

Utilization of Microsoft Excel Matrix Functions Technique for Adsorption Equilibrium Models of Arsenic unto Powdered Eggshells

Amoko J S

Department of Chemistry, Adeyemi
Federal University of Education, Ondo,
Nigeria, temiamoko@gmail.com,
ORCID: 0000-0001-6641-7747

Adekunbi, E A

Department of Chemistry, Adeyemi
Federal University of Education, Ondo,
Nigeria, bemagnified08@yahoo.com
ORCID: 0009-0005-0279-8487

Oke, I.A

Department of Civil Engineering,
Obafemi Awolowo University, Ile-Ife,
Nigeria, okeia@oauife.edu.ng ORCID:
0000-0002-7082-7682

Abstract—This paper utilized Microsoft Excel Matrix Functions in determination of adsorption equilibrium parameters. Adsorption equilibrium data were obtained from our previous and published articles. Unknown engineering design parameters in the frequently utilized 2-parameters adsorption equilibrium models were determined utilising matrix functions and Microsoft Excel Solver in Microsoft Excel. Efficacies of these techniques were evaluated statistically utilising Analysis of Variance, Coefficient of Determination (CD) and correlation coefficient (R). and compared with experimental adsorption equilibrium. The study revealed that there was no significant difference between the adsorption capacities obtained utilising the two techniques at a 95 % confidence level. It was concluded that the CD and R between linear experimental adsorption equilibria, linear Microsoft Excel Solver and matrix simulated adsorption equilibria were between 0.6916 and 0.9535; 0.0492 and 0.9535; and 0.8318 and 0.9765, and 0.2218 and 0.9765, respectively. The paper established that matrix functions and Microsoft Excel Solver in Microsoft Excel are essential tools in the determination of engineering parameters in adsorption process.

Keywords— Adsorbent, Adsorption Isotherm, Arsenic, Matrix Technique, Microsoft Excel Solver.

I. INTRODUCTION

Water, air and land pollutions are currently transcendental issues[1-6]. Numerous methods such as biological, physical and chemical methods or techniques have been utilised to eradicate different contaminants and pollutants that are affecting the environment and aquatic ecosystems [7-15]. There are numerous methods and purification techniques currently utilised for water and wastewater purification. The methods and techniques include electrochemical method (electro-sorption, electro-Fenton process, son electro catalysis, photo electro catalysis, electro-floto-coagulation, electro-de-ionization, electrochemical membrane or electro-filtration processes, photoelectrochemical purification, electrochemical disinfection, electrochemical peroxidation, electrochemical desalination or capacitive deionization, electrochemical reduction, electrochemical advanced oxidation, electrodialysis, electro-flotation, and electrooxidation, electrocoagulation), flocculation, irradiation, membrane separation, ion exchange, and

adsorption (Figure 1) [16- 43]. Although, electrochemical purification methods require fewer addition of chemicals and there is no secondary pollution formation but the techniques are expensive and technically difficult to operate. Compared with all these listed above purification methods, the adsorption purification method has established a lot of consideration due to its high removal efficiency, good and reliable economic efficiency, and flexible in the technical operation [44-67]. In summary, one of these techniques applicable in water and wastewater purification is adsorption technique. Adsorption has been utilized based on its easy to scale-up to industrial prototypes, great efficacy and potential to eliminate typical pollutants from aqueous media and its relatively inexpensive [56–84]. Three key processes of adsorption of pollutants and contaminants present in environment are external diffusion, intraparticle diffusion, and surface reaction (Figure 2). Furthermore, at a dynamic agitation, stages intraparticle diffusion and external diffusion have very little influences on the transportation of contaminant and pollutant from the aqueous solution phase to the central surface of the adsorbent, which is a limiting step in the pollutant reduction or removal, which is the rate-controlling mechanism [85-94] This action is assumed to be the required between the adsorbate (pollutant) and adsorbent (medium) molecules at the liquid–solid interface [23-35]. In this case, several adsorption equilibrium isotherm models have been utilised to describe the binding of these chemical species controlled in aqueous solution to the surface of an adsorbent medium and material [28-57] Table 1 presents adsorption equilibrium for single and multi-components aqueous solutions. . The adsorption equilibrium models provide information and data on the adsorption rate, the weight transfer mechanisms and , the efficacy of the adsorbent utilised, which indicates that accurate adsorption equilibrium parameters are essential tools for the design of the adsorption purification systems [1-94]. This study therefore evaluated the capabilities of Microsoft Excel Matrix Functions Technique for Adsorption Equilibrium Models in relation to experimental and data and simulated equilibrium from Microsoft Excel Solver.

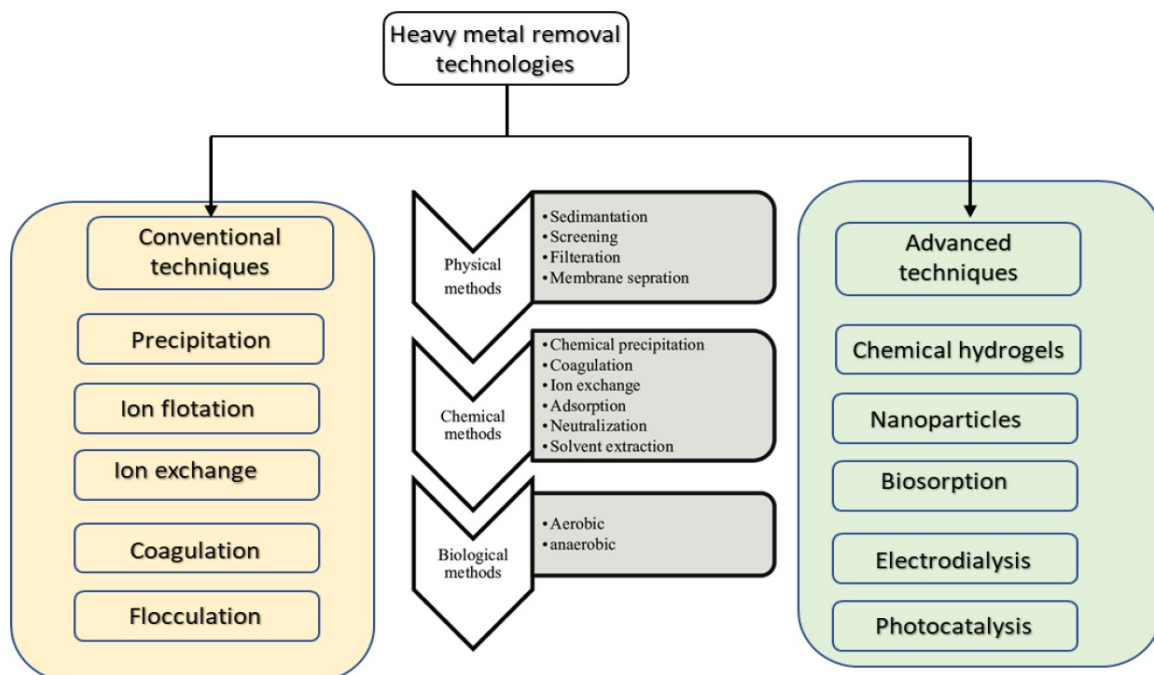


Fig. 1. some of the frequently used treatment techniques for the removal of contaminants and pollutants from the environment (Source: Abiodun et al.[47] and Obijole et al.[48])

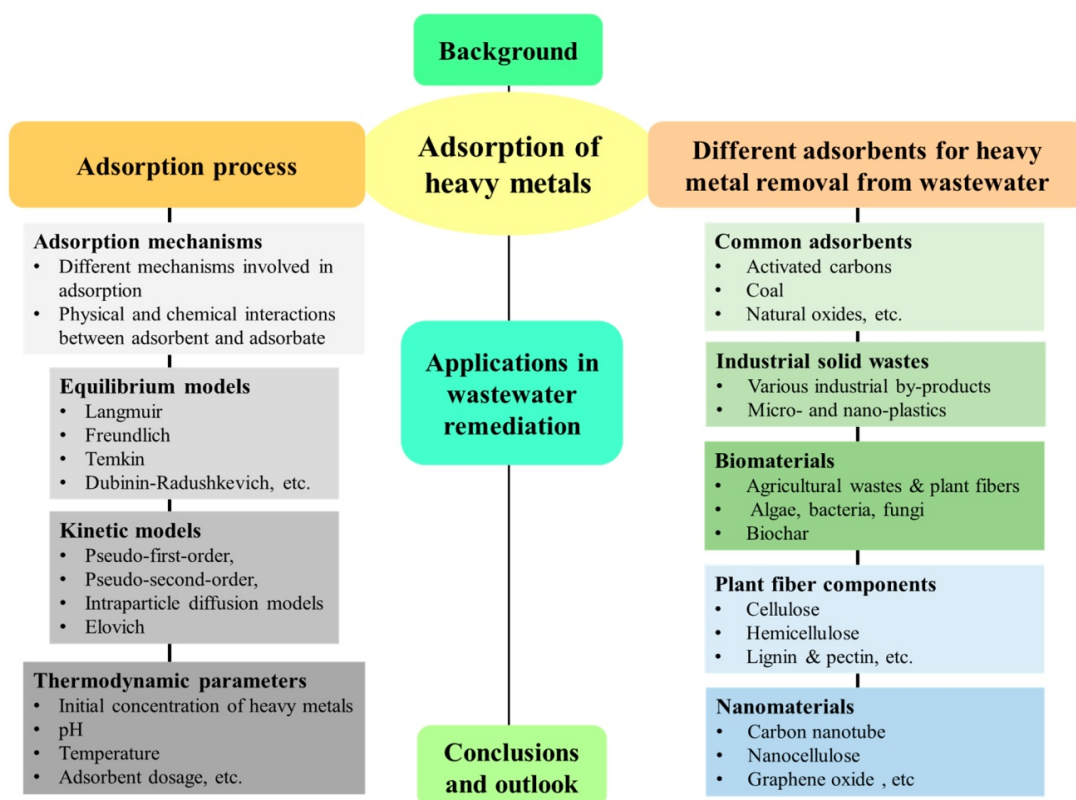


Fig. 2. Schematic and summary of adsorption knowledge available in the literature (Source: Babajide et al. [42]; Raji et al. [76]; Amoko et al.

Table 1a. Adsorption equilibrium isotherm for single component aqueous solutions

Type	Relationship	Parameters
Langmuir	$q_e = \frac{a_L b_L C_e}{1 + a_L C_e}$	a_L and b_L
Freundlich	$q_e = K_f C_e^{1/N_f}$	K_f and N_f
Redlich–Peterson	$q_e = \frac{\alpha_t C_e}{1 + \beta_t C_e^\gamma}$	α_t , γ and β_t
Temkin	$q_e = a_t + 2.3b_t \log C_e$	a_t and b_t
Crombie-Quilty and McLoughlin	$q_e = K_m \left(\frac{C_e}{M} \right)^{1/N_m}$	K_m and N_m
Sips	$q_e = \frac{\alpha_{ts} C_e^{\gamma_{ts}}}{1 + \beta_{ts} C_e^{\gamma_{ts}}}$	α_{ts} , γ_{ts} and β_{ts}
Langmuir-Freundlich	$q_e = \frac{q_m K_t C_e^{K_{LF}}}{1 + K_t C_e^{K_{LF}}}$	q_m , K_{LF} and K_t
Toth	$q_e = \frac{q_m \alpha_{tt}^{\gamma_{tt}} C_e}{\left(1 + \alpha_{tt} C_e^{\gamma_{tt}} \right)^{\left(\frac{1}{\gamma_{tt}} \right)}}$	q_m , α_{tt} and γ_{tt}
	$q_e = \frac{\alpha_{tt} C_e}{\left(\beta_{tt} + C_e^{\gamma_{tt}} \right)^{\left(\frac{1}{\gamma_{tt}} \right)}}$	α_{tt} , β_{tt} and γ_{tt}
Radke-Prausnitz	$\frac{1}{q_e} = \left(\frac{\alpha_{rp}}{C_e} \right) + \frac{\beta_{rp}}{\left(C_e^{\gamma_{rp}} \right)}$	α_{rp} , γ_{rp} and β_{rp}
	$q_e = \frac{q_m \alpha_{rp} C_e}{\left(1 + \alpha_{rp} C_e^{\gamma_{rp}} \right)}$	α_{rp} , γ_{rp} and q_{rp}
Khan	$q_e = \frac{q_{mk} \alpha_k C_e}{\left(1 + \alpha_k C_e \right)^{\gamma_k}}$	α_k , γ_k and q_{mk}
Fritz and Schhunder	$q_e = \frac{q_{mfs} \alpha_{fs} C_e^{\gamma_{fst}}}{\left(1 + \alpha_{fs} C_e^{\gamma_{fst}} \right)}$	α_{fs} , γ_{fst} and q_{mfs}
Linear	$q_e = K_p C_e$	k_p
Loading ratio	$q_e = \frac{q_{mL} (b_{Ll} C_e)^{(1/k_l)}}{1 + (b_{Ll} C_e)^{(1/k_l)}}$	q_{mL} , b_{Ll} and k_l
Four parameters	$C_e = \alpha_1 Q_e^{(\alpha_2 q_m + \alpha_3)}$	α_1 , α_2 , α_3 and q_m
Dubinin–Radushkevich	$q_e = X_m \text{Exp}(-k\varepsilon^2)$	X_m , k and ε
Statistical	$q_e = \left(\frac{k C_e + (k C_e)^2 \frac{\Gamma_{ii}}{2}}{1 + k C_e + (k C_e)^2 \frac{\Gamma_{ii}}{2}} \right)$	k
Halsey	$q_e = \left(\frac{k_H}{C_e} \right)^{n_H}$	k_H and n_H
Koble - Corrigan	$q_e = \frac{\alpha_{kc} C_e^{\gamma_{kc}}}{\left(1 + \beta_{kc} C_e^{\gamma_{kc}} \right)}$	α_{kc} , β_{kc} and γ_{kc}

