Supplementary material

Solar Photo-Assisted Degradation of Bipyridinium Herbicides at Circumneutral pH: A Life Cycle Assessment Approach

Alejandra Teutli-Sequeira [1], Ruben Vasquez-Medrano [2,*], Dorian Prato-Garcia [3] and Jorge G. Ibanez [2]

[1] Cátedras CONACYT - Instituto Interamericano de Tecnología y Ciencias del Agua. Universidad Autónoma del Estado de México. Carretera Toluca-Atlacomulco Km. 14.5 Unidad San Cayetano, Toluca de Lerdo, Mexico; aleteutlis@gmail.com (A.T.-S.)

[2] Departamento de Ingeniería Química, Industrial y de Alimentos, Universidad Iberoamericana Ciudad de México, Prolongación Paseo de la Reforma 880, Lomas de Santa Fe, 01219, Mexico, Mexico; jorge.ibanez@ibero.mx (J.G.I.)

[3] Facultad de Ingeniería y Administración, Universidad Nacional de Colombia, Sede Palmira, Carrera 32 No. 12-00, Chapinero, Vía Candelaria, Palmira, Colombia; dpratog@unal.edu.co (D.P.-G.)

* Correspondence: ruben.vasquez@ibero.mx; Tel.: +52-555-9504-074

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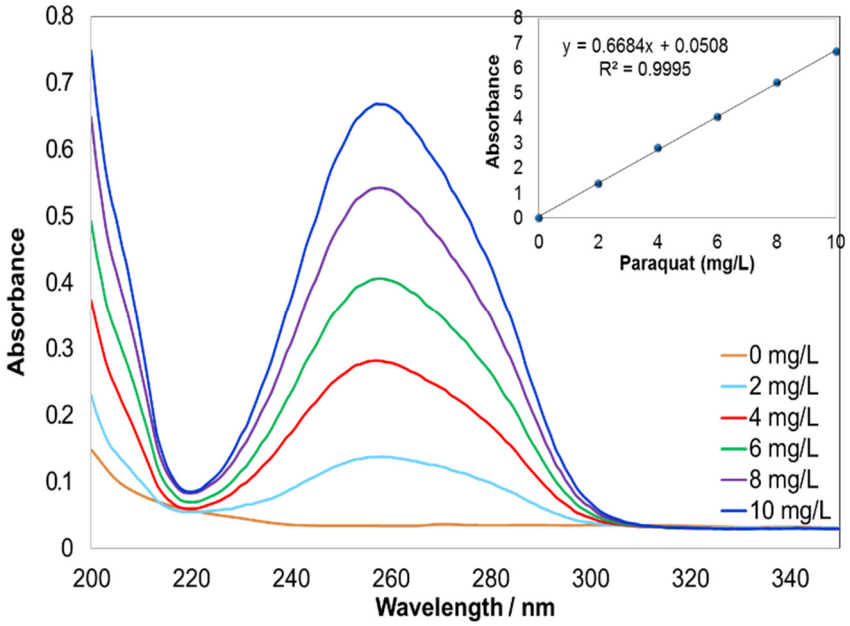
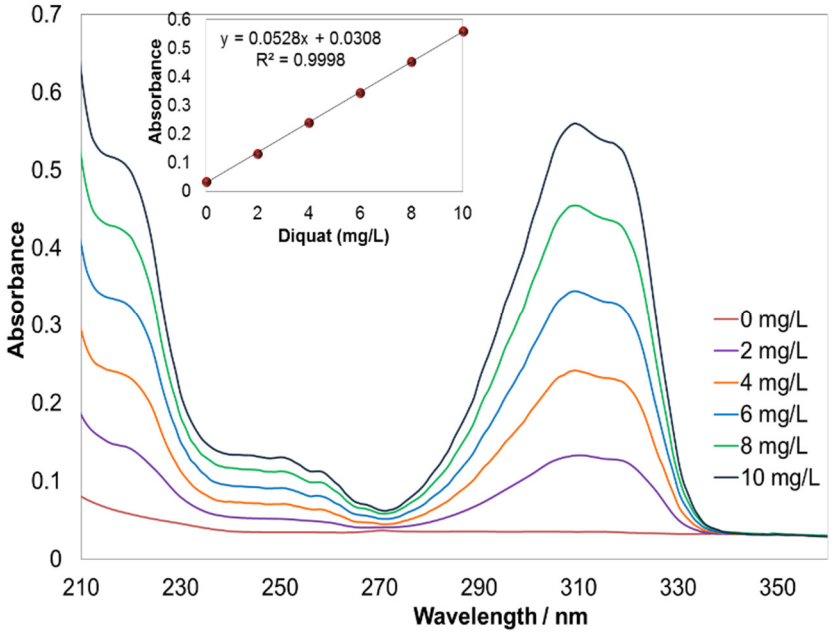


(a)



(b)

Figure S1. Paraquat (**a**) and diquat (**b**) absorbances at different concentrations. Insert: Calibration curve.

