Electronic Supplementary Material (ESI) for Environmental Science: Nano.

-Supporting Information-

Photocatalytic nanoparticles in flow-through annular photoreactors for continuous selenate reduction in industrial wastewater

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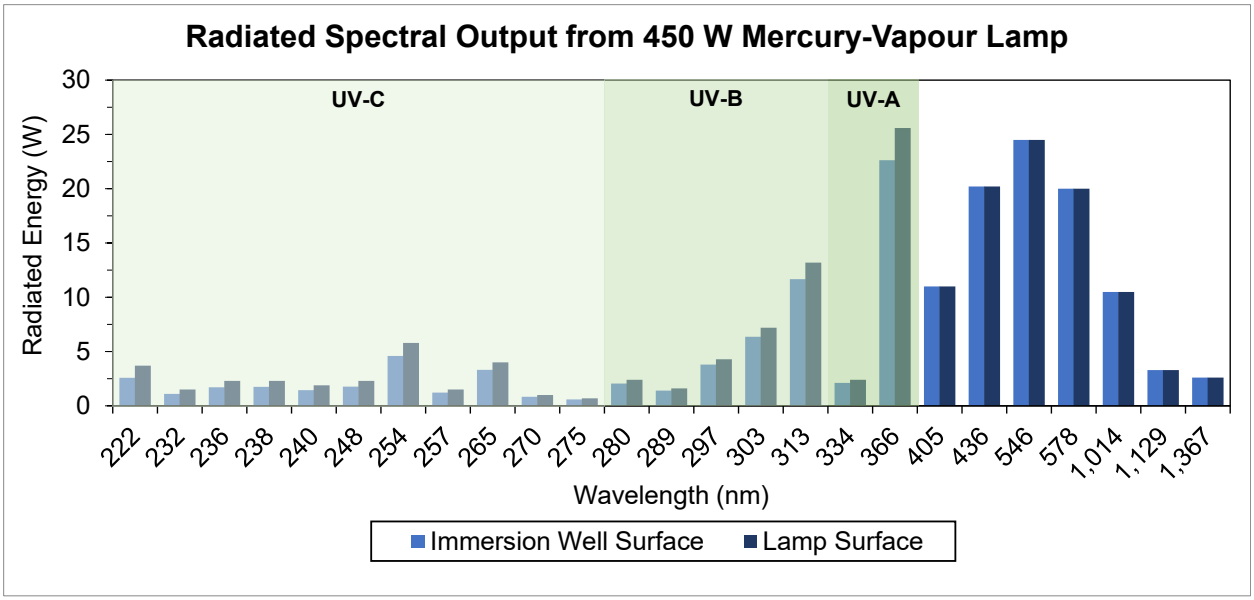

Figure S1: Radiated spectral output of 450W medium pressure UV lamp (Ace Glass Inc.) used throughout the study

