Supplementary Information (SI) for RSC Advances.
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Exploring the Efficacy of *Cystoseira sedoide* alga for Cadmium and Copper Biosorption: An Integrated Experimental and Computational Study

Nadjette BENGOURNA[a], Karima BELGUIDOUM[b], Dounya KHALLA[c], Mouna NACEF[c], Imane KOUADRI[c], Aida BENHAMIDA[a], Habiba AMIRA-GUEBAILIA[b], Alaa eddine BROUK[c], Abed Mohamed AFFOUNE[c], Hamid SATHA[a]

[a] Laboratoire des Silicates, Polymères et des Nanocomposites (LSPN), Université 8 Mai 1945, Guelma, BP 401, Guelma, 24000, Algeria.

[b] Laboratoire de Chimie Appliquée (L.C.A), Université 8 Mai 1945, BP 401, 24000 Guelma, Algeria

[c] Laboratoire d'Analyses Industrielles et Génie des Matériaux (L.A.I.G.M), Université 8 Mai 1945 Guelma, BP 401 Guelma 24000, Algeria.

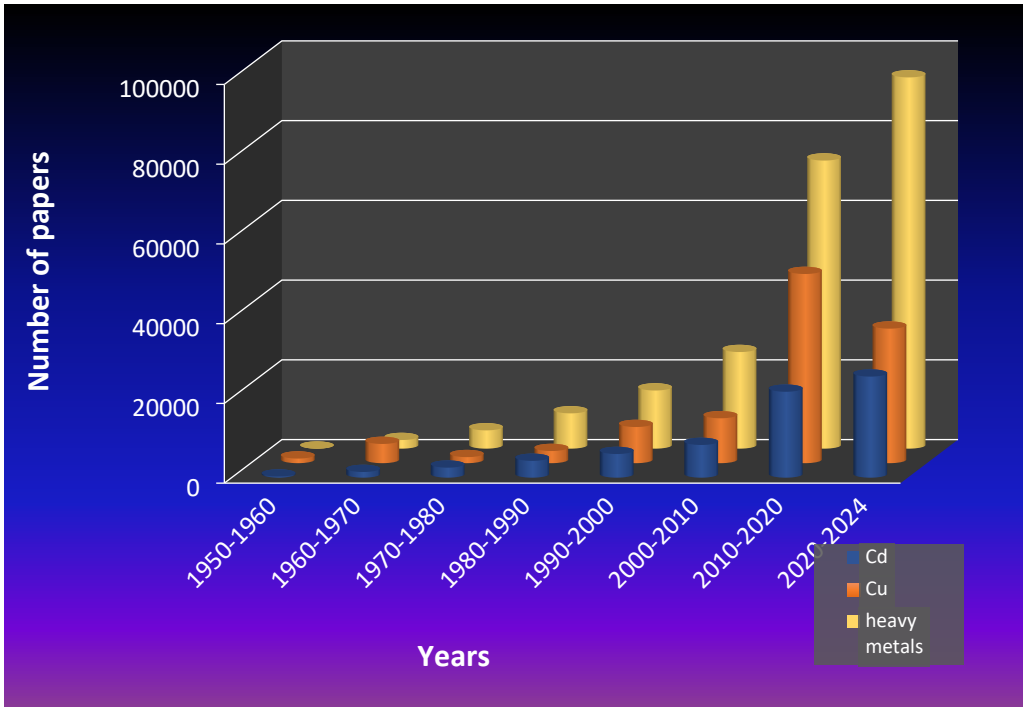


Figure S1. Published documents per year related to heavy metals adsorption (from Science Direct database). Keywords: Heavy metals, Cadmium, Copper, Adsorption.

