Supporting Information (SI) on

Mechanistic insights on the decontamination of Th(IV) on graphene oxide-based composites by EXAFS and modeling techniques

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Pseudo-first-order and pseudo-second-order kinetic models. The linear equations of pseudo-first-order and pseudo-second-order kinetic models were described as Eqns. (S1)[S1] and (S2)[S2]:

$$\ln(q_e - q_t) = \ln q_e - k_1 \times t \qquad (S1)$$

$$t/q_t = 1/(k_2 \times q_e^2) + t/q_e \qquad (S2)$$

where q_e and q_t (mg/g) are the amount of Th(IV) adsorbed at equilibrium and at time t, respectively. k_1 and k_2 are the pseudo-first-order and pseudo-second-order kinetic rate constants, respectively.
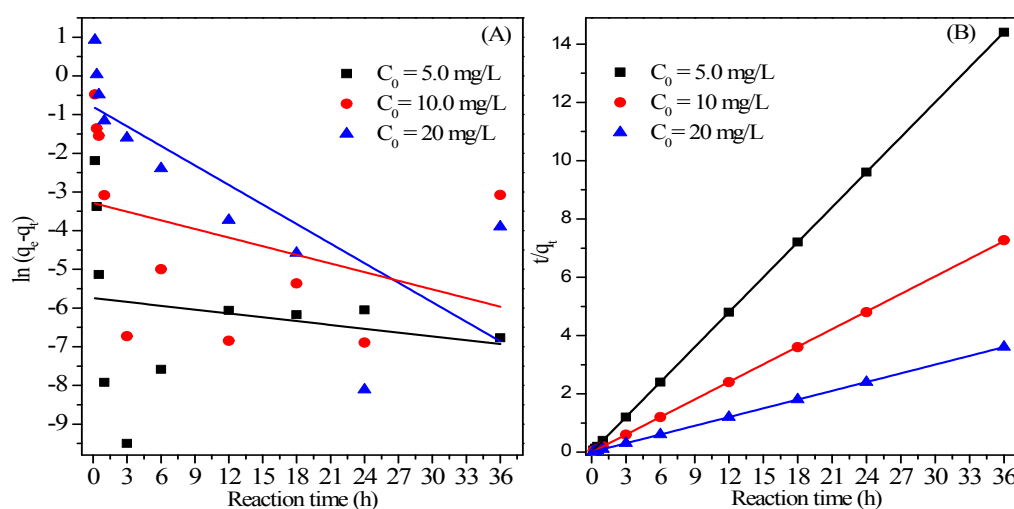

Figure S1. Adsorption kinetics of Th(IV) on amidoxime/graphene oxide composites fitted by pseudo- first-order (A) and pseudo-second-order (B) kinetic models

Table S1 Optimized parameters of pseudo- and pseudo-second-order kinetic model

C_0	Pseudo-first-order kinetic model			Pseudo-second-order kinetic model		
(mg/L)	q_e(mg/g)	k_1(h^{-1})	R^2	q_e(mg/g)	k_2(g/mg/h)	R^2
5.0	0.0032	0.033	0.0362	2.498	160.16	1
10.0	0.0374	0.0744	0.1406	4.97	11.566	1
20.0	0.4501	0.1684	0.6044	10	2.439	1

Distribution of Th(IV) speciation. The distribution of Th(IV) species under different pH conditions was simulated by Visual MINTEQL 2.6 mode.[S3]
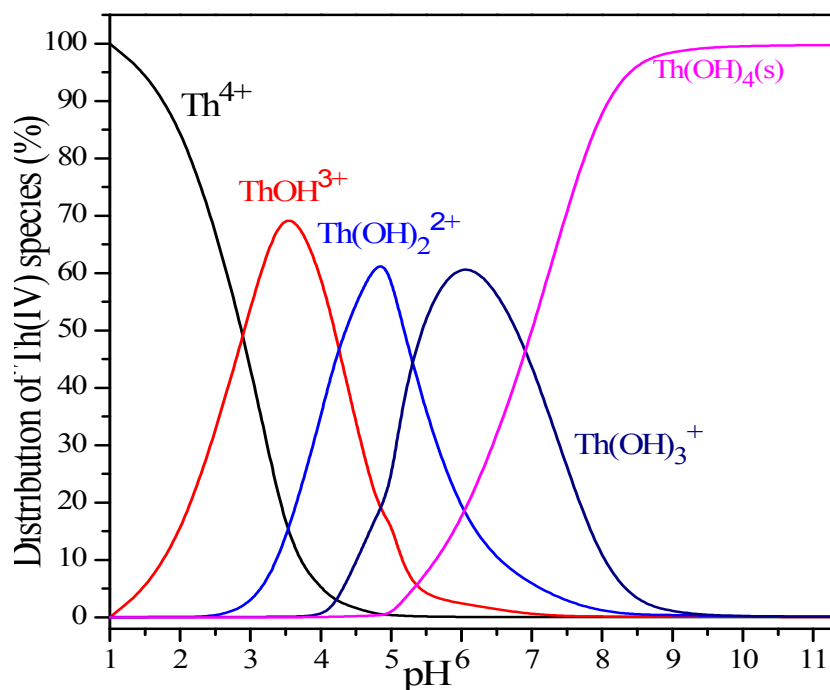

Figure S2. Distribution of Th(IV) species in aqueous solutions, $C_0 = 10$ mg/L.

