Data Article

Experimental and computational data set on adsorption of Cr (VI) from water using an activated carbon

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Abstract

Chromium (Cr) is a widely used metal in metallurgical and chemical industries, whose waste contaminates the surface and groundwater. Cr (VI) is toxic and produces carcinogenic effects owing to its high mobility in water and soil. In this work, computational and experimental studies from the adsorption of Cr(VI) from aqueous solutions on teak wood residues activated with ZnCl2 (AT) are presented. Full interpretation of data can be found in DOI:10.1016/j.jece.2020.103702 [1]. Experimental data were adjusted to Langmuir, Freundlich and Temkin isothermal models and the nonlinear and linear forms of the Pseudo-first and Pseudo-second order kinetic models. Computational data allow to understand the adsorption process of Cr(VI) on carbonaceous materials.

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1. Data description

Data present in this work correspond to the kinetics adsorption process of Cr(VI) on activated carbon obtained from chemical activation (ZnCl₂) of teakwood sawdust [1]. Fig. 1 shows the experimental setup where all adsorption experiments were carried out. Fig. 2 shows a comparison between the removal percentage of Cr(VI) using activated and no-activated teakwood sawdust. Fig. 3 presents the data adjustment for the Langmuir [2], Freundlich [3] and Temkin [4] isothermal models. Table 1 and Fig. 4 show the parameters found by nonlinear and linear forms from the Pseudo-first [5] and Pseudo-second order kinetic models [6]. Finally, Table 2 shows the Cartesian coordinates for the most stable configurations during the adsorption process of Cr³⁺ and HCrO₄⁻ on carbonaceous structures obtaining by Gaussian 09 program. The raw data of all Figures are shared as supplementary material.

2. Experimental design, materials, and methods

2.1. Adsorbent material and chromium solution

Adsorbent material was obtained from teakwood sawdust activated with ZnCl₂ 3 mol L⁻¹ (98% CAS 7646-85-7, Duksan) at 550 °C [7]. By adding a K₂Cr₂O₇ (99% CAS 7778-50-9, Mol Labs) mass of 14.145 g to a 1 L volume, a 5000 mg L⁻¹ Cr (VI) solution was prepared, from which synthetic Cr (VI) solutions were produced at different initial concentrations (35, 50, 100, 170, 250, and 290 mg L⁻¹). The pH level of the solution was adjusted to 2 by using 0.1 mol L⁻¹ NaOH (98% CAS 1310-73-2, Panreac) and 0.1 mol L⁻¹ HCl solutions (37% CAS 7647-01-0, Merck).
Fig. 1. Three-layer glass reactor placed in a constant-temperature bath at 25 °C. The reactor was stirred at 200 rpm with a turbine propeller operated by a rotor.

Fig. 2. Adsorption of Cr (VI) using materials before and after the transformation process. T: teak wood sawdust; AT: activated teak (solution volume 100 mL, pH 2, Cr (VI) concentration 100 mg L⁻¹, adsorbent dose 0.1 g, temperature 25 °C, stirring speed 100 rpm and contact time 3 h).
**Fig. 3.** Cr (VI) adsorption isotherms on AT (solution volume 500 mL, adsorbent dose 0.5 g, Cr (VI) concentrations 35, 50, 100, 170, 290 mg L⁻¹, pH 2, temperature 25 °C, stirring speed 200 rpm, and contact time 72 h).

**Table 1**

Parameters of pseudo-first order and pseudo second-order models.

| Form     | C₀₀ (mg L⁻¹) | qₑₑₚₑₑ (mg g⁻¹) | Pseudo First-Order | Pseudo Second-Order |
|----------|--------------|------------------|--------------------|---------------------|
|          |              |                  | k₁ (min⁻¹) x 10⁻²  | qₑₑ (mg g⁻¹) R²    | k₂ (g mg⁻¹ min⁻¹) x 10⁻² | qₑₑ (mg g⁻¹) R² |
| Nonlinear| 35           | 35.701           | 0.388              | 34.455              | 0.9651                     | 0.015           | 37.017                     | 0.9886 |
| Linear   |              |                  | 0.138              | 26.032              | 0.9643                     | 0.018           | 37.037                     | 0.9985 |
| Nonlinear| 50           | 41.428           | 0.254              | 40.773              | 0.9297                     | 0.008           | 44.276                     | 0.9667 |
| Linear   |              |                  | 0.069              | 33.327              | 0.9815                     | 0.008           | 45.872                     | 0.9916 |
| Nonlinear| 100          | 45.866           | 0.212              | 45.593              | 0.9224                     | 0.008           | 48.421                     | 0.9454 |
| Linear   |              |                  | 0.138              | 37.017              | 0.9639                     | 0.006           | 51.546                     | 0.9881 |
| Nonlinear| 170          | 64.498           | 0.143              | 56.149              | 0.9463                     | 0.003           | 69.685                     | 0.9303 |
| Linear   |              |                  | 0.069              | 54.639              | 0.9888                     | 0.003           | 64.935                     | 0.9733 |
| Nonlinear| 290          | 71.444           | 0.129              | 63.126              | 0.9374                     | 0.002           | 74.685                     | 0.9498 |
| Linear   |              |                  | 0.069              | 70.583              | 0.7681                     | 0.003           | 72.464                     | 0.9521 |
Fig. 4. Cr (VI) adsorption kinetics on AT to Pseudo First-Order and Pseudo Second-Order models (solution volume 500 mL, Cr (VI) concentrations 35, 50, 100, 170, 290 mg L$^{-1}$, pH 2, adsorbent dose 0.5 g, temperature 25 °C, stirring speed 200 rpm, and contact time 30, 60, 120, 180, 300, 420, 1380, 1740, 2640, 3120, 4080, and 4320 min). Nolinear and linear form.
Fig. 4. (continued).
Fig. 4. (continued).
Table 2
Structural details for the optimization of the most stable configurations for Cr3+ and HCrO4-.