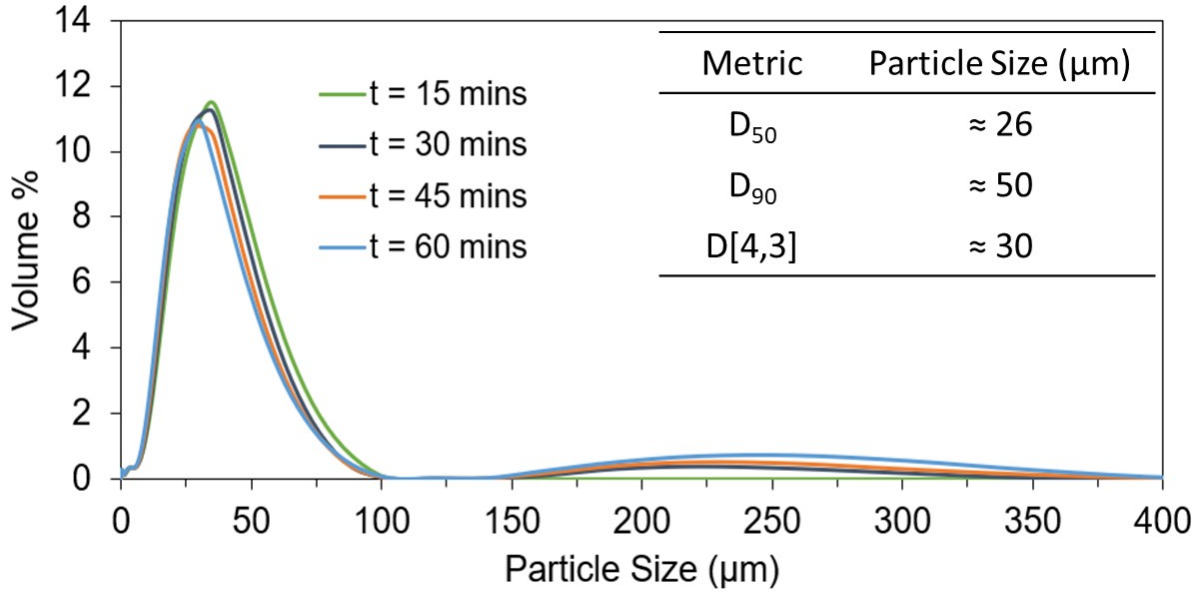

Figure S2: Particle size distribution measured through flow through cell laser light scattering. PSD tested after 15, 30, 45, and 60 minutes of mixing to observe potential changes over time.

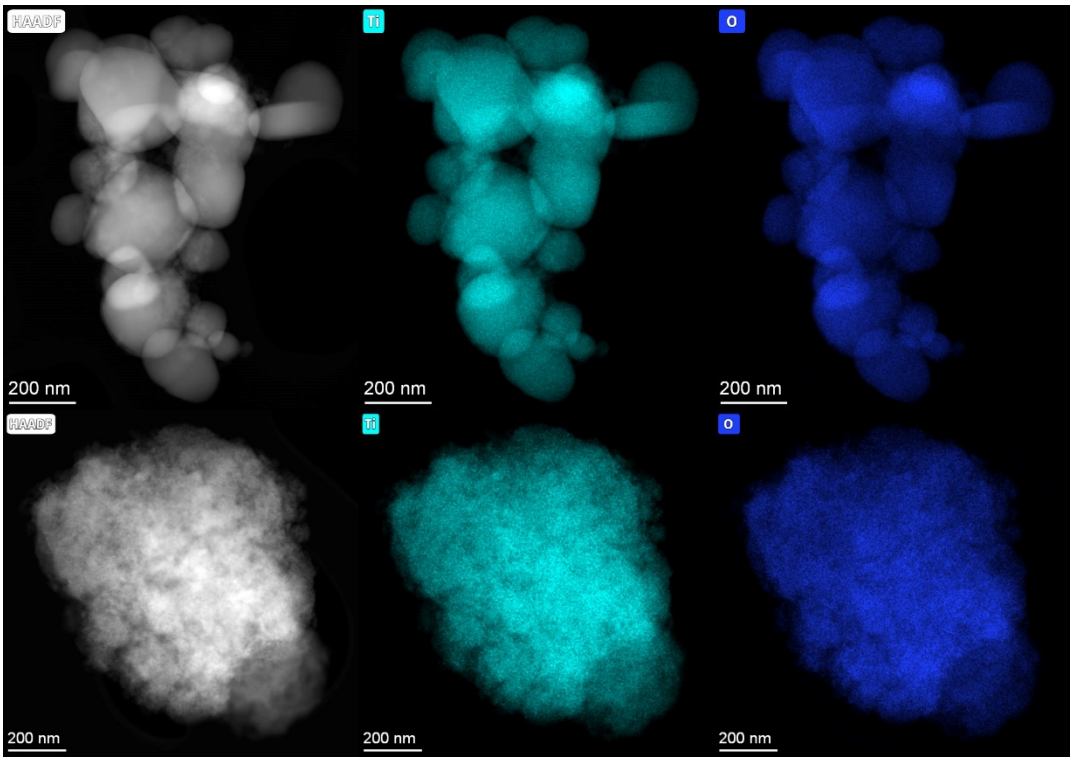

Figure S3: STEM-EDS elemental mapping of KRONOClean 7050 at clusters of large crystallite sizes (top row) and fine crystallites (bottom row). White: HAADF, cyan: Ti, blue: O.

