Supplementary data

Production of modified sunflowers seeds shells for the removal of bisphenol A

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Table S1. Parameters and errors for Canonical and Fractal-like kinetic models at different BPA initial concentration

- **Canonical kinetic models**

		BPA Initial concentration (mg/L)				
Models	Parameters	25	50	75	100	125
	q_e *exp* (mg/g)	15.2632	29.9248	42.9574	53.7343	63.7343
	$t_{0.5}$ *exp* (min)	5.6	7.5	7.4	8.1	8.8
PFO	q_e (mg/g)	14.0397	28.0493	41.1763	51.0404	59.2516
	K_1 (1/min)	0.1463	0.0803	0.0813	0.0694	0.0570
	$t_{0,5}$ (min)	4.7	8.6	8.5	10.0	12.2
	R^2	0.9701	0.9678	0.9763	0.9682	0.9404
	ARE (%)	0.4038	0.5031	0.4220	0.5290	0.7559
	RMSE (%)	0.8728	1.8539	2.3271	3.3892	5.4958
PSO	q_e (mg/g)	14.5838	29.719	43.5184	54.314	63.6471
	k_2 (g/mg min)	0.0182	0.0043	0.0030	0.0020	0.0014
	$t_{0,5}$ (min)	3.8	7.9	7.6	9.2	11.6
	R^2	0.9885	0.9956	0.9984	0.9961	0.9838
	ARE (%)	0.2777	0.1780	0.1090	0.1820	0.3886
	RMSE (%)	0.5421	0.6787	0.6073	1.1699	2.8310

- **Fractal-like kinetic models**

		BPA Initial concentration (mg/L)				
Models	Parameters	25	50	75	100	125
	q_e *exp* (mg/g)	15.2632	29.9248	42.9574	53.7343	63.7343
	$t_{0.5}$ *exp* (min)	5.6	7.5	7.4	8.1	8.8
Weibull	q_e (mg/g)	66.0000	30.2553	43.1313	54.7155	72.4644
	τ	>>	14.0	12.6	16.6	39.0
	α	0	0.4138	0.4812	0.453	0.3518
	$t_{0.5}$ (min)	>>	5.8	5.9	7.4	13.8
	R^2	0.9819	0.9996	0.9998	0.9996	0.9994
	ARE (%)	0.6498	0.0454	0.0247	0.0398	0.0591
	RMSE (%)	0.2181	0.2395	0.2287	0.4197	0.6318
Hill	q_e (mg/g)	64	32.3037	45.0877	58.4639	86.379
	τ	>>	7.7	7.2	9.4	29.1
	α	0	0.6344	0.7864	0.6843	0.4293
	$t_{0.5}$ (min)	>>	7.7	7.2	9.4	29.1
	R^2	0.9987	0.9997	0.9997	0.9997	0.9993
	ARE (%)	0.0851	0.0404	0.0473	0.0433	0.0679
	RMSE (%)	0.2182	0.2031	0.3183	0.4062	0.7092
PFOf	q_e (mg/g)	75.1286	30.2553	43.1313	54.7155	72.4644
	K_{1f} ($1/min^{(1-h)}$)	0.0120	0.1387	0.1424	0.1268	0.0969
	h	0.9074	0.5862	0.5188	0.5470	0.6482
	$t_{0.5}$ (min)	>>	5.8	5.9	7.4	13.8
	R^2	0.9987	0.9996	0.9998	0.9996	0.9994
	ARE (%)	0.0855	0.0454	0.0247	0.0398	0.0591
	RMSE (%)	0.2181	0.2395	0.2287	0.4197	0.6318
PSOf	q_e (mg/g)	110.399	32.3037	45.0877	58.4639	86.3791
	K_{2f} (g/mg $min^{(1-h)}$)	0.0001	0.0054	0.0037	0.0025	0.0012
	h	0.9030	0.3656	0.2136	0.3157	0.5707
	$t_{0.5}$ (min)	>>	7.7	7.2	9.4	29.1
	R^2	0.9932	0.9730	0.9987	0.9969	0.9918
	ARE (%)	4.4274	3.7950	2.5555	1.4419	0.9662
	RMSE (%)	0.2181	0.2031	0.3183	0.4062	0.7092