Table 1b. Adsorption equilibrium isotherm for multi component aqueous solutions

Type	Relationship
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Langmuir, Bulter and Ockrent, Schwlb, Markham and Benton, Moriguch and Kaneniwa	$q_e = \frac{a_L C_e}{1 + \sum_{i=1}^n b_{Li} C_{ei}}$
Myers and Prausnitz	Ideal adsorbed solution theory (iteration method)
Suwanayeen and Danner	Vacancy solution theory (iteration method)
Fritz and Schhunder	$q_e = \frac{\alpha f s_i C_e^{\gamma_{fst}}}{\left(\beta_{fs} + \sum_{i=1}^n \alpha f s_i C_{ei}^{\gamma_{fst}} \right)}$
Yon and Turnock	$q_e = \frac{a_{L_i} (C_e)^{\gamma_{yt}}}{1 + \sum_{i=1}^n b_{L_i} (C_e)^{\gamma_{vy}}}$
Redlich–Peterson	$q_e = \frac{a_L C_e}{1 + \sum_{i=1}^n b_{Li} C_{ei}}$
Ruthven	$q_e = \left(\frac{q_m (C_e)^2}{1 + \sum_{j=1}^n k_j (C_e)^{\gamma_j}} \right)$
Sheindorf et al.[42]	$q_e = a_i (C_{ei}) \left(\sum_{j=1}^n a_{ij} C_{ej} \right)^{(m-1)}$
Ruthven and Wong	$q_e = \frac{K_i p_i \left(1 + \sum_{j=1}^n k_j p_j \Gamma_j \right)}{1 + \sum_{k=1}^n K_k p_k \left(1 + \sum_{j=1}^n k_j p_j \frac{\Gamma_j}{2} \right)}$
Jain and Snoeyink	$q_{e1} = \left(\frac{(q_{m1} - q_{m2}) b_1 C_{e1}}{1 + b_1 C_{e1}} \right) - \left(\frac{(q_{m2}) b_2 C_{e2}}{1 + b_1 C_{e1} + b_2 C_{e2}} \right)$
	$q_{e2} = \left(\frac{(q_{m2}) b_2 C_{e2}}{1 + b_1 C_{e1} + b_2 C_{e2}} \right)$

Abbreviations and Symbols

R is the gas constant (8.31 mol⁻¹ K⁻¹); T is the absolute temperature (K); q_e is the adsorption capacity of the adsorbent at equilibrium(mg/g); C₀ is the initial concentration of arsenic in the aqueous solution (mg/l); C_e is the final concentration of arsenic in the aqueous solution at equilibrium (mg/l); M is the weight of the adsorbent added (g); Γ is the Gamma function symbol; exp or Exp is the exponential and V is the volume of the water sample utilised (300ml = 0.30 litres).

k is the statistical isotherm parameter for the weight of the pollutant per unit weight of the adsorbent (mg/g)

k_p is the isotherm constant for the linear model for the weight of the pollutant per unit weight of the adsorbent (mg/g)

q_e is the equilibrium solid-phase concentration of sorbate t (mg/mg)

α_L and β_L are the Langmuir adsorption constant(L/mg) and Langmuir isotherm parameter (mg/g) respectively

K_f and α_f are the Freundlich isotherm exponents for pollutant weight per unit weight of the adsorbent (g/mg) and Freundlich isotherm parameter for the volume of the solution per unit weight of the pollutant (L/mg) respectively

K_H and α_H are Hasley's isotherm parameters for pollutant weight per unit weight of the adsorbent and for the volume of the solution per unit weight of the pollutant respectively K_m and α_m are constant for activated sludge model as volume of the solution per unit weight of the pollutant) and exponential constant for activated sludge model as pollutant weight per unit weight of the adsorbent respectively

K_{Hr} and α_{Hr} are isotherm parameters for Halsey C (Rangabhashiyum *et al.*, 2014) as volume of the solution per unit weight of the pollutant) and exponential constant for Halsey C model as pollutant weight per unit weight of the adsorbent respectively

K_{Hf} and α_{Hf} are isotherm parameters for Halsey B (Hamdaoui and Naffrechous, 2007) as volume of the solution per unit weight of the pollutant) and exponential constant for Halsey B model as pollutant weight per unit weight of the adsorbent respectively

K_{LV} and α_{LV} are isotherm parameters for Langmur — Vageler as the volume of the solution per unit weight of the pollutant) and exponential constant for the Langmur — Vagel model as pollutant weight per unit weight of the adsorbent respectively

K_{FH} and α_{FH} are isotherm parameters for Flory — Huggins as volume of the solution per unit weight of the pollutant) and exponential constant for the Flory — Huggins model

as pollutant weight per unit weight of the adsorbent respectively

K_{lk} and α_{lk} are isotherm parameters for Kiselev as volume of the solution per unit weight of the pollutant) and exponential constant for Kiselev model as pollutant weight per unit weight of the adsorbent respectively

K_{Hd} and α_{Hd} are isotherm parameters for Hill-de Boer as volume of the solution per unit weight of the pollutant) and exponential constant for Hill-de Boer model as pollutant weight per unit weight of the adsorbent respectively

K_{FG} and α_{FG} are isotherm parameters for Folwer — Guggenhien as volume of the solution per unit weight of the pollutant) and exponential constant for Folwer — Guggenhien model as pollutant weight per unit weight of the adsorbent respectively

K_E and α_E are isotherm parameters for Elovich as the volume of the solution per unit weight of the pollutant) and exponential constant for Elovich model as pollutant weight per unit weight of the adsorbent respectively

K_{jm} and α_{jm} are isotherm parameters for Jovanovic the volume of the solution per unit weight of the pollutant) and exponential constant for Jovanovic model as pollutant weight per unit weight of the adsorbent respectively

K_{fhh} and α_{fhh} are isotherm parameters for Frenkel- Halsey-Hill the volume of the solution per unit weight of the pollutant) and exponential constant for Frenkel- Halsey-Hill model as pollutant weight per unit weight of the adsorbent respectively

K_{hj} and α_{hj} are isotherm parameters for Harkin Jura A the volume of the solution per unit weight of the pollutant) and exponential constant for Harkin Jura A model as pollutant weight per unit weight of the adsorbent respectively

K_{hj} and α_{hj} are isotherm parameters for Harkin Jura B the volume of the solution per unit weight of the pollutant) and exponential constant for Harkin Jura B model as pollutant weight per unit weight of the adsorbent respectively

K_{rw} and α_{rw} are isotherm parameters for Ruthven and Wong the volume of the solution per unit weight of the pollutant) and exponential constant for Ruthven and Wong model as pollutant weight per unit weight of the adsorbent respectively

K_{si} and α_{si} are isotherm parameters for Sheindorf et al. (1983), the volume of the solution per unit weight of the pollutant) and exponential constant for Sheindorf et al. (1983), model as pollutant weight per unit weight of the adsorbent respectively

α_{mLB} and β_{mLB} are isotherm parameters for Langmuir, Bulter and Ockrent, Schwlb, Markham and Benton, Moriguch and Kaneniwa as volume of the solution per unit weight of the pollutant) and exponential constant for Langmuir, Bulter and Ockrent, Schwlb, Markham and Benton, Moriguch and Kaneniwa model as pollutant weight per unit weight of the adsorbent respectively

β_{LF} , K_{LF} and α_{LF} are isotherm parameters for Langmuir-Freundlich isotherm exponents for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the adsorbent (mg/g) and the weight of the pollutant per unit weight of the adsorbent (mg/g), respectively

$\alpha_{t,}$, $\beta_{t,}$ and $\gamma_{t,}$ are the Redlich–Peterson isotherm exponents for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit

weight of the adsorbent (mg/g) and the weight of the pollutant per unit weight of the adsorbent (mg/g), respectively

$\alpha_{fs,}$ γ_{fs} and q_{mfs} are the Fritz and Schhunder's isotherm parameters for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the adsorbent (mg/g) and the weight of the pollutant per unit weight of the adsorbent (mg/g), respectively

$\alpha_k,$ γ_k and q_{mk} are the Khan's isotherm parameters for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the adsorbent (mg/g) and the weight of the pollutant per unit weight of the adsorbent (mg/g), respectively

$\alpha_{kc,}$ β_{kc} and γ_{kc} are the Koble-Corrigan's isotherm parameters for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the adsorbent (mg/g) and the weight of the pollutant per unit weight of the adsorbent (mg/g), respectively

$\alpha_{rp,}$ γ_{rp} and q_{rp} are the Radke-Prausnitz's isotherm parameters for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the adsorbent (mg/g) and the weight of the pollutant per unit weight of the adsorbent (mg/g), respectively

$\alpha_{ts,}$ β_{ts} and γ_{ts} are the Sips isotherm parameters for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the adsorbent (mg/g) and the weight of the pollutant per unit weight of the adsorbent (mg/g), respectively

$\alpha_{tt,}$ β_{tt} and γ_{tt} are the Toth isotherm parameters for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the adsorbent (mg/g) and the weight of the pollutant per unit weight of the adsorbent (mg/g), respectively

$q_m,$ $\alpha_{tt,}$ and γ_{tt} are the Toth isotherm parameters for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the adsorbent (mg/g) and the weight of the pollutant per unit weight of the adsorbent (mg/g), respectively

$q_m,$ K_{LF} and K_t are the Langmuir – Freundlich isotherm constants for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the adsorbent (mg/g) and the weight of the pollutant per unit weight of the adsorbent (mg/g), respectively

$q_{mL},$ b_{Li} and k_i are the Loading ratio's isotherm parameter for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the adsorbent (mg/g) and the weight of the pollutant per unit weight of the adsorbent (mg/g), respectively

$K_{md,}$ α_{md} and ε are the Dubinin-Radushkevich's isotherm parameters for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the adsorbent (mg/g) and the weight of the pollutant per unit weight of the adsorbent (mg/g), respectively

$K_{mRu,}$ α_{mRu} and γ_{mRu} are the Ruthven for the volume of the solution per unit weight of the pollutant (L/mg); the weight

of the pollutant per unit weight of the absorbent (mg/g) and the weight of the pollutant per unit weight of the absorbent (mg/g), respectively

α_{mLRP} , γ_{mLRP} and β_{mLRP} are the Redlich–Peterson for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the absorbent (mg/g) and the weight of the pollutant per unit weight of the absorbent (mg/g), respectively

α_{mFS} ; β_{mFS} and γ_{mFS} are the Yon and Turnock for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the absorbent (mg/g) and the weight of the pollutant per unit weight of the absorbent (mg/g), respectively

α_{mFS} ; β_{mFS} and γ_{mFS} are the Fritz and Schhunder for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the absorbent (mg/g) and the weight of the pollutant per unit weight of the absorbent (mg/g), respectively

K_{scjf} ; β_{scjf} and γ_{scjf} are the Single Component Jovanovic - Freundlich for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the absorbent (mg/g) and the weight of the pollutant per unit weight of the absorbent (mg/g), respectively

K_{BS} , α_{BS} and β_{BS} are isotherm parameters for Brouers-Sotolongo isotherm exponents for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the absorbent (mg/g) and the weight of the pollutant per unit weight of the absorbent (mg/g), respectively

K_{wvv} , α_{wvv} , β_{wvv} and γ_{wvv} are isotherm parameters for Weber-Van Vliet isotherm exponents for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the absorbent (mg/g), exponents for the volume of the solution per unit weight of the pollutant (L/mg) and the weight of the pollutant per unit weight of the absorbent (mg/g), respectively

