

Engineering of Kaolin/SLS-Functionalized Biochar@ β -cyclodextrin Composite for adsorbing o-Nitrophenol; Optimization, Mechanistic study, and Box–Behnken Design

Abdelazeem S. Eltaweil ^{1,2}, Nouf Al Harby ^{3,*}, Mervette El Batouti ², and Eman M. Abd El-Monaem ⁴

¹ Department of engineering, College of Engineering and Technology, University of Technology and Applied Sciences, Ibra, Sultanate of Oman.

² Department of Chemistry, Faculty of Science, Alexandria University 21934, Alexandria, Egypt

³ Department of Chemistry, College of Science, Qassim University, Buraidah 51452, Saudi Arabia.

⁴ Advanced Technology Innovation, Borg El-Arab, Alexandria, Egypt.

* Correspondence: N.F.A. (hrbien@qu.edu.sa).

Figure S1. EDX spectra of (a) pristine BC and the as-fabricated SLS-BC (b) before and (c) after washing.

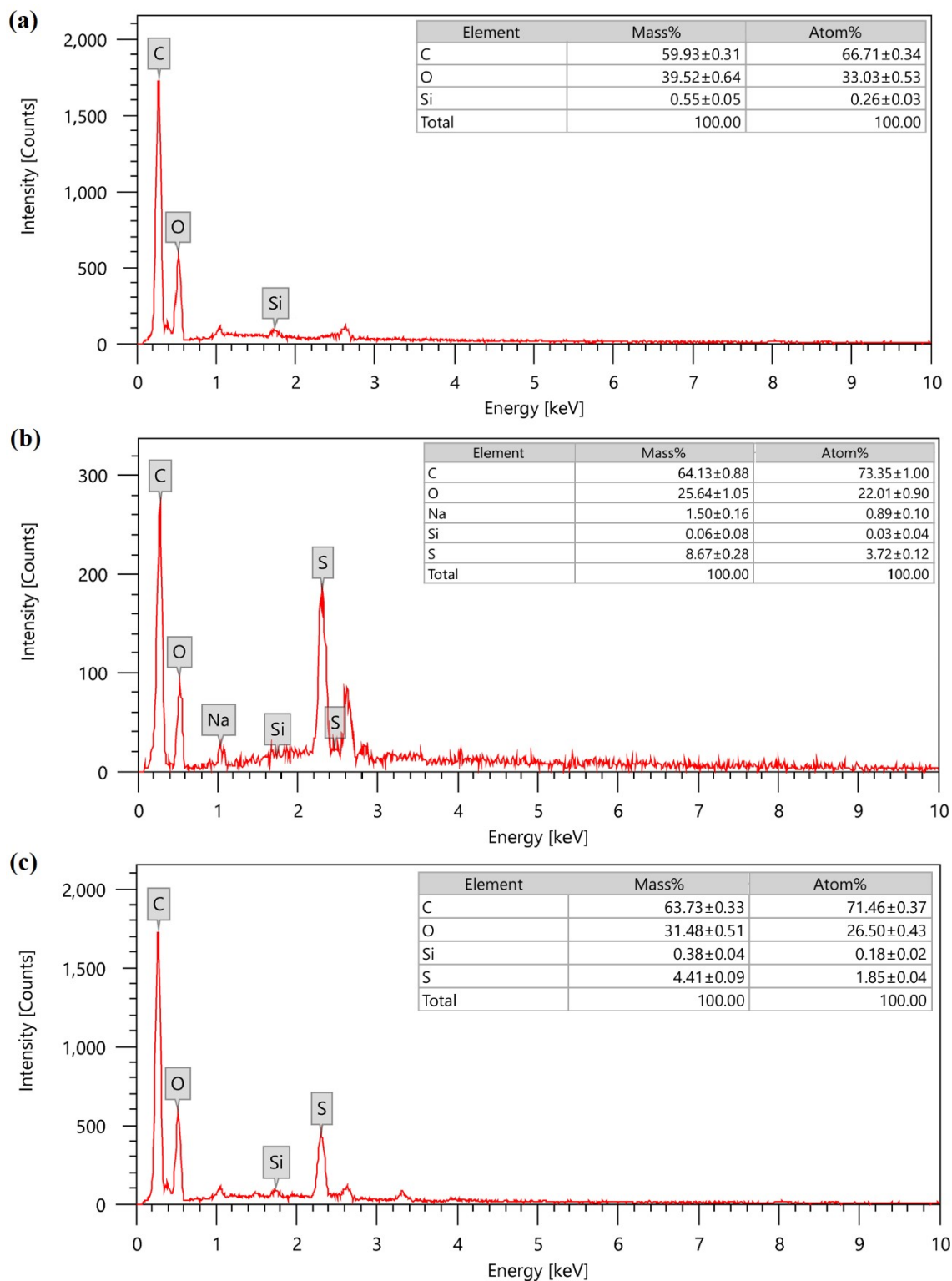


Figure S2. Removal% of different o-NP concentrations by Kaol/SLS-BC_{0.5}/β-CD_{0.5} composite.