Table S2. Parameters and errors for Canonical and Fractal-like kinetic models at different adsorbent dosage

- **Canonical kinetic models**

		m (g/L)			
Models	Parameters	0.5	1	1.5	2
	q_e *exp* (mg/g)	59.3985	39.1353	29.9248	22.6316
	$t_{0.5}$ *exp* (min)	16.5	8.5	7.5	5.4
PFO	q_e (mg/g)	54.0347	36.4220	28.0493	21.8038
	K_1 (1/min)	0.0361	0.0660	0.0803	0.1437
	$t_{0.5}$ (min)	19.2	10.5	8.6	4.8
	R^2	0.9497	0.9491	0.9678	0.9874
	ARE (%)	0.7699	0.6847	0.5031	0.2546
	RMSE (%)	23.3391	9.5002	3.4369	0.7645
PSO	q_e (mg/g)	59.1357	38.9552	29.7190	22.5445
	k_2 (g/mg min)	0.0009	0.0026	0.0043	0.0126
	$t_{0.5}$ (min)	19.0	10.0	7.9	3.5
	R^2	0.9843	0.9879	0.9956	0.9985
	ARE (%)	0.4315	0.3312	0.1780	0.0897
	RMSE (%)	2.6121	1.4918	0.6787	0.3054

- **Fractal-like kinetic models**

		m (g/L)			
Models	Parameters	0.5	1	1.5	2
	q_e *exp* (mg/g)	59.3985	39.1353	29.9248	22.6316
	$t_{0,5}$ *exp* (min)	16.5	8.5	7.5	5.4
Weibull	q_e (mg/g)	67.9712	42.4336	30.2553	22.6732
	τ	67.7	26.0	14.0	4.0
	α	0.4113	0.3627	0.4138	0.3537
	$t_{0.5}$ (min)	27.8	9.5	5.8	1.4
	R^2	0.9990	0.9990	0.9996	0.9993
	ARE (%)	0.0742	0.0712	0.0454	0.0509
	RMSE (%)	0.7533	0.4984	0.2395	0.2354
Hill	q_e (mg/g)	82.6845	48.2244	32.3037	23.2823
	τ	57.2	15.9	7.7	2.4
	α	0.4887	0.4776	0.6344	0.6864
	$t_{0.5}$ (min)	57.2	15.9	7.7	2.4
	R^2	0.9991	0.9990	0.9997	0.9994
	ARE (%)	0.0678	0.0683	0.0404	0.0451
	RMSE (%)	0.7200	0.5075	0.2031	0.2162
PFOf	q_e (mg/g)	67.9712	42.4336	30.2553	22.6732
	K_{1f} ($1/min^{(1-h)}$)	0.0727	0.1112	0.1387	0.2162
	h	0.5887	0.6373	0.5862	0.6463
	$t_{0.5}$ (min)	27.8	9.5	5.8	1.4
	R^2	0.9990	0.9990	0.9996	0.9993
	ARE (%)	0.0742	0.0712	0.0454	0.0509
	RMSE (%)	0.7533	0.4984	0.2395	0.2354
PSOf	q_e (mg/g)	82.6845	48.2244	32.3037	23.2823
	K_{2f} (g/mg $min^{(1-h)}$)	0.0008	0.0026	0.0054	0.0162
	h	0.5113	0.5224	0.3656	0.3136
	$t_{0.5}$ (min)	57.2	15.9	7.7	2.4
	R^2	0.9991	0.9776	0.9947	0.9683
	ARE (%)	0.0678	3.0004	2.1930	1.8639
	RMSE (%)	0.7200	0.5075	0.2031	0.2162

Table S3. Parameters and errors for Canonical and Fractal-like kinetic models at different initial pH

