Supplementary Material

for

Development and Evaluation of Operational Parameter Driven Mechanistic and Empirical Kinetic Models for Photocatalytic Degradation of Emerging Contaminants

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Appendix A: Data used for modeleing

Table S1. Dataset 1 extracted using Plot Digitizer [1]

Material	Time (min)	Dose (g/L)	Initial Concentration (mg/L)	Light Intensity (W)	Removal (%)
P-1	0	0.2	5	50	0
P-1	30	0.2	5	50	12.25806452
P-1	60	0.2	5	50	19.35483871
P-1	90	0.2	5	50	27.09677419
P-1	120	0.2	5	50	30.32258065
P-1	0	0.4	5	50	0
P-1	30	0.4	5	50	14.38848921
P-1	60	0.4	5	50	24.46043165
P-1	90	0.4	5	50	38.84892086
P-1	120	0.4	5	50	46.04316547
P-1	0	0.6	5	50	0
P-1	30	0.6	5	50	36.43410853
P-1	60	0.6	5	50	59.68992248
P-1	90	0.6	5	50	70.54263566
P-1	120	0.6	5	50	78.29457364
P-1	0	0.8	5	50	0
P-1	30	0.8	5	50	52
P-1	60	0.8	5	50	74.4
P-1	90	0.8	5	50	84
P-1	120	0.8	5	50	88.8
P-1	0	1.2	5	50	0
P-1	30	1.2	5	50	33.96226415
P-1	60	1.2	5	50	47.16981132
P-1	90	1.2	5	50	63.20754717
P-1	120	1.2	5	50	67.9245283
P-1	0	0.8	1	50	0
P-1	30	0.8	1	50	22.83950617
P-1	60	0.8	1	50	45.0617284
P-1	90	0.8	1	50	57.40740741
P-1	120	0.8	1	50	63.58024691
P-1	0	0.8	2	50	0
P-1	30	0.8	2	50	31.12582781
P-1	60	0.8	2	50	54.96688742
P-1	90	0.8	2	50	69.53642384
P-1	120	0.8	2	50	74.17218543
P-1	0	0.8	5	50	0
P-1	30	0.8	5	50	52.41935484
P-1	60	0.8	5	50	74.19354839
P-1	90	0.8	5	50	83.87096774
P-1	120	0.8	5	50	88.70967742
P-1	0	0.8	8	50	0
P-1	30	0.8	8	50	40.625
P-1	60	0.8	8	50	60.15625

P-1	90	0.8	8	50	72.65625
P-1	120	0.8	8	50	78.125
P-1	0	0.8	10	50	0
P-1	30	0.8	10	50	34.32835821
P-1	60	0.8	10	50	50
P-1	90	0.8	10	50	61.19402985
P-1	120	0.8	10	50	66.41791045

Table S2. Dataset 2 extracted using Plot Digitizer [1]

Material	Time (min)	Dose (g/L)	Initial Concentration (mg/L)	Light Intensity (W)	Removal (%)
P-1	0	0.2	5	50	0
P-1	30	0.2	5	50	11.53846154
P-1	60	0.2	5	50	15.38461538
P-1	90	0.2	5	50	19.23076923
P-1	120	0.2	5	50	23.71794872
P-1	0	0.4	5	50	0
P-1	30	0.4	5	50	30
P-1	60	0.4	5	50	44.66666667
P-1	90	0.4	5	50	54
P-1	120	0.4	5	50	60.66666667
P-1	0	0.4	5	50	0
P-1	30	0.6	5	50	43.88489209
P-1	60	0.6	5	50	69.78417266
P-1	90	0.6	5	50	82.01438849
P-1	120	0.6	5	50	86.33093525
P-1	0	0.8	5	50	0
P-1	30	0.8	5	50	63.07692308
P-1	60	0.8	5	50	83.07692308
P-1	90	0.8	5	50	91.53846154
P-1	120	0.8	5	50	94.61538462
P-1	0	1.2	5	50	0
P-1	30	1.2	5	50	48.71794872
P-1	60	1.2	5	50	65.81196581
P-1	90	1.2	5	50	76.92307692
P-1	120	1.2	5	50	82.90598291
P-1	0	0.8	1	50	0
P-1	30	0.8	1	50	25.30120482
P-1	60	0.8	1	50	52.40963855
P-1	90	0.8	1	50	63.25301205
P-1	120	0.8	1	50	69.27710843
P-1	0	0.8	2	50	0
P-1	30	0.8	2	50	28.48101266
P-1	60	0.8	2	50	61.39240506
P-1	90	0.8	2	50	74.6835443
P-1	120	0.8	2	50	79.74683544
P-1	0	0.8	5	50	0