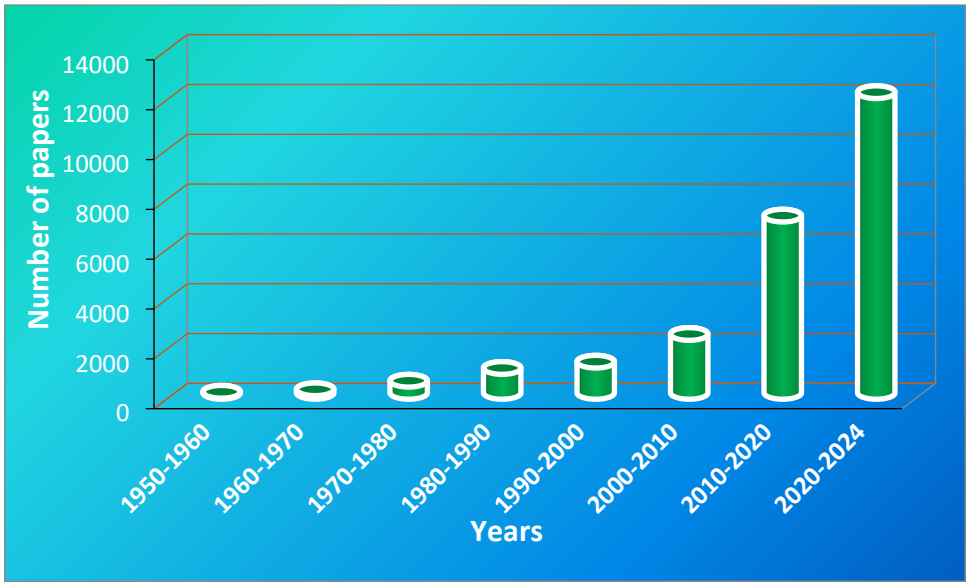


Figure S2. Published documents per year related to the use of algae in the adsorption (from Science Direct database). Keywords: Algae, Adsorption.

Table S1. Functional groups of *Cystoseira sedoide* alga before and after Cd^{2+} and Cu^{2+}biosorption.

Wavelength (cm^{-1})			Functional groups
C. sedoide	Cu /*C. sedoide*	Cd/ *C. sedoide*	
868.34	866.48	864.62	C-H out of plane bending vibrations in aromatic groups
1011.77	1009.90	1011.77	C-O bonds of saccharide structure
1410.37	1410.37	1408.51	-COO- symmetric stretching vibrations
1596.63	1585.46	1596.63	-COO- asymmetric stretching vibrations
2919.10	------	------	-CH stretching vibrations (υCH, alkyl).
3265	3265	3265	-OH stretching vibration

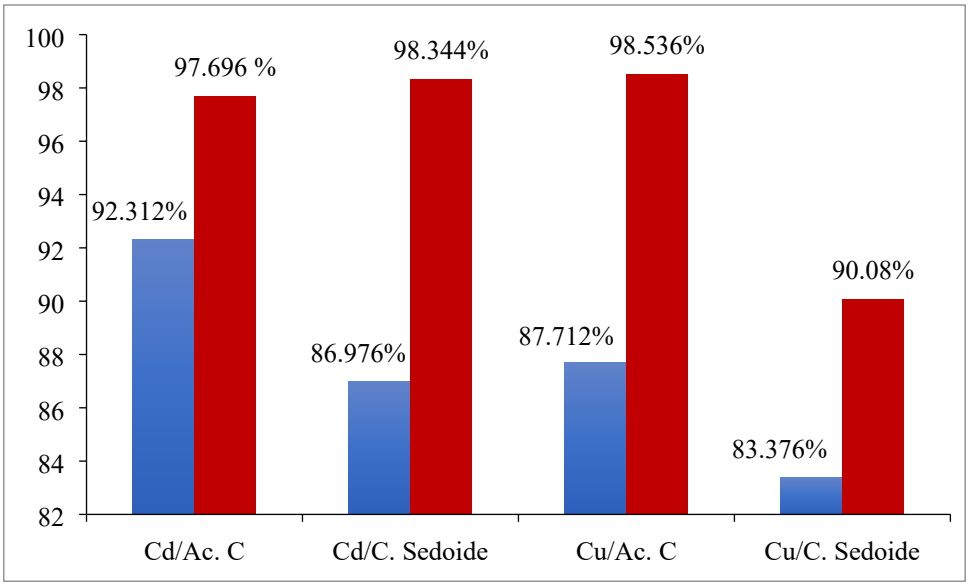


Figure S3. Effect of the solution stirring on the adsorption of Cd^{+2} and Cu^{+2} on *C. sedoide* and Ac.C. Blue: without stirring and red: with stirring at 300 rpm.