K_{bu} , β_{bu} , γ_{bu} and α_{bu} are isotherm parameters for Bauder isotherm exponents for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the absorbent (mg/g), exponents for the volume of the solution per unit weight of the pollutant (L/mg) and the weight of the pollutant per unit weight of the absorbent (mg/g), respectively

K_{msj} , γ_{msj} , α_{msj} and β_{msj} are isotherm parameters for Marczewsk- Jaroniec isotherm exponents for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the absorbent (

mg/g), exponents for the volume of the solution per unit weight of the pollutant (L/mg) and the weight of the pollutant per unit weight of the absorbent (mg/g), respectively

K_{FS4} γ_{FS4} , α_{FS4} and β_{FS4} are isotherm parameters for Fritz-Schhunder isotherm exponents for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the absorbent (mg/g) and the weight of the pollutant per unit weight of the absorbent (mg/g), respectively

q_{fs5} , K_{fs5} , α_{fs5} , γ_{fs5} and β_{fs5} are isotherm parameters for Fritz-Schhunder isotherm exponents for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the absorbent (mg/g) and the weight of the pollutant per unit weight of the absorbent (mg/g), respectively

α_1 , α_2 , α_3 and q_m are isotherm parameters for Four parameters' isotherm parameter exponents for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the absorbent (mg/g) and the weight of the pollutant per unit weight of the absorbent (mg/g), respectively

K_{mjs2} ; K_{mjs1} ; β_{mjs1} and β_{mjs2} are isotherm parameters for Jain and Snoeyink exponents for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the absorbent (mg/g) and the weight of the pollutant per unit weight of the absorbent (mg/g), respectively

K_{mejf2} ; γ_{mejf1} K_{mejf1} ; β_{mejf1} γ_{mejf2} and β_{mejf2} are isotherm parameters for Extended Jovanovic -Freundlich exponents for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the absorbent (mg/g) and the weight of the pollutant per unit weight of the absorbent (mg/g), respectively

K_{melf2} ; γ_{melf1} K_{melf1} ; β_{melf1} γ_{melf2} and β_{melf2} are isotherm parameters for Extended Langmuir -Freundlich exponents for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the absorbent (mg/g) and the weight of the pollutant per unit weight of the absorbent (mg/g), respectively

K_{mel2} ; K_{mel1} ; β_{mel1} and β_{mel2} are isotherm parameters for Extended Langmuir exponents for the volume of the solution per unit weight of the pollutant (L/mg); the weight of the pollutant per unit weight of the absorbent (mg/g) and the weight of the pollutant per unit weight of the absorbent (mg/g), respectively

documented that the functionality of Microsoft Excel can significantly increase the robustness of numerical data analysis [42-46], but literature on utilization of matrix functions in Microsoft Excel is rare. It is well stated that utilising matrices for solving numerical problems offers numerous advantages in handling complexity, improving computational efficiency, facilitating data analysis, and enhancing the accuracy of models and predictions. This approach is particularly beneficial for multicomponent systems, dynamic processes, and optimization tasks, making it a powerful tool in both research and industrial applications of adsorption technology. The main focus of this paper is to [42]:

II. LITERATURE REVIEW

Analysis of the adsorption equilibrium data can be conducted through linearized, non-linear, and least squares analysis utilising software such as Sigma Plot, Origin, Microsoft Excel Solver, MATLAB, Mathematica, Mathcad, Spreadsheet, Maple, GAUSS, Freemate, Flepro, Dataplot, Ardnial and SPSS. Figure 3 presents in details adsorption equilibrium. With reference to the cost of some of these software, there is a need to utilize tools and software that can be utilised to analyse data at no additional cost such as calc spread sheet on Libre Office, Microsoft Add-ins and Microsoft Excel . It has been

- solve selected adsorption equilibrium models utilising matrix functions in Microsoft Excel
- establish the accurateness and preciseness of matrix transformation of the technique in solving commonly utilised adsorption equilibrium models with specific consideration to the utilization of least squares transformed and built-in matrix functions in Microsoft Excel, and
- compare the results with experimental adsorption equilibrium, and simulated adsorption equilibrium from Microsoft Excel Solver with a

III. METHODOLOGY

Data on arsenic removal from surface water utilising Aponmu River, Ilara-Mokin, Nigeria by adsorption process utilising powdered eggshells and the adsorption properties of powdered eggshells were extracted from previous and published studies such as Amoko et al.[50]; Amoko et al. [51]; Fehintola et al.[52]; Obijole et al. [53] and Oke et al.[54]. Adsorption equilibrium models (Langmuir and Freundlich) were analysed utilising transformed linear and least squares form of the models. The Langmuir, Langmuir – Vageler, Flory – Huggins, Freundlich, Halsey B, and Halsey A equations are as follows [42]:

Langmuir

$$q_e = \frac{a_L b_L C_e}{1 + a_L C_e} \quad (1)$$

Freundlich

$$q_e = K_f C_e^{1/N_f} \quad (2)$$

Flory – Huggins

$$\frac{\theta}{C_e} = K_{FH} (1 - \theta)^{N_{FH}}; \quad (3a)$$

$$\theta = 1 - \frac{C_e}{C_0} \quad (3b)$$

Halsey B

$$q_e = K_{Hf} \left(\frac{C_e}{C_0} \right)^{\frac{1}{N_{Hf}}} \quad (4)$$

Halsey A

$$q_e = \left(\frac{K_H}{C_e} \right)^{\frac{1}{N_H}} \quad (5)$$

Temkin

$$q_e = \frac{RT}{b_t} \ln(a_t C_e) \quad (6)$$

Frenkel- Halsey- Hill

$$q_e = \text{Exp} \left(\frac{\ln((K_{fhh}) - \ln(C_e))}{N_{fhh}} \right) \quad (7)$$

Elovich

$$\left(\frac{q_e}{q_{mE}} \right) = K_E C_e \left(\exp^{-\frac{q_e}{q_{mE}}} \right) \quad (8)$$

critical aim of attaining sustainable development goals 3 (good health and well-being), 6 (clean water and sanitation); 14 (life below water) and 15 (life on land) [49] and to further knowledge in computer education.

Matrix was selected based on accessibility, availability at no additional and easy to utilise

Elovich

$$\left(\frac{q_e}{q_{mE}} \right) = K_E C_e \left(\exp^{-\frac{q_e}{q_{mE}}} \right) \quad (9)$$

Where;

q_e and C_e are adsorption equilibrium capacity and adsorption equilibrium concentration.

a_L and b_L are Langmuir adsorption constants

K_f and N_f are Freundlich adsorption constants

a_t and b_t are Temkin's adsorption constants

K_H and N_H are Halsey A's adsorption constants

K_{Hf} and N_{Hf} are Halsey B's adsorption constants

K_{fhh} and N_{fhh} are Frenkel- Halsey- Hill's adsorption constants

K_E and q_{mE} are Elovich's adsorption constants

K_{FG} and W are Folwer –Guggenhiem's adsorption constants

K_{Hd} and K_2 are Hill-de Boer 's adsorption constants

K_1 and K_n are Kiselev's adsorption constants

K_{FH} and N_{FH} are Flory – Huggins's adsorption constants

q_{max} and K_{LV} are Langmuir – Vageler's adsorption constants

The matrix arrays were solved with matrix functions in Microsoft Excel. The results were evaluated statistically utilising Analysis of Variance (ANOVA), Coefficient of Determination (CD) and Correlation Coefficient (R) and compared with linear and non-linear experimental adsorption equilibrium and simulated equilibrium values from Microsoft Excel Solver. Figures 4 and 5 present the flowchart of the procedures for matrix and Microsoft Excel Solver techniques respectively. The mathematical and matrix transformation are as presented in equations (9) to (12). The details of the transformation are as presented in the appendix

$$Y = mX + C \quad (9)$$

$$\sum_{i=1}^n Y_i = m \sum_{i=1}^n X_i + nC \quad (10)$$

$$\sum_{i=1}^n X_i Y_i = m \sum_{i=1}^n X_i^2 + C \sum_{i=1}^n X_i \quad (11)$$

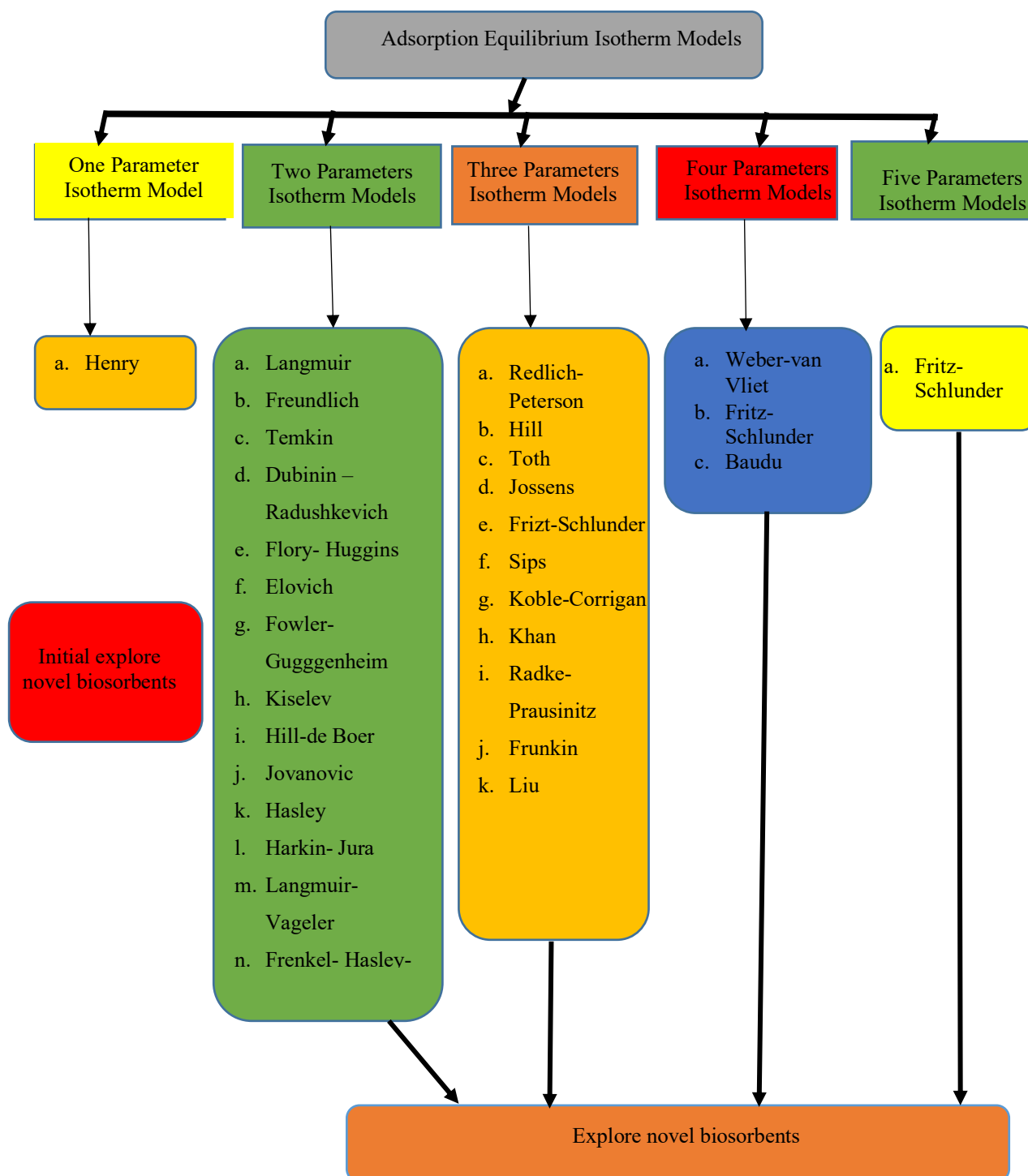


Fig. 3: The significance of adsorption equilibrium isotherm models in use to establish performance of adsorbents (Adopted from Rangabhashiyam *et al.* [56])

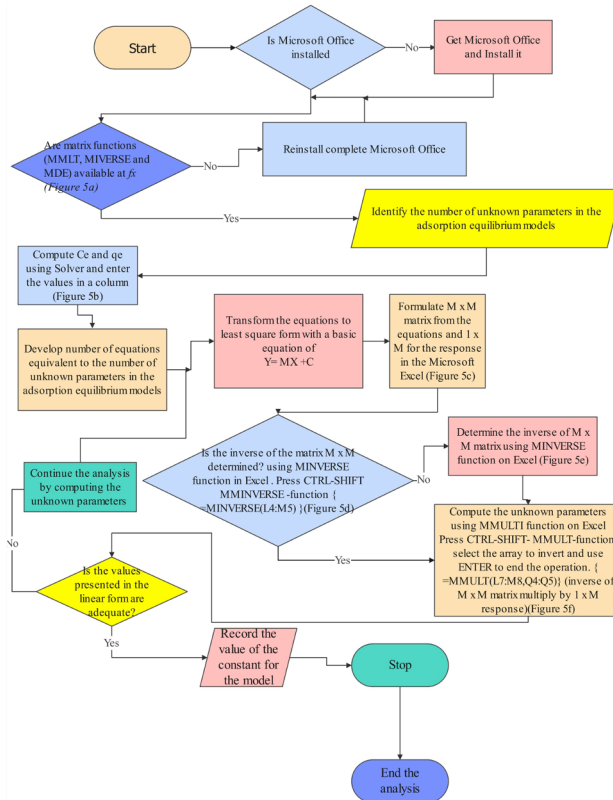


Fig. 4: Procedure for using the Matrix technique on Microsoft Excel in the computation of the Isotherm's parameters

Matrix transformation of

$$\begin{pmatrix} \sum_{i=1}^n X_i & n \\ \sum_{i=1}^n X_i^2 & \sum_{i=1}^n X_i \end{pmatrix} \begin{pmatrix} m \\ C \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^n Y_i \\ \sum_{i=1}^n X_i Y_i \end{pmatrix} \quad (12)$$

IV. RESULTS AND DISCUSSION

Results from the study are presented as follows: properties of the powdered eggshell, adsorption equilibrium capacities, Step-by step of Microsoft Excel Matrix Functions techniques, Adsorption equilibrium model and parameters, efficacies assessments of the technique.

