Cs = 133.09 # Aqueous solubility (mg L^(-1))
V3_2 = 2 # Micropore volume for pores with diameter < 3.2 nm (mL g^(-1))
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 2 # Exponential constant for the biochar surface (adjusted as specified)

# Calculate Wo
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms for Sewage Sludge BC
W = DA_equation(C, Cs, Wo, N, n)

# Plotting for Sewage Sludge BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg L^(-1))')
plt.ylabel('Volume of Phosphate Adsorbed (mg g^(-1))')
plt.title('Sewage Sludge BC Isotherm Simulation (pH 4, 30 °C, T: 5 h)')
plt.grid(False)
plt.show()

# Plotting for Sewage Sludge BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg/L)')
plt.ylabel('Volume of Phosphate Adsorbed (mg/g)')
plt.title('Sewage Sludge BC Isotherm Simulation (pH 7, 25 °C)')
plt.grid(False)
plt.show()

import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
```

```
R = 8.314 # J K^(-1) mol^(-1)
T = 298.15 # K (25 °C)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Pine Sawdust BC
C = np.linspace(10, 60, 100) # Concentrations (mg L^(-1))
Cs = 133.09 # Aqueous solubility (mg L^(-1))
V3_2 = 2 # Micropore volume for pores with diameter < 3.2 nm (mL g^(-1))
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 1 # Exponential constant for the biochar surface (adjusted as specified)

# Calculate Wo
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms for Pine Sawdust BC
W = DA_equation(C, Cs, Wo, N, n)

# Plotting for Pine Sawdust BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg L^(-1))')
plt.ylabel('Volume of Phosphate Adsorbed (mg g^(-1))')
plt.title('Pine Sawdust BC Isotherm Simulation (pH: - , 25 °C, T: 120 min)')
plt.grid(False)
plt.show()

import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 303.15 # K (30 °C)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Ca-Alginate Granular Beads
C = np.linspace(1, 242.34, 100) # Concentrations (mg L^(-1)) - Adjusted the upper limit
Cs = 133.09 # Aqueous solubility (mg L^(-1))
V3_2 = 2 # Micropore volume for pores with diameter < 3.2 nm (mL g^(-1))
```

```
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 1 # Exponential constant for the biochar surface (adjusted as specified)

# Calculate Wo
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms for Ca-Alginate Granular Beads
W = DA_equation(C, Cs, Wo, N, n)

# Plotting for Ca-Alginate Granular Beads
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg L^(-1))')
plt.ylabel('Volume of Phosphate Adsorbed (mg g^(-1))')
plt.title('Ca-Alginate Granular Beads Isotherm Simulation')
plt.grid(False)
plt.show()

import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 298.15 # K (25 °C)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Sugar Cane Bagasse BC
C = np.linspace(25, 400, 100) # Concentrations (mg L^(-1))
Cs = 133.09 # Aqueous solubility (mg L^(-1))
V3_2 = 2 # Micropore volume for pores with diameter < 3.2 nm (mL g^(-1))
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 1 # Exponential constant for the biochar surface (adjusted as specified)

# Calculate Wo
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms for Sugar Cane Bagasse BC
W = DA_equation(C, Cs, Wo, N, n)

# Plotting for Sugar Cane Bagasse BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg L^(-1))')
```

```
plt.ylabel('Volume of Phosphate Adsorbed (mg g^(-1))')
plt.title('Sugar Cane Bagasse BC Isotherm Simulation (pHopt: 3 - 4, 25°C, T: -)')
plt.grid(False)
plt.show()


import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 298.15 # K (25°C)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Rice Hull BC
C = np.linspace(10, 200, 100) # Concentrations (mg L^(-1))
Cs = 133.09 # Aqueous solubility (mg L^(-1))
V3_2 = 2 # Micropore volume for pores with diameter < 3.2 nm (mL g^(-1))
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 1 # Exponential constant for the biochar surface (adjusted as specified)

