

Supplementary Materials

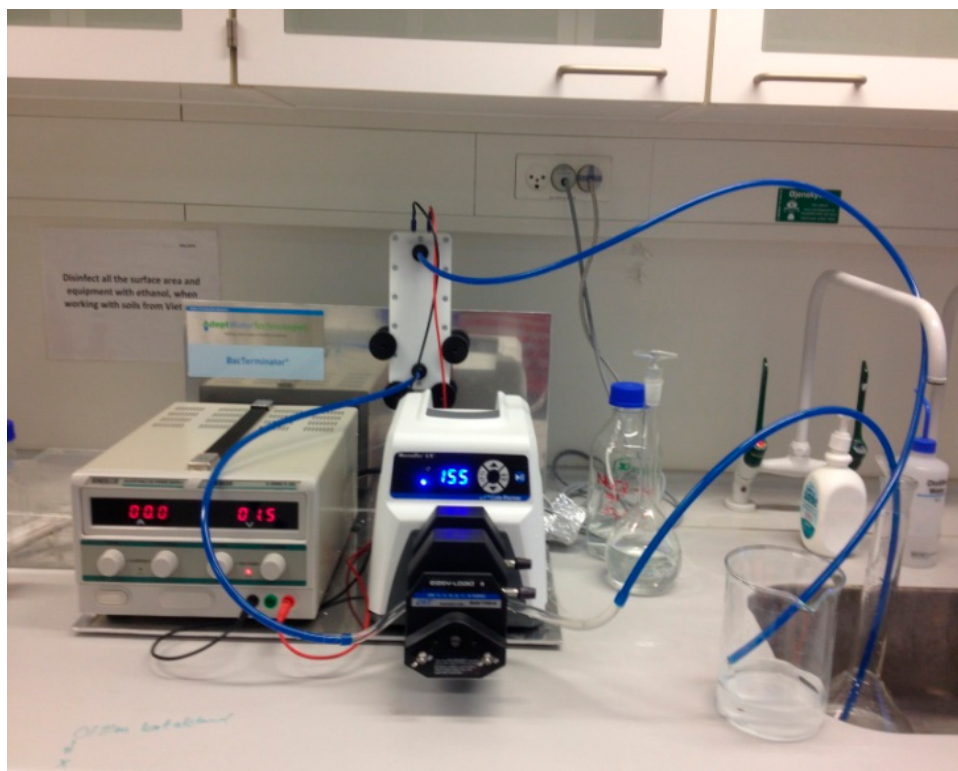


Figure S1. The electrochemical system of Adept Water Technology.



Figure S2. SEM image of electrode.