- Properties of Powdered eggshell:** The properties of the eggshell (physical, chemical, scanning electron microscope (SEM) and Energy Dispersive Spectroscopy (EDS)) were presented in literature such as Amoko et al.[50]; Amoko et al. [51]; Fehintola et al.[52]; Obijole et al. [53] and Oke et al.[54].
- Step-by step of Microsoft Excel Matrix Functions and Microsoft Excel solver techniques:** The results and the steps required to obtained and utilised these two techniques are

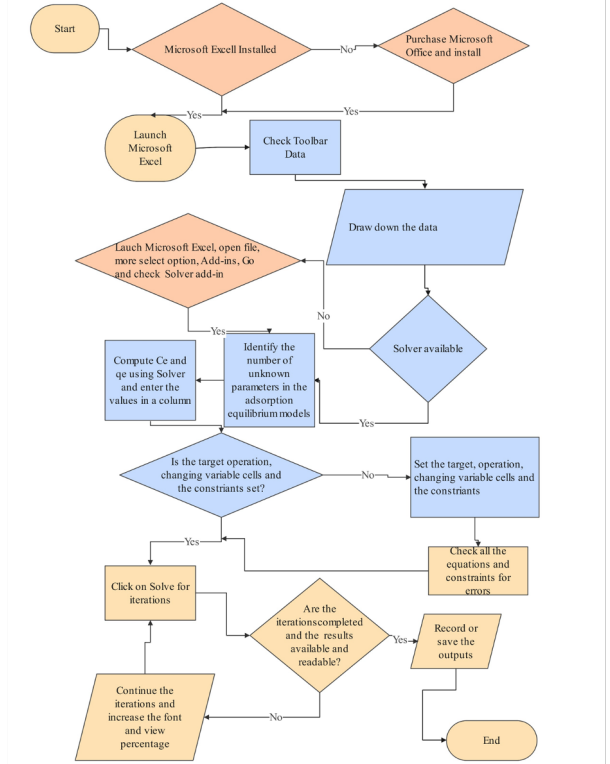


Fig. 5: Procedure for using Microsoft Excel Solver technique on Microsoft Excel in the computation of the Isotherm's parameters

provided in literature such as Fehintola et al.[52]; Obijole et al. [53] and Oke et al.[54].

- Adsorption Equilibrium capacities:** Table 2 presents the results of adsorption equilibrium capacities of powdered eggshell. The Table revealed that the adsorption equilibrium capacities properties of the eggshell was between 0.1868 and 0.4783 (mg of the pollutant per gram of the adsorbent) at 0.85 g of the adsorbent with initial concentration of the pollutant between 0.60 mg/l and 1.5 mg/l of arsenic. The equilibrium concentrations were between 0.0992 and 0.3170 mg/l of arsenic. Detailed adsorption results and influences of selected operational factors are presented in literature such as Amoko et al.[50]; Amoko et al. [51]; Fehintola et al.[52]; Obijole et al. [53] and Oke et al.[54]. Table 3 shows the influences of initial concentrations on adsorption equilibrium capacities and adsorption equilibrium concentration.

Table 2: Results of adsorption equilibrium capacities of powdered eggshell

Initial Concentration of the pollutants (mg/l)	adsorption equilibrium concentration (C_e , mg/l)	adsorption equilibrium capacities (q_e , mg/g)
1.5	0.3170	0.4732
1.3	0.1577	0.4569
1.1	0.0992	0.4003
0.6	0.1331	0.1868

Table 3: Effects of initial concentrations on adsorption equilibrium capacities and adsorption equilibrium concentration

Source of Variation	Sum of Squares	Degree of freedom	Mean Sum of square	F-value	P-value	F crit
Between the adsorption equilibrium capacities	0.059	3	0.020	2.702	0.218	9.277
Between adsorption equilibrium capacities and adsorption equilibrium concentration	0.082	1	0.082	11.348	0.043	10.128
Error	0.022	3	0.007			
Total	0.162	7				

The Table revealed that there is no significant adsorption equilibrium capacities at 95 % ($F_{1,3} = 2.7018$ and $p = 0.2180$, which is greater than 0.05). In addition, the Table established that there is significant difference between adsorption equilibrium concentration at 95 % confidence level ($F_{1,3} = 11.348$ and $p = 0.043$, which is less than 0.05).

- d) **Adsorption equilibrium model and parameters:** Table 4 presents the selected adsorption equilibrium models with 2-parameters constants. The Table revealed that the values of adsorption equilibrium parameters vary with the adsorption equilibrium models, methods and techniques utilised (matrix and Microsoft Excel Solver), but the values were similar in magnitudes. This result indicates that the matrix technique in Microsoft Excel (in-built functions) can be utilised to solve numerical problems of 2-parameters adsorption equilibrium models. The Table also established that these 2-parameters adsorption equilibrium models must be linearized and transformed into matrix arrays for easier applications. The detail of the computations for the two techniques are presented at the Appendices. Table 5 shows the influences of the technique of adsorption equilibria. The Table revealed that there was no significant difference between experimental adsorption equilibria and simulated adsorption equilibria (matrix and Microsoft Excel Solver) at a 95 % confidence level ($F_{1,38} = 3.341$, $p = 0.075$ which is greater than 0.05). for the matrix technique. Table 6 shows the result of the influences of the technique of adsorption equilibria capacities. There was no significant difference between the adsorption capacities obtained utilising the two techniques at a 95 %

confidence level ($F_{15,32} = 0.867$; $p = 0.604$ which is greater than 0.05).

Table 7 shows the result of the influences of the techniques (Matrix and MES) of adsorption equilibria parameters. There was no significant difference between the adsorption capacities obtained utilising the two techniques at a 95 % confidence level ($F_{1,30} = 1.9534$; $p = 0.172$ which is greater than 0.05).

- e) **Efficacies assessments of the technique:** Table 8 presents the results of the efficacies assessment for both matrix and Microsoft Excel Solver techniques when compared with non- linear experimental adsorption equilibria and non- linear simulated adsorption equilibria. These values of R established that the relationship between linear experimental adsorption equilibria and linear simulated adsorption equilibria was between 0.2218 (Langmuir A) and 0.9765 (Langmuir D), which indicates that the relationship was between below average to good relationship as stated in literature such as Babajide et al. [42]; Loveday[63]; Oke [64]; Oke et al.[65]. In addition, the Table also established that these 2-parameters adsorption equilibrium models must be linearized and transformed into matrix arrays for easier applications and effective efficacys.
- f) Table 9 shows the result of the influences of the technique on linear experimental adsorption equilibria and linear simulated adsorption equilibria. It was established that there was no significant difference between the adsorption capacities obtained utilising the two techniques at a 95 % confidence level ($F_{2,45} = 1.283$; $p = 0.287$ which is greater than 0.05).

Table 4 the selected adsorption equilibrium models with 2-parameters constants

Summary	Matrix	MES	Parameters
Freundlich	0.6732	0.6732	K
	2.8809	2.8809	N
Langmuir A	0.4892	78.6780	bL
	13.9252	0.0350	aL
Langmuir B	0.7541	3.7197	bL
	5.1106	0.2786	aL
Langmuir C	0.2859	78.9000	bL
	26.3074	0.0374	aL
Langmuir D	0.3363	121.8379	bL
	3.4345	0.0202	aL
Langmuir E	0.0959	84.9035	bL
	5.2452	0.0230	aL
Flory-Huggins	0.6741	0.6741	Kfh
	1.8616	1.8617	Nfh
Hasley B	0.1476	0.1671	KHb
	2.1479	2.4980	NHb
Frenkel-Hasley-Hill	0.6571	0.2390	Kfhh
	0.3495	1.2313	Nfhh
Elovich	2.7579	0.2390	Ke
	1.5163	1.2313	qmax

Table 8 Statistical evaluation of both matrix and Microsoft Excel Solver techniques

Techniques	Coefficient of Determination	Correlation Coefficient
Matrix	0.037	0.193
MES	0.040	0.200

Table 9 Effects of Techniques on statistical evaluation of linear experimental and linear simulated adsorption capacities

Source of Variation	Sum of Squares	Degree of freedom	Mean Sum of square	F-value	P-value	F crit
Between Experimental and the two Techniques	0.074	2	0.037	1.283	0.287	3.204
Within Experimental and the two Techniques	1.290	45	0.029			
Total	1.364	47				

Table 10 Effects of Techniques on non-linear Experimental and simulated adsorption equilibrium capacities

Source of Variation	Sum of Squares	Degree of freedom	Mean Sum of square	F-value	P-value	F crit
Within Techniques	2.12E-05	1	2.12 x 10 ⁻⁵	5.26	0.26	161.45
Between Evaluations	0.024914	1	0.024914	6173.49	0.01	161.45
Error	4.04E-06	1	4.04 x 10 ⁻⁶			
Total	0.024939	3				

Table 5 Effects of the technique of adsorption equilibria

Source of Variation	Sum of Squares	Degree of freedom	Mean Sum of square	F-value	P-value	F crit
Between Techniques	2511.946	1	2511.946	3.341496	0.075412	4.098172
Within Groups	28566.234	38	751.743			
Total	31078.18	39				

Table 6 Effects of the technique of adsorption equilibria capacities

Source of Variation	Sum of Squares	Degree of freedom	Mean Sum of square	F-value	P-value	F crit
Between adsorption equilibrium capacities	0.394	15	0.026	0.867	0.604	1.992
Within adsorption equilibrium capacities	0.970	32	0.030			
Total	1.364	47				

Table 7 Effects of the technique (MES and Matrix) on adsorption equilibria parameters.

Source of Variation	Sum of Squares	Degree of freedom	Mean Sum of square	F-value	P-value	F crit
Between Techniques	0.0703574	1	0.070357	1.953395	0.172472	4.170877
Within Groups	1.0805399	30	0.036018			
Total	1.1508973	31				

Table 10 shows the influences of techniques (MES and Matrix) on non-linear Experimental and simulated adsorption equilibrium capacities. The Table revealed that there was no significant difference between the adsorption capacities obtained utilising the two techniques at a 95 % confidence level ($F_{1,1} = 5.26$; $p =$

0.260 which is greater than 0.05), but between the statistical assessments (Correlation Coefficient and Coefficient of Determination) there was significant difference at a 95 % confidence level ($F_{1,1} = 6173.49$; $p = 0.010$ which is less than 0.05).

V. CONCLUSION

The Based on the study and the findings, the following key conclusions can be drawn:

- Matrix technique with the Microsoft Excel function tools can be utilized to solve adsorption equilibrium equations.
- Utilizing the matrix is flexible (the technique can take $N \times N$ matrix arrays of N greater than 100) and faster due to its capacities as in-built functions.
- Results from the simulation of the adsorption equilibrium based on the parameters from the matrix technique were precise and accurate with a coefficient of correlation of 0.9765 with the experimental values.
- The efficacy of the evaluated adsorption equilibrium models was reliable.