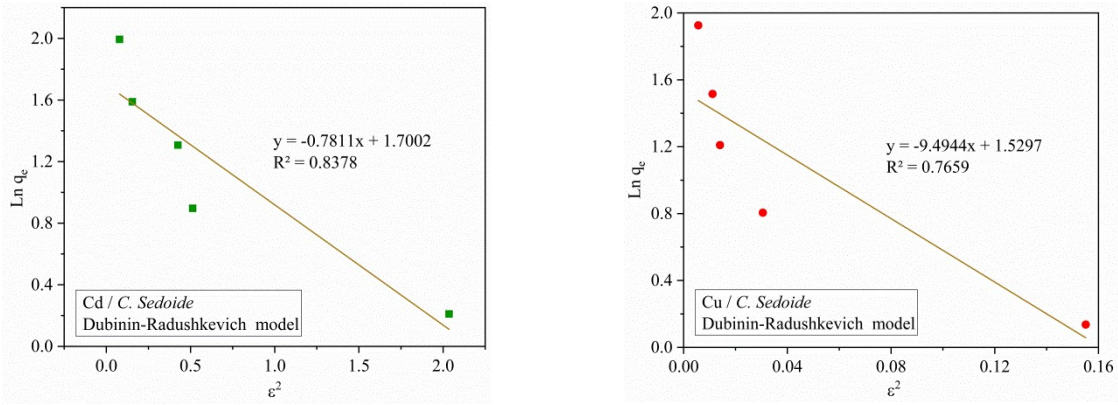
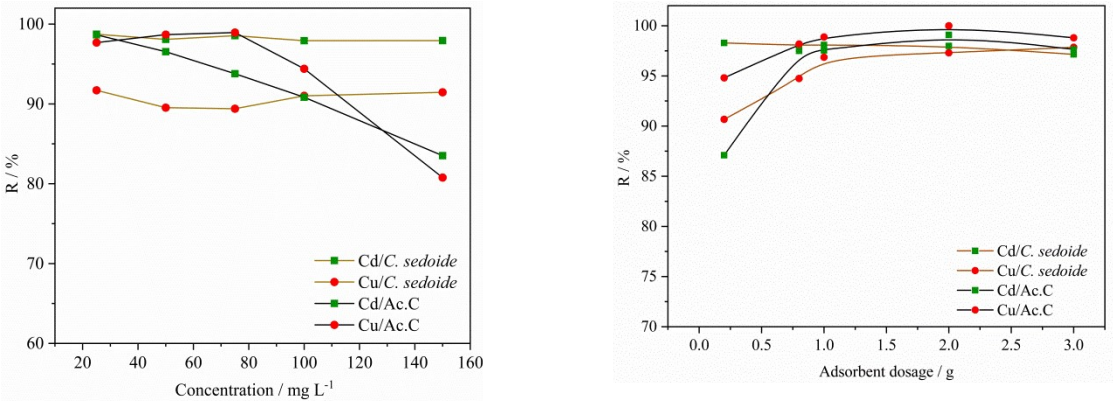


Figure S4. Linearized plots of Dubinin-Radushkevich (D-R) model for different isotherm models for Cd^{2+} ions biosorption on *C. sedoide*