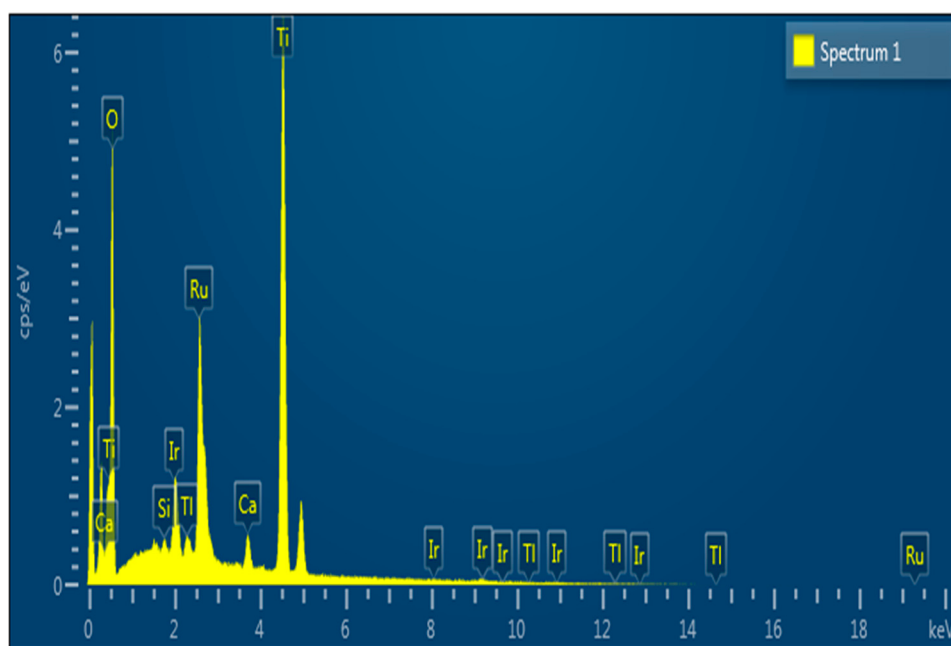
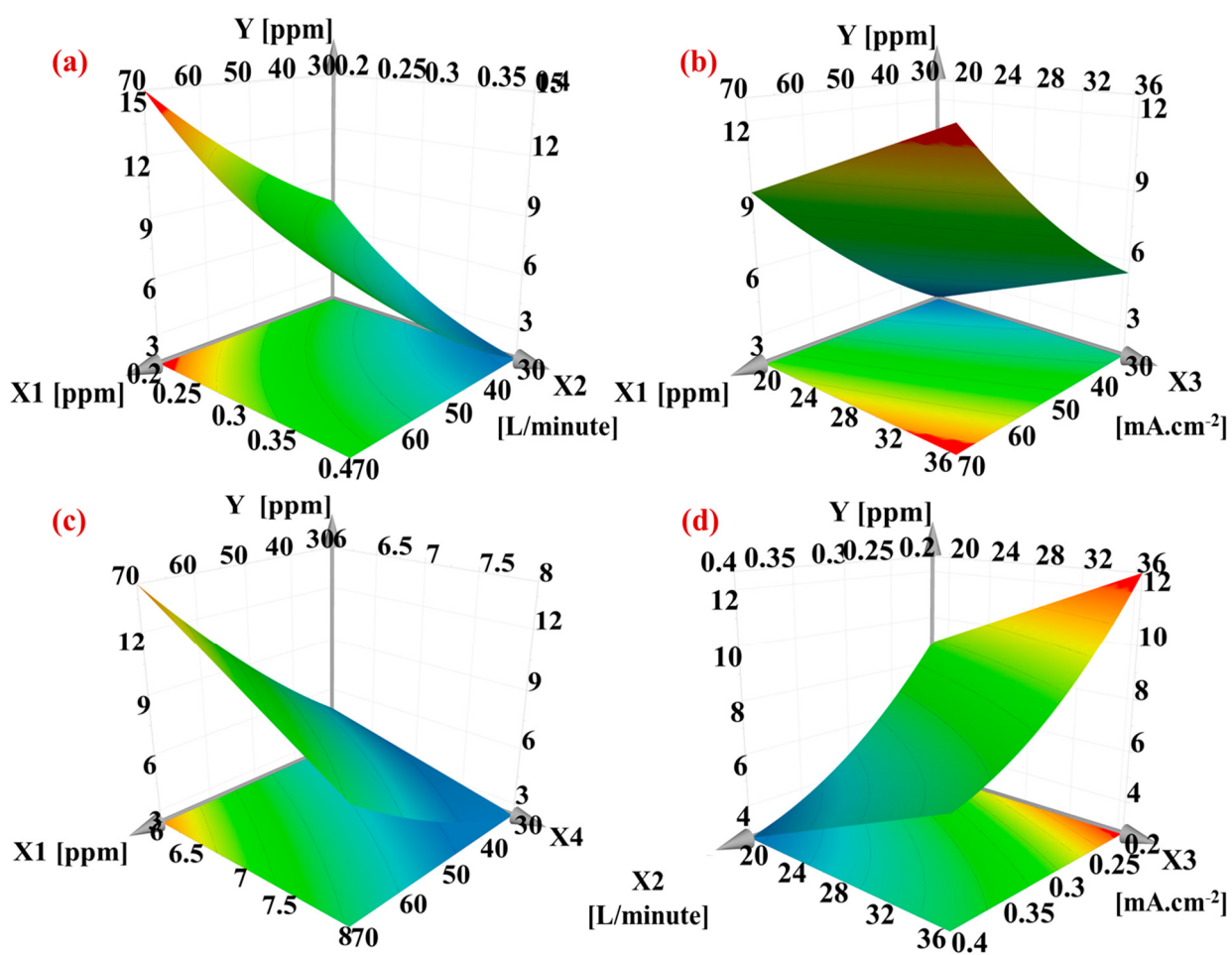


Figure S3. EDX spectra analysis of Ti-RuO₂ electrode.