P-1	30	0.8	5	50	62.79069767
P-1	60	0.8	5	50	82.94573643
P-1	90	0.8	5	50	91.47286822
P-1	120	0.8	5	50	94.57364341
P-1	0	0.8	8	50	0
P-1	30	0.8	8	50	51.85185185
P-1	60	0.8	8	50	68.88888889
P-1	90	0.8	8	50	82.22222222
P-1	120	0.8	8	50	85.18518519
P-1	0	0.8	10	50	0
P-1	30	0.8	10	50	36.55172414
P-1	60	0.8	10	50	57.93103448
P-1	90	0.8	10	50	71.72413793
P-1	120	0.8	10	50	75.17241379

Table S3. Dataset 3 extracted using Plot Digitizer [2]

Material	Time (min)	Dose (g/L)	Initial Concentration (mg/L)	Light Intensity (W)	Removal (%)
P-2	0	0.5	5	50	0
P-2	20	0.5	5	50	69.82758621
P-2	40	0.5	5	50	100
P-2	60	0.5	5	50	101.7241379
P-2	80	0.5	5	50	101.7241379
P-2	0	0.5	10	50	0
P-2	20	0.5	10	50	70.83333333
P-2	40	0.5	10	50	100
P-2	60	0.5	10	50	101.1904762
P-2	80	0.5	10	50	98.80952381
P-2	0	0.5	20	50	0
P-2	20	0.5	20	50	65.40540541
P-2	40	0.5	20	50	88.10810811
P-2	60	0.5	20	50	96.21621622
P-2	80	0.5	20	50	98.91891892
P-2	0	0.5	50	50	0
P-2	20	0.5	50	50	42.26804124
P-2	40	0.5	50	50	57.21649485
P-2	60	0.5	50	50	73.19587629
P-2	80	0.5	50	50	75.77319588
P-2	0	0.5	75	50	0
P-2	20	0.5	75	50	35.02538071
P-2	40	0.5	75	50	47.71573604
P-2	60	0.5	75	50	56.85279188
P-2	80	0.5	75	50	64.97461929
P-2	0	0.5	100	50	0
P-2	20	0.5	100	50	18.27411168
P-2	40	0.5	100	50	33.50253807
P-2	60	0.5	100	50	44.16243655

P-2	80	0.5	100	50	49.23857868
P-2	0	0.1	20	50	0
P-2	20	0.1	20	50	36.50793651
P-2	40	0.1	20	50	57.14285714
P-2	60	0.1	20	50	68.78306878
P-2	80	0.1	20	50	78.83597884
P-2	0	0.25	20	50	0
P-2	20	0.25	20	50	61.95652174
P-2	40	0.25	20	50	79.89130435
P-2	60	0.25	20	50	86.95652174
P-2	80	0.25	20	50	92.93478261
P-2	0	0.5	20	50	0
P-2	20	0.5	20	50	66.12903226
P-2	40	0.5	20	50	89.78494624
P-2	60	0.5	20	50	98.92473118
P-2	80	0.5	20	50	100
P-2	0	0.75	20	50	0
P-2	20	0.75	20	50	64.80446927
P-2	40	0.75	20	50	84.3575419
P-2	60	0.75	20	50	93.29608939
P-2	80	0.75	20	50	97.20670391
P-2	0	1	20	50	0
P-2	20	1	20	50	53.84615385
P-2	40	1	20	50	73.96449704
P-2	60	1	20	50	85.79881657
P-2	80	1	20	50	92.30769231
P-2	0	2	20	50	0
P-2	20	2	20	50	48.04469274
P-2	40	2	20	50	65.92178771
P-2	60	2	20	50	78.2122905
P-2	80	2	20	50	84.3575419

