Supplementary Material for

Effect of Oxycations in Clay Mineral on Adsorption—Vanadyl Exchange Bentonites and Their Ability for Amiloride Removal

Leandro Oliveira [1], Josy Osajima [2], Ramon Raudel Peña-Garcia [3,4], Edson Cavalcanti Silva-Filho [2] and Maria Gardennia Fonseca [1,*]

[1] Research and Extension Center—Fuels and Materials Laboratory, Federal University of Paraiba, João Pessoa 58051-085, Paraiba, Brazil; leandro_oliveira008@hotmail.com
[2] Interdisciplinary Laboratory of Advanced Materials, CCN, Federal University of Piaui, Teresina 64049-550, Piaui, Brazil; josy_osajima@yahoo.com.br (J.O.); edsonfilho@ufpi.edu.br (E.C.S.-F.)
[3] Academic Unit of Santo Agostinho, Federal Rural University of Pernambuco, Cabo de Santo Agostinho 52171-900, Pernambuco, Brazil; ramon.raudel@ufrpe.br
[4] Materials Science and Engineering Graduate Program, Federal University of Piaui, Teresina 64049-550, Piauí, Brazil
* Correspondence: mgardennia@quimica.ufpb.br; Tel.: +55-83-3216-7433

Kinetic and equilibrium models

For kinetics, experimental data were adjusted to fit the three kinetic models (as shown in Equations 1 to 3 in Supplementary Material SI1): pseudo-first-order [68], pseudo-second-order [69], and simplified Elovich equation [70], assuming $\alpha\beta t \gg 1$.

Pseudo-first-order $$q_t = q_e(1 - e^{-k_1 t}) \quad (1)$$

Pseudo-second-order $$q_t = \frac{{q_e}^2 k_e t}{1 + k_2 t} \quad (2)$$

Elovich $$q_t = \frac{1}{\beta}\ln(\alpha\beta t) \quad (3)$$

where q_e and q_t are the sorption capacities (mg g^{-1}) at equilibrium and at time t (min), respectively; and k_1 (min^{-1}) and k_2 (g mg^{-1} min^{-1}) are the pseudo-first-order and pseudo-second-order rate constants, respectively. In the Elovich model, α (mg g^{-1} min^{-1}) and β (g mg^{-1}) are the initial adsorption rate and Elovich constant, related to the extent of surface coverage and the activation energy involved in chemisorption, respectively.

The equilibrium isotherms were analyzed using the Langmuir [71], Freundlich [72], and Temkin [73] models (following Equations 4-6 in Supplementary Material SI1).

Langmuir $$q_e = \frac{q_{max} K_L C_e}{1 + K_L C_e} \quad (4)$$

Freundlich $$q_e = K_F C_e^{\frac{1}{n}} \quad (5)$$

Temkin $$q_e = \frac{RT}{b_T} \ln(A_T C_e) \quad (6)$$

where C_e (mg L^{-1}) is the drug equilibrium concentration and q_e (mg g^{-1}) is the equilibrium amiloride amount adsorbed on the samples. In the Langmuir equation, q_{max} (mg g^{-1}) is the maximum adsorption capacity of the adsorbent, assuming monolayer drug uptake by the adsorbent, and K_L (L mg^{-1}) is the Langmuir constant.

In the Freundlich model, K_F (mg g^{-1}) (mg $L^{-1})^{-1/n}$ and n are Freundlich constants related to the capacity and intensity of adsorption, respectively [72], while in the Temkin model, b_T is the constant related to the sorption heat (J mol^{-1}), A_T is the isotherm constant (L mg^{-1}), R is the gas constant (8.314 J mol^{-1} K) and T is the absolute temperature (K) [73].