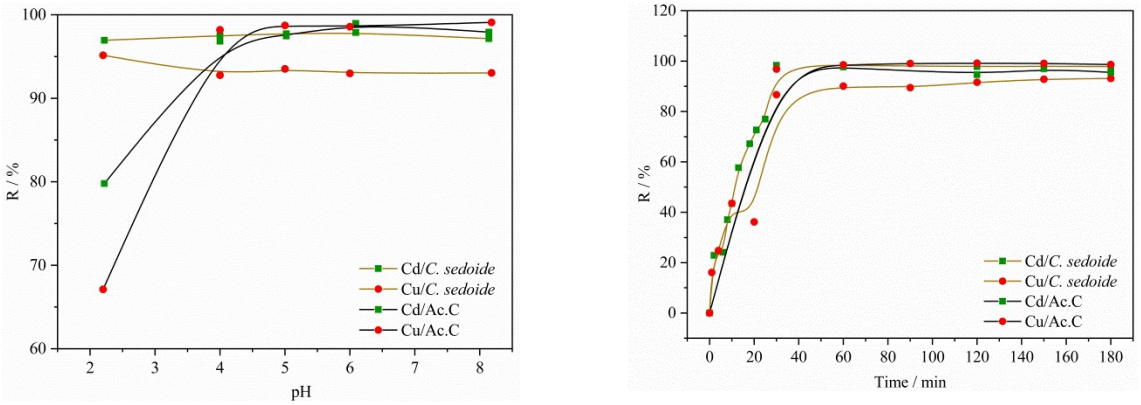


Figure S5. Effect of initial concentration, *C. sedoide* alga and Ac.C doses, pH, and temperature on the removal rate of Cd^{2+} and Cu^{2+} ions