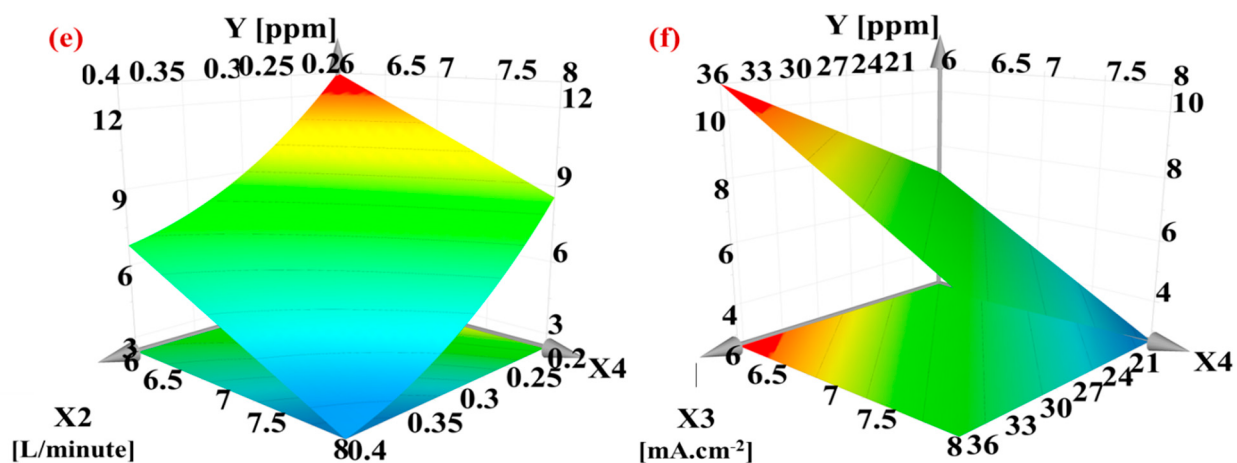


Figure S4. Three-dimensional response surface for active chloride formation.