# Calculate Wo
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms for Rice Hull BC
W = DA_equation(C, Cs, Wo, N, n)

# Plotting for Rice Hull BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg L^(-1))')
plt.ylabel('Volume of Phosphate Adsorbed (mg g^(-1))')
plt.title('Rice Hull BC Isotherm Simulation (pHopt: -, 25°C, T: 24 h)')
plt.grid(False)
plt.show()

import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 298.15 # K (25 °C in Kelvin)
epsilon = R * T * np.log(Cs/C)
```

```
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for CO_(2) activated Thalia dealbata BC
C = np.linspace(0, 223.1, 100) # Concentrations (mg/L)
Cs = 0.0 # Aqueous solubility (Assumed to be zero mg/L)
V3_2 = 0.0 # Assumed to be zero for simplicity (micropore volume)
N = 0.0 # Assumed to be zero for simplicity (molecular descriptor)
n = 4 # Exponential constant (You can adjust this as needed)

# Calculate Wo (Assumed to be zero)
Wo = Wo_from_PSD(V3_2)
# Simulate isotherms for CO_(2) activated Thalia dealbata BC
W = DA_equation(C, Cs, Wo, N, n)

# Plotting for CO_(2) activated Thalia dealbata BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg/L)')
plt.ylabel('Volume of Phosphate Adsorbed (mg/g)')
plt.title('CO_(2) Activated Thalia dealbata BC Isotherm Simulation')
plt.grid(False)
plt.show()

import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 298 # K (25 °C)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Eggshell and Rice Straw BC Composite
C = np.linspace(1, 50, 100) # Concentrations (mg L^(-1)) - Adjusted the lower limit
Cs = 133.09 # Aqueous solubility (mg L^(-1))
V3_2 = 2 # Micropore volume for pores with diameter < 3.2 nm (mL g^(-1))
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 1.14 # Exponential constant for the biochar surface (original value)

# Calculate Wo
```

```
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms for Eggshell and Rice Straw BC Composite
W = DA_equation(C, Cs, Wo, N, n)

# Plotting for Eggshell and Rice Straw BC Composite
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg L^(-1))')
plt.ylabel('Volume of Phosphate Adsorbed (mg g^(-1))')
plt.title('Eggshell and Rice Straw BC Composite Isotherm Simulation')
plt.grid(False)
plt.show()

import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 298.15 # K (25 °C)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Pine BC
C = np.linspace(10, 60, 100) # Concentrations (mg L^(-1))
Cs = 133.09 # Aqueous solubility (mg L^(-1))
V3_2 = 2 # Micropore volume for pores with diameter < 3.2 nm (mL g^(-1))
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 1 # Exponential constant for the biochar surface (adjusted as specified)

# Calculate Wo
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms for Pine BC
W = DA_equation(C, Cs, Wo, N, n)

# Plotting for Pine BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg L^(-1))')
plt.ylabel('Volume of Phosphate Adsorbed (mg g^(-1))')
plt.title('Pine BC Isotherm Simulation (pH: - , 25°C, T: RT)')
plt.grid(False)
plt.show()
```

```
import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 293.15 # K (20 °C in Kelvin)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Wood BC
C = np.linspace(25, 150, 100) # Concentrations (mg/L)
Cs = 133.09 # Aqueous solubility (mg/L)
V3_2 = 147 # Micropore volume for pores with diameter < 3.2 nm (mL/g)
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 1.25 # Exponential constant for the biochar surface (adjusted as specified)

# Calculate Wo
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms for Wood BC
W = DA_equation(C, Cs, Wo, N, n)

# Plotting for Wood BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg/L)')
plt.ylabel('Volume of Phosphate Adsorbed (mg/g)')
plt.title('Wood BC Isotherm Simulation (pHopt: -, 20°C, T: 10 h)')
plt.grid(False)
plt.show()


import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 298 # K (25 °C)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W
```

