

Supplementary Information

Aqueous Ibuprofen Sorption by Activated Walnut Shell Biochar: Process optimization and Cost Estimation

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S1. Preparation and analysis of ibuprofen solutions

Freshly prepared solutions of ibuprofen were used to avoid any photodegradability. Ibuprofen solutions were made by dissolving ibuprofen in ethanol and double distilled water (DDW). E.g. 50 mg L⁻¹ solution of ibuprofen was made by taking 50 mg of ibuprofen in 100 ml of ethanol followed by DDW addition to 1 liter using volumetric flask. Ibuprofen solutions were analyzed using a UV-VIS spectrometer at λ_{\max} of 264 nm.

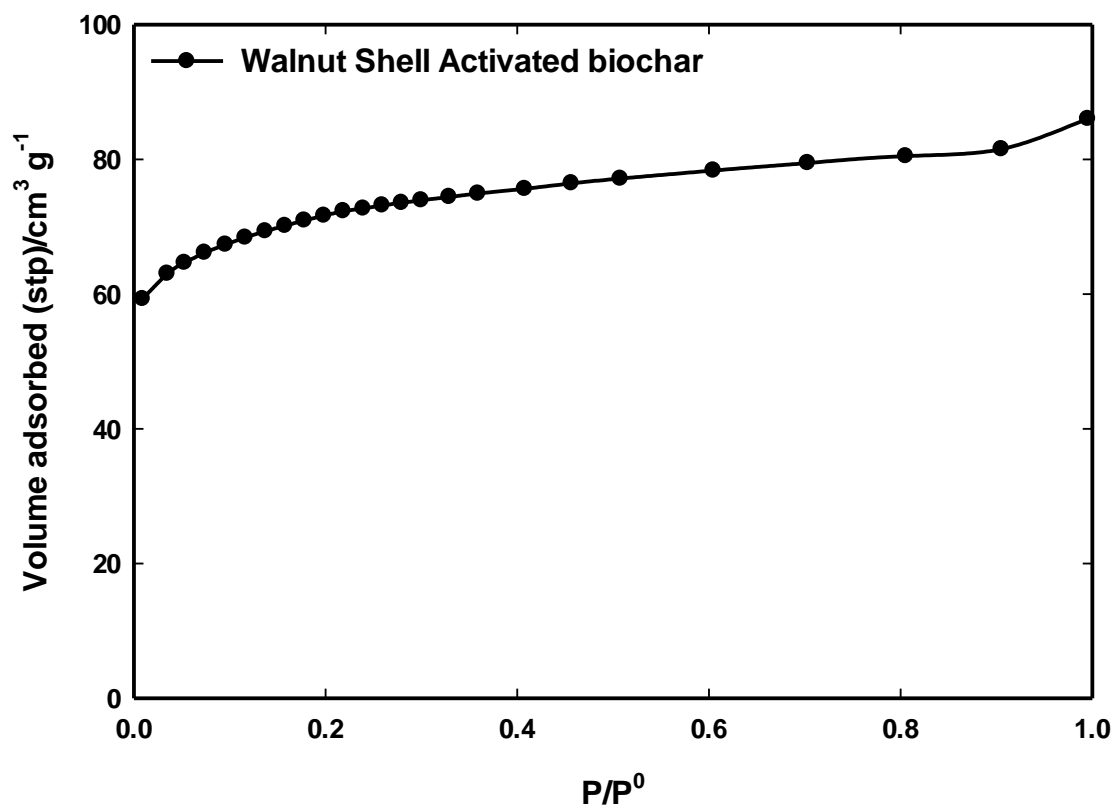
Table S1. Kinetic equations & isotherm parameters applied for sorption data fitting.