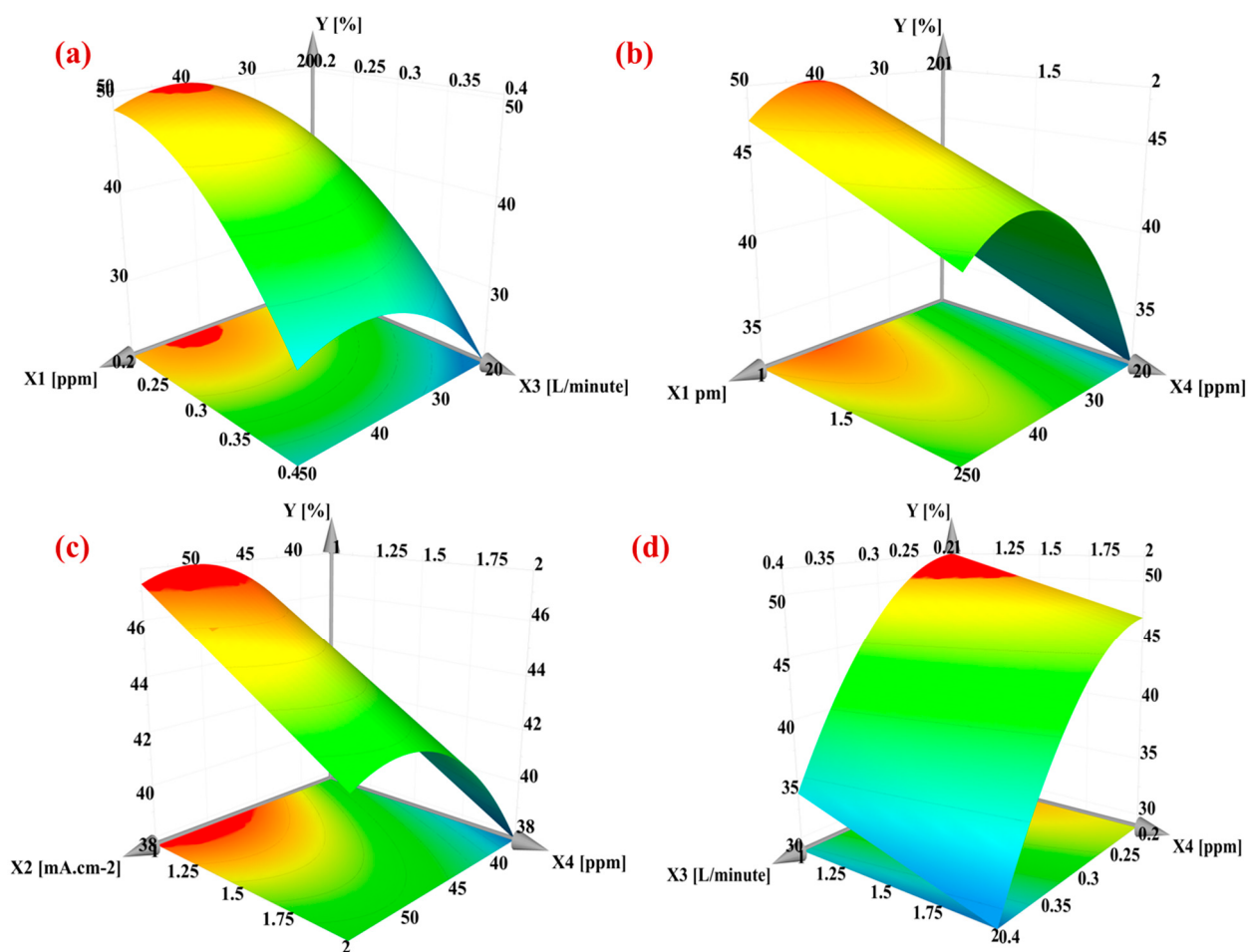


Figure S5. Three-dimensional response surface for fenobucarb removal efficiency.

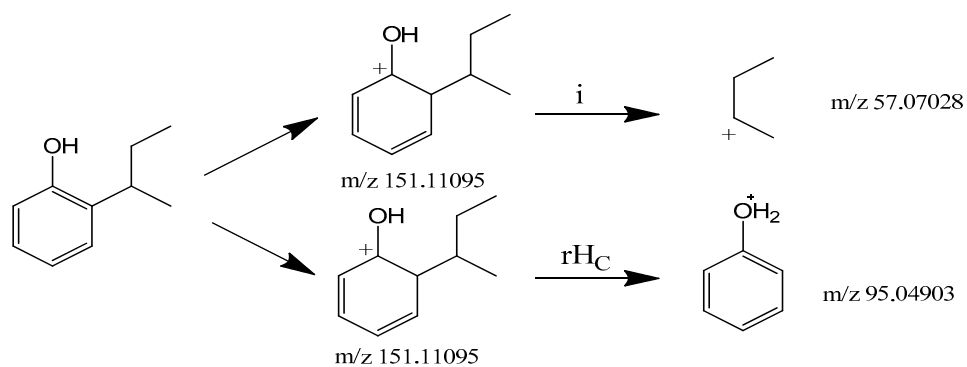


Figure S6. 2-(sec-butyl) phenol and fragmentation.

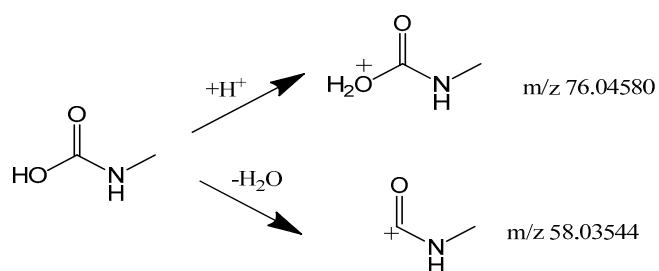


Figure S7. Methylcarbamic and fragmentation.