Table S4. Dataset 4 extracted using Plot Digitizer [3]

Material	Time (min)	Dose (g/L)	Initial Concentration (mg/L)	Light Intensity (W)	Removal (%)
P-3	0	0.1	10	50	0
P-3	30	0.1	10	50	14.74358974
P-3	60	0.1	10	50	26.28205128
P-3	90	0.1	10	50	34.61538462
P-3	120	0.1	10	50	37.17948718
P-3	0	0.25	10	50	0
P-3	30	0.25	10	50	30.40540541
P-3	60	0.25	10	50	47.97297297
P-3	90	0.25	10	50	56.75675676
P-3	120	0.25	10	50	61.48648649
P-3	0	0.5	10	50	0
P-3	30	0.5	10	50	41.72661871

P-3	60	0.5	10	50	64.74820144
P-3	90	0.5	10	50	73.38129496
P-3	120	0.5	10	50	82.01438849
P-3	0	0.75	10	50	0
P-3	30	0.75	10	50	47.79411765
P-3	60	0.75	10	50	72.79411765
P-3	90	0.75	10	50	84.55882353
P-3	120	0.75	10	50	93.38235294
P-3	0	0.75	10	50	0
P-3	30	1	10	50	40.76923077
P-3	60	1	10	50	66.15384615
P-3	90	1	10	50	81.53846154
P-3	120	1	10	50	87.69230769
P-3	0	0.75	1	50	0
P-3	30	0.75	1	50	30.26315789
P-3	60	0.75	1	50	53.28947368
P-3	90	0.75	1	50	66.44736842
P-3	120	0.75	1	50	75
P-3	0	0.75	5	50	0
P-3	30	0.75	5	50	38.29787234
P-3	60	0.75	5	50	63.82978723
P-3	90	0.75	5	50	75.17730496
P-3	120	0.75	5	50	80.85106383
P-3	0	0.75	10	50	0
P-3	30	0.75	10	50	47.05882353
P-3	60	0.75	10	50	72.05882353
P-3	90	0.75	10	50	84.55882353
P-3	120	0.75	10	50	92.64705882
P-3	0	0.75	15	50	0
P-3	30	0.75	15	50	29.57746479
P-3	60	0.75	15	50	54.22535211
P-3	90	0.75	15	50	69.71830986
P-3	120	0.75	15	50	77.46478873
P-3	0	0.75	20	50	0
P-3	30	0.75	20	50	28.18791946
P-3	60	0.75	20	50	48.99328859
P-3	90	0.75	20	50	63.75838926
P-3	120	0.75	20	50	70.46979866

Table S5. Dataset 5 extracted using Plot Digitizer [4]

Material	Time (min)	Dose (g/L)	Initial Concentration (mg/L)	Light Intensity (W)	Removal (%)
P-4	0	0.25	20	50	0
P-4	20	0.25	20	50	58.57142857
P-4	40	0.25	20	50	74.28571429
P-4	60	0.25	20	50	80
P-4	80	0.25	20	50	85.71428571