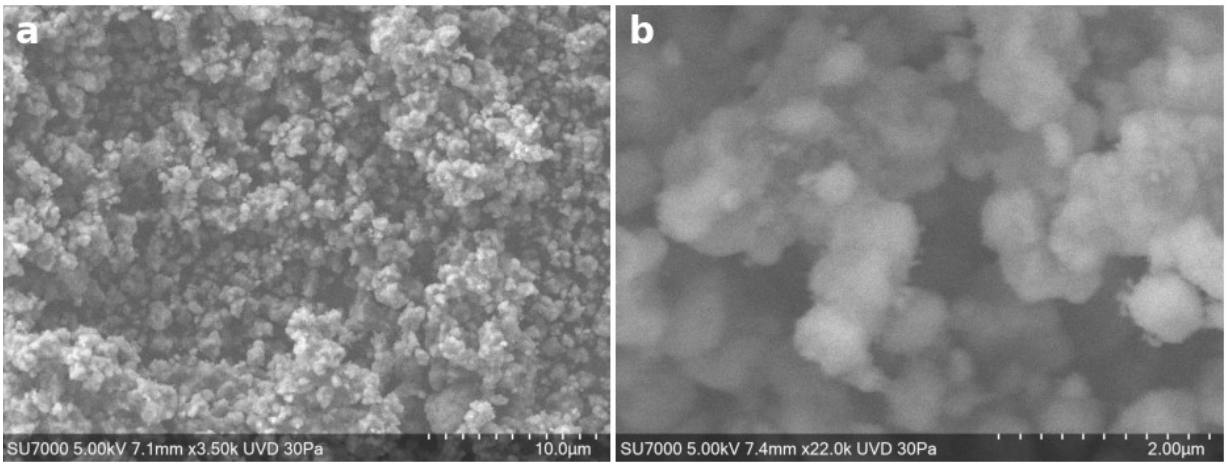

Figure S4: SEM images of bulk KRONOClean 7050 photocatalyst material at (**a)** 3500x magnification and (**b)** 22000x magnification.

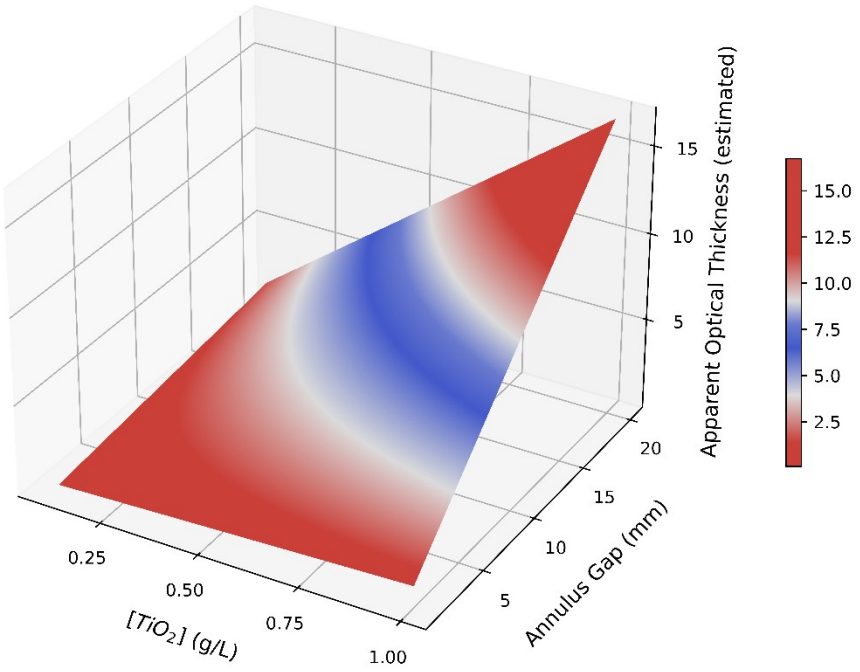

Figure S5: Surface response plot describing the effect of [TiO_2] and annulus gap on estimated apparent optical thickness, calculated using literature values for photocatalyst optical properties and SFM parameters (Table S2). Suggested values for efficient photon/photocatalyst usage represented in blue, while inefficient photon/photocatalyst usage represented in red.

