chemengineering

Supplementary Materials

Electrochemical Degradation of Diuron by Anodic Oxidation on DSA in Sulfate Medium

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Figure S1 shows the percentages of removed Diuron for the different initial Diuron concentrations and current densities. As can be observed, the highest percentage of Diuron removed corresponds to D40-19, different from the absolutes values (maximum removal D40-38), which could be indicative of a more efficient degradation, i.e., better use of the oxidants conditions (direct oxidation and oxidants generated). It is also interesting to note that a high Diuron removal is also attained for the condition D10-9.5. In this condition, the operation at higher current densities results in the massive development of ineffective secondary reactions.

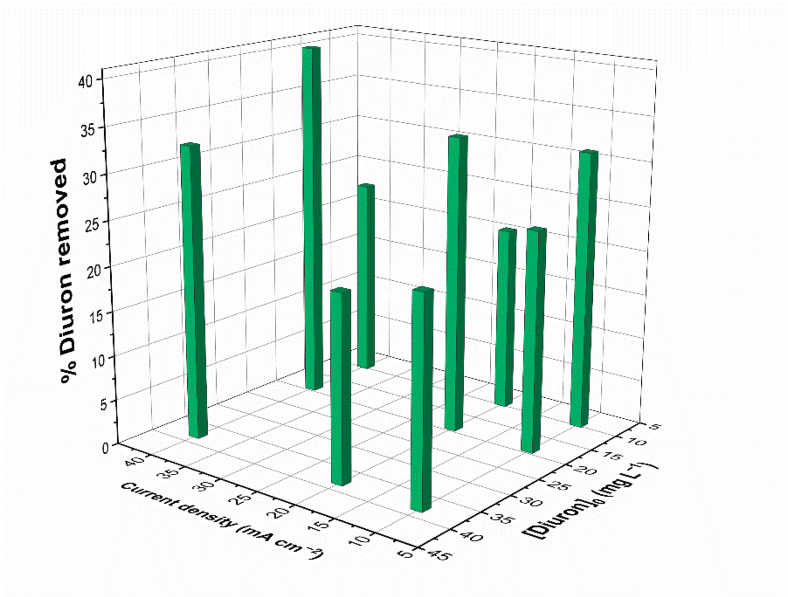
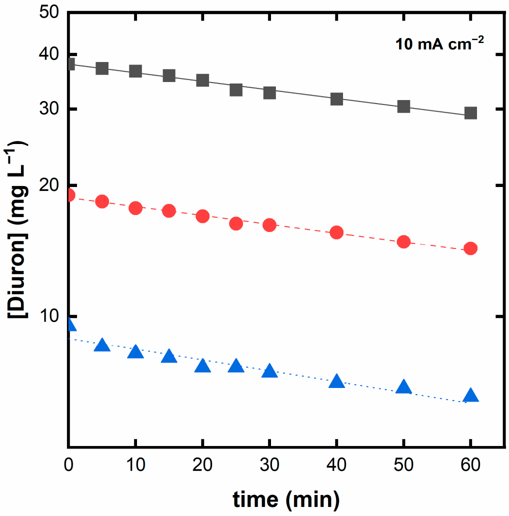


Figure S1. Final percentages of Diuron removed for the different initial Diuron concentrations and current densities studied

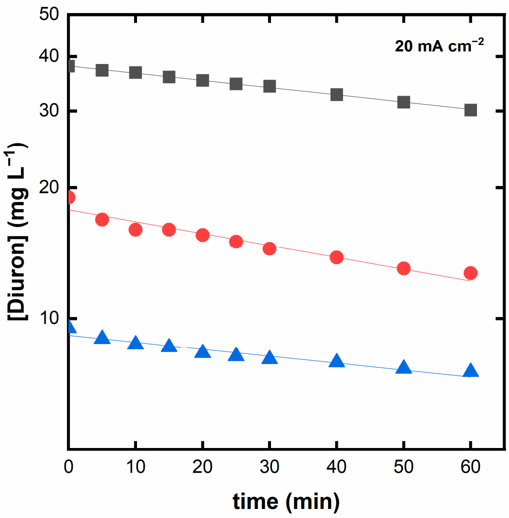
Figure S2 shows the corresponding concentration profiles and fitting to the first-order kinetic model (Equation S1) where C is the Diuron concentration at any time, C_0 is the initial Diuron concentration, and k is the rate constant. The statistical parameters standard error and t value and Prob>|t| for the model parameters and the R^2 values and Prob > F are also presented to assess the statistical significance of the parameters and the entire model. As can be seen, all the experimental data fit well with a first-order kinetics model, where all the model parameters are significant along with the entire model. The rate constant values are used for depicting Fig. 3 with the corresponding discussion.

