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Data Article

Data for experimental and calculated values of the adsorption of Pb(II) and Cr(VI) on APTES functionalized magnetite biochar using Langmuir, Freundlich and Temkin equations

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ABSTRACT

Adsorption isotherms are indispensable tools for the description of sorption processes of pollutants on adsorbents. The closeness of the equilibrium concentration (qe) to the calculated solid phase concentration (qe_{cal}) of the adsorbate, together with the co-efficient of determination (R^2) and associated errors are important in determining the best goodness-of-fit model. In this work we have investigated the adsorption of Pb(II) and Cr(VI) on a nanocomposite that was prepared using magnetite nanoparticles capped with locally prepared biochar and functionalized using 3-(aminopropyl) triethoxysilane (APTES) at 3 different temperatures. Detailed discussion of data can be found in DOI:10.1016/j.micromeso.2020.110573. The sorption processes were equally analyzed utilizing both the linear and non-linear forms of Langmuir, Freundlich and Temkin equations.

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Specifications Table

Subject	Chemical Engineering
Specific subject area	Adsorption studies
Type of data	Figures, tables, Image
How data were acquired	EVOLS15, ZEISS equipped with INCA software was used to obtain both scanning electron microscope (SEM) and energy-dispersive x-ray spectroscopy (EDS) data while Inductively coupled plasma optical emission spectrometry (ICP-OES: 720 ICP-OES VARIAN) was utilized to determine the residual concentrations of metal ions after the adsorption process. Origin 9.1 software was employed for data analysis.
Data format	Raw, analyzed
Parameters for data collection	Pilot adsorption studies was investigated using batch process method in a laboratory sonicator bath (SCIENTECH). Reaction vials were anchored on a wooden support and placed in the sonicator at different working temperatures.
Description of data collection	The experimental data for the adsorption of Cr(VI) and Pb(II) were obtained manually after the sorption process using ICP-OES. Adsorption isotherms were obtained using initial concentrations of 10 – 100 mg/L for each cation at 20, 30 and 50 °C respectively after 1 h equilibration time. 0.01 g of adsorbent and 0.01 L of adsorbate were employed for the studies. De-ionized water of resistivity value 10.7 Ωcm^{-1} was used as diluent. Solution pH was 2.00 ± 0.20 for both cations.
Data source location	University of Kwazulu-Natal, Pietermaritzburg, South Africa.
Data accessibility	The data is found only in this article
Related research article	Ebenezer C. Nnadozie, Peter A. Ajibade, Adsorption, Kinetic and mechanistic studies of Pb(II) and Cr(VI) ions using APTES functionalized magnetic biochar. *Microporous Mesoporous Mater.* Published. https://doi.org/10.1016/j.micromeso.2020.110573.

Value of the Data

- Calculated adsorption data presented at different temperatures are important in determining the adsorption capacity and process of Pb(II) and Cr(VI) on APTES functionalized magnetite biochar from aqueous solutions.
- Data from linear and non-linear isotherms models are useful in predicting and adopting model(s) for the interpretation of the adsorptions of Pb(II) and Cr(VI) on magnetite functionalized biochar from aqueous solution.
- Data shows the inadequacy of mono-predictors such as R^2 or% removal in predicting goodness-of-fit isotherm for cations adsorption. They can also serve as useful guide for the pilot adsorption studies of other cations.
- Adsorption data are useful tools for the ergonomic design of pollutants detoxification for industrial scale up process for wastewater treatment and overall water quality.

1. Data Description

Data presented in this work describes the adsorption of Cr(VI) and Pb(II) on magnetite nanoparticles capped and functionalized using biochar prepared from *C. odorata* and APTES respectively (Fe_3O_4@BC/APTES) [1]. Adsorption is an effective and popular process for the removal of pollutants from wastewater [2–4]. Adsorption isotherms are important tools for the description of the interaction between adsorbate and adsorbents. However, to effectively determine a choice model, it is desirable to do a comparative analysis of the sorption process and associated error analysis prior to determination of best goodness-of-fit [5,6]. The linear and non-linear adsorption parameters such as the equilibrium solid phase concentration (qe), residual sum of squares (RSS) and R^2 have been reported for the linear and non-linear forms of the isotherm equations.

