Supporting Materials

Excellent Cr(VI) adsorbent made from pyrolyzed green coconut trash with parametric modelling and optimization using RSM and experimental data

Supplementary Tables

Table S1 - Nonlinear models of kinetics and adsorption isotherms.

Kinetic Models	Equations
Pseudo-first order	$q_t = q_e\left[1-\exp^{-k_1 t}\right]$
Pseudo-second order	$q_t = \frac{q_e^{\,2} k_2 t}{1+q_e k_2 t}$
Intraparticle diffusion	$q_t = k_{\text{int}} t^{0.5} + \beta$
Isotherm Models	**Equations**
Langmuir	$q_e = \frac{q_m K_L C_e}{1+K_L C_e}$ $\mathrm{R_L} = \frac{1}{1+K_L \mathrm{C_0}}$
Freundlich	$q_e = K_F C_e^{\frac{1}{n_f}}$
Temkin	$q_e = \frac{RT}{b_t}\ln(a_t C_e)$
Toth	$q_e = \frac{q_m K_t C_e}{\left(1+\left(K_t C_e\right)^t\right)^{\frac{1}{t}}}$

q_t (mg g^{-1}) gives adsorption capacity of Cr(VI) at any time t (min); q_e (mg g^{-1}) gives theoretical adsorption capacity in equilibrium which was calculated using the kinetic models; k_1 (min^{-1}), k_2 (g mg^{-1} min^{-1}), and k_{int} (mg g^{-1} min$^{-0.5}$) are adsorption rate constants for given kinetic models; β constant relates to the thickness of the boundary layer.

In the above equations C_e (mg/L) equilibrium Cr(VI) concentration, C_0 (mg/L) gives initial Cr(VI) concentration, q_e (mg/g) gives adsorption capacity for equilibrium, q_m (mg/g) gives maximum monolayer adsorption capacity, K_L (L/mg) gives Langmuir constant, K_F (mg/g). $(mg/L)^{-1/n_f}$ as Freundlich isotherm equilibrium constant related to Cr(VI) adsorption capacity, and n_f depicts factor heterogeneity, R_L is separation factor, b_t (J/mol) denotes Temkin constant, a_t (L/mg) gives Temkin isotherm constant, and R was used as universal gas constant (8.314 J/mol.K), also T (K) gives temperature, K_t (L/mg) Toth constant related to binding affinity which is specific to the adsorbate and adsorbent pair and t is surface heterogeneity parameter.

Table S2 BBD matrix of three factors and the results**.**

Run count	pH	The temperature in (°C)	Dosage (g/L)	Actual, Removal %	Predicted, Removal %
1	4	40	6.5	46.31	47.41
2	4	35	5	66.98	65.55
3	3.25	30	8	92.87	92.54
4	3.25	35	6.5	73.63	73.59
5	2.5	35	8	80.21	81.64
6	3.25	35	6.5	73.54	73.59
7	2.5	30	6.5	99.99	98.89
8	4	35	8	72.65	71.47
9	3.25	35	6.5	73.62	73.59
10	3.25	40	5	44.98	45.31
11	2.5	35	5	74.52	75.70
12	4	30	6.5	78.36	79.87
13	3.25	35	6.5	73.46	73.59
14	3.25	40	8	52.87	52.95
15	3.25	30	5	88.41	88.33
16	2.5	40	6.5	50.23	48.72
17	3.25	35	6.5	73.68	73.59

Table S3 Adequacy of the given model tested for Cr(VI) removal.

The sequential model with the sum of squares						
Source	**Sum of Squares**	**df**	**Mean Square**	**F-value**	**p-value**	**Remarks**
Mean vs Total	87024.12	1	87024.12			
Linear vs Mean	3689.86	3	1229.95	90.17	< 0.0001	
2FI vs Linear	81.35	3	27.12	2.83	0.0929	
Quadratic vs 2FI	**81.85**	**3**	**27.28**	**13.52**	**0.0027**	**Suggested**
Cubic vs Quadratic	14.10	3	4.70	628.38	< 0.0001	Aliased
Residual	0.0299	4	0.0075			
Total	90891.31	17	5346.55			
Model Summary fit Statistics						
Source	**Std. Dev.**	**R^2**	**Adjusted R^2**	**Predicted R^2**	**PRESS**	
Linear	3.69	0.9541	0.9436	0.9092	351.14	
2FI	3.10	0.9752	0.9603	0.8941	409.72	
Quadratic	**1.42**	**0.9963**	**0.9916**	**0.9416**	**225.66**	**Suggested**
Cubic	0.0865	1.0000	1.0000		*	Aliased