Model/Equation	Equation	Parameters explanations	Reference
Kinetic equations			
Pseudo-first order	$q_t = q_e(1 - e^{-k_1 t})$	K_1 (time ⁻¹) is pseudo-first order rate constant, q_e and q_t (mg/g) are the ibuprofen amount adsorbed at equilibrium and at any time (t)	(Lagergren 1898)
Pseudo-second order	$\frac{dq_t}{dt} = k_2(q_e - q_t)^2$	k_2 (g mg ⁻¹ min ⁻¹) is the pseudo-second order rate constant, q_e and q_t (mg/g) are the ibuprofen amount adsorbed at equilibrium and at any time (t)	(Ho and McKay 1999)
Isotherm models			
Langmuir	$q_e = \frac{Q^0 b C_e}{1 + b C_e}$	q_e (mg/g) is the ibuprofen amount adsorbed per unit WSAB weight, C_e (mg/L) is equilibrium ibuprofen concentration, Q^0 (mg/g) is the monolayer adsorption capacity and b is the constant related to net enthalpy of adsorption (L mg ⁻¹)	(Langmuir 1916)
Freundlich	$q_e = K_F C_e^{1/n}$	q_e (mg/g) is the ibuprofen amount adsorbed per unit WSAB weight, C_e (mg/L) is the equilibrium ibuprofen concentration in the solution, K_F (mg/g) is a constant indicating the relative adsorption capacity of the biochar and $1/n$ is the constant representing adsorption intensity	(Freundlich 1906)

Table S2: Determination of point of zero charge (pH_{zpc})

Points of reference		Walnut shell activated biochar (WSAB)	
$\text{pH}_{(\text{initial})}$	$\text{pH}_{(\text{final})}$	$\text{pH}_{(\text{initial})}$	$\text{pH}_{(\text{final})}$
0	0		
2	2	2	2.01[*]
4	4	4	2.61
6	6	6	2.64
8	8	8	2.62
10	10	10	2.66
12	12	-	-

pH_{ZPC} for walnut shell activated biochar is 2.0

Figure S1. N_2 adsorption isotherm curve of walnut shell activated biochar.

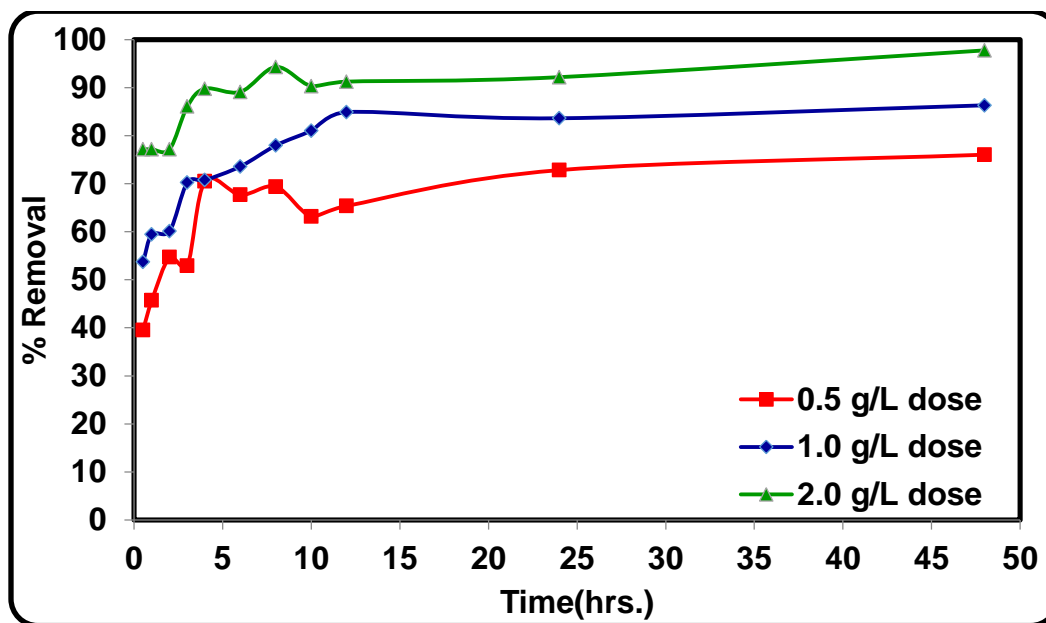


Figure S2. Effect of WSAB dose on ibuprofen adsorption rate [Initial pH = 4.0, temperature = 25 °C and initial concentration = 50 mg L⁻¹].

