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Supplementary Information

Supporting Information for

Removal efficiency and reaction kinetics of phenolic compounds in refinery wastewater by nano catalytic wet oxidation

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Supplementary Tables

Table S1
Optimal values of kinetic parameters are optimized using the nonlinear method of CAT-1

Parameter	Value	Unit
n	3.36	_
E_A	30.080	kJ/mol.
k_o	2.059578×10^{6}	$wt^{-2.268057}.min^{-1}$
SSE	2.450×10^{-5}	_

Table S 2
Optimal values of kinetic parameters are optimized using the nonlinear method of CAT-2

Parameter	Value	Unit
n	2.75	_
E_A	27.599	kJ/mol.
k_o	2.07113×10^{5}	$wt^{-1.756145}.min^{-1}$
SSE	1.375×10^{-5}	_

Table S3
Optimal values of kinetic parameters are optimized using the nonlinear method of CAT-3

Parameter	Value	Unit
n	1.98	_
E_A	26.254	kJ/mol.
k_o	20952	$wt^{-0.984583}.min^{-1}$
SSE	$8.70578*10^{-6}$	_

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Table S4
Experimental and simulation results using the nonlinear method of CAT-1

Temperature (°C)	Time (min)	Phenol concentration (ppm)		Conversion %		Error %
		Experimental	Predicted	Experimental	Predicted	
30	20	496	480.682	21.4619	23.84417	3.088
30	40	420	407.238	33.28149	35.26625	3.039
30	60	361	361.639	42.45723	42.35785	0.177
30	80	316	329.66	49.45568	47.33126	4.323
30	100	304	305.568	51.32193	51.07807	0.516
30	120	298	286.536	52.25505	54.03795	3.847
45	20	405	421.662	35.61431	33.02302	4.114
45	40	340	344.004	45.72317	45.10047	1.178
45	60	290	300.031	53.49922	51.93919	3.459
45	80	258	270.627	58.47589	56.51213	4.894
45	100	250	249.114	59.72006	59.85785	0.354
45	120	244	232.455	60.65319	62.44868	4.732
60	20	376	364.209	40.12442	41.95816	3.136
60	40	300	288.887	51.94401	53.67232	3.704
60	60	260	248.958	58.16485	59.88212	4.247
60	80	232	223.073	62.51944	63.90778	3.848
60	100	215	204.475	65.1633	66.80016	4.895
60	120	200	190.244	67.49611	69.01337	4.878
75	20	320	312.544	48.83359	49.99316	2.330
75	40	253	243.122	59.2535	60.78974	3.904
75	60	218	207.917	64.69673	66.26485	4.625
75	80	177	185.537	71.07309	69.74541	4.823
75	100	163	169.635	73.25039	72.21851	4.071
75	120	159	157.554	73.87247	74.09736	0.909

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Table S 5
Experimental and simulation results using the nonlinear method of CAT-2

Temperature (°C)	Time (min)	Phenol concentration (ppm)		Conversion %		Error %
		Experimental	Predicted	Experimental	Predicted	
30	20	435	427.219	30.94868	32.15879	1.789
30	40	354	339.13	43.54588	45.85848	4.201
30	60	293	287.883	53.03266	53.82846	1.746
30	80	243	253.529	60.80871	59.17123	4.333
30	100	237	228.526	61.74184	63.05972	3.576
30	120	218	209.321	64.69673	66.0465	3.981
45	20	345	361.889	44.94557	42.31897	4.895
45	40	272	274.337	56.2986	55.93515	0.859
45	60	226	227.881	63.45257	63.16003	0.832
45	80	189	198.167	69.20684	67.78118	4.850
45	100	176	177.153	71.22862	71.0493	0.655
45	120	167	161.132	72.6283	73.5409	3.514
60	20	312	301.733	50.07776	51.67449	3.291
60	40	228	220.941	63.14152	64.23935	3.096
60	60	187	180.842	69.51788	70.47558	3.293
60	80	161	155.984	73.56143	74.34152	3.116
60	100	143	138.723	76.36081	77.02597	2.991
60	120	130	125.873	78.38258	79.02442	3.175
75	20	258	250.031	58.47589	59.71524	3.089
75	40	183	178.634	70.13997	70.81897	2.386
75	60	150	144.8	75.27216	76.08087	3.467
75	80	119	124.248	80.09331	79.27714	4.410
75	100	108	110.141	81.80404	81.47107	1.982
75	120	98	99.718	83.35925	83.09207	1.753

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Table S 6
Experimental and simulation results using the nonlinear method of CAT-3

Temperature (°C)	Time (min)	Phenol concentration (ppm)		Conversion %		Error %
		Experimental	Predicted	Experimental	Predicted	
30	20	333	346.516	46.812	44.7098	4.059
30	40	250	237.862	59.720	61.60778	4.855
30	60	188	180.868	69.362	70.47154	3.794
30	80	140	145.801	76.827	75.92519	4.144
30	100	127	122.064	78.849	79.6168	3.887
30	120	110	104.954	81.493	82.27776	4.587
45	20	257	268.673	58.631	56.81602	4.542
45	40	178	169.857	70.918	72.18398	4.575
45	60	124	124.007	79.316	79.31462	0.006
45	80	93	97.553	84.137	83.42877	4.896
45	100	80	80.335	86.159	86.10653	0.419
45	120	69	68.283	87.869	87.98087	1.039
60	20	211	202.363	65.785	67.12862	4.093
60	40	125	119.847	79.160	79.96159	4.122
60	60	81	84.968	86.003	85.386	4.899
60	80	63	65.747	88.802	88.37527	4.360
60	100	55	53.583	90.047	90.26703	2.576
60	120	47	45.197	91.291	91.57123	3.836
75	20	157	150.242	74.184	75.23453	4.304
75	40	87	84.724	85.070	85.42395	2.616
75	60	59	58.872	89.425	89.44448	0.217
75	80	44	45.057	91.757	91.593	2.402
75	100	36	36.468	93.002	92.92877	1.300
75	120	30	30.615	93.935	93.83904	2.050