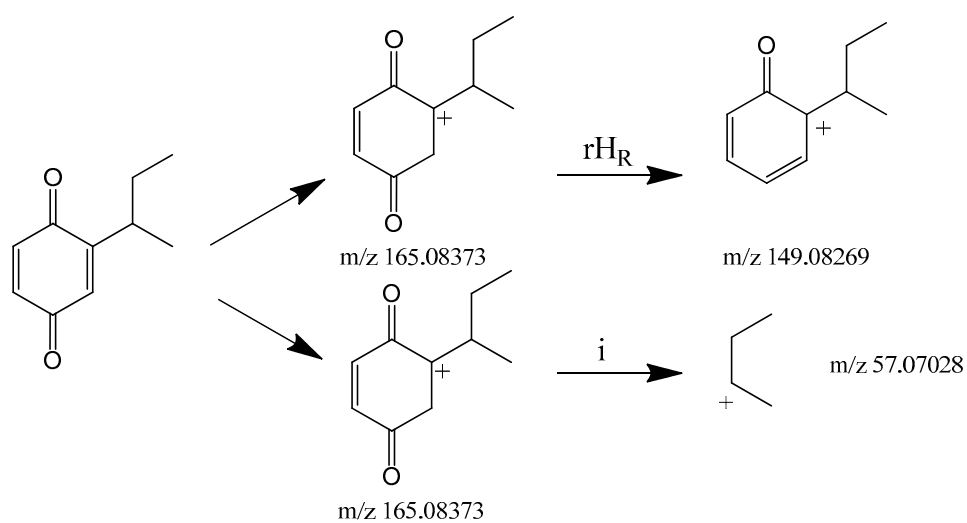


Figure S8. 2-(sec-butyl) cyclohexane-2,5-diene-1,4-dione fragmentation.

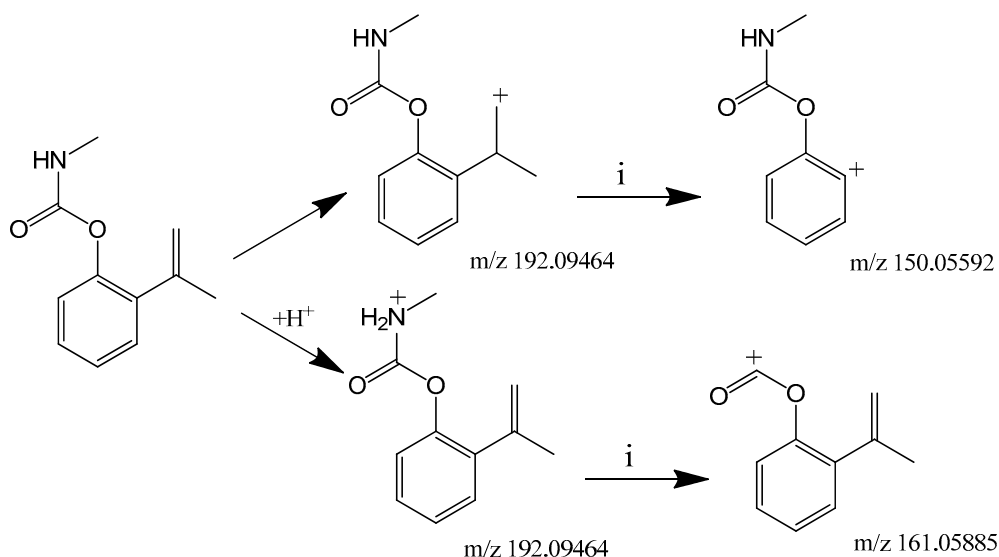


Figure S9. 2-(prop-1-en-2-yl) phenyl methylcarbamate fragmentation.

Table 1. Components percentage of elements.

Spectrum 1				
Element	Line Type	Weight %	Weight % Sigma	Atomic %
O	K series	48.37	0.37	77.94
Ti	K series	31.79	0.26	17.11
Ru	L series	12.57	0.22	3.21
Ir	M series	4.63	0.17	0.62
Si	K series	0.21	0.03	0.19
Tl	M series	1.21	0.18	0.15
Ca	K series	1.21	0.05	0.78
Total		100.00		100.00

Table S2. Reactions at electrode and solution.

