# Hydrothermal Carbonization of Agan Nut Shell: Functional Mesoporous Carbon with Excellent Performance in the Adsorption of Bisphenol A and Diuron

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**Supplementary Information**

**(Equation 3-12)**

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* ***Calculations***

The amount of BPA and diuron adsorbed per unit mass of adsorbent at any time *t, Qt* (mg g−1) and at equilibrium, Q*e* (mg g−1) was calculated using the following mass-balance equations:

(3)

(4)

The percent (%) BPA and diuron removal was estimated using Eq. (5):

(5)

* **Theory**
* ***Adsorption isotherms***

The Langmuir, Freundlich, and isotherm models were used to describe the temperature dependent equilibrium adsorption data of BPA and diuron [1, 2].

Langmuir :

(6)

Freundlich:

(7)

Adsorption feasibility:

(8)

* ***Adsorption kinetics***

In the present study, three most commonly used rate equations, namely the pseudo-first-order (PFO), the pseudo-second-order (PSO), and intra-particle diffusion, were applied to understand the adsorption kinetics [3, 4].

Pseudo-first-order:

(9)

Pseudo-second-order:

(10)

Intra-particle diffusion :

(11)

* ***Thermodynamic parameters***

Thermodynamic parameters such as Gibbs free energy change (∆*G*O, kJ mol−1), enthalpy (∆*H*O, kJ mol−1) and entropy (∆*S*O, J mol−1 K−1) were calculated using Eqs. (12) and (13) [5].

(12)

(13)

**References**

1. Langmuir, I.: The adsorption of gases on plane surfaces of glass, mica and platinum. J. Am. Chem. Soc. 40, 1361 (1918)

2. Freundlich, H.M.F.: Over the adsorption in solution. J. Phys. Chem. 57, 385–471 (1906)

3. G.M., M.: Pseudo-second order model for sorption process. Proc. Biochem. 34, 451 (1999)

4. S. Lagergren, B.K.: Zur Theorie der sogenannten Adsorption gelöster Stoffe. Zeitschrift für Chemie und Ind. der Kolloide. 2, 15 (1907). doi:10.1007/BF01501332

5. Chowdhury, S., Mishra, R., Saha, P., Kushwaha, P.: Adsorption thermodynamics, kinetics and isosteric heat of adsorption of malachite green onto chemically modified rice husk. Desalination. 265, 159–168 (2011). doi:http://dx.doi.org/10.1016/j.desal.2010.07.047