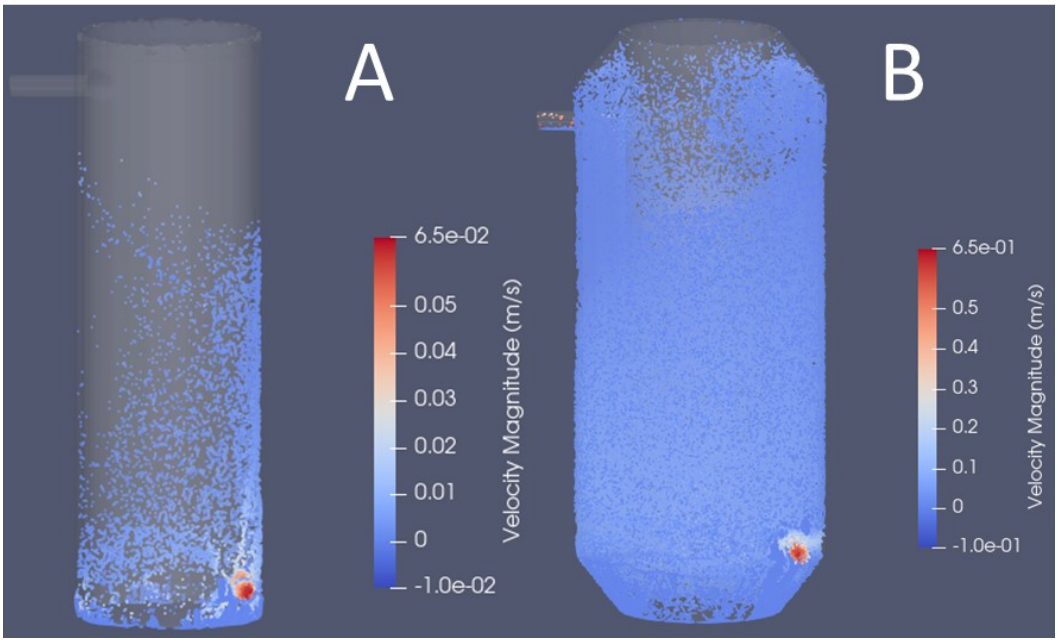

Figure S6: Snapshot of CFD modelling of (A) 47 mL reactor and (B) 502 mL reactor comparing photocatalyst particle positions at equal residence times and vertical velocities (0.39 cm/s). Snapshot taken after 60 seconds of simulation (~1.6 residence times).

Table S1: Characteristics of the three reactor vessels used to probe the effect of annulus thickness on photoreactor performance.

Specifications	**Units**	**Reactor #1**	**Reactor #2**	**Reactor #3**
Reactor Length	cm	15	15	15
Reactor Volume	mL	47	257	502
Annulus thickness	mm	2	9.5	16.5
Cross-sectional surface area	cm^2	3.14	17.16	33.43
UV Power per Working Volume	W/L	1781	326	167
UV Intensity	mW/cm^2	422	422	422

Table S2: Full Box-Behnken Design experimental results reporting measured Se removal % and calculated E_{EO} (from lamp specifications and residence time) as a function of the four factors of study: [TiO_2], [Formic acid], Annulus gap, and Velocity.

Factors (independent)				**Outputs (dependent)**	
[TiO2] (g/L)	**[FA] (mg/L)**	**Annulus Gap (mm)**	**Velocity (cm/s)**	**% Se Removal**	**E_{EO}**
1	600	9.5	0.39	77%	5.4
0.5	300	9.5	0.39	62%	8.4
0.5	600	9.5	0.39	72%	6.3
1	600	9.5	0.25	81%	7.4
0.25	600	9.5	0.25	67%	11.3
1	600	9.5	0.50	74%	4.6
0.25	600	9.5	0.50	63%	6.2
0.5	300	9.5	0.50	65%	6.0
0.5	900	9.5	0.50	74%	4.7
1	300	9.5	0.39	80%	4.9
0.25	900	9.5	0.39	62%	8.2
0.5	900	9.5	0.25	82%	7.3
0.5	300	9.5	0.25	70%	10.4
1	900	9.5	0.39	85%	4.3
0.25	300	9.5	0.39	45%	13.3
0.5	600	9.5	0.39	70%	6.6
0.5	900	16.5	0.39	54%	5.4
1	600	16.5	0.39	63%	4.1
0.5	600	16.5	0.50	44%	5.5
0.5	300	16.5	0.39	48%	6.2
0.5	600	16.5	0.25	64%	6.3
0.5	600	16.5	0.50	45%	5.4