P-4	0	0.5	20	50	0
P-4	20	0.5	20	50	76.19047619
P-4	40	0.5	20	50	88.88888889
P-4	60	0.5	20	50	93.65079365
P-4	80	0.5	20	50	95.23809524
P-4	0	0.75	20	50	0
P-4	20	0.75	20	50	81.96721311
P-4	40	0.75	20	50	93.44262295
P-4	60	0.75	20	50	96.72131148
P-4	80	0.75	20	50	98.36065574
P-4	0	1	20	50	0
P-4	20	1	20	50	87.5
P-4	40	1	20	50	96.42857143
P-4	60	1	20	50	100
P-4	80	1	20	50	96.42857143
P-4	0	2	20	50	0
P-4	20	2	20	50	57.35294118
P-4	40	2	20	50	67.64705882
P-4	60	2	20	50	72.05882353
P-4	80	2	20	50	73.52941176
P-4	0	0.5	5	50	0
P-4	20	0.5	5	50	80.76923077
P-4	40	0.5	5	50	100
P-4	60	0.5	5	50	100
P-4	80	0.5	5	50	100
P-4	0	0.5	10	50	0
P-4	20	0.5	10	50	79.31034483
P-4	40	0.5	10	50	91.37931034
P-4	60	0.5	10	50	94.82758621
P-4	80	0.5	10	50	98.27586207
P-4	0	0.5	20	50	0
P-4	20	0.5	20	50	77.77777778
P-4	40	0.5	20	50	90.47619048
P-4	60	0.5	20	50	93.65079365
P-4	80	0.5	20	50	96.82539683
P-4	0	0.5	25	50	0
P-4	20	0.5	25	50	63.63636364
P-4	40	0.5	25	50	83.33333333
P-4	60	0.5	25	50	87.87878788
P-4	80	0.5	25	50	90.90909091
P-4	0	0.5	40	50	0
P-4	20	0.5	40	50	44.87179487
P-4	40	0.5	40	50	69.23076923
P-4	60	0.5	40	50	76.92307692
P-4	80	0.5	40	50	80.76923077

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37 **Table S6. Dataset 6 extracted using Plot Digitizer** [5]

Material	Time (min)	Dose (g/L)	Initial Concentration (mg/L)	Light Intensity (W)	Removal (%)
P-5	0	0.4	100	16	0
P-5	40	0.4	100	16	64.61538462
P-5	50	0.4	100	16	74.87179487
P-5	60	0.4	100	16	80
P-5	75	0.4	100	16	86.66666667
P-5	90	0.4	100	16	88.71794872
P-5	105	0.4	100	16	89.74358974
P-5	120	0.4	100	16	90.25641026
P-5	135	0.4	100	16	91.79487179
P-5	150	0.4	100	16	93.84615385
P-5	0	0.4	150	16	0
P-5	40	0.4	150	16	58.97435897
P-5	50	0.4	150	16	68.71794872
P-5	60	0.4	150	16	74.35897436
P-5	75	0.4	150	16	82.56410256
P-5	90	0.4	150	16	83.58974359
P-5	105	0.4	150	16	84.61538462
P-5	120	0.4	150	16	85.64102564
P-5	135	0.4	150	16	86.15384615
P-5	150	0.4	150	16	88.20512821
P-5	0	0.4	200	16	0
P-5	40	0.4	200	16	47.17948718
P-5	50	0.4	200	16	57.43589744
P-5	60	0.4	200	16	63.07692308
P-5	75	0.4	200	16	70.25641026
P-5	90	0.4	200	16	73.84615385
P-5	105	0.4	200	16	74.35897436
P-5	120	0.4	200	16	74.35897436
P-5	135	0.4	200	16	74.87179487
P-5	150	0.4	200	16	75.38461538
P-5	0	0.4	250	16	0
P-5	40	0.4	250	16	43.58974359
P-5	50	0.4	250	16	52.82051282
P-5	60	0.4	250	16	56.92307692
P-5	75	0.4	250	16	61.02564103
P-5	90	0.4	250	16	63.58974359
P-5	105	0.4	250	16	63.07692308
P-5	120	0.4	250	16	62.56410256
P-5	135	0.4	250	16	62.56410256
P-5	150	0.4	250	16	62.05128205
P-5	**0**	0.2	150	16	0
P-5	30	0.2	150	16	37.03703704
P-5	40	0.2	150	16	56.61375661