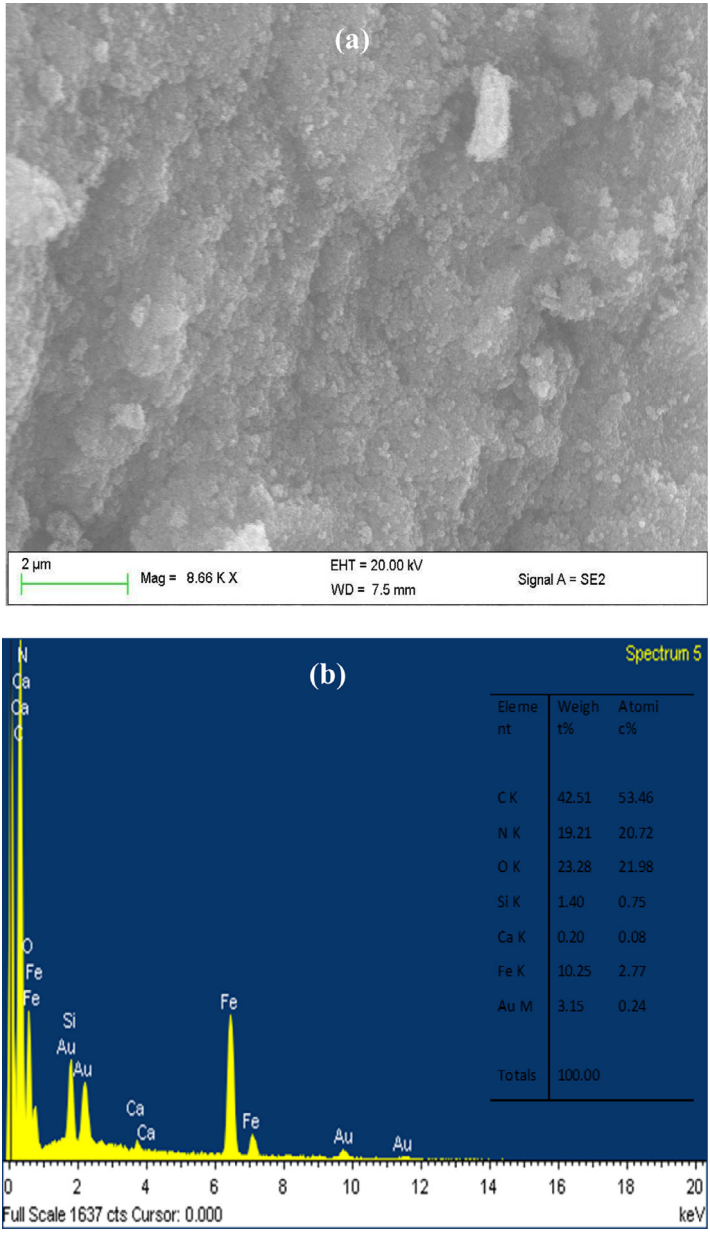

Fig. 1. (a) SEM micrograph of Fe_3O_4@BC/APTES (b) EDS spectrum of Fe_3O_4@BC/APTES.

Fig. 1 is the EDS and SEM of the magnetic nanocomposite. Table 1 and 2 are raw datasets for the adsorption of Pb(II) and Cr(VI) on Fe_3O_4@BC/APTES at different temperatures. Table 3 is the calculated and experimented value of equilibrium solid phase concentration of Pb(II) on Fe_3O_4@BC/APTES at 50 °C using linear and non-linear forms of the isotherm equation. Table 4 is calculated and experimented value of equilibrium solid phase concentration of Cr(VI) on Fe_3O_4@BC/APTES at 30 °C using linear and non-linear forms of the isotherm equation. Raw data

Table 1
Adsorption data for Pb(II) on Fe_3O_4@BC/APTES at different temperatures; Co = 10 – 100 mg/L, adsorbent = 0.01 g, adsorbate volume = 0.01 L, equilibration time = 1 h.

	20 °C		30 °C		50 °C	
C_o mg/L	C_e (mg/L)	q_e	C_e (mg/L)	q_e	C_e (mg/L)	q_e
10	0.61	9.40	1.26	8.74	1.60	8.41
25	1.42	23.59	1.31	23.69	3.24	21.76
50	17.15	32.85	18.60	31.40	13.30	36.70
75	40.80	34.20	28.10	46.90	24.10	50.90
100	39.85	60.15	49.25	50.75	45.40	54.60

Table 2
Adsorption data for Cr(VI) on Fe_3O_4@BC/APTES at different temperatures; Co = 10 – 100 mg/L, adsorbent = 0.01 g, adsorbate volume = 0.01 L, equilibration time = 1 h.