Table S2. The thermodynamic equilibrium parameters of Th(IV) in aqueous solutions

Reactions	Log K	Ref.
$Th^{4+} + H_2O = ThOH^{3+} + H^+$	-3.86	(S4)
$Th^{4+} + 2H_2O = Th(OH)_2^{2+} + 2H^+$	-8.01	(S4)
$Th^{4+} + 3H_2O = Th(OH)_3^+ + 3H^+$	-12.99	(S4)
$Th^{4+} + 4H_2O = Th(OH)_4^0(aq) + 4H^+$	-17.16	(S4)

Langmuir and Freundlich Equations. The Langmuir and the Freundlich equation can be expressed by Eqns. (S3)[S5] and (S4)[S6]:

$$\frac{C_e}{Q_e} = \frac{1}{Q_m \times K_L} + \frac{C_e}{Q_m} \qquad (S3)$$

$$Q_e = K_f \times C^n \qquad (S4)$$

where Qe (mg/g) and Ce (mg/L) are the amount of adsorbed Th(IV) by amidoxime/graphene oxide composites and the equilibrium concentration in solution. K_f (mg^{1-n}g^{-1}L^n) and n refer to an empirical constants related to adsorption capacity and the Freundlich exponent related to isotherm nonlinearity.

Table S3. Parameters of Langmuir and Freundlich models for Th(IV) adsorption on amidoxime/graphene oxide composites at pH 2.0 and I = 0.01 mol/L NaCl

	Langmuir			Freundlich		
	K_a (L/mg)	q_{max} (mg/g)	R^2	ln K_F (mg/g)/(mg/g)^n	$1/n$	R^2
293 K	1.095	123.46	0.996	4.08	0.405	0.987
313 K	0.947	140.84	0.999	4.13	0.413	0.967
333 K	0.859	163.93	0.999	4.24	0.403	0.967

Calculation of Thermodynamic Parameters. The thermodynamic parameters (e.g., ΔG^0, ΔH^0 and ΔS^0) of Th(IV) sorption on amidoxime/graphene oxide composites were calculated by Eqns. (S5) and (S6):

$$\Delta G^0 = - RTlnK_d^0 = \Delta H^0 - T \times \Delta S^0 \qquad \text{(S5)}$$

$$\ln K_d^0 = \frac{\Delta S^0}{R} - \frac{\Delta H^0}{RT} \qquad \text{(S6)}$$

where R and T are the ideal gas constant (8.314 J/(mol·K)) and temperature in Kelvin, respectively. The value of ln K_d^0 can be calculated from the plot of ln K_d vs. 1/T (Figure S3).
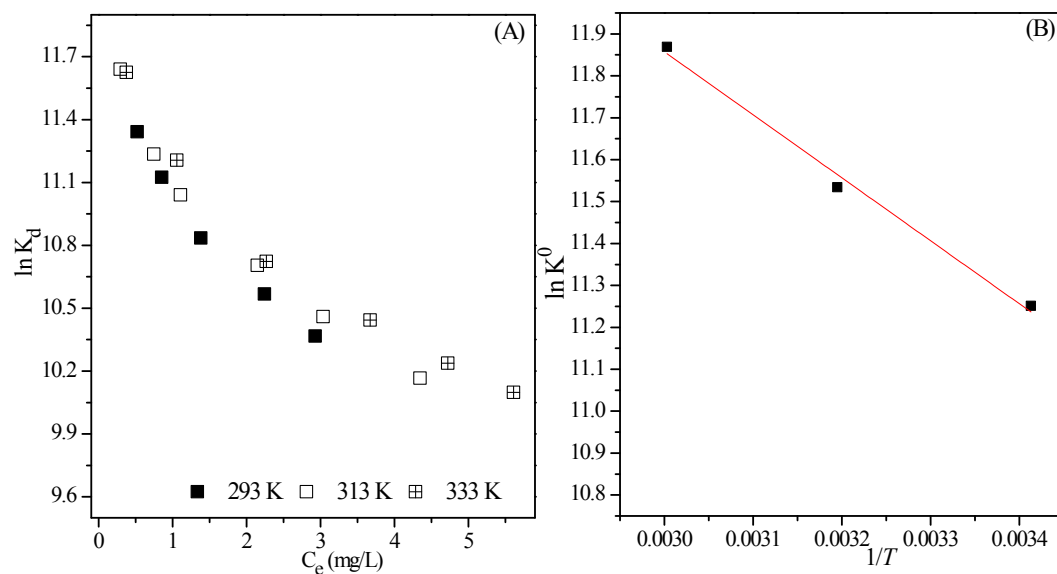
Figure S3. The plot of ln K_d vs Ce (A) and Ln K^0 vs. $1/T$ (B) of Th(IV) adsorption on

amidoxime/ graphene oxide composites

Table S4 Thermodynamic parameters of the adsorption of Th(IV) on amidoxime/

graphene oxide composites at pH 2.0 and $I = 0.01$ mol/L NaCl

Temperature	ΔG^0(kJ/mol)	ΔH^0(kJ/mol)	ΔS^0(J/(mol·K))
293 K	-27.41		
313 K	-30.01	12.493	136.06
333 K	-32.86		

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