P-5	50	0.2	150	16	67.72486772
P-5	60	0.2	150	16	71.42857143
P-5	75	0.2	150	16	74.6031746
P-5	90	0.2	150	16	74.6031746
P-5	105	0.2	150	16	75.13227513
P-5	120	0.2	150	16	77.77777778
P-5	135	0.2	150	16	79.36507937
P-5	150	0.2	150	16	78.30687831
P-5	**0**	0.4	150	16	-1.058201058
P-5	30	0.4	150	16	37.03703704
P-5	40	0.4	150	16	56.61375661
P-5	50	0.4	150	16	67.72486772
P-5	60	0.4	150	16	75.66137566
P-5	75	0.4	150	16	83.06878307
P-5	90	0.4	150	16	85.18518519
P-5	105	0.4	150	16	86.77248677
P-5	120	0.4	150	16	88.35978836
P-5	135	0.4	150	16	86.77248677
P-5	150	0.4	150	16	89.94708995
P-5	**0**	0.5	150	16	-1.058201058
P-5	30	0.5	150	16	44.97354497
P-5	40	0.5	150	16	59.78835979
P-5	50	0.5	150	16	75.13227513
P-5	60	0.5	150	16	82.01058201
P-5	75	0.5	150	16	88.35978836
P-5	90	0.5	150	16	90.47619048
P-5	105	0.5	150	16	91.53439153
P-5	120	0.5	150	16	92.06349206
P-5	135	0.5	150	16	93.12169312
P-5	150	0.5	150	16	94.17989418
P-5	**0**	0.6	150	16	-0.529100529
P-5	30	0.6	150	16	44.97354497
P-5	40	0.6	150	16	59.78835979
P-5	50	0.6	150	16	77.77777778
P-5	60	0.6	150	16	84.12698413
P-5	75	0.6	150	16	88.35978836
P-5	90	0.6	150	16	92.59259259
P-5	105	0.6	150	16	93.65079365
P-5	120	0.6	150	16	94.70899471
P-5	135	0.6	150	16	93.12169312
P-5	150	0.6	150	16	96.82539683
P-5	**0**	0.7	150	16	0
P-5	30	0.7	150	16	50.79365079
P-5	40	0.7	150	16	67.72486772
P-5	50	0.7	150	16	77.77777778
P-5	60	0.7	150	16	84.12698413
P-5	75	0.7	150	16	91.53439153
P-5	90	0.7	150	16	92.59259259

P-5	105	0.7	150	16	93.65079365
P-5	120	0.7	150	16	94.70899471
P-5	135	0.7	150	16	96.82539683
P-5	150	0.7	150	16	96.82539683
P-5	**0**	0.9	150	16	0
P-5	30	0.9	150	16	75.66137566
P-5	40	0.9	150	16	93.12169312
P-5	50	0.9	150	16	96.2962963
P-5	60	0.9	150	16	97.35449735
P-5	75	0.9	150	16	97.35449735
P-5	90	0.9	150	16	98.94179894
P-5	105	0.9	150	16	98.94179894
P-5	120	0.9	150	16	100
P-5	135	0.9	150	16	100.5291005
P-5	150	0.9	150	16	100.5291005
P-5	**0**	0.6	150	8	1.477832512
P-5	30	0.6	150	8	44.82758621
P-5	40	0.6	150	8	57.63546798
P-5	50	0.6	150	8	65.51724138
P-5	60	0.6	150	8	72.90640394
P-5	75	0.6	150	8	74.38423645
P-5	90	0.6	150	8	76.84729064
P-5	105	0.6	150	8	77.33990148
P-5	120	0.6	150	8	79.31034483
P-5	135	0.6	150	8	79.31034483
P-5	150	0.6	150	8	79.80295567
P-5	**0**	0.6	150	16	1.477832512
P-5	30	0.6	150	16	44.82758621
P-5	40	0.6	150	16	63.05418719
P-5	50	0.6	150	16	74.87684729
P-5	60	0.6	150	16	81.28078818
P-5	75	0.6	150	16	86.20689655
P-5	90	0.6	150	16	88.1773399
P-5	105	0.6	150	16	91.13300493
P-5	120	0.6	150	16	91.62561576
P-5	135	0.6	150	16	93.10344828
P-5	150	0.6	150	16	94.58128079

Table S7. Dataset 7 extracted using Plot Digitizer [6]

Material	Time (min)	Dose (g/L)	Initial Concentration (mg/L)	Light Intensity (mW/cm^2)	Removal (%)
P-6	0	0.05	10	60	0
P-6	5	0.05	10	60	9.683257919
P-6	10	0.05	10	60	15.38461538
P-6	15	0.05	10	60	18.37104072
P-6	30	0.05	10	60	27.87330317
P-6	45	0.05	10	60	28.95927602