REFERENCES

- Sossou, K., Prasad, S. B., Agbotsou, E. K., and Souley, H. S. (2024). Evaluation of the performance of magnetic zeolite nanocomposites in removing various water contaminants as heavy metals, organic pollutants, and emerging contaminants: A review. *Next Nanotechnology*, 6, 100075.
- Abewaa, M., Mengistu, A., Takele, T., Fito, J., and Nkambule, T. (2023). Adsorptive removal of malachite green dye from aqueous solution using Rumex abyssinicus derived activated carbon. *Scientific Reports*, 13(1), 14701.
- Antúnez-García, J., Ponce-Ruiz, J. L., Núñez-González, R., Petranovskii, V., Murrieta-Rico, F. N., Serrato, A. R., ... and Zamora, J. (2024). Theoretical investigation of Fe and Cu cations hosted within the MOR zeolite framework. *Materials Today Communications*, 41, 110418.
- Bahmanzadegan, F., Pordsari, M. A., and Ghaemi, A. (2023). Improving the efficiency of 4A-zeolite synthesized from kaolin by amine functionalization for CO₂ capture. *Scientific Reports*, 13(1), 12533.
- Bakhran, Z., Baiysbai, O., Azimov, A., Dairabay, D., and Brener, A. (2024). Theoretical Description and Simulation of the Hydrodynamics and Porous Layer Structure during Mass Transfer in an Adsorption Apparatus with Ion-exchange Resins. *Chemical Engineering Transactions*, 110, 67-72.
- Chebbi, M., Ounoki, S., Youcef, L., and Amrane, A. (2023). Synthesis and characterization of pine cones biochar for the removal of an antibiotic (Metronidazole) from aqueous solutions. *Journal of Industrial and Engineering Chemistry*, 126, 327-339.
- Chebbi, M., Ounoki, S., Youcef, L., and Amrane, A. (2023). Synthesis and characterization of pine cones biochar for the removal of an antibiotic (Metronidazole) from aqueous solutions. *Journal of Industrial and Engineering Chemistry*, 126, 327-339.
- Fathalian, F., Moghadamzadeh, H., Hemmati, A., and Ghaemi, A. (2024). Efficient CO₂ adsorption using chitosan, graphene oxide, and zinc oxide composite. *Scientific Reports*, 14(1), 3186.
- Georgin, J., Franco, D. S. P., Meili, L., Dehmani, Y., dos Reis, G. S., and Lima, E. C. (2023). Main advances and future prospects in the remediation of the antibiotic amoxicillin with a focus on adsorption technology: A critical review. *Journal of Water Process Engineering*, 56, 104407.
- Hirpaye, B. Y., Mena, A. A., Kumar, A., Aborisade, M. A., and Oba, B. T. (2024). Hydrothermal synthesis of zeolite-a from natural rhyolite for effective removal of Cr (VI) from wastewater. *International Journal of Environmental Science and Technology*, 1-16.
- Hu, Q., Huang, L., Li, Y., Yang, X., Ma, S., and Pei, X. (2024). Statistical analysis and application of binary breakthrough models developed by Gudermannian, error and hyperbolic tangent functions in a fixed-bed column. *Journal of Water Process Engineering*, 60, 105273.
- Hu, Q., Lan, R., He, L., Liu, H., and Pei, X. (2023). A critical review of adsorption isotherm models for aqueous contaminants: Curve characteristics, site energy distribution and common controversies. *Journal of Environmental Management*, 329, 117104.
- Hu, Q., Pang, S., and Wang, D. (2022). In-depth insights into mathematical characteristics, selection criteria and common mistakes of adsorption kinetic models: A critical review. *Separation and Purification Reviews*, 51(3), 281-299.
- Hu, Q., Pang, S., Li, Y., Huang, L., Zhang, Y., Xu, X., and Pei, X. (2024). Enhanced removal of phosphate from aqueous solutions by oxygen vacancy-rich MgO microspheres: Performance and mechanism. *Chemosphere*, 355, 141776.
- Jagiello, J. (1994). Stable numerical solution of the adsorption integral equation using splines. *Langmuir*, 10(8), 2778-2785.
- Jia, Y., Li, J., Zeng, X., Zhang, N., Wen, J., Liu, J., ... and Su, S. (2022). The performance and mechanism of cadmium availability mitigation by biochars differ among soils with different pH: Hints for the reasonable choice of passivators. *Journal of Environmental Management*, 312, 114903.
- Kačur, J., Malengier, B., and Remešikova, M. (2005). Solution of contaminant transport with equilibrium and non-equilibrium adsorption. *Computer methods in applied mechanics and engineering*, 194(2-5), 479-489.
- Khumalo, S. M., Bakare, B. F., and Rathilal, S. (2024). Single and multicomponent adsorption of amoxicillin, ciprofloxacin, and sulfamethoxazole on chitosan-carbon nanotubes hydrogel beads from aqueous solutions: Kinetics, isotherms, and thermodynamic parameters. *Journal of Hazardous Materials Advances*, 13, 100404.
- Kim, D. G., Boldbaatar, S., and Ko, S. O. (2022). Enhanced adsorption of tetracycline by thermal modification of coconut shell-based activated carbon. *International Journal of Environmental Research and Public Health*, 19(21), 13741.
- Lach, J. (2024). Kinetics, statics and thermodynamics of ampicillin adsorption on microporous carbon sorbents. *Desalination and Water Treatment*, 317, 100144.
- Lima, E. C., Hosseini-Bandegharai, A., Moreno-Piraján, J. C., and Anastopoulos, I. (2019). A critical review of the estimation of the thermodynamic parameters on adsorption equilibria. Wrong use of equilibrium constant in the Van't Hoff equation for calculation of thermodynamic parameters of adsorption. *Journal of molecular liquids*, 273, 425-434.
- Marey, A., Gado, W. S., Soliman, A. G., Masoud, A. M., El-Zahhar, A. A., Al-Hazmi, G. A., ... and El Naggat, A. M. (2024). Efficient removal of methylene blue dye from wastewater specimen using polystyrene coated nanoparticles of silica. *Inorganic Chemistry Communications*, 160, 112018.
- Mudhoo, A., and Pittman Jr, C. U. (2023). Adsorption data modeling and analysis under scrutiny: A clarion call to redress recently found troubling flaws. *Chemical Engineering Research and Design*, 192, 371-388.
- Qin, Y., Zhao, Z., Xu, H., Liu, W., Wu, F., Zhou, Y., and Duan, W. (2022). Numerical solution of three mathematical models of gas adsorption in coal particle based on finite difference method. *Fuel*, 308, 122036.
- Ramos-Guivar, J. A., Checchia-Huaman, N. R., Litterst, F. J., and Passamani, E. C. (2023). Synergetic effect between zeolite 5 A and maghemite nanoparticles for fast lead uptake from the Peruvian river Cumbaza: Study of surface adsorption mechanism using X-ray photoelectron spectroscopy. *Applied*

- Surface Science Advances*, 18, 100489.
- [26] Ramos-Guivar, J. A., Checca-Huaman, N. R., Litterst, F. J., and Passamani, E. C. (2023). Synergetic effect between zeolite 5 A and maghemite nanoparticles for fast lead uptake from the Peruvian river Cumbaza: Study of surface adsorption mechanism using X-ray photoelectron spectroscopy. *Applied Surface Science Advances*, 18, 100489.
- [27] Ramos-Guivar, J. A., Rueda-Vellamin, R., Manrique-Castillo, E. V., Mendoza-Villa, F., Checca-Huaman, N. R., and Passamani, E. C. (2024). Synthesis and Characterization of Maghemite Nanoparticles Functionalized with Poly (Sodium 4-Styrene Sulfonate) Saloplastic and Its Acute Ecotoxicological Impact on the Cladoceran *Daphnia magna*. *Polymers*, 16(11), 1581.
- [28] Remešiková, M. (2007). Numerical solution of two-dimensional convection–diffusion–adsorption problems using an operator splitting scheme. *Applied mathematics and computation*, 184(1), 116-130.
- [29] Remešiková, M. A. R. I. A. N. A. (2005). Numerical solution of contaminant transport problems with non-equilibrium adsorption in 2D. In *Proceedings of ALGORITHM* (pp. 159-166).
- [30] Richter, E., Wilfried, S., and Myers, A. L. (1989). Effect of adsorption equation on prediction of multicomponent adsorption equilibria by the ideal adsorbed solution theory. *Chemical engineering science*, 44(8), 1609-1616.
- [31] Saleh, T. A. (2022). Kinetic models and thermodynamics of adsorption processes: Classification. In *Interface science and technology* (Vol. 34, pp. 65-97). Elsevier.
- [32] Soudani, A., Youcef, L., Bulgariu, L., Youcef, S., Toumi, K., and Soudani, N. (2022). Characterizing and modeling of oak fruit shells biochar as an adsorbent for the removal of Cu, Cd, and Zn in single and in competitive systems. *Chemical Engineering Research and Design*, 188, 972-987.
- [33] Souza, P. R., Dotto, G. L., and Salau, N. P. G. (2017). Detailed numerical solution of pore volume and surface diffusion model in adsorption systems. *Chemical Engineering Research and Design*, 122, 298-307.
- [34] Tang, X., Xiong, J., Zhu, Y., He, R., Chen, X., Chen, Q., ... and Ma, L. (2024). Adsorption Characteristics of Illite and Kerogen Oil Phase: Thermodynamics Experiments. *Minerals*, 14(6), 579.
- [35] Timilsina, A., Adhikari, K., Yadav, A. K., Joshi, P., Ramena, G., and Bohara, K. (2023). Effects of microplastics and nanoplastics in shrimp: Mechanisms of plastic particle and contaminant distribution and subsequent effects after uptake. *Science of the Total Environment*, 894, 164999.
- [36] Von Heynitz, C., Bachmann, F., Hofmann, T. F., and Glas, K. (2024). Toward Higher Resource Efficiency in Solid–Fluid Reactions: Dye Adsorption Study on the Planetary Rotating Bed Reactor. *ACS Sustainable Resource Management*.
- [37] Wang, J., and Guo, X. (2020). Adsorption kinetic models: Physical meanings, applications, and solving methods. *Journal of Hazardous materials*, 390, 122156.
- [38] Wang, Y., Wang, C., Huang, X., Zhang, Q., Wang, T., and Guo, X. (2023). Guideline for modeling solid-liquid adsorption: kinetics, isotherm, fixed bed, and thermodynamics. *Chemosphere*, 140736.
- [39] Wang, Y., Wang, C., Huang, X., Zhang, Q., Wang, T., and Guo, X. (2023). Guideline for modeling solid-liquid adsorption: kinetics, isotherm, fixed bed, and thermodynamics. *Chemosphere*, 140736.
- [40] Zarria-Romero, J. Y., and Ramos-Guivar, J. A. (2024). Cytotoxicity and Genotoxicity Effects of a Magnetic Zeolite Composite in *Daphnia magna* (Straus, 1820). *International Journal of Molecular Sciences*, 25(14).
- [41] Zauška, L., Beňová, E., Urbanová, M., Brus, J., Zeleňák, V., Hornebecq, V., and Almáši, M. (2022). Adsorption and release properties of drug delivery system naproxen-SBA-15: Effect of surface polarity, sodium/acid drug form and pH. *Journal of Functional Biomaterials*, 13(4), 275.
- [42] Babajide J.O., Obijole O.A. Fehintola, E.O., Adekunbi, E A and Oke, I.A (2024). Towards An Understanding of Adsorption Kinetics: Solving Numerical Problems Using Matrix Functions In Microsoft Excel. Paper presented at 17th International Multi-Conference On ICT Applications tagged AICTTRA 2024 held between 27th - 30th October 2024 at Africa Centre of Excellence (OAK-Park), Obafemi Awolowo University, Ile-Ife, Nigeria
- [43] Hamayun, M., Mahmood, T., Naeem, A., Muska, M., Din, S. U., and Waseem, M. (2014). Equilibrium and kinetics studies of arsenate adsorption by FePO₄. *Chemosphere*, 99, 207–215. doi:10.1016/j.chemosphere.2013.10
- [44] Lin, L., Zhou, S., Huang, Q., Huang, Y., Qiu, W., and Song, Z. (2018). Capacity and mechanism of arsenic adsorption on red soil supplemented with ferromanganese oxide–biochar composites. *Environmental Science and Pollution Research*, 25(20), 20116–20124. doi:10.1007/s11356-018-2188-7
- [45] Wang, J., and Guo, X. (2023). Adsorption kinetics and isotherm models of heavy metals by various adsorbents: An overview. *Critical Reviews in Environmental Science and Technology*, 53(21), 1837–1865. <https://doi.org/10.1080/10643389.2023.2221157>
- [46] Outram, J.G, Sara J. C., Wayde, M., and Graeme J. M.. (2021). Application of non-linear regression analysis and statistical testing to equilibrium isotherms: Building an Excel template and interpretation. *Separation and Purification Technology* 258, 118005
- [47] Abiodun, O.-A.O.; Oluwaseun, O.; Oladayo, O.K.; Abayomi, O.; George, A.A.; Opatola, E.; Oras, R.F.; Isukuru, E.J.; Ede, I.C.; Oluwayomi, O.T.; Jude A. O. and Ibrahim A. O. (2023) Remediation of Heavy Metals Using Biomass-Based Adsorbents: Adsorption Kinetics and Isotherm Models. *Clean Technol.* 2023, 5, 934–960. <https://doi.org/10.3390/cleantechnol5030047>
- [48] Obijole, O.A, Adekunbi, E. A , Babajide, O.J, Sani, B.S, Idi, M.D and Oke, I.A 2022. A Review of Techniques for Arsenic Removal From Water. Book Series Published in the United States of America by IGI Global, <https://doi.org/10.4018/978-1-7998-7356-3.ch015>
- [49] Dalampira, E., and Nastis, S. A. 2019. Mapping Sustainable Development Goals: A network analysis framework. *Sustainable Development*. <https://doi.org/10.1002/sd.1964>
- [50] Amoko, J. S., Obijole O. A., Fehintola, E. O, Oke, I. A., Adeosun, O.O., Ojo, S. O., Bolorunduro, K. A., Foghi, P., Amele S. O., and Adegbite, A. A 2015. Evaluation of Linear Regression Equations and Methods of Solving linear Equations: Adsorption Kinetics Model Direct Research *Journal of Engineering and Information Technology* . 3 (2), 7-30,
- [51] Amoko JS, Ojo BM, Babatolu AO, Demehin AI, Oke IA. 2023. Linear and Non-Linear of 2-Parameters Adsorption Equilibrium Isotherm Models of Synthetic Arsenic Wastewaters. *Fundamental and Applied Agriculture*, 8(4): 684–697. <https://doi.org/10.5455/faa.14338>
- [52] Fehintola, E.O; Amoko, J.S; Demehin, A.I ;Akanni A. O; Akinmusere O. K and Oke, I.A. Adsorption Mechanisms and Structures of Arsenic Removed. *Science Forum (Journal Of Pure And Applied Sciences)* 24 (2024)
- [53] Adekunbi, E., Babajide, J., Oloyede, H., Amoko, J., Obijole, O. and Oke, I. A. 2019. Evaluation of Microsoft Excel Solver as a tool for adsorption kinetics determination. *IFE J. Sci.* 21, 169–183.
- [54] Oke, I. A. ; Olarinoye, N.O. and Adewusi, S.R.A. (2008) Adsorption Kinetics for Arsenic Removal by Untreated Powdered Eggshell from Aqueous Solutions. *Adsorption*, 14,(1), 85-92
- [55] Hamadaoui, Q and Naffrechoux, E (2007). Modeling of adsorption isotherms of phenol and chlorophenols onto granular activated carbon Part I. Two-parameter models and equations allowing determination of thermodynamic parameters. *Journal of Hazardous Materials* 147, 381–394
- [56] Rangabhashiyam, S. Anu, N. M.S. Giri, N. and Selvaraju, N. (2014). Review: Relevance of isotherm models in biosorption of pollutants by agricultural by-products. *Journal of Environmental Chemical Engineering* 2, 398–414
- [57] Vishali, S. and Mullai, P. (2016): Analysis of two-parameter and three-parameter isotherms by nonlinear regression for the treatment of textile effluent using immobilized *Trametes Versicolor*: comparison of various error functions, *Desalination and Water Treatment*, DOI: 10.1080/19443994.2016.1167127
- [58] Karri, R. R., Sahu, J.N. and Jayakumar, N.S. (2017). Optimal isotherm parameters for phenol adsorption from aqueous solutions onto coconut shell based activated carbon: Error analysis of linear and non-linear methods. *Journal of the Taiwan Institute of Chemical Engineers* 12(2), 1–16.
- [59] Ayawei N., Newton, A E., and Wankasi, D. (2017) Review

