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Corrigendum to “Efficient adsorption of Mn(II) by layered double hydroxides intercalated with diethylenetriaminepentaacetic acid and the mechanistic study” [J. Environ. Sci. 85 (2019) 56–65]

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The authors regret to inform that there were some mistakes in the part of thermodynamics studies, the calculated enthalpy, entropy and Gibbs energy were wrong due to the misunderstanding of the equilibrium constant (K_{ads}).

As we know, the free energy change, ΔG , of adsorption is given by Zhou et al., 2012:

$$\Delta G = -R \times T \times \ln K_{ads} \quad (1)$$

where, R (8.314 J/(mol·K)) is the gas constant, T (K) is the solution temperature, and K_{ads} is the equilibrium constant.

The unit of ΔG is J/mol. Since the unit for the term RT is also J/mol, the equilibrium constant K_{ads} in Eq. (1) and (2) must be dimensionless, while it was L/mg in our original

paper. In order to obtain the dimensionless constant K_{ads} , a correct Langmuir model was reported previously:

$$\theta = \frac{K_{ads} C_e}{1 + K_{ads} C_e} \quad (2)$$

where, θ is the fraction of the surface covered at equilibrium, dimensionless. $\theta = q_e/q_m$, q_e is the equilibrium adsorption capacity of adsorbent; q_m is the maximum sorption capacity of adsorbent; C_e (mol/L) is the solute concentration at the equilibrium; C^0 is the molar concentration of the standard reference solution, 1 mol/L. The standard equilibrium constant K_{ads} (dimensionless) can be calculated by the modified Langmuir equation. In this regard, the correct thermodynamic parameters were recalculated and listed in Table 1.

Table 1 – Thermodynamic parameters for the adsorption of Mn(II) by LDHs-DTPA.

Temperature (K)	K_{ads} (dimensionless)	ΔG (kJ/mol)	ΔH (kJ/mol)	ΔS (kJ/mol)	R^2
293.15	708.7	–16.00	20.40	0.124	0.994
303.15	966.9	–17.33			
313.15	1208.6	–18.48			

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As the thermodynamic parameters were recalculated, the related corrections were also made in the pristine paper and given below.

- (1) **Abstract:** “Thermodynamics study results also showed that the adsorption process of Mn(II) by LDHs-DTPA was endothermic indicated by the positive ΔH value.”
- (2) **Section 2.5 (P. 61).** Table 3 (Thermodynamic parameters for the adsorption of Mn(II) by LDHs-DTPA) in the pristine paper was replaced by the above Table 1 (**P. 62**) “The calculated thermodynamic parameters are listed in Table 3. The negative values of ΔG meant the adsorption processes were spontaneous in temperature range from 20 to 40 °C. The ΔH value was 20.40 kJ/mol, indicating the adsorption of Mn(II) by LDHs-DTPA was endothermic. That meant the bond formation energy between Mn(II) and the function groups of the adsorbents was smaller than the bond breaking energy might be associated with the displacement of previously adsorbed molecules from the surface of the adsorbents, such as water or other functional groups like H^+ or OH^- (Kan et al., 2013). The ΔH value of 20.40 kJ/mol indicated that the physisorption

characteristic of Mn(II), since physisorption involves enthalpy changes in the range of 2.1–20.9 kJ/mol while chemisorption involved enthalpy changes in the range of 100–500 kJ/mol (Ferreiro and de Bussetti, 2007). Moreover, the positive value of ΔS suggested the increased randomness in the system as the Mn(II) ions got adsorbed onto the adsorbents (Kan et al., 2013).”

- (3) **Conclusion.** “Besides, it was observed that the adsorption processes were spontaneous in temperatures ranging of 20–40 °C and the process was endothermic for the positive value of ΔH .”

The authors regretfully apologize for any inconvenience caused.

REFERENCE

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- Zhou, X., Liu, H., Hao, J., 2012. How to calculate the thermodynamic equilibrium constant using the Langmuir equation. *Adsorption Science and Technology* 30, 647–649.