P-6	60	0.05	10	60	30.58823529
P-6	75	0.05	10	60	30.58823529
P-6	90	0.05	10	60	30.58823529
P-6	0	0.15	10	60	0
P-6	5	0.15	10	60	20.54298643
P-6	10	0.15	10	60	27.87330317
P-6	15	0.15	10	60	34.9321267
P-6	30	0.15	10	60	49.86425339
P-6	45	0.15	10	60	53.12217195
P-6	60	0.15	10	60	53.93665158
P-6	75	0.15	10	60	55.56561086
P-6	90	0.15	10	60	55.83710407
P-6	0	0.3	10	60	0
P-6	5	0.3	10	60	29.23076923
P-6	10	0.3	10	60	47.69230769
P-6	15	0.3	10	60	59.36651584
P-6	30	0.3	10	60	71.58371041
P-6	45	0.3	10	60	77.28506787
P-6	60	0.3	10	60	82.44343891
P-6	75	0.3	10	60	88.41628959
P-6	90	0.3	10	60	89.77375566
P-6	0	0.4	10	60	0
P-6	5	0.4	10	60	34.38914027
P-6	10	0.4	10	60	49.59276018
P-6	15	0.4	10	60	61.26696833
P-6	30	0.4	10	60	87.87330317
P-6	45	0.4	10	60	91.13122172
P-6	60	0.4	10	60	92.760181
P-6	75	0.4	10	60	94.9321267
P-6	90	0.4	10	60	95.47511312
P-6	0	0.8	10	60	0
P-6	5	0.8	10	60	34.38914027
P-6	10	0.8	10	60	49.59276018
P-6	15	0.8	10	60	61.26696833
P-6	30	0.8	10	60	87.87330317
P-6	45	0.8	10	60	93.03167421
P-6	60	0.8	10	60	94.66063348
P-6	75	0.8	10	60	96.83257919
P-6	90	0.8	10	60	97.37556561
P-6	0	0.3	100	60	0
P-6	5	0.3	100	60	8.791208791
P-6	10	0.3	100	60	15.10989011
P-6	15	0.3	100	60	21.15384615
P-6	30	0.3	100	60	29.12087912
P-6	45	0.3	100	60	30.76923077
P-6	60	0.3	100	60	33.79120879
P-6	75	0.3	100	60	35.98901099
P-6	90	0.3	100	60	36.26373626

P-6	0	0.3	75	60	0
P-6	5	0.3	75	60	21.97802198
P-6	10	0.3	75	60	35.71428571
P-6	15	0.3	75	60	44.50549451
P-6	30	0.3	75	60	53.57142857
P-6	45	0.3	75	60	57.96703297
P-6	60	0.3	75	60	62.08791209
P-6	75	0.3	75	60	68.40659341
P-6	90	0.3	75	60	68.40659341
P-6	0	0.3	50	60	0
P-6	5	0.3	50	60	25.27472527
P-6	10	0.3	50	60	41.20879121
P-6	15	0.3	50	60	51.37362637
P-6	30	0.3	50	60	62.08791209
P-6	45	0.3	50	60	66.48351648
P-6	60	0.3	50	60	71.7032967
P-6	75	0.3	50	60	78.02197802
P-6	90	0.3	50	60	78.57142857
P-6	0	0.3	25	60	0
P-6	5	0.3	25	60	27.74725275
P-6	10	0.3	25	60	44.50549451
P-6	15	0.3	25	60	55.76923077
P-6	30	0.3	25	60	66.20879121
P-6	45	0.3	25	60	71.7032967
P-6	60	0.3	25	60	76.37362637
P-6	75	0.3	25	60	82.96703297
P-6	90	0.3	25	60	83.79120879
P-6	0	0.3	10	60	0.549450549
P-6	5	0.3	10	60	30.49450549
P-6	10	0.3	10	60	48.35164835
P-6	15	0.3	10	60	59.61538462
P-6	30	0.3	10	60	71.42857143
P-6	45	0.3	10	60	77.74725275
P-6	60	0.3	10	60	82.41758242
P-6	75	0.3	10	60	88.73626374
P-6	90	0.3	10	60	90
P-6	0	0.4	10	45	0
P-6	5	0.4	10	45	25.75757576
P-6	10	0.4	10	45	36.36363636
P-6	15	0.4	10	45	46.71717172
P-6	30	0.4	10	45	59.09090909
P-6	45	0.4	10	45	69.19191919
P-6	60	0.4	10	45	70.70707071
P-6	75	0.4	10	45	73.98989899
P-6	90	0.4	10	45	74.74747475
P-6	0	0.4	10	60	0.757575758
P-6	5	0.4	10	60	33.83838384
P-6	10	0.4	10	60	49.24242424