$$C = C_0 \exp(-kt) \qquad \text{(S1)}$$



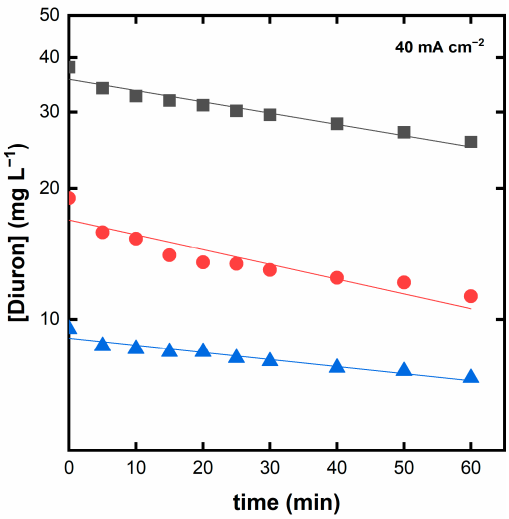
		Value	Standard Error	t-Value	Prob>|t|	Dependency
38 mg/L	C0	38.0	0.223	170	1.58E-15	0.615
	k	0.00451	2.05E-4	22.0	1.89E-8	0.615
19 mg/L	C0	18.7	0.0990	189	6.82E-16	0.613
	k	0.00471	1.85E-4	25.4	6.12E-9	0.613
9.5 mg/L	C0	8.89	0.161	55.3	1.28E-11	0.605
	k	0.00572	6.48E-4	8.82	2.14E-5	0.605

ANOVA Prob > F much below 0.05 for the three fittings, values of R^2 of 0.9844, 0.9882 and 0.9785 for 38, 19 and 9.5 mg L^{-1} of initial Diuron concentration



		Value	Standard Error	t-Value	Prob>|t|	Dependency
38 mg/L	C0	38.0	0.0697	546	1.42E-19	0.620
	k	0.00380	6.29E-5	60.5	6.23E-12	0.620
19 mg/L	C0	17.8	0.321	55.4	1.25E-11	0.601
	k	0.00630	6.54E-4	9.63	1.12E-5	0.601
9.5 mg/L	C0	9.14	0.101	90.2	2.54E-13	0.621
	k	0.00368	3.79E-4	9.69	1.08E-5	0.621

ANOVA Prob > F much below 0.05 for the three fittings, values of R^2 of 0.9822, 0.9899 and 0.9912 for 38, 19 and 9.5 mg L^{-1} of initial Diuron concentration

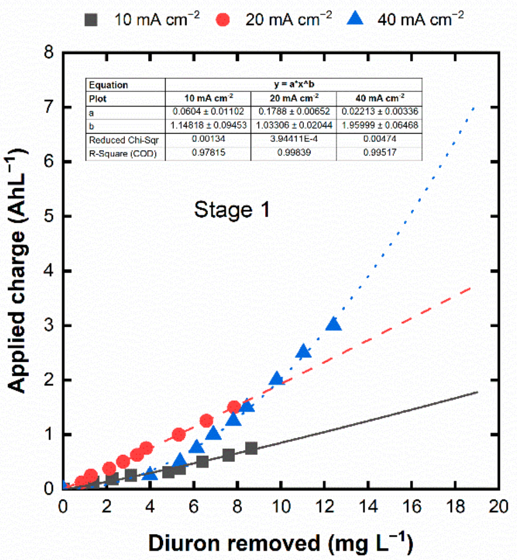


		Value	Standard Error	t-Value	Prob>|t|	Dependency
38 mg/L	C0	35.6	0.600	59.4	7.14E-12	0.603
	k	0.00595	6.06E-4	9.83	9.68E-6	0.603
19 mg/L	C0	16.9	0.590	28.7	2.38E-9	0.589
	k	0.00781	0.00131	5.97	3.35E-4	0.589
9.5 mg/L	C0	9.04	0.114	79.5	6.96E-13	0.621
	k	0.00375	4.31E-4	8.70	2.37E-5	0.621

ANOVA Prob > F much below 0.05 for the three fittings, values of R^2 of 0.9263, 0.8852 and 0.9065 for 38, 19 and 9.5 mg L^{-1} of initial Diuron concentration

Figure S2. Concentration profiles for the different current densities, along with the fitting parameter to a first-order kinetics

In order to estimate the required volumetric charges for each stage of the Diuron removal, Figure S3a and b presents the corresponding experimental fitting of the applied charge *vs*. the applied volumetric charge.