- **Canonical kinetic models**

		pH			
Model	Parameters	2	3	5	7
	q_e *exp* (mg/g)	29.9248	27.3580	23.8718	22.5867
	$t_{0.5}$ *exp* (min)	7.6	8.7	5.5	5.6
PFO	q_e (mg/g)	28.0493	26.5686	23.8784	22.5036
	K_1 (1/min)	0.08027	0.06513	0.12069	0.12382
	$t_{0.5}$ (min)	8.6	10.6	5.7	5.6
	R^2	0.9678	0.9777	0.9808	0.9878
	ARE (%)	0.5031	0.4515	0.3195	0.2192
	RMSE (%)	1.8539	1.4842	1.1905	0.8909
PSO	q_e	29.7190	28.2686	24.8750	23.3327
	K_2 (g/mg min)	0.0043	0.0036	0.0087	0.0102
	$t_{0.5}$ (min)	7.9	9.7	4.6	4.2
	R^2	0.9956	0.9986	0.9963	0.9964
	ARE (%)	0.1780	0.1127	0.1601	0.1497
	RMSE (%)	0.6787	0.3737	0.5204	0.4840

- **Fractal-like kinetic models**

		pH			
Model	Parameters	2	3	5	7
	q_e *exp* (mg/g)	29.9248	27.3580	23.8718	22.5866
	$t_{0.5}$ *exp* (min)	7.6	8.7	5.5	5.6
Weibull	q_e (mg/g)	30.2553	27.6631	24.801	22.9315
	τ	14.0313	16.3181	6.5185	6.5049
	α	0.4138	0.5453	0.4185	0.5197
	$t_{0.5}$ (min)	5.8	8.3	2.7	3.2
	R^2	0.9996	0.9997	0.9976	0.9970
	ARE (%)	0.0454	0.0376	0.1103	0.1361
	RMSE (%)	0.2395	0.1869	0.4930	0.5189
Hill	q_e (mg/g)	32.3037	28.956	25.5368	23.3327
	τ	7.7025	9.636	3.8095	4.2059
	α	0.6344	0.8638	0.7672	1
	$t_{0.5}$ (min)	7.7	9.6	3.8	4.2
	R^2	0.9997	0.9992	0.9972	0.9964
	ARE (%)	0.0404	0.0762	0.1195	0.1497
	RMSE (%)	0.2031	0.3231	0.5361	0.5727
PFOf	q_e (mg/g)	30.2553	27.6631	24.8010	22.9315
	K_{1f} ($1/min^{(1-h)}$)	0.1387	0.1190	0.1910	0.1964
	h	0.5862	0.4548	0.5815	0.4803
	$t_{0.5}$ (min)	5.8	8.3	2.7	3.2
	R^2	0.9996	0.9997	0.9976	0.9970
	ARE (%)	0.0454	0.0376	0.1103	0.1361
	RMSE (%)	0.2395	0.1869	0.4930	0.5189
	q_e	32.3037	28.956	25.5368	23.331
	K_{2f}(g/mg $min^{(1-h)}$)	0.0054	0.0042	0.0108	0.0102
PSOf	h	0.3656	0.1362	0.2328	0.0000
	$t_{0.5}$ (min)	7.7025	9.6360	3.8095	4.2071
	R^2	0.9997	0.9992	0.9972	0.9964
	ARE (%)	0.0404	0.0762	0.1195	0.1498
	RMSE (%)	0.2031	0.3231	0.5361	0.5727

Table S4. Values of the diffusivities, of adjustments errors and R^2 of the Vermeulen and Fractal Vermeulen models.