P-6	15	0.4	10	60	61.11111111
P-6	30	0.4	10	60	86.36363636
P-6	45	0.4	10	60	91.41414141
P-6	60	0.4	10	60	93.93939394
P-6	75	0.4	10	60	95.45454545
P-6	90	0.4	10	60	96.46464646
P-6	0	0.4	10	75	0
P-6	5	0.4	10	75	37.12121212
P-6	10	0.4	10	75	54.7979798
P-6	15	0.4	10	75	67.42424242
P-6	30	0.4	10	75	89.64646465
P-6	45	0.4	10	75	95.95959596
P-6	60	0.4	10	75	98.98989899
P-6	75	0.4	10	75	100.2525253
P-6	90	0.4	10	75	100.5050505

Table S8. Validation Dataset extracted using Plot Digitizer [7]

Time (min)	Dose (g/L)	Initial Concentration (mg/L)	Removal Efficiency (%)
0	0.01	10	0
12	0.01	10	18.13953488
24	0.01	10	26.04651163
36	0.01	10	34.41860465
48	0.01	10	41.39534884
60	0.01	10	51.62790698
72	0.01	10	65.58139535
0	0.02	10	0
12	0.02	10	29.76744186
24	0.02	10	40.93023256
36	0.02	10	61.86046512
48	0.02	10	73.02325581
60	0.02	10	83.72093023
72	0.02	10	93.02325581
0	0.04	10	0
12	0.04	10	40
24	0.04	10	53.02325581
36	0.04	10	75.81395349
48	0.04	10	86.04651163
60	0.04	10	94.88372093
72	0.04	10	99.53488372
0	0.02	5	0
12	0.02	5	0
24	0.02	5	1.449275362
36	0.02	5	7.246376812
48	0.02	5	8.695652174

60	0.02	5	14.00966184
72	0.02	5	16.42512077
0	0.02	10	0
12	0.02	10	26.57004831
24	0.02	10	38.16425121
36	0.02	10	57.00483092
48	0.02	10	65.2173913
60	0.02	10	83.57487923
72	0.02	10	92.2705314
0	0.02	20	0
12	0.02	20	31.40096618
24	0.02	20	46.37681159
36	0.02	20	67.63285024
48	0.02	20	76.32850242
60	0.02	20	90.33816425
72	0.02	20	95.65217391

Table S9. Sensitivity Parameters for different Datasets across Different Models

		Model 1	Model 2	Model 3	Model 4	Model 5	Model 6
Dataset 1	Time	0.7295	0.7339	0.7376	0.7050	0.6648	0.7249
	Dose	0.3419	0.4435	0.4914	0.6579	0.4520	0.4845
	IC	-0.0472	0.0000	0.0466	0.0412	0.0582	0.0363
Dataset 2	Time	0.5696	0.5827	0.6174	0.7603	0.6777	0.5994
	Dose	0.3563	0.3717	0.5235	0.7018	0.4997	0.3667
	IC	-0.0397	0.0840	0.0677	0.0580	0.0816	0.0628
Dataset 3	Time	0.4492	0.4701	0.4567	0.8274	0.2872	0.3510
	Dose	0.4354	0.0677	0.1730	-0.0205	0.0335	0.2776
	IC	-0.4511	-0.3710	-0.3574	-0.3190	-0.2197	-0.2679
Dataset 4	Time	0.7337	0.7355	0.7362	0.7807	0.7068	0.7248
	Dose	0.1302	0.2833	0.2832	0.5590	0.3061	0.3964
	IC	-0.1464	0.0000	-0.0475	-0.0440	0.0171	-0.0616
Dataset 5	Time	0.3295	0.3383	0.3454	10.0000	0.1807	0.3915
	Dose	0.2608	0.0000	0.1293	-20.8333	-0.0149	-0.1805
	IC	-0.2863	-0.2313	-0.2750	-21.9167	-0.1132	-1.4353
Dataset 6	Time	0.1921	0.2521	0.2600	0.3638	0.3315	0.2984
	Dose	0.1921	0.1705	0.2000	0.4026	0.2350	0.2249
	IC	-0.2224	-0.3412	-0.3799	-0.3224	0.0000	0.0000
	Light	0.1921	0.1752	0.2000	0.2649	0.1977	0.0847
Dataset 7	Time	0.0382	0.0286	0.0493	0.6361	0.2997	0.0843
	Dose	0.0379	0.0296	0.0513	0.2240	0.3311	0.0831
	IC	0.0352	-0.0183	-0.0148	-0.0257	-0.1507	0.0000
	Light	0.0379	0.0510	0.0513	0.1902	0.6385	0.0017