Reaction	E ⁰ (V)	k
Anode		
$2\text{Cl}^- \rightarrow \text{Cl}_2 + 2\text{e}^-$ (1)	1.36	
$2\text{H}_2\text{O} \rightarrow \text{O}_2 + 4\text{H}^+ + 2\text{e}^-$ (2)	1.23	
$\text{H}_2\text{O} + \text{O}_2 \rightarrow \text{O}_3 + 2\text{H}^+ + 2\text{e}^-$ (3)		
$3\text{H}_2\text{O} + \text{O}_2 \leftrightarrow \text{O}_3 + 6\text{H}^+ + 6\text{e}^-$ (4)	1.51	
$6\text{HOCl} + 3\text{H}_2\text{O} \rightarrow 2\text{ClO}_3^- + 4\text{Cl}^- + 12\text{H}^+ + 3/2\text{O}_2 + 6\text{e}^-$ (5)		
$6\text{OCl}^- + 3\text{H}_2\text{O} \rightarrow 2\text{ClO}_3^- + 4\text{Cl}^- + 6\text{H}^+ + 3/2\text{O}_2 + 6\text{e}^-$ (6)	0.46	
$\text{Cl}^- + 3\text{H}_2\text{O} \rightarrow \text{ClO}_3^- + 6\text{H}^+ + 6\text{e}^-$ (7)		
$\text{ClO}_2^- + 2\text{OH}^- \rightarrow \text{ClO}_3^- + \text{H}_2\text{O} + 2\text{e}^-$ (8)		
$\text{ClO}_3^- \rightarrow \text{ClO}_3^\bullet + \text{e}^-$ (9)		
$\text{ClO}_3^\bullet + \text{OH}^- \rightarrow \text{ClO}_4^- + \text{H}^+ + \text{e}^-$ (10)		
$\text{ClO}_3^- + \text{H}_2\text{O} \rightarrow \text{ClO}_4^- + 2\text{H}^+ + 2\text{e}^-$ (11)	1.19	
$\text{H}_2\text{O} + \text{M} \rightarrow \text{MOH}^\bullet + \text{H}^+ + \text{e}^-$ (12)		
$\text{MOH}^\bullet + \text{R} \rightarrow \text{M} + \text{RO} + \text{H}^+ + \text{e}^-$ (13)		
$2\text{Cl}^- + \text{H}_2\text{O} \rightarrow \text{Cl}_2 + 2\text{e}^-$ (14)		
Cathode		

$\text{H}_2\text{O} \rightarrow \text{OH}^\bullet + \text{H}^+ + \text{e}^-$ (15)	2.59
$\text{OCl}^- + \text{H}_2\text{O} + 2\text{e}^- \rightarrow \text{Cl}^- + 2\text{OH}^-$ (16)	
$\text{OCl}^- + 2\text{OH}^- \rightarrow \text{ClO}_2^- + \text{H}_2\text{O} + 2\text{e}^-$ (17)	
Side reactions in solution	
$\text{Cl}_2 + \text{H}_2\text{O} \leftrightarrow \text{HOCl} + \text{H}^+ + \text{Cl}^-$ (18)	
$\text{HOCl} \leftrightarrow \text{OCl}^- + \text{H}^+$ (19)	7.47 M^{-1}
$\text{OCl}^- + \text{ClO}_2^- \rightarrow \text{ClO}_3^- + \text{Cl}^-$ (20)	
$\text{ClO}_3^\bullet + \text{OH}^\bullet \rightarrow \text{ClO}_4^- + \text{H}^+$ (21)	
$\text{OH}^\bullet + \text{OH}^\bullet \rightarrow \text{H}_2\text{O}_2$ (22)	
$\text{HClO} + \text{ClO}^- \rightarrow \text{ClO}^\bullet + \text{Cl}^\bullet + \text{OH}^\bullet$ (23)	
$\text{ClO}^\bullet + \text{ClO}^- + \text{OH}^- \rightarrow 2\text{Cl}^- + 2\text{O} + \text{OH}^\bullet$ (24)	
$2\text{HClO} + \text{ClO}^- \rightarrow \text{ClO}_3^- + 2\text{Cl}^- + 2\text{H}^+$ (25)	$0.76 \text{ L}^2/\text{mol}^2$ at 70°C
Organics + $\text{OCl}^- \rightarrow$ Intermediates $\rightarrow \text{CO}_2 + \text{Cl}^- + \text{H}_2\text{O}$ (26)	