	20 °C		30 °C		50 °C	
C_o mg/L	C_e (mg/L)	q_e	C_e (mg/L)	q_e	C_e (mg/L)	q_e
10	4.72	5.28	4.50	5.51	5.13	4.88
25	13.55	11.45	11.25	13.75	13.95	11.05
50	23.70	26.30	22.50	27.50	22.95	27.05
75	49.70	25.30	46.55	28.45	48.55	26.45
100	64.30	35.70	63.65	36.35	66.90	33.10

Table 3
Calculated and experimented value of equilibrium solid phase concentration of Pb(II) on Fe_3O_4@BC/APTES at 50 °C using linear and non-linear forms of the isotherm equation; Co = 10 – 100 mg/L, adsorbent = 0.01 g, adsorbate volume = 0.01 L, equilibration time = 1 h.

Isotherm		Langmuir		Freundlich		Temkin	
Forms	qe (exp)	Linear qe (cal)	Non-linear qe (cal)	Linear qe (cal)	Non-linear qe (cal)	Linear qe (cal)	Non-linear qe (cal)
	8.41	5.8152	10.5628	(1.2582)	14.8053	(0.1052)	115.8202
	21.76	11.0480	18.3737	(0.8467)	19.8199	(0.2439)	231.8813
	36.70	32.4899	40.1453	(0.0268)	35.4437	(0.5203)	463.1505
	50.90	45.1319	48.4274	0.3184	45.2689	(0.6366)	560.5010
	54.60	58.2207	54.9808	0.6860	58.7498	(0.7606)	664.2143
RSS	44.09	88.67	33.26	0.05	79.03	0.01	3744.33
R^2	0.96	0.94	0.97	0.98	0.92	0.98	0.98

Table 4
Calculated and experimented value of equilibrium solid phase concentration of Cr(VI) on Fe_3O_4@BC/APTES at 30 °C using linear and non-linear forms of the isotherm equation; Co = 10 – 100 mg/L, adsorbent = 0.01 g, adsorbate volume = 0.01 L, equilibration time = 1 h.

Isotherm		Langmuir		Freundlich		Temkin	
Forms	qe (exp)	Linear qe (cal)	Non-linear qe (cal)	Linear qe (cal)	Non-linear qe (cal)	Linear qe (cal)	Non-linear qe (cal)
	4.875	1.2808	8.3336	1.0023	9.7876	0.2326	123.2120
	11.05	3.3780	17.5334	1.7459	16.5191	0.3171	325.2947
	27.05	5.3867	23.4221	2.1156	21.4288	0.3590	425.7637
	26.45	10.4804	32.2836	2.6720	31.7021	0.4222	576.9755
	33.10	13.6556	35.5952	2.9101	37.4859	0.4493	641.6769
RSS	54.27	21.71	55.19	0.26	80.11	0.00	19,346.96
R^2	0.87	0.72	0.85	0.85	0.79	0.79	0.85