- Article: Modelling and Interpretation of Adsorption Isotherms. Hindawi Journal of Chemistry. <https://doi.org/10.1155/2017/3039817>
- [60] Garba, Z.N. (2019). The Relevance of Isotherm and Kinetic Models to Chlorophenols Adsorption: A Review. *Avicenna Journal Environmental Health Engineering*. 6(1), 55 – 65
- [61] Al-Ghouti, M.A. and Da'ana, D.A. (2020). Guidelines for the use and interpretation of adsorption isotherm models: A review, *J. Hazard. Mater.* 393, 122383
- [62] Garba, Z.N. (2019). The Relevance of Isotherm and Kinetic Models to Chlorophenols Adsorption: A Review. *Avicenna Journal Environmental Health Engineering*. 6(1), 55 – 65
- [63] Loveday, R. (1980). *Statistics, a Second Course in Statistics*, 2nd ed. New York: Cambridge University Press.
- [64] Oke, I. A (2008) Utilization of Weibull Techniques For Short Term Data In Environmental Engineering. *Environmental Engineering and Sciences*. 25 (7), 1099- 1107.
- [65] Oke, I. A.; Lukman, S; Amoko, J. S, and Fehintola E.. O (2018) An Evaluation of Solutions to Moment Method Of Biochemical Oxygen Demand Kinetics. *NIJOTECH*. 37(1), 1 – 12
- [66] Suwannahong, K.; Wongcharee, S.; Kreetachart, T.; Sirilamduan, C.; Riyo, J.; Wongphat, A. Evaluation of the Microsoft Excel Solver Spreadsheet-Based Program for Nonlinear Expressions of Adsorption Isotherm Models onto Magnetic Nanosorbent. *Appl. Sci.* 2021, 11, 7432. <https://doi.org/10.3390/app11167432>
- [67] Aslan, S., Polat, A., and Topcu, U. S. (2015). Assessment Of The Adsorption Kinetics, Equilibrium And Thermodynamics For The Potential Removal Of Ni^{2+} From Aqueous Solution Using Waste Eggshell. *Journal Of Environmental Engineering And Landscape Management*, 23(3), 221–229.
- [68] Choi, H. (2019). *Assessment of the adsorption kinetics, equilibrium and thermodynamic for Pb(II) removal using a low cost hybrid biowaste adsorbent, eggshell/coffee ground/sericite*. *Water Environment Research*. doi:10.1002/wer.1158
- [69] Choi, H.-J. (2019). *Assessment of the adsorption kinetics, equilibrium and thermodynamic for Pb(II) removal using a hybrid adsorbent, eggshell and sericite, in aqueous solution*. *Water Science and Technology*. doi:10.2166/wst.2019.191
- [70] De Freitas, F., Battistola, L. D., Arruda, R., and de Andrade, R. L. T. (2019). *Assessment of the Cu(II) and Pb(II) removal efficiency of aqueous solutions by the dry biomass Aguapé: kinetics of adsorption*. *Environmental Monitoring and Assessment*, 191(12). doi:10.1007/s10661-019-7933-y
- [71] Elkady, M. F., Ibrahim, A. M., and El-Latif, M. M. A. (2011). *Assessment of the adsorption kinetics, equilibrium and thermodynamic for the potential removal of reactive red dye using eggshell biocomposite beads*. *Desalination*, 278(1-3), 412–423. doi:10.1016/j.desal.2011.05.063
- [72] Li, R., Li, Q., Gao, S., and Shang, J. K. (2012). *Exceptional arsenic adsorption performance of hydrous cerium oxide nanoparticles: Part A. Adsorption capacity and mechanism*. *Chemical Engineering Journal*, 185-186, 127–135.
- [73] Liu H, Chen C, Li X and Yang P (2024), Meta-analysis compares the effectiveness of modified biochar on cadmium availability. *Front. Environ. Sci.* 12:1413047. doi: 10.3389/fenvs.2024.1413047
- [74] Liu, B., Liu, Z., Wu, H., Pan, S., Cheng, X., Sun, Y., and Xu, Y. (2020). *Effective and simultaneous removal of organic/inorganic arsenic using polymer-based hydrated iron oxide adsorbent: Capacity evaluation and mechanism*. *Science of The Total Environment*, 742, 140508. doi:10.1016/j.scitotenv.2020.140
- [75] Liu, Y., Liu, Z., Dai, J., Gao, J., Xie, J., and Yan, Y. (2011). *Selective Adsorption of Co(II) by Mesoporous Silica SBA-15-Supported Surface Ion Imprinted Polymer: Kinetics, Isotherms, and Thermodynamics Studies*. *Chinese Journal of Chemistry*, 29(3), 387–398. doi:10.1002/cjoc.201190093
- [76] Raji, Z.; Karim, A.; Karam, A.; Khalloufi, S. Adsorption of Heavy Metals: Mechanisms, Kinetics, and Applications of Various Adsorbents in Wastewater Remediation—A Review. *Waste* 2023, 1, 775–805. <https://doi.org/10.3390/waste1030046>
- [77] Sohrabi, H., and Ameri, E. (2015). *Adsorption equilibrium, kinetics, and thermodynamics assessment of the removal of the reactive red 141 dye using sesame waste*. *Desalination and Water Treatment*, 57(38), 18087–18098.
- [78] Tang J, Han Y, Zha Y and Li X (2024), Distribution, seasonal characteristics, ecological risks and human health risks of 9 antibiotics in the main water environment of Anhui province, China. *Front. Environ. Sci.* 12:1408363. doi: 10.3389/fenvs.2024.1408363
- [79] Wang, J., and Guo, X. (2020). Adsorption kinetic models: Physical meanings, applications, and solving methods. *Journal of Hazardous Materials*, 390, 122156. doi:10.1016/j.jhazmat.2020.122156
- [80] Xu, Z., Wu, Y., Zhang, J., Zhang, L., and Wang, L. (2010). *Equilibrium and kinetic data of adsorption and separation for zirconium and hafnium onto MIBK extraction resin*. *Transactions of Nonferrous Metals Society of China*, 20(8), 1527–1533. doi:10.1016/s1003-6326(09)60333-2
- [81] Yang Q, Chen J, Liu Y, Li Y, Zhang H, Zhang J, Sun X, Lu M, Ma R and Wu Y (2024), Analysis of changes in water quality and treatment effectiveness of seven major river basins in China from 2001 to 2020. *Front. Environ. Sci.* 12:1340994. doi: 10.3389/fenvs.2024.1340994
- [82] Yazdani, M. (Roza), Tuutijärvi, T., Bhatnagar, A., and Vahala, R. (2016). *Adsorptive removal of arsenic(V) from aqueous phase by feldspars: Kinetics, mechanism, and thermodynamic aspects of adsorption*. *Journal of Molecular Liquids*, 214, 149–156. doi:10.1016/j.molliq.2015.12.002
- [83] Yin, Y., Zhou, T., Luo, H., Geng, J., Yu, W., and Jiang, Z. (2019). *Adsorption of arsenic by activated charcoal coated zirconium-manganese nanocomposite: Performance and mechanism*. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*. doi:10.1016/j.colsurfa.2019.04.09
- [84] Rodríguez-Narciso, S., Lozano-Álvarez, J. A., Salinas-Gutiérrez, R., and Castañeda-Leyva, N. (2021). A stochastic model for adsorption kinetics. *Adsorption Science and Technology*, 2021, 5522581.
- [85] Yaroshchuk, L., and Tiurina, Y. (2022). Simulation of the Industrial Oil Adsorption Purification Process for Automation Tasks. *Modelling and Simulation in Engineering*, 2022(1), 2738654.
- [86] Chen, J., Liu, Y., Liu, J., Duan, Q., Wang, Z., Song, J., ... and Sun, J. (2024). Effects of carbonization on the structure and sorption properties of coffee grounds for Pb (II) and Ni (II) in various metal systems. *Desalination and Water Treatment*, 320, 100623.
- [87] Andreu-Vilarroig, C., Cortésa, J. C., Navarro-Quiles, A., and Sferle, S. M. (2023). Statistical analysis of a general adsorption kinetic model with randomness in its formulation. An application to real data. *MATCH Communications in Mathematical and in Computer Chemistry*.
- [88] Zhang, Z., and Luo, W. (2024). Preparation of amidogen-rich monolithic corn bract via surface graft modification for efficient separation of acid red from wastewater. *Chemical Papers*, 1-13.
- [89] Wei, X., Luo, M., Wang, T., Yu, S., Dong, Y., Che, T., and Chen, F. (2024). Preparation of Biochar Composite Graphene Oxide for the Removal of Boron in Simulated Fracturing Flowback Fluid. *Arabian Journal for Science and Engineering*, 1-10.
- [90] Xu, H., Li, S., Wang, J., Deng, J., Huang, G., Sang, Q., and Cui, J. (2023). Removal of Pyridine from Aqueous Solutions Using Lignite, Coking Coal, and Anthracite: Adsorption Kinetics. *Processes*, 11(11), 3118.
- [91] Duan, S., Huang, K., and Tao, M. (2022). Equilibrium and kinetic adsorption of hydrogen fluoride onto zeolite 3A. *Adsorption Science and Technology*, 2022, 5790408.
- [92] Guo, X., Rao, L., and Shi, Z. (2022). Preparation of High-Porosity B-TiO₂/C3N4 Composite Materials: Adsorption–Degradation Capacity and Photo-Regeneration Properties. *International Journal of Environmental Research and Public Health*, 19(14), 8683.
- [93] Cortés, J. C., Navarro-Quiles, A., Santonja, F. J., and Sferle, S. M. (2023). Statistical analysis of randomized pseudo-first/second order kinetic models. Application to study the adsorption on cadmium ions onto tree fern. *Chemometrics and Intelligent Laboratory Systems*, 240, 104910.
- [94] Zhang, W., Xu, Y., Mu, X., Li, S., Liu, X., and Lei, Z. (2023). Research progress of polysaccharide-based natural polymer hydrogels in water purification. *Gels*, 9(3), 249.