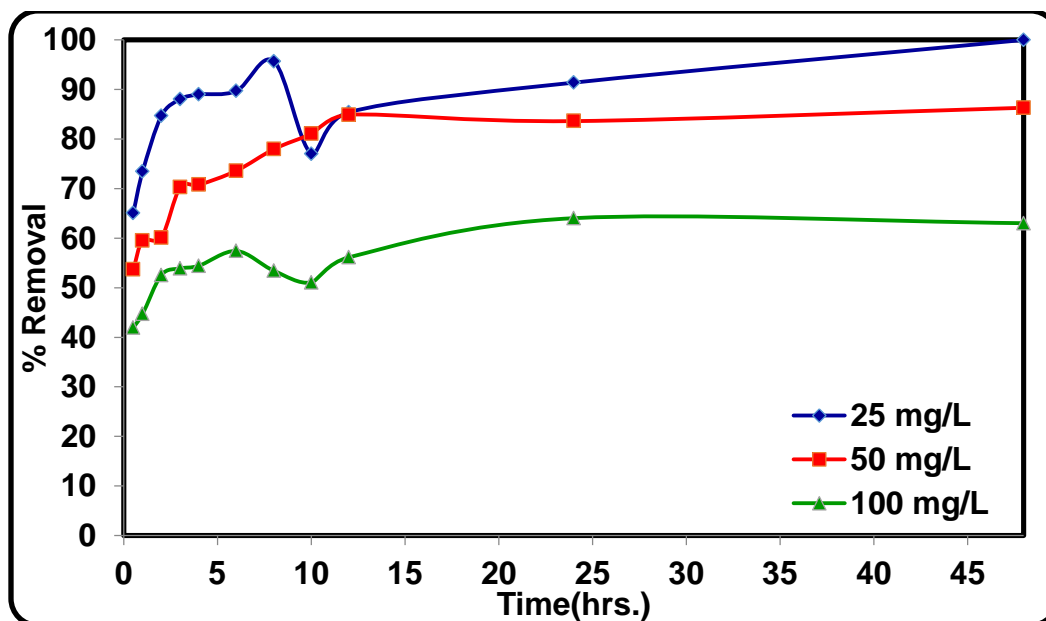


Figure S3. Effect of initial ibuprofen concentration on adsorption rate [Initial pH = 4.0, temperature = 25 °C and dose = 1.0 g L⁻¹].