Table S10. Experimental study used for model validation purpose

Time (min)	Dose (g/L)	Initial Concentration (mg/L)	Light Intensity (W/m^2)	Removal (%)	Model Application
0	0.5	20	0	39	Training
30	0.5	20	31	39	Training
60	0.5	20	62	39	Training
90	0.5	20	77	39	Validation
120	0.5	20	81	39	Training
0	1	20	0	39	Training
30	1	20	43	39	Training
60	1	20	72	39	Validation
90	1	20	87	39	Training
120	1	20	91	39	Training
0	2	20	0	39	Validation
30	2	20	52	39	Training
60	2	20	71	39	Training
90	2	20	83	39	Training
120	2	20	89	39	Validation
0	1	10	0	39	Training
30	1	10	56	39	Training
60	1	10	85	39	Training
90	1	10	93	39	Training
120	1	10	97	39	Training
0	1	50	0	39	Training
30	1	50	36	39	Training
60	1	50	57	39	Training
90	1	50	73	39	Validation
120	1	50	79	39	Training
0	1	20	0	49	Training
30	1	20	56	49	Validation
60	1	20	78	49	Training
90	1	20	92	49	Training
120	1	20	98	49	Training
0	1	20	0	66	Training
30	1	20	57	66	Validation
60	1	20	81	66	Training
90	1	20	93	66	Training
120	1	20	97	66	Training

Appendix B: Optimization Code

```
% ====================================================
% Decision variables:
```

```
% x(1) = time (t)
% x(2) = dose (D)
% x(3) = light intensity (I0)
% x(4) = initial concentration (C)
% ============================================================

% ------------------ Bounds ------------------
lb = [0    0.5   39   10];
ub = [120  2.0   66   50];

x0 = [30  1.0   50   20];

opts = optimoptions('fmincon','Display','off');

% ------------------ Constants ------------------
k = 0.0009;
a = 0.3002;
b = 0.8276;
c = 0.4464;
d = 0.2354;

% ------------------ MODEL (anonymous function) ------------------
removal = @(x) (1 - exp( ...
    -x(1) * (k * (x(2)^a * x(3)^b) / (x(4)^c * d)) ...    )) * 100;

% ============================================================
% CASE 1: Maximize removal at lowest time
wt = 0.05;
obj1 = @(x) -removal(x) + wt*x(1);

[x1,~] = fmincon(obj1,x0,[],[],[],[],lb,ub,[],opts);
R1 = removal(x1);

disp('--- Max Removal at Lowest Time ---')
```

```
disp(' Time   Dose   Intensity   Concentration   Removal')
disp([x1 R1])

% ========================================================
% CASE 2: Maximize removal at minimum dose
wd = 5;
obj2 = @(x) -removal(x) + wd*x(2);

[x2,~] = fmincon(obj2,x0,[],[],[],[],lb,ub,[],opts);
R2 = removal(x2);

disp('--- Max Removal at Minimum Dose ---')
disp(' Time   Dose   Intensity   Concentration   Removal')
disp([x2 R2])
```

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