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Table S 7
Experimental and simulation results using the linear method of CAT-1

Temperature (°C)	Time (min)	Phenol concentration (ppm)		Conversion %		Error %
		Experimental	Predicted	Experimental	Predicted	
30	20	496	474.402	21.4619	24.82084	4.354
30	40	420	401.264	33.28149	36.19533	4.461
30	60	361	356.532	42.45723	43.1521	1.238
30	80	316	325.38	49.45568	47.99689	2.968
30	100	304	301.997	51.32193	51.63344	0.659
30	120	298	283.564	52.25505	54.50016	4.844
45	20	405	418.293	35.61431	33.54697	3.282
45	40	340	342.101	45.72317	45.39642	0.618
45	60	290	299.239	53.49922	52.06236	3.186
45	80	258	270.628	58.47589	56.51198	4.895
45	100	250	249.698	59.72006	59.76703	0.121
45	120	244	233.484	60.65319	62.28865	4.310
60	20	376	386.037	40.12442	38.56345	2.669
60	40	300	310.826	51.94401	50.26034	3.609
60	60	260	270.078	58.16485	56.59751	3.876
60	80	232	243.355	62.51944	60.7535	4.894
60	100	215	224.008	65.1633	63.76236	4.190
60	120	200	209.122	67.49611	66.07745	4.561
75	20	320	308.434	48.83359	50.63235	3.614
75	40	253	241.307	59.2535	61.07201	4.622
75	60	218	207.306	64.69673	66.35988	4.906
75	80	177	185.662	71.07309	69.72597	4.894
75	100	163	170.256	73.25039	72.12193	4.452
75	120	159	158.531	73.87247	73.94541	0.295

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Table S 8
Experimental and simulation results using the linear method of CAT-2

Temperature (°C)	Time (min)	Phenol concentration (ppm)		Conversion %		Error %
		Experimental	Predicted	Experimental	Predicted	
30	20	435	427.922	30.94868	32.04946	1.627
30	40	354	338.93	43.54588	45.88958	4.257
30	60	293	286.997	53.03266	53.96625	2.049
30	80	243	252.165	60.80871	59.38336	3.772
30	100	237	226.882	61.74184	63.3154	4.269
30	120	218	207.37	64.69673	66.34992	4.876
45	20	345	361.89	44.94557	42.31882	4.896
45	40	272	273.193	56.2986	56.11306	0.439
45	60	226	226.105	63.45257	63.43624	0.046
45	80	189	196.024	69.20684	68.11446	3.716
45	100	176	174.782	71.22862	71.41804	0.692
45	120	167	158.803	72.6283	73.90311	4.908
60	20	312	324.171	50.07776	48.18491	3.901
60	40	228	239.067	63.14152	61.42037	4.854
60	60	187	195.858	69.51788	68.14028	4.737
60	80	161	168.883	73.56143	72.33546	4.896
60	100	143	149.994	76.36081	75.27309	4.891
60	120	130	135.937	78.38258	77.45925	4.567
75	20	258	250.458	58.47589	59.64883	2.923
75	40	183	177.783	70.13997	70.95132	2.851
75	60	150	143.42	75.27216	76.29549	4.387
75	80	119	122.604	80.09331	79.53281	3.029
75	100	108	108.352	81.80404	81.7493	0.326
75	120	98	98.463	83.35925	83.28725	0.472

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Table S 9
Experimental and simulation results using the linear method of CAT-3

Temperature (°C)	Time (min)	Phenol concentration (ppm)		Conversion %		Error %
		Experimental	Predicted	Experimental	Predicted	
30	20	333	346.465	46.812	44.71773	4.044
30	40	250	237.728	59.720	61.62862	4.909
30	60	188	180.691	69.362	70.49907	3.888
30	80	140	145.605	76.827	75.95568	4.004
30	100	127	121.86	78.849	79.64852	4.047
30	120	110	104.748	81.493	82.3098	4.775
45	20	257	268.953	58.631	56.77247	4.651
45	40	178	169.988	70.918	72.16361	4.501
45	60	124	124.056	79.316	79.307	0.045
45	80	93	97.557	84.137	83.42815	4.900
45	100	80	80.331	86.159	86.10715	0.414
45	120	69	68.243	87.869	87.98709	1.097
60	20	211	201.24	65.785	67.30327	4.626
60	40	125	118.964	79.160	80.09891	4.829
60	60	81	84.251	86.003	85.49751	4.014
60	80	63	65.142	88.802	88.46936	3.400
60	100	55	53.059	90.047	90.34852	3.529
60	120	47	44.733	91.291	91.64339	4.823
75	20	157	149.437	74.184	75.35972	4.817
75	40	87	84.13	85.070	85.51633	3.299
75	60	59	58.4	89.425	89.51788	1.017
75	80	44	44.664	91.757	91.65412	1.509
75	100	36	36.13	93.002	92.98134	0.361
75	120	30	30.317	93.935	93.88538	1.057

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