```
def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Broussonetia Papyrifera Leaves BC
C = np.linspace(1, 50, 100) # Concentrations (mg L^(-1)) - Adjusted the lower limit
Cs = 133.09 # Aqueous solubility (mg L^(-1))
V3_2 = 2 # Micropore volume for pores with diameter < 3.2 nm (mL g^(-1))
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 5 # Exponential constant for the biochar surface (adjusted as specified)

# Calculate Wo
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms for Broussonetia Papyrifera Leaves BC
W = DA_equation(C, Cs, Wo, N, n)

# Plotting for Broussonetia Papyrifera Leaves BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg L^(-1))')
plt.ylabel('Volume of Phosphate Adsorbed (mg g^(-1))')
plt.title('Broussonetia Papyrifera Leaves BC Isotherm Simulation')
plt.grid(False)
plt.show()

import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 298.15 # K (25 °C)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Sesame Straw BC
C = np.linspace(0, 400, 100) # Concentrations (mg L^(-1))
Cs = 133.09 # Aqueous solubility (mg L^(-1))
V3_2 = 2 # Micropore volume for pores with diameter < 3.2 nm (mL g^(-1))
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 1 # Exponential constant for the biochar surface (adjusted as specified)

# Calculate Wo
Wo = Wo_from_PSD(V3_2)
```

```
# Simulate isotherms for Sesame Straw BC
W = DA_equation(C, Cs, Wo, N, n)

# Plotting for Sesame Straw BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg L^(-1))')
plt.ylabel('Volume of Phosphate Adsorbed (mg g^(-1))')
plt.title('Sesame Straw BC Isotherm Simulation (pHopt: -, 25 °C, T: -)')
plt.grid(False)
plt.show()

import numpy as np
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 298.15 # K (25 °C)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2

# Parameters for Maize Straw BC
C = np.linspace(100, 2000, 100) # Concentrations (mg L^(-1))
Cs = 133.09 # Aqueous solubility (mg L^(-1))
V3_2 = 2 # Micropore volume for pores with diameter < 3.2 nm (mL g^(-1))
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 1 # Exponential constant for the biochar surface (adjusted as specified)

# Calculate Wo
Wo = Wo_from_PSD(V3_2)

# Simulate isotherms for Maize Straw BC
W = DA_equation(C, Cs, Wo, N, n)

# Plotting for Maize Straw BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg L^(-1))')
plt.ylabel('Volume of Phosphate Adsorbed (mg g^(-1))')
plt.title('Maize Straw BC Isotherm Simulation (pH: - , 25 °C, T: 120 min)')
plt.grid(False)
plt.show()

import numpy as np
```

```
import matplotlib.pyplot as plt

def DA_equation(C, Cs, Wo, N, n):
R = 8.314 # J K^(-1) mol^(-1)
T = 298.15 # K (25°C)
epsilon = R * T * np.log(Cs/C)
W = Wo * np.exp(-((epsilon/(100*N))**n))
return W

def Wo_from_PSD(V3_2):
return 0.055 + V3_2
# Parameters for Sugar Cane Bagasse BC
C = np.linspace(25, 400, 100) # Concentrations (mg L^(-1))
Cs = 133.09 # Aqueous solubility (mg L^(-1))
V3_2 = 2 # Micropore volume for pores with diameter < 3.2 nm (mL g^(-1))
N = 0.336 # Molecular descriptor for phosphate (PO_(4)^(3-))
n = 1 # Exponential constant for the biochar surface (adjusted as specified)
# Calculate Wo
Wo = Wo_from_PSD(V3_2)
# Simulate isotherms for Sugar Cane Bagasse BC
W = DA_equation(C, Cs, Wo, N, n)
# Plotting for Sugar Cane Bagasse BC
plt.figure(figsize=(10, 6))
plt.plot(C, W)
plt.xlabel('Concentration (mg L^(-1))')
plt.ylabel('Volume of Phosphate Adsorbed (mg g^(-1))')
plt.title('Sugar Cane Bagasse BC Isotherm Simulation (pHopt: 3 - 4, 25°C, T: -)')
plt.grid(False)
plt.show()
import numpy as np
import matplotlib.pyplot as plt