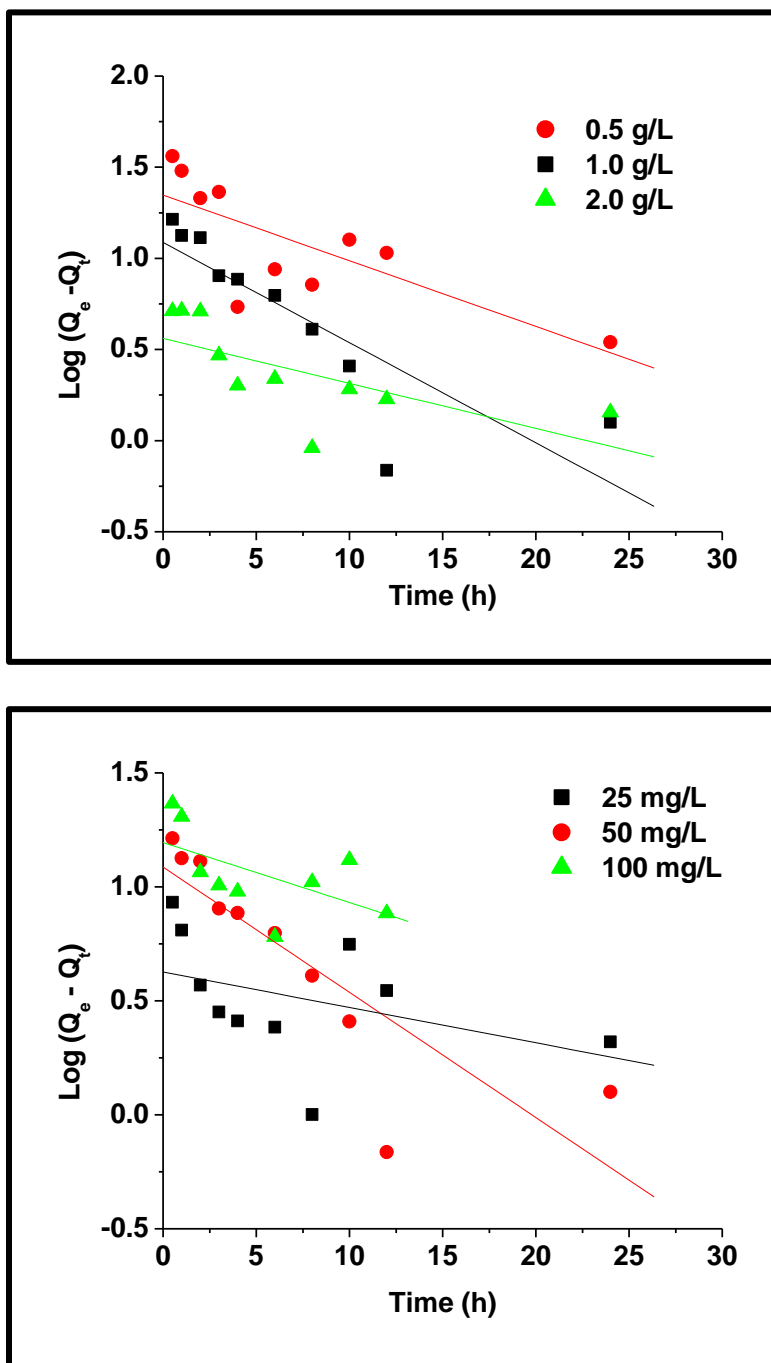


Figure S4. Pseudo-first order fitting curves of ibuprofen adsorption (A) effect of WSAB dose (B) effect of initial ibuprofen concentration [Initial pH = 4.0, temperature = 25 °C].

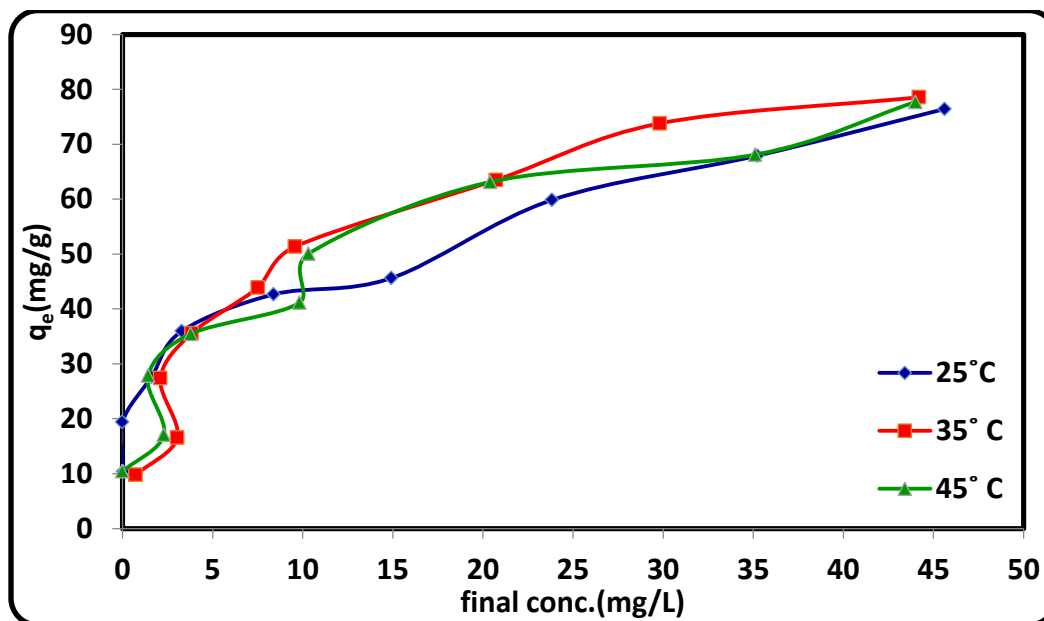


Figure S5. Ibuprofen adsorption isotherms at 25, 35, 45 °C [Initial pH = 4.0, temperature = 25 °C and dose = 1.0 g L⁻¹].

