Electronic Supplementary Information (ESI)

Machine-Learning Assisted Optimisation During Heterogeneous Photocatalytic Degradation Utilising a Static Mixer under Continuous Flow

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1. Additional figures and data

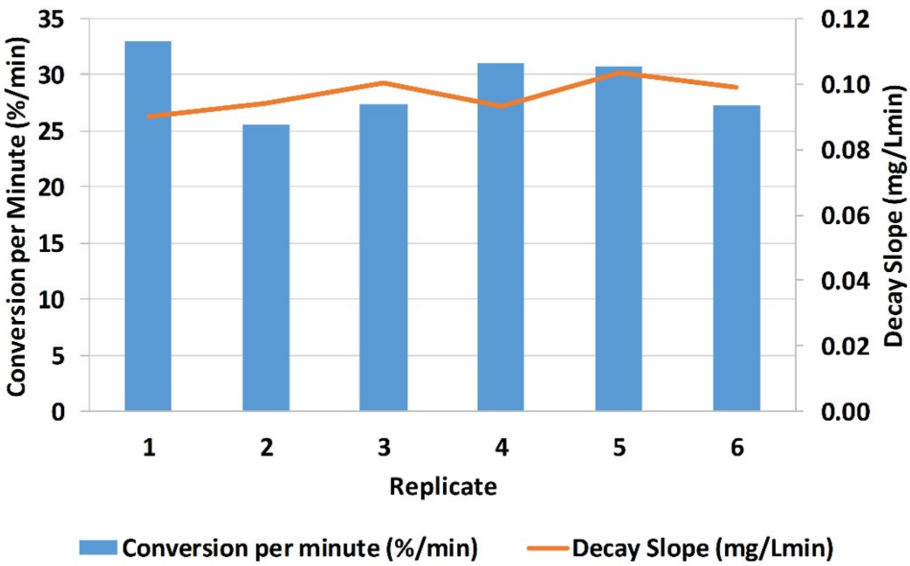

Figure S1 – Replicate experiments processing 0.7 – 1.0 L of Reactive Orange 16 dye through the continuous photoreactor with catalyst regeneration carried out at the end of each experiment. Conditions: residence time = 3.22 min, temperature = 20 °C and reactor pressure = 10 bar.

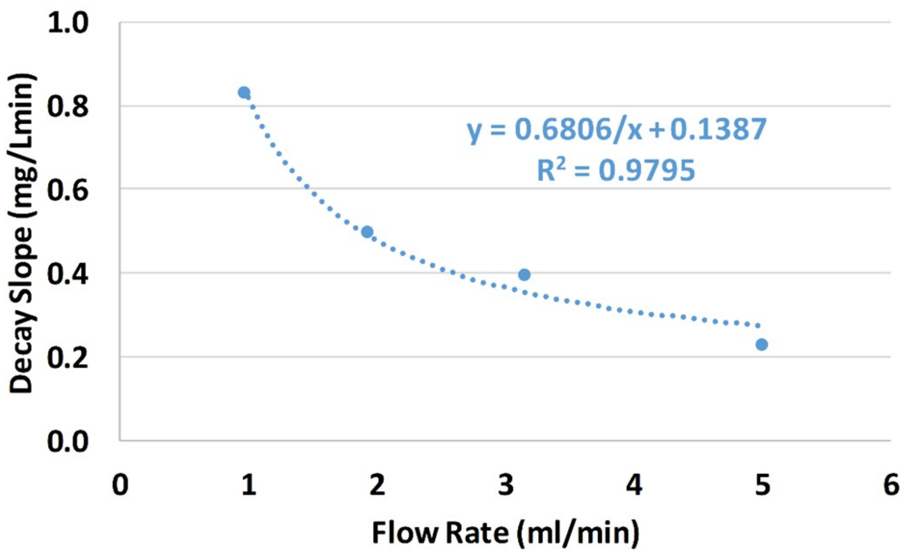

Figure S2 – Variation in the catalyst activity decay slope observed at different flow rates of Reactive Orange 16. A reciprocal function fitted over the observed flow rate range is shown. Conditions: temperature = 20 °C and reactor pressure = 10 bar.

Table S1 – Summary of experimental data from the experiments carried out during ML training (light blue. # 1 – 6) and optimisation (# 7 – 17) of the continuous flow photocatalytic degradation of the azo-dye Reactive Orange 16. Dye C_I is the initial Reactive Orange dye concentration, Q_S indicates the set flow rate, Q_M indicates the measured flow rate, τ indicates the residence time, T_S indicates the set temperature, T_M indicates the measured temperature, catalyst regen indicates if the catalyst was regenerated prior to the experiment or not, X indicates conversion and dye over catalyst is the amount of dye that had passed over the catalyst prior to the start of the reaction (UV lights on, steady state conditions).

#	Dye C_I (mg/L)	Q_S (ml/min)	Q_M (ml/min)	τ (min)	T_S (°C)	T_M (°C)	Catalyst (Regen.)	X (%)	X (%/min)	Dye over catalyst (mg)
1	84	3.00	3.13	1.99	20	19.9	Yes	77	38.6	13.2
2	75	0.98	1.00	6.24	24.4	23.0	Yes	96	15.4	12.2
3	75	10.00	7.10	0.88	20.0	20.5	Yes	50	56.9	0.0
4	75	3.00	3.09	2.02	20.0	19.1	Yes	80	39.6	9.0
5	75	1.00	1.02	6.12	20.0	19.8	No	97	15.9	23.0
6	75	3.00	3.13	1.99	80.0	68.9	No	93	46.6	30.8
7	74	7.50	6.94	0.90	20.0	19.0	Yes	57	63.4	10.4
8	74	7.30	7.27	0.86	38.6	35.5	No	50	58.3	32.9
9	74	8.99	8.92	0.70	20.0	19.4	No	29	41.5	71.7
10	85	9.01	7.92	0.79	79.9	67.5	Yes	73	92.7	12.8
11	85	9.96	8.60	0.73	78.1	66.3	No	63	86.8	24.4
12	85	8.05	7.43	0.84	79.5	67.5	No	60	71.4	38.2
13	85	9.96	9.64	0.65	57.6	49.4	No	39	60.3	62.0
14	81	9.99	8.99	0.69	80.0	67.4	No	62	89.3	92.6
15	81	7.47	7.59	0.82	79.9	67.3	Yes	84	102.2	15.7
16	81	7.26	7.34	0.85	71.2	60.8	No	74	87.0	28.2
17	81	9.98	10.00	0.62	58.3	50.5	No	52	83.3	39.8