## Electronic Supplementary Material (ESI) for Materials Advances. This journal is © The Royal Society of Chemistry 2022

## **Supplementary Information**

Isotherm model	Linearized Equation	Parameter	Significance	References
Langmuir	$\frac{C_e}{q_e} = \frac{1}{q_m b} + \frac{C_e}{q_m}$	q <sub>m</sub>	Maximum dye adsorption capacity (mg g <sup>-1</sup> )	Langmuir 1018 [1]
	Monolayer adsorption on homogeneous adsorbent surface	b	Constant related to affinity of binding sites (L mg <sup>-1</sup> )	& Dabrowski
	$R_L = \frac{1}{1 + bC_0}$	R <sub>L</sub>	Dimensionless separation factor ( $R_L$ < 1 represents favourable adsorption)	2001[2]
Freundlich	$\log q_e = \log K_F + \frac{1}{n} \log C_e$	K <sub>F</sub>	Adsorption capacity $(mg^{1-1/n} g^{-1} L^{-1})$	Ayawei <i>et al</i> . 2015
	Multilayer adsorption on heterogeneous adsorption surface	n	Adsorption intensity (1 <n<10 interaction)<="" represents="" strong="" td=""><td>[3]</td></n<10>	[3]
Temkin	$q_e = \frac{RT}{b} lnK_T + \frac{RT}{b} lnC_e$	K <sub>T</sub>	Temkin constant (L mg <sup>-1</sup> )	
	Heat of adsorption decreases linearly with increase in adsorbent coverage The Temkin isotherm is valid for only an intermediate range of ion concentration	b	Constant related to heat of adsorption (J mol <sup>-1</sup> )	Ringot <i>et al.</i> 2007 [4] & Shahbeig <i>et</i> <i>al.</i> 2013 [5]
D-R Isotherm	The D-R isotherm expresses Gaussian energy distribution on	q <sub>m</sub>	Maximum monolayer adsorption	Ayawei <i>et al</i> . 2015
	heterogeneous surface.	β	exponent that lies between 0 and 1	[3]

Supplementary Table S1: Linearized equations of the four adsorption isotherm models studied.

$lnq_e = lnq_m - \beta \varepsilon^2$			
$\varepsilon = RT ln \left( 1 + \frac{1}{C_e} \right)$	E	Mean adsorption energy (J mol <sup>-1</sup> )	
$E = \frac{1}{\sqrt{2\beta}}$			

## Supplementary Table S2: Linearized equations of the three adsorption kinetic models studied.

Kinetic model	Linearized Equation	Parameter	Significance	References
Pseudo first- order Kinetics	$log(q_e - q_t) = logq_e - \left(\frac{k_1}{2.303}t\right)$	q <sub>e</sub>	Quantity of dye adsorbed at equilibrium (mg g <sup>-1</sup> )	Lagergren 1898 [8]
	Lagergren's equation describes	q <sub>t</sub>	Quantity of dye adsorbed at time, t (mg g <sup>-1</sup> )	and Annadurai &
	adsorption in solid – liquid systems based on sorption capacity of solids	k <sub>1</sub>	Rate constant of pseudo first-order adsorption (min <sup>-1</sup> )	Krishnan 1997 [9]
Pseudo second- order Kinetics	$\frac{t}{-} = \frac{1}{-} + \frac{1}{-t}$	k <sub>2</sub>	Rate constant of pseudo second-order adsorption	
	$q_t  k_2 q_e^2  q_e$		$(g mg^{-1} min^{-1})$	
	It predicts the behaviour of molecules over the whole range of adsorption process. Also useful for calculation of $q_e$	q <sub>e</sub>	Equilibrium adsorption capacity (mg g <sup>-1</sup> )	Mckay & Ho 1999 [10]
Intra – particle diffusion	$q_t = k_i t^{0.5} + C$	k <sub>i</sub>	Intra – particle diffusion rate constant (mg g <sup>-1</sup> min <sup>-0.5</sup> )	
	Weber – Morris model is important to describe the overall mechanism of adsorption. It assumes that if the plot of $q_t$ versus $t^{0.5}$ is linear and passes through origin, then intra – particle diffusion is the sole rate – limiting step.	С	Intercept	Weber & Morris 1964 [11]

Supplementary Table S3: Linearized equations and their significance studied for evaluation of adsorption thermodynamics.