|      | ^5Carboxyl-Cr(III) | ^7Phenol-Cr(III) |
|------|--------------------|-------------------|
| 6    | -4.187693          | 0.0000000        |
| 6    | -3.509319          | -0.366274        |
| 6    | -1.751557          | 0.049901         |
| 6    | -1.577438          | -0.674547        |
| 6    | -2.737338          | 0.21925          |
| 6    | -4.025747          | 1.001473         |
| 6    | -0.591101          | -1.532645        |
| 6    | -0.273356          | 1.283455         |
| 6    | 0.889799           | 0.435463         |
| 6    | 0.703552           | -0.97137         |
| 6    | 2.174201           | 1.085489         |
| 6    | 2.278795           | 2.473631         |
| 6    | 1.136990           | 3.279379         |
| 6    | -0.136811          | 2.710488         |
| 6    | -1.308493          | 3.543158         |
| 6    | -2.558343          | 2.998116         |
| 6    | 3.437526           | 3.633266         |
| 1    | 1.174260           | 4.619354         |
| 1    | -5.183318          | -0.797106        |
| 1    | -1.226743          | 4.583827         |
| 1    | -2.254023          | 0.909955         |
| 1    | -4.229697          | -0.091449        |
| 1    | -2.245023          | -0.001042        |
| 1    | 3.255824           | 2.938739         |
| 1    | 1.246445           | 4.358287         |
| 1    | -3.226744          | -2.638844        |
| 1    | -2.116819          | -3.507648        |
| 1    | -0.894664          | 0.057851         |
| 1    | -4.229697          | -0.105010        |
| 1    | -2.245023          | 1.201151         |
| 1    | 3.420958           | 0.329044         |
| 1    | 5.304314           | 0.432081         |
| 1    | 4.522211           | 1.016636         |
| 8    | 3.508512           | -0.933218        |
| 24   | 2.255664           | -2.312482        |

|      | ^5Lactone-Cr(III)  | ^6Semiquinone-Cr(III) |
|------|--------------------|-----------------------|
| 6    | -0.832776          | 3.504155              |
| 6    | 0.303668           | 2.651118              |
| 6    | 0.056159           | 2.160611              |
| 6    | -1.238811          | 0.674113              |
| 6    | -2.354110          | 1.573249              |
| 6    | -2.100766          | 2.982992              |
| 6    | 1.147262           | 0.323950              |
| 6    | -1.411384          | -0.734125             |
| 6    | -0.265677          | -1.631638             |
| 6    | 1.019198           | -1.063121             |
| 6    | -0.585170          | -2.988919             |
| 6    | -1.832904          | -3.553477             |
| 6    | -2.924352          | -2.661115             |
| 6    | -2.730857          | -1.262966             |
| 6    | -3.833508          | -0.350581             |
| 6    | -3.655416          | 1.019409              |
| 8    | -4.516540          | 1.678002              |
| 1    | -4.838897          | -0.759476             |
| 1    | -0.670292          | 4.576210              |
| 1    | -2.952188          | 3.660513              |
| 1    | -1.993908          | -4.626049             |
| 1    | -3.934731          | -3.059489             |
| 1    | 1.615465           | 3.024882              |
| 1    | 2.466010           | 0.835923              |
| 1    | 1.960223           | 4.050641              |
| 8    | 2.665972           | 2.156415              |
| 8    | 3.467721           | 0.060663              |

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Table 2 (continued)

| 5Lactone-Cr(III) | 6Semiquinone-Cr(III) |
|------------------|---------------------|
|                  |                     |
|                  |                     |

| 6Carboxyl-HCrO₅ - a | 6Carboxyl-HCrO₅ - b |
|---------------------|---------------------|
|                     |                     |
|                     |                     |

| 2Phenol-HCrO₅ - a | 2Phenol-HCrO₅ - b |
|------------------|------------------|
|                  |                  |
|                  |                  |