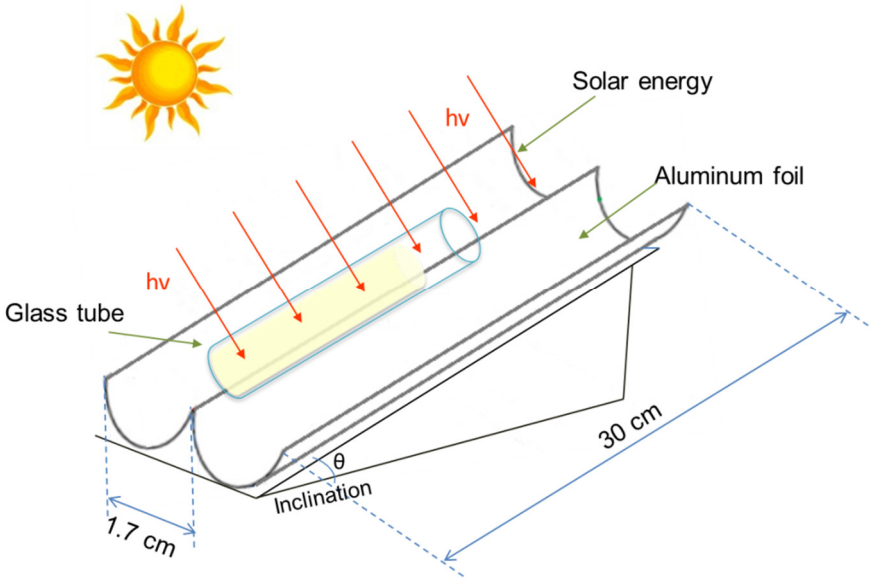


Figure S2 Schematic representation of a two-slot compound parabolic collector (CPC). θ is the geographic latitude.

Table S1 Coded levels and actual values for central composite design and response surface methodology analysis of photo-Fenton treatments of 100 mg L^{-1} PQ and DQ solutions.

Herbicide	Experiment	Coded value		Actual values			Observed Responses	
				[Fe^{3+}]	[H_2O_2]	[$Na_2C_2O_4$]	% Removal	
		A	B	mg/L	mg/L	mg/L	COT	Herbicide
PQ	1	-1	-1	10	84.4	200	52.98	47.01
	2	1	-1	30	84.4	600	87.30	57.30
	3	-1	1	10	253.1	200	58.49	57.93
	4	1	1	30	253.1	600	74.65	33.53
	5	-1.41	0	5.9	168.7	118	29.15	43.96
	6	1.41	0	34.1	168.7	682	77.17	36.87
	7	0	-1.41	20	49.4	400	69.82	39.02
	8	0	1.41	20	288.0	400	78.64	73.35
	9	0	0	20	168.7	400	79.02	58.06
	10	0	0	20	168.7	400	79.43	53.72
	11	0	0	20	168.7	400	85.07	59.06
	12	0	0	20	168.7	400	82.65	68.07
	13	0	0	20	168.7	400	87.07	64.10
DQ	1	-1	-1	10	140	200	79.60	15.85
	2	1	-1	30	140	600	74.07	27.48
	3	-1	1	10	420	200	75.08	37.34
	4	1	1	30	420	600	73.67	27.47
	5	-1.41	0	5.9	280	118	32.42	23.23
	6	1.41	0	34.1	280	682	73.68	41.83
	7	0	-1.41	20	82.01	400	57.92	14.23
	8	0	1.41	20	477.99	400	75.47	13.25
	9	0	0	20	280	400	72.38	21.25
	10	0	0	20	280	400	73.07	23.53
	11	0	0	20	280	400	79.88	22.33
	12	0	0	20	280	400	64.36	19.18
	13	0	0	20	280	400	72.42	21.57

Table S2 General inventory of the Fenton treatment process during its useful lifetime (Diquat).

Product	kg/FU (Diquat)	kg/FU (Paraquat)
Ceramic tile	0.082	0.082
Brick	0.850	0.850
Cement	0.488	0.488
Sand	1.420	1.420
Gravel	0.620	0.620
Polyethylene, Linear Low-Density Polyethylene (LLDPE)	0.022	0.022
polyvinylidenchloride, PVC	0.055	0.055
Cast Iron	0.046	0.046
H_2O_2 (50%, solution)	1.040	0.300
Iron chloride (98%)	0.083	0.083
Steel	0.015	0.015
Aluminum	0.037	0.037

Table S3 Cost analysis for the Fenton treatment process.

Baseline information	Unit	DQ	PQ	Source
Treatment capacity (TC)	(m^3/d)	10		
Annual operation (AO)	(day/year)	330		
Facility cost	(US/m^2)	320		
Electricity cost	(US/kWh)	0.20		
Project contingency	12% of C_1			
Engineering and setup	50% of (C_1+C_2)			Blanco and Malato, 2003
Spare parts	0.5% of (C_1+C_2)			
Treatment cost calculation				
Facility cost (C_1)	(US)	67200		-
Project contingency (C_2)	(US)	8064		-
Engineering and setup (C_3)	(US)	37632		-
Spare parts (C_4)	(US)	376		-
Total installed cost (TIC) (C_1+C_2+C_3+C_4)	(US)	113272		-
Electricity (C_5)	(US/year)	2442		
Reagents (C_6)	(US/year)	2560	1468	
Maintenance material cost (C_7)	(US/year)	65.0		
Personnel (C_8)	(US/year)	800.0		
Total operating cost (OC) (C_5+C_6+C_7+C_8)	(US/year)	7308	6215	
Annual levelized cost (ALC) ALC=TIC×FCR+OC FCR=17% (Fixed Charge Rate)	(US)	25564	25472	Blanco and Malato, 2003
Annual treatment cost (ATC) ATC=ALC/ YLC YLC=yearly treated volume YLC=3300 (m^3/year) YLC=TC×AO	(US/m^3)	8.05	7.72	Blanco and Malato, 2003