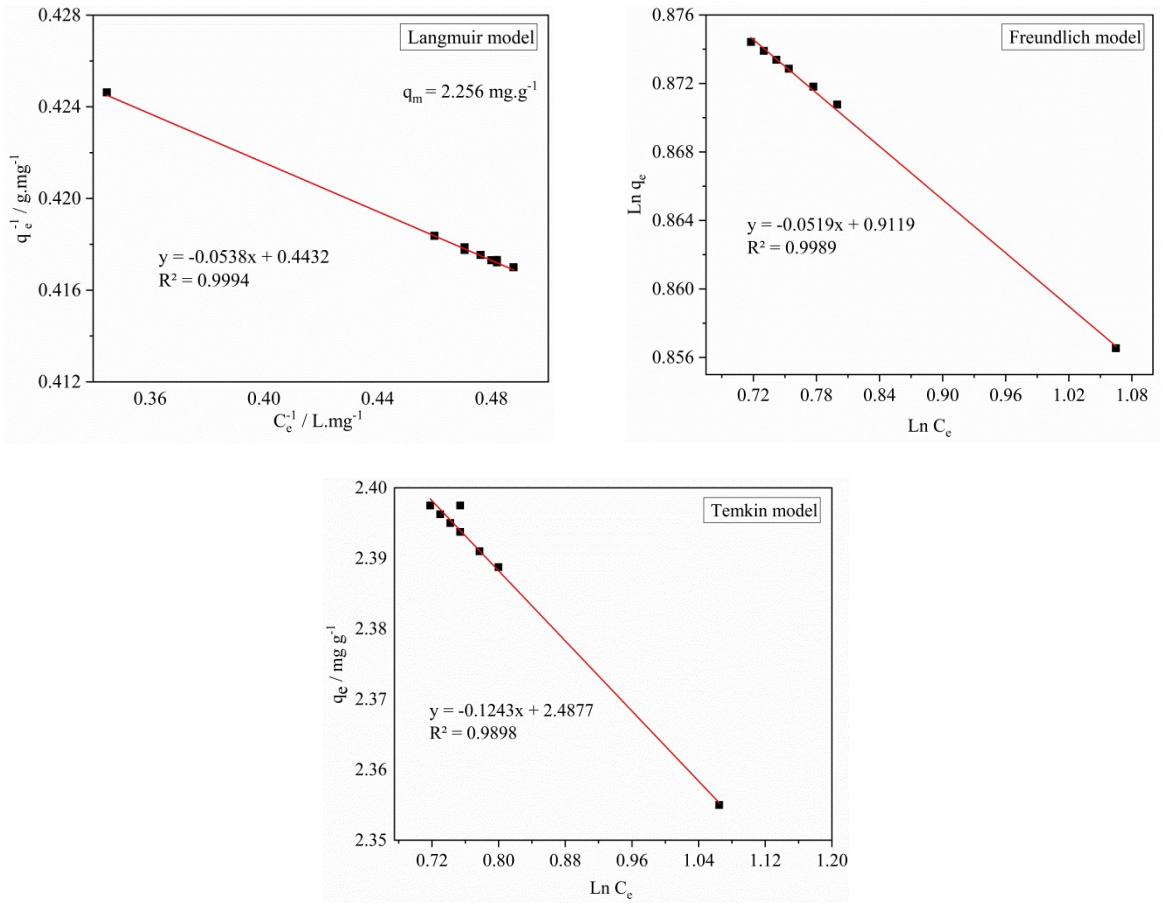


Figure S6. Linearized plots of different isotherm models for Cd^{2+} ionsbiosorptionon *C. sedoise* in the presence of Cu^{2+} ions.

Table S2. Summary of Dubinin-Radushkevich (D-R) model used for the adsorption of Cd^{2+} and Cu^{2+}.

Dubinin-Radushkevich equation	$q_e = q_{DR}\, exp\left((- B_{DR}\, \varepsilon_{DR}^2\right)$
Dubinin-Radushkevich linearized equation	$\ln q_e = \ln q_{DR}\, \beta\varepsilon^2$
Polanyi potential	$\varepsilon_{DR} = RT\ln\left(\frac{C_s}{C_e}\right)$
The mean free energy of biosorption(E)	$E = \frac{1}{\sqrt{2\,\beta_{DR}}}$
E significance	8 kJ/mol<E<16 kJ/mol→Chemisorption E<8 kJ/mol→Physisorption
Results	Cd^{2+}/ *C. Sedoide*: E= 14.2 kJ/mol Cu^{2+}/ *C. Sedoide*: E= 8.45 kJ/mol Cd^{2+}/ Ac.C : E= 11.2 kJ/mol Cu^{2+}/ Ac.C : E= 15.58 kJ/mol

Table S3. Thermodynamic parameters of Cd^{2+} and Cu^{2+}biosorption on *C. Sedoide*

Thermodynamic parameters		Cadmium	Copper
ΔH^0 (kJ.mol^{-1})		3.0899	9.36
ΔS^0 (kJ.mol^{-1}.K^{-1})		0.042	0.050
ΔG^0(kJ.mol^{-1})	293 K	- 9.234	-5.227
	303 K	- 9.674	-5.931
	313 K	-10.106	-6.046
	323 K	-10.540	-6.559
	333 K	-10.902	-7.427

Figure S7. Linearized plots of different isotherm models for Cd^{2+} ions biosorption on *C. sedoise* in the presence of Cu^{2+} ions

Table S4. Competitive biosorption parameters of Cd^{2+} on *C. sedoide* in the binary-metal system

		Biosorption capacity ratio	Biosorption reduction rate
Metal	Adsorption systems	$q_{ratio} = \frac{q_{m,i}^{mix}}{q_{m,i}^{0}}$	$\Delta Y = \frac{q_{m,i}^{0} - q_{m,i}^{mix}}{q_{m,i}^{0}} X100\ \%$
Cd^{2+}	Cd^{2+}, Cu^{2+}	0.208	79.25

Table S5. The Mulliken charge of Cd^{2+} and Cu^{2+} before and after complexation with alginate in different configurations.

Metal	**Charge**	
	Before complexation	**After complexation**
$Cu(ALG)^{+2}$/Symetrie	2	0.969
$Cu(ALG)^{+2}$/Inverse	2	1.096
$Cd(ALG)^{+2}$/Symetrie	2	1.682
$Cd(ALG)^{+2}$/Inverse	2	1.676
$(Cu\text{-}ALG\text{-}Cu)^{+4}$	4	Cu_{45} :0.809 Cu_{44}: 0.815
$(Cd\text{-}ALG\text{-}Cd)^{+4}$	4	Cd_{45}:1.871 Cd_{44}: 1.849
$(Cu\text{-}ALG\text{-}Cd)^{+4}$	4	Cd_{44}:1.868 Cu_{45}: 0.802