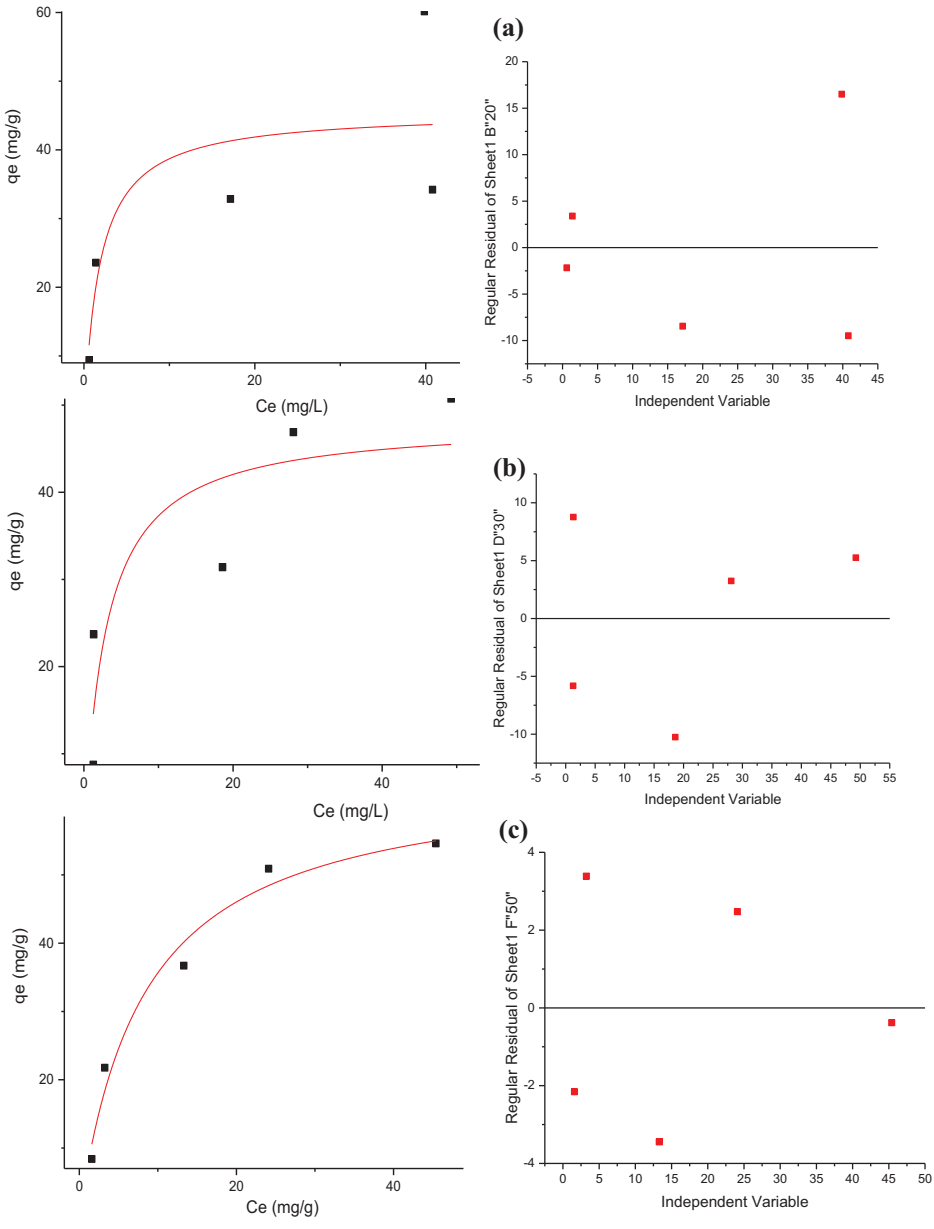

Fig. 2. (Left): Langmuir adsorption isotherms of Pb(II) on Fe_3O_4@BC/APTES (a) 20 (b) 30 and (c) 50 °C (Right) Residual sum of squares plots for the non-linear fitting of Pb(II) on Fe_3O_4@BC/APTES (a) 20 (b) 30 and (c) 50 °C; Co = 10 – 100 mg/L, adsorbent = 0.01 g, adsorbate volume = 0.01 L, equilibration time = 1 h.

for Tables 3 and 4 are available in the supplementary files as Tables S1-S6. Fig. 2 shows the adsorption isotherms and residual sum of squares plots of Pb(II) on Fe_3O_4@BC/APTES at (a) 20 (b) 30 and (c) 50 °C while Fig. 3 is adsorption isotherms and residual sum of squares plots of Cr(VI) on Fe_3O_4@BC/APTES (a) 20 (b) 30 and (c) 50 °C respectively. Raw data for Figs. 2 and 3 are available in the supplementary files as excel spreadsheet.