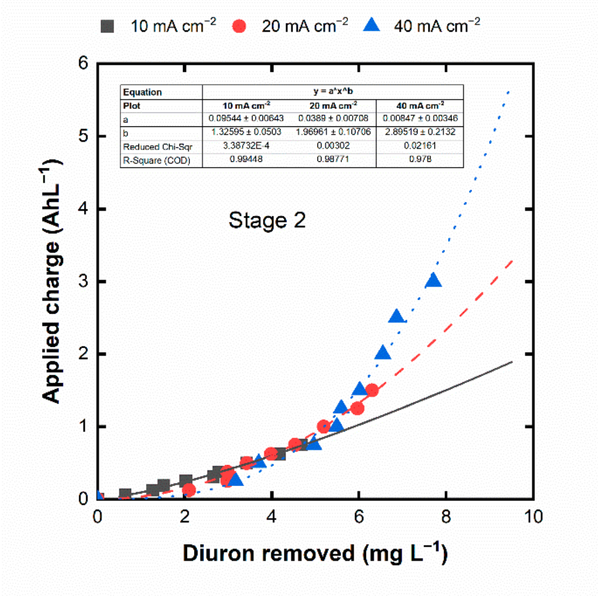


Figure S3. Fitting of the applied charges versus the Diuron removed to estimate the required volumetric charges for designing the treatment system

Based on the equations presented here, Table S1 collects the corresponding required volumetric charges for each stage (stage 1, 38 → 19 mg L^{-1}, stage 2, 19 → 9.5 mg L^{-1}).

Table S1. Required volumetric charges (AhL^{-1}) for each stage of Diuron removal for each applied current density

Stage	Current density (mA cm^{-2})		
	10	**20**	**40**
1	1.77	3.74	7.10
2	1.89	3.28	5.74
Total	3.66	7.02	12.84

Figure S4 shows in detail the regions of the initial applied volumetric charges where the most efficient performance corresponds to the current density of 40 mA cm^{-2}. The corresponding charges in which the curves cross are 0.25 AhL^{-1} and 0.735 AhL^{-1}. Thus, the design will be divided into four steps, an initial stage at 40 mA cm^{-2} up to 0.25 AhL^{-1} and the subsequent return to 10 mA cm^{-2}, and in the second stage, an initial stage at 40 mA cm^{-2} up to 0.735 AhL^{-1} and the subsequent return to 10 mA cm^{-2}. Calculations are presented in Table 5.

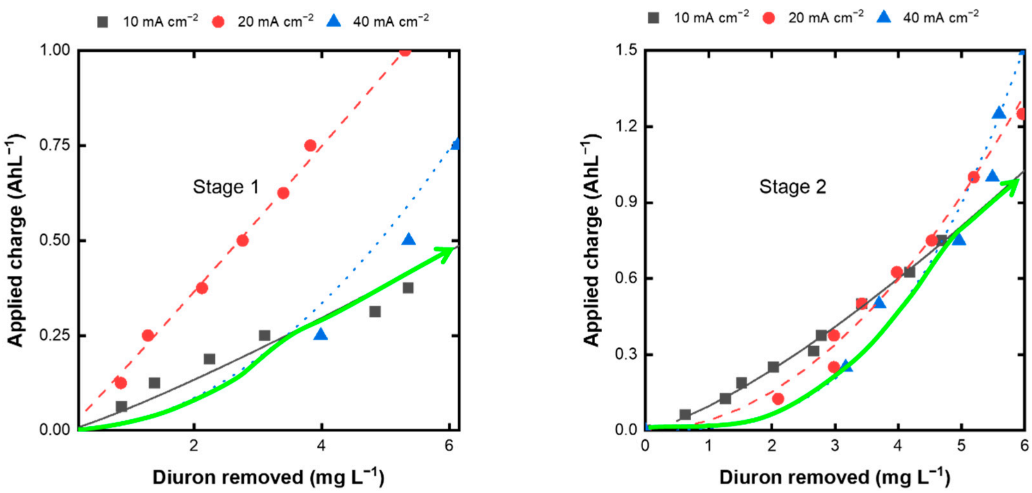


Figure S4. Fitting of the applied charges versus the Diuron removed to estimate the required volumetric charges for designing the treatment system in the combined current approach