Table S3. Experiments matrix and results for model Y₁

Exp No	Run Order	Chloride concentration	Flow rate	Current density	pH	Active Chlorine concentration (mg/L)	
						Exp	Pred
		X ₁	X ₂	X ₃	X ₄		
1	15	-1	-1	-1	-1	7.21	6.68
2	1	1	-1	-1	-1	17.19	16.00
3	24	-1	1	-1	-1	3.71	2.40
4	16	1	1	-1	-1	9.12	8.69
5	17	-1	-1	1	-1	11.25	10.91
6	14	1	-1	1	-1	24.18	23.31
7	27	-1	1	1	-1	4.27	3.70
8	20	1	1	1	-1	14.51	13.08
9	25	-1	-1	-1	1	3.89	3.67
10	5	1	-1	-1	1	9.18	9.15
11	11	-1	1	-1	1	1.32	1.58
12	31	1	1	-1	1	5.35	4.04
13	21	-1	-1	1	1	6.98	6.80
14	3	1	-1	1	1	15.71	15.37
15	10	-1	1	1	1	2.25	1.79
16	28	1	1	1	1	7.42	7.34
17	8	-2	0	0	0	0.81	1.36
18	18	2	0	0	0	14.52	16.23
19	19	0	-2	0	0	15.71	16.43
20	29	0	2	0	0	2.58	4.12
21	2	0	0	-2	0	2.96	4.22
22	7	0	0	2	0	10.74	11.74
23	12	0	0	0	-2	8.76	10.96
24	13	0	0	0	2	2.15	2.20
25	26	0	0	0	0	8.10	6.23
26	9	0	0	0	0	7.64	6.23
27	22	0	0	0	0	6.48	6.23
28	4	0	0	0	0	4.11	6.23
29	6	0	0	0	0	6.70	6.23
30	30	0	0	0	0	6.14	6.23
31	23	0	0	0	0	4.41	6.23

Table S4. Regression coefficient of model Y₁

Active Chlorine	Coeff. SC	Std. Err.	P	Conf. int (±)
b₀	6.2257	0.5680	7.56162 × 10 ⁻⁹	1.2042
b₁	3.7167	0.3067	1.79116 × 10 ⁻⁹	0.6503
b₂	-3.0792	0.3068	2.60853 × 10 ⁻⁸	0.6503
b₃	1.8817	0.3068	1.4404 × 10 ⁻⁵	0.6503
b₄	-2.1900	0.3068	2.35191 × 10 ⁻⁶	0.6503
b₁₁	0.6419	0.2810	0.0363711	0.5958
b₂₂	1.0119	0.2810	0.00239664	0.5958
b₃₃	0.4382	0.2810	0.138551	0.5958
b₄₄	0.0894	0.2810	0.754513	0.5958
b₁₂	-0.7550	0.3757	0.0616653	0.7965
b₁₃	0.7725	0.3757	0.0564724	0.7965
b₁₄	-0.9588	0.3757	0.0213275	0.7965
b₂₃	-0.7312	0.3757	0.0694042	0.7965
b₂₄	0.5500	0.3757	0.162606	0.7965
b₃₄	-0.2725	0.3757	0.47876	0.7965
N = 31	Q ² = 0.832		Cond. no =4.686	
DF = 16	R ² = 0.959		RSD =1.503	
	R ² adj. = 0.923			
			Confidence =	0.95