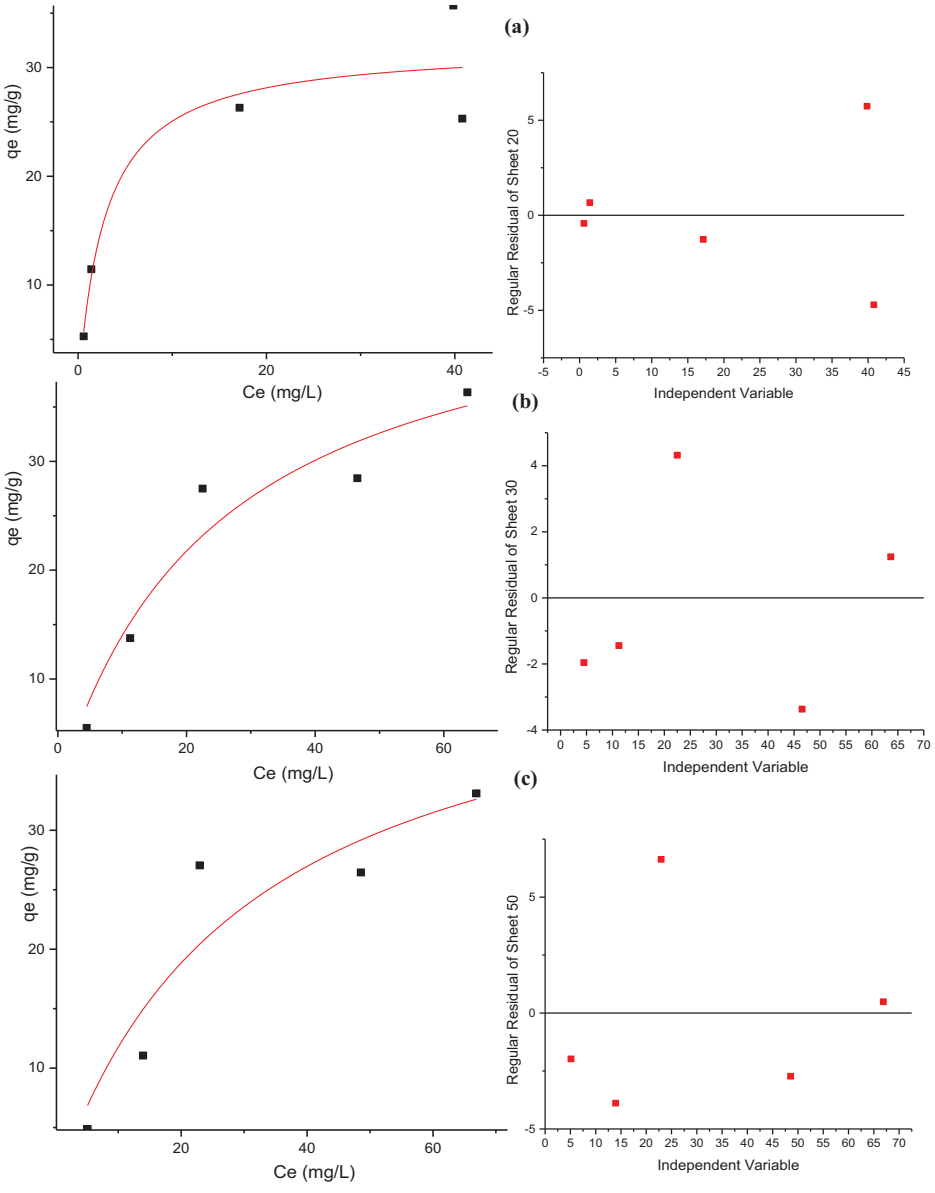

Fig. 3. (Left): Langmuir adsorption isotherms of Cr(VI) on Fe_3O_4@BC/APTES (a) 20 (b) 30 and (c) 50 °C (Right) Residual sum of squares plots for the non-linear fitting of Cr(VI) on Fe_3O_4@BC/APTES (a) 20 (b) 30 and (c) 50 °C; Co = 10 – 100 mg/L, adsorbent = 0.01 g, adsorbate volume = 0.01 L, equilibration time = 1 h.

2. Experimental Design, Materials and Methods

2.1. Materials

Iron (III) chloride hexahydrate ($FeCl_3 \cdot 6H_2O$: CAS-10025–77-1); Iron (II) chloride tetrahydrate ($FeCl_2 \cdot 4H_2O$: CAS-13478); 3-aminopropryl triethoxysilane (APTES: CAS-919-30-2); $Pb(NO_3)_2$

(CAS: 10099-74-8) and aqueous ammonia (NH_3•H_2O) 28–30% were purchased from Merck South Africa. Potassium dichromate ($K_2Cr_2O_7$: 504320) was purchased from Saarchem South Africa. De-ionized water with resistivity value of 10.7 Ωcm^{-1} from the Department of Chemistry, University of Kwazulu-Natal South Africa was used as solvent throughout the study. Surface area (S_{BET}) of Fe_3O_4@BC/APTES was 35.66 m^2/g; with average pore size of 20.82 nm and pore volume of 0.2035 cm^3/g.

2.2. Experimental

Adsorption data were generated using 10 – 100 mg/L of the metal solutions. 10 mg of the adsorbent and 10 ml of single adsorbate at each concentration were quantitatively transferred to 15 ml centrifuge tube. Samples were run in duplicates and the average taken. The adsorption process was initiated by sonicating in a water bath for 1 h. After adsorption the residual concentrations of the metal ions was determined by ICP-OES.

2.3. Analytical techniques

ICP-OES was used to measure equilibrium concentrations of the metal after the adsorption process at wavelengths of 267.72 and 217 nm for Cr(VI) and Pb(II) respectively. Calibration curves were obtained by investigating the relationship between the instrument response and prepared concentrations between 1 – 100 mg/L for each analyte. De-ionized water was used as diluent and blank. The standard curve covered the range of expected concentrations.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships which have, or could be perceived to have, influenced the work reported in this article.

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Supplementary Materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.dib.2020.106292.

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