Appendix A: Derivations of Adsorption equilibrium -Linear Equations and General Form of Least Square For Matrix Transformations

A. Langmuir linear equation A Model (unknown parameters)

are a_L and b_L : $q_e = \frac{a_L b_L C_e}{1 + a_L C_e}$ which indicates that

$$\frac{1}{q_e} = \frac{1 + a_L C_e}{a_L b_L C_e} = \frac{1}{a_L b_L C_e} + \frac{a_L C_e}{a_L b_L C_e} = \frac{1}{a_L b_L C_e}$$

$$\frac{1}{q_e} = \frac{1}{a_L b_L} \left(\frac{1}{C_e} \right) + \frac{1}{b_L} \text{ which indicates that}$$

$$\frac{1}{q_e} = \frac{1}{a_L b_L} \left(\frac{1}{C_e} \right) + \frac{1}{b_L} \text{ equivalent to}$$

$Y = mX + C$ where X stand for independent variables and Y stands for dependent variables

B. Langmuir linear equation B Model: $q_e = \frac{a_L b_L C_e}{1 + a_L C_e}$

which indicates that $\frac{1}{q_e} = \frac{1 + a_L C_e}{a_L b_L C_e} = \frac{1}{a_L b_L C_e} + \frac{a_L C_e}{a_L b_L C_e} = \frac{1}{a_L b_L C_e}$

indicates that $\frac{C_e}{q_e} = \left(\frac{1}{b_L} \right) C_e + \frac{1}{a_L b_L}$

C. Langmuir linear equation C Model: $q_e = \frac{a_L b_L C_e}{1 + a_L C_e}$

which indicates that $\frac{1}{q_e} = \frac{1 + a_L C_e}{a_L b_L C_e} = \frac{1}{a_L b_L C_e} + \frac{a_L C_e}{a_L b_L C_e} = \frac{1}{a_L b_L C_e} +$

$$b_L = \frac{b_L q_e}{a_L b_L C_e} + q_e \equiv q_e = b_L - \frac{q_e}{a_L C_e}$$

D. Langmuir linear equation D Model: $q_e = \frac{a_L b_L C_e}{1 + a_L C_e}$

which indicates that $\frac{1}{q_e} = \frac{1 + a_L C_e}{a_L b_L C_e} = \frac{1}{a_L b_L C_e} + \frac{a_L C_e}{a_L b_L C_e} = \frac{1}{a_L b_L C_e} +$

$$\frac{q_e}{C_e} = a_L b_L - (a_L) q_e$$

E. Langmuir linear equation E Model:

$$\frac{1}{q_e} = \frac{1 + a_L C_e}{a_L b_L C_e} = \frac{1}{a_L b_L C_e} + \frac{a_L C_e}{a_L b_L C_e} = \frac{1}{a_L b_L C_e}$$

$$\frac{1}{C_e} = a_L b_L \left(\frac{1}{q_e} \right) - a_L \text{ which indicates that}$$

$$\frac{1}{C_e} = a_L b_L \left(\frac{1}{q_e} \right) - a_L \text{ equivalent to}$$

$Y = mX + C$ where X stand for independent variables and Y stands for dependent variables

F. Freundlich Model: $q_e = K_f C_e^{1/N_f}$

$$\text{Linear equation Freundlich Model} \quad \log(q_e) = \log(K_f) + \frac{1}{N_f} \log(C_e) \text{ which}$$

indicates that

$$\log(q_e) = \log(K_f) + \frac{1}{N_f} \log(C_e) \text{ is}$$

equivalent to $Y = mX + C$ where X stand for independent variables and Y stands for dependent variables

G. Langmuir – Vageler: Linear equation Freundlich Model

$$\log(q_e) = \log(C_f q_{\max}) - \log(C_f + K_{LV})$$

which indicates that

$$\log(q_e) = \log(C_f q_{\max}) - \log(C_f + K_{LV})$$

equivalent to $Y = mX + C$ where X stand for independent variables and Y stands for dependent variables

H. Flory – Huggins Linear equation Freundlich Model

$$\log\left[\frac{\theta}{C_e}\right] = \log(K_{FH}) + N_{FH} \log(1 - \theta)$$

which indicates that

$$\log\left[\frac{\theta}{C_e}\right] = \log(K_{FH}) + N_{FH} \log(1 - \theta)$$

equivalent to $Y = mX + C$ where X stand for independent variables and Y stands for dependent variables

I. Halsey B Linear equation Freundlich Model

$$\log(q_e) = \log K_H - \frac{1}{N_{Hf}} \log\left(\frac{C_e}{C_0}\right)$$

which indicates that

$$\log(q_e) = \log K_H - \frac{1}{N_{Hf}} \log\left(\frac{C_e}{C_0}\right)$$

equivalent to $Y = mX + C$ where X stand for independent variables and Y stands for dependent variables

J. Halsey A Linear equation Freundlich Model

$$\log(q_e) = \left(\frac{1}{N_H} \right) \log K_H - \frac{1}{N_H} \log C_e$$

which indicates that

$$\log(q_e) = \left(\frac{1}{N_H} \right) \log K_H - \frac{1}{N_H} \log C_e$$

equivalent to $Y = mX + C$ where X stand for independent variables and Y stands for dependent variables

K. Temkin Linear equation Freundlich Model

$$q_e = a_t + 2.3b_t \log C_e \quad \text{which}$$

indicates that $q_e = a_t + 2.3b_t \log C_e$

equivalent to $Y = mX + C$ where X stand for independent variables and Y stands for dependent variables

L. Frenkel- Halsey- Hill Linear equation Freundlich Model

$$\ln(q_e) = \left(\frac{1}{N_{fhh}} \right) \ln K_{fhh} - \frac{1}{N_{fhh}} \ln C_e$$

which indicates that

$$\ln(q_e) = \left(\frac{1}{N_{fhh}} \right) \ln K_{fhh} - \frac{1}{N_{fhh}} \ln C_e$$

equivalent to $Y = mX + C$ where X stand for independent variables and Y stands for dependent variables

M. Elovich Linear equation Freundlich Model

$$\ln \left(\frac{q_e}{C_e} \right) = \ln(K_E q_{mE}) - \frac{q_e}{q_{mE}} \quad \text{which}$$

indicates that

$$\ln \left(\frac{q_e}{C_e} \right) = \ln(K_E q_{mE}) - \frac{q_e}{q_{mE}} \quad \text{equivalent}$$

to $Y = mX + C$ where X stand for independent variables and Y stands for dependent variables

N. Folwer –Guggenhiem

$$\ln \left(\frac{C_e(1-\theta)}{\theta} \right) = -\ln(K_{FG}) + \frac{2\theta W}{RT}$$

which indicates that

$$\ln \left(\frac{C_e(1-\theta)}{\theta} \right) = -\ln(K_{FG}) + \frac{2\theta W}{RT}$$

equivalent to $Y = mX + C$ where X stand for independent variables and Y stands for dependent variables

O. Hill-de Boer

$$\ln \left[C_e \frac{(1-\theta)}{\theta} \right] - \frac{\theta}{(1-\theta)} = -\ln(K_{Hd}) - \frac{K_2 \theta}{RT}$$

which indicates that

$$\ln \left[C_e \frac{(1-\theta)}{\theta} \right] - \frac{\theta}{(1-\theta)} = -\ln(K_{Hd}) - \frac{K_2 \theta}{RT}$$

equivalent to $Y = mX + C$ where X stand for independent variables and Y stands for dependent variables

P. Kiselev

$$\frac{1}{C_e(1-\theta)} = \frac{K_1}{\theta} + K_1 K_n \quad \text{which indicates}$$

$$\text{that } \frac{1}{C_e(1-\theta)} = \frac{K_1}{\theta} + K_1 K_n \quad \text{equivalent to}$$

$Y = mX + C$ where X stand for independent variables and Y stands for dependent variables

APPENDIX B: Matrix Array of Linear Equations and Computations

Table B1Matrix

Matrix Computations																										
	Y = log qe	X = logCe	XY	X ²	Matrix		Variable		Y																	
15	-0.3249553	-0.4989407	0.1621334	0.2489419	-3.181	4	M= 1/N		-1.791																	
16	-0.3401472	-0.8022601	0.2728865	0.6436213	2.667	-3.181	Z= log Kf		1.472																	
17	-0.3975797	-1.0036197	0.3990188	1.0072525	Inverse																					
18	-0.7287129	-0.8758332	0.638231	0.7670838	5.7720976	7.2590078	M= 1/N	0.3471103																		
19					4.839761	5.7720976	Z= log Kf	-0.1718393																		
20																										
21																										
22	Sum	-1.791	-3.181	1.472	2.667	4	2.881	N	Kf	0.673																
23																										
24	Langmuir A																									
25		Y =1/qe	X =1/Ce	XY	X ²	Matrix		Variable		Y																
26		2.1133	3.1546	6.6665	9.9513	27.094	4	M= 1/(aL*bL)		12.154																
27		2.1885	6.3425	13.8806	40.2272	208.310	27.094	Z=(1/bL)		85.965																
28		2.4979	10.0837	25.1883	101.6809	Inverse																				
29		5.3544	7.5133	40.2296	56.4503	-0.2732677	0.0403435	M= 1/(aL*bL)	0.1467981																	
30						2.1009861	-0.2732677	Z=(1/bL)	2.0441908																	
31																										
32		Sum		12.154	27.094	85.965	208.310	4	13.925	aL	bL	0.489														
33																										
34																										

Equilibrium MES and Matrix

Kinetics MES | Kinetics Matrix | +

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Table B2Matrix

Used AICTRA 24 Computations Journal Articles 2 - Microsoft Excel + Analys...																		
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Font Alignment Number Styles Cells Editing Add-ins																		
man 8 A A Wrap Text General Conditional Formatting Format as Table Cell Styles Insert Delete Format Sum Sort & Filter Find & Select Add-ins																		
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AH AI AJ AK AL AM AN AO AP AQ AR AS AT AU AV AW																		
40	Langmuir B																	
41		Y = Ce/qe	X = Ce	XY	X ²					Matrix		Variable		Y				
42		0.6699	0.3170	0.2124	0.1005			0.707	4			M = 1/bL		1.975				
43		0.3451	0.1577	0.0544	0.0249			0.153	0.707			Z = (1/aL*bL)		0.386				
44		0.2477	0.0992	0.0246	0.0098			Inverse										
45		0.7127	0.1331	0.0949	0.0177			-6.3212691	35.767278			M = 1/bL	1.3260615					
46		0.0000	0.0000	0.0000	0.0000			1.3671788	-6.3212691			Z = (1/aL*bL)	0.2594748					
47		0.0000	0.0000	0.0000	0.0000													
48		Sum	1.975	0.707	0.386	0.153		4	0.754	bL		aL		5.111				
49																		
50																		
51																		
52	Langmuir C																	
53		Y = qe	X = qe/Ce	XY	X ²					Matrix		Variable		Y				
54		0.4732	1.4927	0.7064	2.2283			9.831	4			M = 1/aL		1.517				
55		0.4569	2.8981	1.3242	8.3990			28.892	9.831			Z = bL		3.909				
56		0.4003	4.0368	1.6161	16.2960			Inverse										
57		0.1868	1.4032	0.2621	1.9690			-0.519526	0.2113856			M = 1/aL	0.0380122					
58		0.0000		0.0000	0.0000			1.5268481	-0.519526			Z = bL	0.2858835					
59		0.0000		0.0000	0.0000													
60		Sum	1.517	9.831	3.909	28.892		4	26.307	aL		bL		0.286				
61																		
Equilibrium MES and Matrix Kinetics MES Kinetics Matrix +																		
11:42 17/11/2024 100%																		