# Constants and properties
pine_bc_weight = 97.2 # Weight of Pine biochar in grams
temperature = 25 # Temperature in Celsius (room temperature)

# DA isotherm constants specific to Pine biochar at the given conditions
Q = # Adsorption capacity (mg/g)
beta = # DA isotherm constant (mol²/J²)

# Phosphate concentration range (mg/L)
phosphate_concentration = np.linspace(0, 200, 100)

# Calculate phosphate adsorption using the DA equation
def adsorption_da(concentration):
epsilon = np.sqrt(-np.log(1 - concentration / Q))
return Q * np.exp(-beta * epsilon ** 2)
```

```
# Calculate phosphate adsorption for Pine BC
phosphate_adsorption = adsorption_da(phosphate_concentration)
# Plot the adsorption isotherm
plt.figure(figsize=(10, 6))
plt.plot(phosphate_concentration, phosphate_adsorption, label='Phosphate Adsorption')
plt.xlabel('Phosphate Concentration (mg/L)')
plt.ylabel('Phosphate Adsorption (mg/g)')
plt.legend()
plt.title('Phosphate Adsorption Isotherm for Pine BC')
plt.grid(True)
plt.show()
```

Supplementary Material S4: Simulating Software/Website under development (80%)

```
<html>
<head>
<title>EricJames Isotherm Simulation</title>
<script src="https://cdn.plot.ly/plotly-1.58.4.min.js"></script>
</head>
<body>
<h1>EricJames Isotherm Simulation</h1>
<div id="plot"></div>
<form id="inputForm">
<label for="Cs">Aqueous solubility (mg L^(-1)):</label>
<input type="number" id="Cs" name="Cs" step="0.01" placeholder="Enter aqueous solubility (mg L^(-1))" required><br>

<label for="Qm">Maximum adsorption capacity (mg/g):</label>
<input type="number" id="Qm" name="Qm" step="0.01" placeholder="Enter maximum adsorption capacity (mg/g)" required><br>

<label for="Kd">Adsorption rate constant (L/mg):</label>
<input type="number" id="Kd" name="Kd" step="0.01" placeholder="Enter adsorption rate constant (L/mg)" required><br>

<input type="submit" value="Simulate">
</form>

<script>
// Function to calculate DA equation
function DA_equation(C, Cs, Qm, Kd) {
return Qm * (1 - (Cs / C) * Math.exp(-Kd * C));
}

// Function to handle form submission
function handleForm(event) {
event.preventDefault();

// Get form values
var Cs = parseFloat(document.getElementById("Cs").value);
var Qm = parseFloat(document.getElementById("Qm").value);
var Kd = parseFloat(document.getElementById("Kd").value);
```

```
// Generate new C values
var C = Array.from({ length: 100 }, (_, i) => 10 + i * (50 - 10) / 99);

// Calculate W values
var W = C.map(c => DA_equation(c, Cs, Qm, Kd));

// Call plotly to generate the plot
var data = [{
x: C,
y: W,
type: 'scatter'
}];
var layout = {
xaxis: { title: 'Concentration (mg L^(-1))' },
yaxis: { title: 'Adsorption Capacity (mg/g)' },
title: 'EricJames Isotherm Simulation'
};
Plotly.newPlot('plot', data, layout);
}

// Add form submission event listener
document.getElementById("inputForm").addEventListener("submit", handleForm);
</script>
</body>
</html>
```

Author Contributions

The authors confirm contribution to the paper as follows: study conception and design: Eric York, Silas Owusu Antwi; Data collection: Eric York; analysis and interpretation of results: Eric York; draft manuscript preparation: James Tadio. All authors reviewed the results and approved the final version of the manuscript.

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Conflict of Interest

The authors declare no conflict of interest.

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