Parameters			Vermeulen model				Fractal Vermeulen model				
pH	m_s (g/L)	C_0 (mg/L)	D_v*1e12 (m^2/s)	*RMSE* (%)	R^2	*ARE* (%)	D_{vf}*1e12 (m^2/s)	*h*	*RMSE* (%)	R^2	*ARE* (%)
2	1.5	25	1.945	0.0822	0.9665	0.6250	11.707	0.63	0.0203	0.9968	0.1300
2	1.5	50	1.133	0.0506	0.9869	0.3998	4.046	0.40	0.0086	0.9995	0.0586
2	1.5	75	1.305	0.0342	0.9933	0.2577	3.454	0.31	0.0058	0.9998	0.0347
2	1.5	100	1.050	0.0404	0.9906	0.3069	2.943	0.32	0.0088	0.9995	0.0538
2	1.5	125	0.740	0.0571	0.9801	0.4641	2.492	0.33	0.0185	0.9978	0.1317
2	0.5	50	0.447	0.0488	0.9873	0,4808	1.236	0.25	0.0176	0.9978	0.1185
2	1	50	0.862	0.0574	0.9804	0.4435	3.033	0.36	0.0166	0.9981	0.1197
2	1.5	50	1.133	0.0506	0.9869	0.3998	4.046	0.40	0.0086	0.9995	0.0586
2	2	50	2.606	0.0411	0.9907	0.2812	10.550	0.52	0.0100	0.9993	0.0556
2	1.5	50	1.133	0.05060	0.9869	0.3998	4.046	0.40	0.0086	0.9995	0.0586
3	1.5	50	1.114	0.02239	0.9966	0.1563	2.052	0.19	0.0068	0.9997	0.0400
5	1.5	50	2.477	0.03834	0.9893	0.2683	5.782	0.32	0.0313	0.9959	0.1528
7	1.5	50	2.583	0.02761	0.9942	0.1724	4.847	0.24	0.0235	0.9969	0.1347

Table S5. Values of the intra-particle diffusivities in the treated adsorbent and the mass transfer coefficient in the liquid film.

Parameters			Film mass transfer (m/s)		Diffusivities (m^2/s)		D_m/D_{app}	*Biot*
pH	m_s (g/L)	C_0 (mg/L)	k_{MW}	k_{FS} *X10^6*	D_{app} *X10^12*	D_{st}		
2	1.5	25	1.9522	3.6531	2.0458	0.9412	288	68
		50	1.2108	2.3304	1.5275	0.7299	386	58
		75	1.1707	2.1912	1.5481	0.7779	380	58
		100	0.9124	1.8846	1.4144	0.6965	416	52
		125	0.7237	1.7904	1.3018	0.5962	452	48
	0.5	50	1.1602	2.9343	0.6943	0.4190	848	61
	1		1.2144	2.8244	1.3478	0.6475	437	50
	1.5		1.2108	2.3304	1.5275	0.7299	386	58
	2		1.6330	2.6956	2.1215	1.0391	278	74
2	1.5		1.2108	2.3304	1.5074	0.7299	391	59
3			0.9546	1.7580	1.3168	0.7079	447	58
5			1.0852	2.5892	2.0830	1.0281	283	48
7			0.9788	2.4122	2.0458	1.0453	288	46

Table S6. Parameters values of canonical isotherms models and the corresponding adjustment errors and determination coefficient.

Isotherm models	Parameters	Values	RMSE (%)	ARE (%)	R^2
Temkin	B_T (J/mol)	20.2375	0.8676	0.0937	0.9985
	K_T (L/g)	0.7518			
Langmuir	$q_{m\,L}$ (mg/g)	88.9451	0.9575	0.1313	0.9979
	K_L (L:mg)	0.08207			
	R_L	0.299 - 0.827			
Freundlich	K_F (mg/g) $(L/g)^n$	11.7899	3.9786	0.4861	0.9692
	n_F	1.98			
D-R	$q_{m\,D\text{-}R}$ (mg/g)	57.7855	7.5238	0.9788	0.9056
	$B_{D\text{-}R}$	3.7 E-06			
	E (KJ/mol)	0.367			
Jovanovich	q_{mJ} (mg/g)	66.0573	0.8955	0.0809	0.9978
	b (mg/L)	10.445			

Table S7. Parameters values of like-fractal isotherms models and the corresponding adjustment errors and determination coefficient.

Isotherm models	q_{max} (mg/g)	$Ce_{0,5}$ (min)	*a*	*b*	*c*	*RMSE* (%)	*ARE* (%)	R^2
GBS	106.7490	18.07	1.4	8.7	3.4	0.8738	0.0451	0.9995
BG	73.1083	8.36	1.1	10.0	0.5	0.9039	0.0632	0.9975
BS	67.2558	7.44	1.0	10.9	0.0	1.1990	0.1019	0.9981
HS	79.1344	9.48	1.2	9.5	1.0	0.7604	0.0458	0.9992