Linearized equation	Parameters	Significance
Change in free energy equation	ΔG	Change in free energy, $\Delta G$ is the measure of spontaneity and feasibility of the process. If the value of $\Delta G$ is negative, the process is spontaneous in nature.
$\Delta G = -RT lnK$	K	Equilibrium constant, k is obtained from the ratio of concentration of adsorbate on the surface of adsorbent to the concentration of adsorbate in the solution and is important for determining $\Delta G$ .
Van't Hoff equation	ΔΗ	Change in enthalpy, $\Delta H$ gives an indication of whether the process is exothermic or endothermic in nature.
$lnK = (\Delta S/R) - (\Delta H/RT)$	ΔS	Change in entropy, $\Delta S$ is the measure of increase or decrease of randomness of the adsorbate – adsorbent system.

## References

- I. Langmuir, The adsorption of gases on plain surfaces of Glass, Mica and Platinum, J. Am. Chem. Soc. 40 (1918) 1361-1403.https://doi.org/10.1021/ja02242a004
- [2] A. Dabrowski, Adsorption from theory to practice, Adv. Colloid Interface Sci. 93 (2001) 135-224.<u>https://doi.org/10.1016/S0001-8686(00)00082-8</u>
- [3] N. Ayawei, A. T. Ekubo, D. Wankasi, E. D. Dikio, Adsorption of Congo red by Ni/Al-CO<sub>3</sub>: Equilibrium, Thermodynamic and Kinetic Studies. Orient J. Chem. 31 (2015) 1307-1318.<u>http://dx.doi.org/10.13005/ojc/310307</u>
- [4] D. Ringot, B. Lerzy, K. Chaplain, J. P. Bonhoure, E. Auclair, and Y. Larondelle, In vitro biosorption of ochratoxin A on the yeast industry by-products: Comparison of isotherm models, Bioresour. Technol. 98 (2007) 1812-1821.<u>https://10.1016/j.biortech.2006.06.015</u>
- [5] H. Shahbeig, N. Bagheri, S. A. Ghorbanian, A. Hallajisani, and S. Poorkarimi, A new adsorption isotherm model of aqueous solutions on granular activated carbon, World J. Modell. Simullation. 9 (2013) 243-254.
- [6] O. Redlich and D. L. Peterson, A useful adsorption isotherm, J. Phys. Chem. 63 (1959) 1024-1024. <u>https://doi.org/10.1021/j150576a611</u>
- [7] F. C. Wu, B. L. Liu, K. T. Wu, and R. L. Tseng, A new linear form analysis of Redlich-Peterson isotherm equation for the adsorption of dyes, Chem. Eng. J. 162 (2010) 21-27.<u>https://doi.org/10.1016/j.cej.2010.03006</u>
- [8] S. Lagergren, About the Theory of So-Called Adsorption of Soluble Substances, *K*. Sven Vetenskapsakad Handl 24 (1898) 1-39.
- [9] G. Annadurai and M. R. V. Krishnan, Adsorption of acid dye from aqueous solution by chitin: Equilibrium studies. Indian J. Chem. Technol. 4, (1997) 217-222.
- [10] Y.S. Ho and G. McKay, Pseudo-second order model for sorption processes, Process Biochem 34 (1999) 451-465.<u>https://doi.org/10.1016/S0032-9592(98)00112-5</u>
- [11] W. J. Weber and J. C. Morris, Equilibria and capacities for adsorption on carbon, J Sanit Eng Div 90 (1964) 79-108.