Table S5. Coefficient adjustment of model Y₁

Y1	Coeff. SC	Std. Err.	P	Conf. int (±)
b ₀	6.7127	0.5006	2.33838 × 10 ⁻¹²	1.0356
b ₁	3.7167	0.3684	6.48394 × 10 ⁻¹⁰	0.7622
b ₂	-3.0792	0.3684	2.01059 × 10 ⁻⁸	0.7622
b ₃	1.8817	0.3684	3.57792 × 10 ⁻⁵	0.7622
b ₄	-2.1900	0.3684	4.64083 × 10 ⁻⁶	0.7622
b ₁₁	0.5912	0.3341	0.0900471	0.6911
b ₂₂	0.9612	0.3341	0.00851059	0.6911
b ₁₄	-0.9588	0.4512	0.0445785	0.9335
N = 31	Q ² = 0.821		Cond. no. = 2.955	
DF = 23	R ² = 0.915		RSD = 1.805	
	R ² adj. = 0.889			
			Confidence = 0.95	

Table S6. Analysis of variance Y₁

Active Chlorine	DF	SS	MS (variance)	F	P	SD
Total	31	2825.160	91.130			
Constant	1	1941.830	1941.830			
Total corrected	30	883.329	29.444			5.426
Regression	7	808.395	115.485	35.4467	0.000	10.746
Residual	23	74.934	3.258			1.805
Lack of Fit	17	61.351	3.608	1.59411	0.293	1.899
(Model error)						
Pure error	6	13.583	2.265			1.505
(Replicate error)						
N = 31		Q ² =0.821		Cond. no =2.955		

DF = 23	R ² =0.915 R ² adj. =0.889	RSD =1.805
---------	---	------------

Table S7. Experiments matrix and results of Y₂

Run	Chloride	Current density	Flow rate	Fenobucarb	% Removal Efficiency	
					Exp	Pred
	X ₁ '	X ₂ '	X ₃ '	X ₄ '		
1	-1	-1	-1	-1	40.10	37.28
2	1	-1	-1	-1	47.36	46.64
3	-1	1	-1	-1	48.73	41.83
4	1	1	-1	-1	54.44	51.19
5	-1	-1	1	-1	19.22	19.13
6	1	-1	1	-1	23.99	28.49
7	-1	1	1	-1	25.37	23.69
8	1	1	1	-1	31.42	33.04
9	-1	-1	-1	1	27.27	32.32
10	1	-1	-1	1	36.27	41.68
11	-1	1	-1	1	38.07	36.88
12	1	1	-1	1	44.27	46.23
13	-1	-1	1	1	18.47	14.17
14	1	-1	1	1	22.86	23.53
15	-1	1	1	1	16.47	18.73
16	1	1	1	1	21.46	28.09
17	-2	0	0	0	7.40	13.13
18	2	0	0	0	39.36	31.84
19	0	-2	0	0	34.27	31.32
20	0	2	0	0	39.26	40.43
21	0	0	-2	0	43.72	45.84
22	0	0	2	0	13.46	9.55
23	0	0	0	-2	41.27	49.63
24	0	0	0	2	44.26	39.71
25	0	0	0	0	43.26	44.67
26	0	0	0	0	45.25	44.67
27	0	0	0	0	48.28	44.67
28	0	0	0	0	39.37	44.67
29	0	0	0	0	46.15	44.67
30	0	0	0	0	45.38	44.67
31	0	0	0	0	50.61	44.67

Table S8. Coefficient adjustment of Y₂

Y ₂	Coeff. SC	Std. Err.	P	Conf. int (±)
b' ₀	44.6716	1.5380	1.24915 × 10 ⁻¹⁹	3.1816
b' ₁	4.6788	0.9625	6.58892 × 10 ⁻⁵	1.9911
b' ₂	2.2779	0.9625	0.0267524	1.9911
b' ₃	-9.0738	0.9625	2.30026 × 10 ⁻⁹	1.9911
b' ₄	-2.4796	0.9625	0.0168888	1.9911

b'11	-5.5461	0.8768	1.87114×10^{-6}	1.8138
b'22	-2.1999	0.8768	0.0196029	1.8138
b'33	-4.2436	0.8768	6.94167×10^{-5}	1.8138
N = 31	Q ² = 0.726		Cond. no. = 3.783	
DF = 23	R ² = 0.890		RSD = 4.715	
	R ² adj. = 0.856		Confidence = 0.95	