Table B3 Matrix

	AH	AI	AJ	AK	AL	AM	AN	AO	AP	AQ	AR	AS	AT	AU	AV	AW
64		Langmuir E														
65			$Y = 1/C_e$	$X = 1/q_e$	XY	X^2		Matrix			Variable		Y			
66			3.1546	2.1133	6.6665	4.4659		12.154	-4		$M = aL * bL$		27.094			
67			6.3425	2.1885	13.8806	4.7895		44.165	-12.154		$Z = aL$		85.965			
68			10.0837	2.4979	25.1883	6.2396		Inverse								
69			7.5133	5.3544	40.2296	28.6699		-0.4200188	0.1382308		$M = aL * bL$	0.5029815				
70								-1.5262405	0.4200188		$Z = aL$	-5.2452015				
71																
72			Sum	27.094	12.154	85.965	44.165	4	-5.245	aL		bL	-0.096			
73																
74																
75																
76			Langmuir D													
77			$Y = q_e/C_e$	$X = q_e$	XY	X^2		Matrix			Variable		Y			
78			1.4927	0.4732	0.7064	0.2239		-1.517	4		$M = aL$		9.831			
79			2.8981	0.4569	1.3242	0.2088		-0.628	1.517		$Z = bL * aL$		3.909			
80			4.0368	0.4003	1.6161	0.1603		Inverse								
81			1.4032	0.1868	0.2621	0.0349		7.2445379	-19.099421		$M = aL$	-3.4345318				
82								2.9979016	-7.2445379		$Z = bL * aL$	1.1549766				
83																
84			Sum	9.831	1.517	3.909	0.628	4	-3.435	aL		bL	-0.336			
85																

Table B4 Matrix

	AH	AI	AJ	AK	AL	AM	AN	AO	AP	AQ	AR	AS	AT	AU	AV	AW
85																
86			Temkin	$Y = q_e$	$X = \log C_e$	XY	X^2		Matrix		Variable		Y			
87				0.473	-0.499	-0.2361	0.2489		3.181	4	$M = 2.3bt$		1.517			
88				0.457	-0.802	-0.3666	0.6436		-2.667	-3.181	$C = at$		-1.168			
89				0.400	-1.004	-0.4018	1.0073		Inverse							
90				0.187	-0.876	-0.1636	0.7671		-5.7720976	-7.2590078	$M = 2.3bt$	-0.2788342				
91									4.839761	5.7720976	$C = at$	0.6010255				
92																
93			Sum	1.517	-3.181	-1.168	2.667	4	-0.121	bt		at	0.601			
94			Flory-Huggins													
95				$Y = Tita/C_e$	$X = \log(1 - Tita)$	XY	X^2		Matrix		Variable		Y			
96				-0.176	-0.103	0.0182	0.0106		0.309	4	$M = NfH$		-0.110			
97				-0.114	-0.056	0.0064	0.0032		-0.027	-0.309	$C = \log(Kfh)$		0.002			
98				-0.041	-0.041	0.0017	0.0017		Inverse							
99				0.222	-0.109	-0.0242	0.0119		-22.545937	-291.65523	$M = NfH$	1.8616088				
100									1.9928773	22.545937	$C = \log(Kfh)$	-0.1713033				
101																
102			Sum	-0.110	-0.309	0.002	0.027	4	1.862	NfH		Kfh	0.674			
103			Hasley B													
104				$Y = \log(q_e)$	$X = \log(C_e/C_0)$	XY	X^2		Matrix		Variable		Y			

Table B5 Matrix

	AH	AI	AJ	AK	AL	AM	AN	AO	AP	AQ	AR	AS	AT	AU	AV	AW
103		Hasley B														
104			Y=log(qe)	X=log(ce/C0)	XY	X ²							Y			
105			-0.325	-0.675	0.2194	0.4557		3.290	4				-1.791			
106			-0.340	-0.916	0.3116	0.8394		-2.815	-3.290				1.423			
107			-0.398	-1.045	0.4155	1.0921		Inverse								
108			-0.729	-0.654	0.4766	0.4277		-7.5856287	-9.2219977							
109								6.4896202	7.5856287							
110																
111		Sum	-1.791	-3.290	1.423	2.815	4	2.148	Nfh							
112		Hasley A														
113			Y=Log(qe)	X=log(Ce)	XY	X ²							Y			
114			-0.176	-0.499	0.0879	0.2489		3.181	4				-0.110			
115			-0.114	-0.802	0.0914	0.6436		-2.667	-3.181				0.027			
116			-0.041	-1.004	0.0415	1.0073		Inverse								
117			0.222	-0.876	-0.1943	0.7671		-5.7720976	-7.2590078							
118								4.839761	5.7720976							
119																
120		Sum	-0.110	-3.181	0.027	2.667	4	2.272	Nfh							
121		Frenkel-Hasley-Hill														
122			Y=ln(qe)	X=ln(Ce)	XY	X ²							Y			

Table B 6 Matrix

	AH	AI	AJ	AK	AL	AM	AN	AO	AP	AQ	AR	AS	AT	AU	AV	AW
121		Frenkel-Hasley-Hill														
122			Y=ln(qe/Ce)	X=ln(Ce)	XY	X ²							Y			
123			-0.748	-0.237	0.1776	0.0564		0.712	4				-4.125			
124			-0.783	-0.129	0.1013	0.0167		-0.145	-0.712				0.786			
125			-0.915	-0.094	0.0865	0.0089		Inverse								
126			-1.678	-0.251	0.4208	0.0629		-9.792	-55.010							
127								1.993	9.792							
128																
129		Sum	-4.125	-0.712	0.786	0.145	4	0.349	Nfh							
130		Elovich														
131			Y=ln(qe/Ce)	X=ln(qe)	XY	X ²							Y			
132			1.149	-0.405	-0.4658	0.1644		0.252	4				7.324			
133			1.847	-0.262	-0.4847	0.0688		-0.503	-0.252				-0.141			
134			2.311	-0.095	-0.2203	0.0091		Inverse								
135			2.017	0.511	1.0302	0.2609		-0.129	-2.052							
136								0.258	0.129							
137																
138		Sum	7.324	-0.252	-0.141	0.503	4	1.516	qmax							
139																
140																
141																

APPENDIX B: MES Computations

Table C1 MES

Table C1 MES													
	A	B	C	D	E	F	G	H	I	J	K	L	M
64				Langmuir E			Observed	Cal					
65		Qe	Ce			Chi Squared	1/ce	ME Solver					
66	1	0.473	0.317			0.901	3.155	4.1038					
67	2	0.457	0.158			4.376	6.342	4.2507					
68	3	0.400	0.099	bL	84.9035	27.340	10.084	4.8549					
69	4	0.187	0.133	aL	0.023	8.525	7.513	10.4330					
70	5					0.000	0.000	0.0000					
71	6					0.000		0.0000					
72	Average	0.379			Target	41.141		0.0000					
73						Average	5.419	3.940					
74													
75	Langmuir D												
76				Langmuir D			Observed	Cal					
77		Qe	Ce			Chi Squared	qe/ce	ME Solver					
78	1	0.473	0.317			0.913	1.493	2.4485					
79	2	0.457	0.158			0.202	2.898	2.4488					
80	3	0.400	0.099	bL	121.8379	2.518	4.037	2.4500					
81	4	0.187	0.133	aL	0.020	1.105	1.403	2.4543					
82	5					0.000		0.0000					
83	6					0.000		0.0000					
84	Average	0.379			Target	4.738		9.802					
85													

Table C2 MES

Table C2 MES													
	A	B	C	D	E	F	G	H	I	J	K	L	M
40				Langmuir B			Observed	Cal					
41		Qe	Ce			Chi Squared	ce/qe	ME Solver					
42	1	0.473	0.317			0.044	0.669907	0.8798					
43	2	0.457	0.158			0.334	0.345054	0.9226					
44	3	0.400	0.099	bL	-3.7197	0.477	0.2477194	0.9383					
45	4	0.187	0.133	aL	-0.279	0.047	0.7126556	0.9292					
46	5					0.000	0	0.0000					
47	6					0.000		0.0000					
48	Average	0.379			Target	0.902		0.000					
49						Average	0.329	0.612					
50													
51	Langmuir C												
52				Langmuir C			Observed	Cal					
53		Qe	Ce			Chi Squared	qe	ME Solver					
54	1	0.473	0.317			1486.389	0.473	39.0269					
55	2	0.457	0.158			1.063	0.457	1.4882					
56	3	0.400	0.099	bL	78.9000	860.192	0.400	-28.9287					
57	4	0.187	0.133	aL	0.037	1700.072	0.187	41.4187					
58	5					0.000	0.000	0.0000					
59	6					0.000	0.000	0.0000					
60	Average	0.379			Target	4047.717		0.000					
61						Average	0.253	8.834					

Table C 3 MES

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
85														
86	Temkin	qe	Ce			Chi Squared	qe	ME Solver						
87		0.473	0.317	at	0.601	0.000	0.473	0.462						
88		0.457	0.158	bt	0.121	0.006	0.457	0.377						
89		0.400	0.099			0.006	0.400	0.321						
90		0.187	0.133			0.029	0.187	0.357						
91														
92														
93					Target	0.042		1.517						
94	Flory-Huggins													
95	Tita	Tita/Ce	1-Tita			Chi Squared		ME Solver						
96	0.211	0.667	0.789	Kfh	0.674	0.039		0.021						
97	0.121	0.769	0.879	Nfh	-1.862	0.002		-0.067						
98	0.090	0.909	0.910			0.003		-0.095						
99	0.222	1.667	0.778			0.036		0.031						
100														
101														
102					Target	0.080		-0.110						
103	Hasley B													
104		qe	Ce/C0			Chi Squared		ME Solver						

Table C 4 MES

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
103	Hasley B													
104		qe	Ce/C0			Chi Squared		ME Solver						
105		0.473	0.211	KHb	0.167	0.033		-0.507						
106		0.457	0.121	NHb	2.498	0.005		-0.410						
107		0.400	0.090			0.002		-0.359						
108		0.187	0.222			0.046		-0.515						
109														
110														
111					Target	0.085		-1.791						
112	Hasley A													
113		qe	Ce			Chi Squared		ME Solver						
114		0.667	0.317	KHb	0.139	0.000		-0.158						
115		0.769	0.158	NHb	2.272	0.008		-0.024						
116		0.909	0.099			0.011		0.064						
117		1.667	0.133			0.046		0.008						
118														
119														
120					Target	0.065		-0.110						
121	Frenkel-Hasley-Hill													
122		qe	Ce			Chi Squared		ME Solver						

Table C5 MES

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
121	Frenkel-Haasley-Hill													
122		qe	Ce			Chi Squared		ME Solver						
123		0.473	0.789	Kfh	0.239	0.049		-0.970						
124		0.457	0.879	Nfh	1.231	0.075		-1.057						
125		0.400	0.910			0.029		-1.086						
126		0.187	0.778			0.517		-0.959						
127														
128					Target	0.670		-4.072						
129														
130	Elovich													
131		qe	Ce			Chi Squared		ME Solver						
132		0.667	0.211	Ke	0.239	1.100		0.100						
133		0.769	0.121	qmax	1.231	1.680		0.551						
134		0.909	0.090			2.308		0.792						
135		1.667	0.222			3.826		0.061						
136														
137														
138					Target	8.915		1.503						
139														
140		Summary												
141	Summary	Matrix	MES	Parameters										

Table C6 MES

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
85														
86	Temkin	Qe	Ce			Chi Squared	qe	ME Solver						
87		0.473	0.317	at	0.601	0.000	0.473	0.462						
88		0.457	0.158	bt	0.121	0.006	0.457	0.377						
89		0.400	0.099			0.006	0.400	0.321						
90		0.187	0.133			0.029	0.187	0.357						
91														
92					Target	0.042		1.517						
93														
94	Flory-Huggins													
95	Tita	Tita/Ce	1-Tita			Chi Squared		ME Solver						
96	0.211	0.667	0.789	Kfh	0.674	0.039		0.021						
97	0.121	0.769	0.879	Nfh	-1.862	0.002		-0.067						
98	0.090	0.909	0.910			0.003		-0.095						
99	0.222	1.667	0.778			0.036		0.031						
100														
101														
102					Target	0.080		-0.110						
103	Hasley B													
104		qe	Ce/CO			Chi Squared		ME Solver						