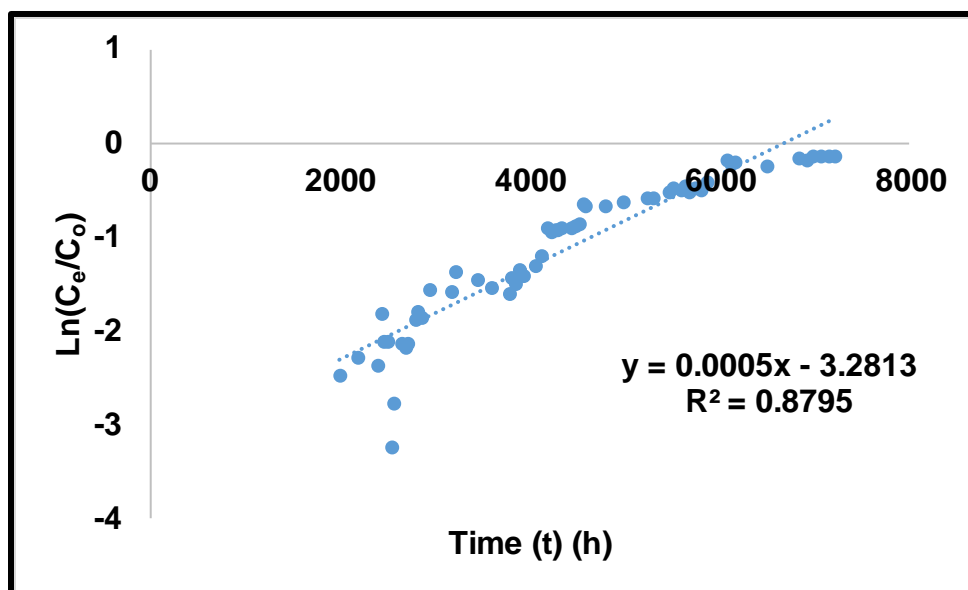


Figure S6. Adams-Bohart model fitting for ibuprofen sorption column data.

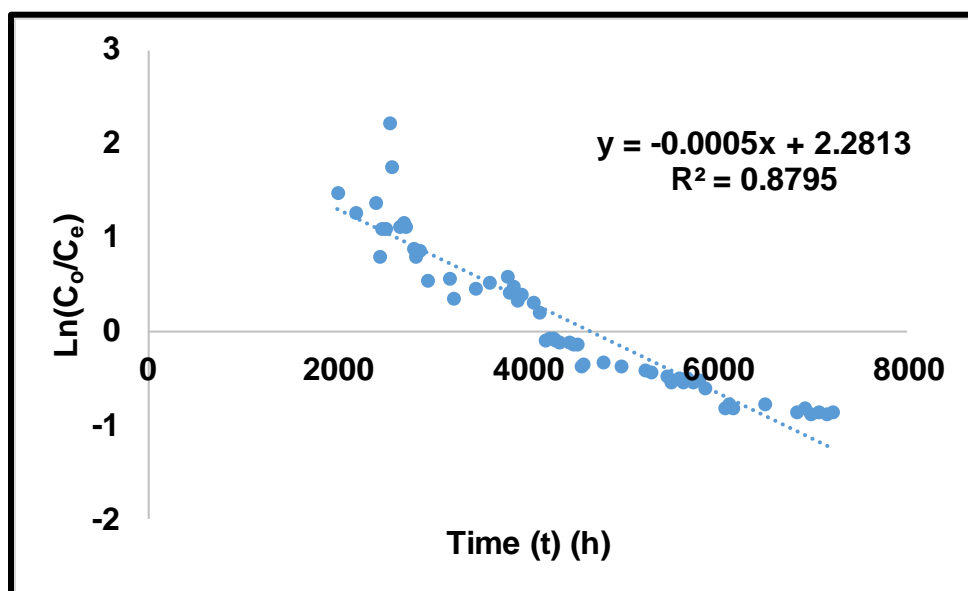


Figure S7. Thomas model fitting for ibuprofen sorption column data.

References

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