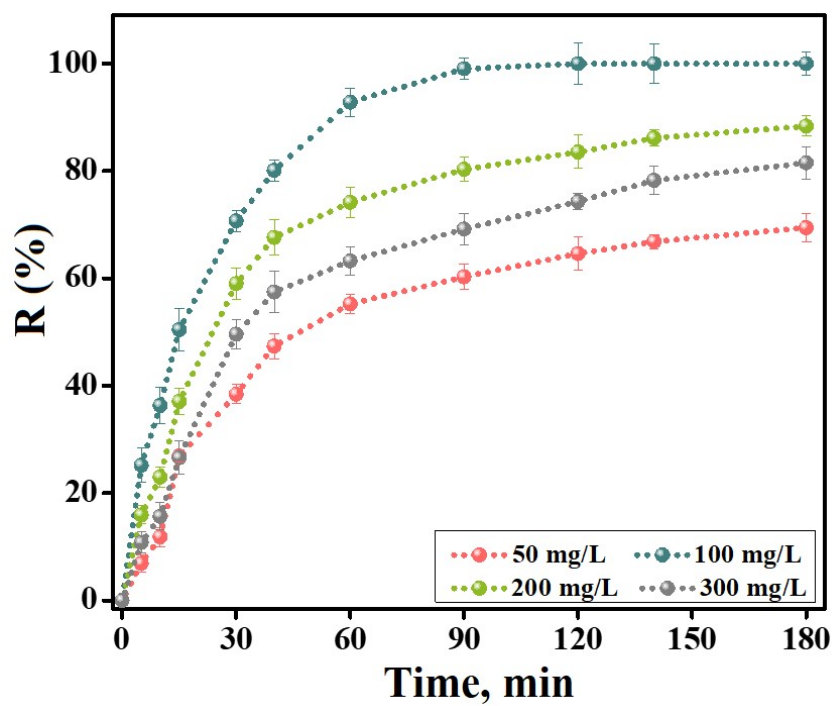


Table S1. Equations of the applied adsorption kinetic models

| Kinetic Model | Equation |
|---------------------|---|
| Pseudo–First order | $\ln (q_e - q_t) = \ln q_e - \left(\frac{k_1}{2.303}\right)t \quad (1)$ |
| Pseudo–Second order | $t/q_t = 1/k_2 q_e^2 + 1/q_e(t) \quad (2)$ |
| Elovich model | $q_t = \frac{1}{\beta} \ln (\alpha\beta) + \frac{1}{\beta} \ln (t) \quad (3)$ |

Where, q_t and q_e are amounts of adsorbed o-NP at time t and equilibrium, respectively. k_1 and k_2 are the rate constants of Pseudo first order and Pseudo second order, respectively. α and β are Elovich coefficients that represent the initial adsorption rate and the desorption coefficient, respectively, also related to the extent of surface coverage and activation energy for chemisorption.

Table S2: Equations of the applied adsorption isotherm models

| Model | Equation |
|-------------------|--|
| Langmuir | $\frac{C_e}{q_e} = \frac{1}{K_L q_{max}} + \frac{C_e}{q_{max}} \quad (4)$ |
| Freundlich | $\ln q_e = \ln K_f + \frac{1}{n} \ln C_e \quad (5)$ |
| Temkin | $q_e = B \ln K_T + B \ln C_e \quad (6)$ |
| DR | $\ln q_e = \ln q_s - K_{DR} \varepsilon^2, \quad \varepsilon = RT \ln \left(1 + \frac{1}{C_e} \right) \quad (7, 8)$ |

Where, q_e and C_e are the adsorption capacity and the concentration of the un-adsorbed o-NP at equilibrium, respectively. q_{max} and K_L are the monolayer adsorption capacity and Langmuir constant, respectively. n and K_f are Freundlich constants. K_T is the equilibrium binding constant and $B = \frac{RT}{b}$, b is Temkin constant related to heat of adsorption. R is the gas constant (8.314 J/mol.k) and T is the absolute temperature. Q_s is the saturation capacity, ε is the Polanyi potential and K_{DR} is a constant related to the mean free energy of adsorption per mole of the adsorbate.

Table S3: Elemental composition of the pure and recyclable of Kaol/SLS-BC_{0.5}/β-CD_{0.5} composite.

| Elements | Atomic % of pure composite | Atomic % of recyclable composite |
|----------|----------------------------|----------------------------------|
| Si | 13.15 | 12.86 |
| Al | 11.87 | 11.15 |
| C | 19.45 | 18.93 |
| S | 3.31 | 3.27 |
| O | 52.22 | 52.78 |
| N | — | 1.01 |