(continued on next page)
Table 2 (continued)

|    | 2Phenol-HCrO₄ - a | 2Phenol-HCrO₄ - b | 2Lactone-HCrO₄ | 1Semicinnoline-HCrO₄ |
|----|------------------|------------------|----------------|-------------------|
| 1  | -1.105350        | 4.119932         | 0.007065       | -0.283158         |
| 1  | -3.575146        | 4.021258         | 0.041123       | 5.131505          |
| 1  | -5.367336        | -4.087113        | 0.020294       | 2.136731          |
| 1  | -6.702654        | -1.978656        | 0.059654       | 1.236731          |
| 1  | 0.587069         | 2.011333         | -0.055900      | 3.863727          |
| 1  | 1.347639         | 0.864164         | -0.079587      | 2.854921          |
| 1  | 0.721461         | -0.410362        | -0.075964      | 1.499081          |
| 1  | 1.085282         | 2.978973         | -0.058720      | 4.900484          |
| 1  | 2.431945         | 0.927767         | -0.098514      | 3.089391          |
| 1  | 1.465945         | -1.510551        | -0.101349      | 0.536696          |
| 8  | 2.446166         | -1.310754        | -0.121907      | 0.956579          |
| 24 | 5.314699         | -0.194865        | -0.042447      | 3.539618          |
| 24 | 4.082524         | -1.248419        | -0.185694      | 2.180890          |
| 24 | 6.373228         | -0.422293        | -1.219336      | 4.653838          |
| 24 | 6.130892         | -0.417093        | 1.545304       | 3.479072          |
| 24 | 4.768133         | 1.306612         | -0.037038      | 3.611580          |
| 24 | 6.695113         | -1.228992        | 1.594148       | -4.365320         |

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2.2. Reactive system

Fig. 1 shows the reaction systems used during the adsorption experiments of Cr (VI) on activated teak (AT). 500 mL of each solution, at pH 2 and 0.5 g of AT, was brought in contact with a three-layer glass reactor placed in a constant-temperature bath at 25 °C. The reactor was stirred at 200 rpm with a turbine propeller operated by a rotor. Samples were taken at 30, 60, 120, 180, 300, 420, 1380, 1740,
2640, 3120, 4080, and 4320 min, until reaching equilibrium. The Cr (VI) concentration of each sample was measured using a Shimadzu UV 1900 UV/VIS spectrophotometer at 542-nm wavelength.

2.3. Experimental adsorption

Fig. 2 shows that the activation process of teakwood sawdust with ZnCl₂ improves the adsorption of Cr (VI). The removal rate increased for AT 8 times respect to T.

Fig. 3 shows the linear fit of the experimental data to the Langmuir, Freundlich and Temkin isotherm models. Equilibrium experiments were carried out using Cr (VI) solutions at different initial concentrations (35, 50, 100, 170, 250 and 290 mg L⁻¹), adsorbent dose of 0.5 g, temperature of 25 °C, stirring speed of 200 rpm and adjusted the solution pH at 2 with an optimal contact time of 4500 min. The experimental data were treated mathematically using the Excel 2013 software to calculate the isotherm parameters, as follows: when plotting Ce/qₑ based on Ce, K₁ and qₑ two parameters (K₁ and qₑmax) can be obtained by using the slope and the intercept (Langmuir constants). When plotting Log qₑ against Log Ce, Kᵢ and 1/n (Freundlich constants) are estimated. By plotting qₑ against Ln Ce, Kₜ and b (Temkin constants) are calculated.

Table 1 and Fig. 4 present the obtained parameters from the experimental data adjusted to nonlinear and linear kinetics models (Pseudo-first and Pseudo second order). The experimental data were treated mathematically using the Excel 2013 software. Constants from linear form were calculated as follows: for the PFO model, a Log (qₑ-q₁) graph was developed as a function of time (t), from which the values of qₑ and k₁ were calculated. In addition, for the PSO model, qₑ and k₂ were calculated by plotting t/q₁ against t. To calculate nonlinear shape constants of the kinetic models, the least squares model derived from the Rosenbrock–Newton optimization algorithm was applied through the Statistical software.

CA₀ (mg L⁻¹) is the initial Cr (VI) concentration of the solution; k₁ (min⁻¹) is the pseudo first-order rate constant; qₑ is the amounts of Cr (VI) adsorbed in the equilibrium (mg g⁻¹); k₂ (g mg⁻¹ min⁻¹) is the pseudo second-order rate constant; R² is the correlation coefficient.

Table 2 shows the Cartesian coordinates for the most stable configurations during the adsorption process of Cr³⁺ and HCrO₄⁻ on carbonaceous structures.

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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dib.2020.105292.

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