1	600	16.5	0.50	59%	3.6
0.25	600	16.5	0.39	37%	8.8
0.5	600	2	0.39	55%	53.7
0.5	900	2	0.39	71%	35.4
1	600	2	0.39	86%	21.9
0.5	300	2	0.39	63%	43.1
0.25	600	2	0.39	44%	74.0
0.5	600	2	0.25	76%	48.4
0.5	600	2	0.50	55%	42.4
0.5	600	9.5	0.39	71%	6.42
0.5	600	9.5	0.39	73%	6.13
0.5	600	9.5	0.39	74%	5.98
1	600	9.5	0.39	82%	4.68
1	600	9.5	0.39	82%	4.70
1	600	9.5	0.39	82%	4.74
1	600	9.5	0.39	81%	4.80
0.25	600	9.5	0.39	60%	8.72
0.25	600	9.5	0.39	62%	8.37
0.25	600	9.5	0.39	63%	8.17
0.25	600	9.5	0.39	61%	8.45
0.5	900	9.5	0.39	75%	5.71
0.5	900	9.5	0.39	77%	5.45
0.5	900	9.5	0.39	77%	5.50
0.5	900	9.5	0.39	78%	5.24
0.5	300	9.5	0.39	49%	11.98
0.5	300	9.5	0.39	49%	11.98
0.5	300	9.5	0.39	55%	10.03
0.5	300	9.5	0.39	54%	10.28
0.5	600	16.5	0.39	50%	5.92
0.5	600	16.5	0.39	51%	5.76
0.5	600	16.5	0.39	54%	5.26
0.5	600	16.5	0.39	52%	5.501
0.5	600	2	0.39	56%	44.12
0.5	600	2	0.39	56%	43.53
0.5	600	2	0.39	60%	38.91
0.5	600	2	0.39	56%	43.45
0.5	600	9.5	0.5	72%	4.97
0.5	600	9.5	0.5	70%	5.14
0.5	600	9.5	0.5	85%	3.29
0.5	600	9.5	0.5	87%	3.09
0.5	600	9.5	0.25	90%	5.41
0.5	600	9.5	0.25	87%	6.03
0.5	600	9.5	0.25	87%	6.10

0.5	600	9.5	0.25	86%	6.30

Table S3: ANOVA results for response surface methodology and regression analysis for BBD data of continuous photocatalytic treatment of SMIB

Parameter	% Se Reduction			$E_{EO,UV}$		
	Parameter Estimate	t Value	Pr(>|t|)	Parameter Estimate	t Value	Pr(>|t|)
Intercept	40.52	1.20	0.24	99.14	4.38	< 0.00010
[TiO_2]	103.80	3.14	0.0028	-60.17	-2.72	0.0088
[FA]	0.099	2.23	0.030	-0.029	-0.99	0.33
Annulus Gap	5.94	3.76	0.00040	-11.32	-10.72	< 0.00010
Velocity	-309.56	-3.01	0.0040	33.29	0.48	0.63
[TiO_2] * [TiO_2]	-40.32	-2.71	0.0092	17.40	1.74	0.087
[FA] * [TiO_2]	-0.031	-1.17	0.25	0.011	0.61	0.54
[FA] * [FA]	-4.24E-5	-2.10	0.041	4.41E-6	0.33	0.75
A.G. * [TiO_2]	-1.53	-1.56	0.13	3.34	5.07	< 0.00010
A.G. * [FA]	-0.00016	-0.11	0.91	0.00079	0.84	0.41
A.G. * A.G.	-0.30	-8.87	< 0.00010	0.33	14.82	< 0.0010
Velocity * [TiO_2]	25.54	0.44	0.66	-30.87	-0.80	0.43
Velocity * [FA]	-0.011	-0.14	0.89	0.011	0.20	0.84
Velocity * A.G.	-0.65	-0.21	0.83	0.62	0.30	0.76
Velocity * Velocity	355.30	3.09	0.0032	-56.72	-0.74	0.46
Response Mean		66.62			12.88	
R-Square		0.84			0.94	
Coefficient of Variation		9.24			31.98	

Table S4: Literature values for photocatalyst optical properties and SFM parameters acquired from several studies using similar photocatalysts (Colina-Márquez et al., 2015, 2010, 2009), which are also close in value with those used in other studies (Grčić and Li Puma, 2013; Toepfer et al., 2006)

Parameter	**Value**
Absorption coefficient (κ)	174.7 m^2 / kg
Scattering coefficient (σ)	1295.8 m^2 / kg
Scattering albedo (ω)	0.881
Forward scattering probability (p_f)	0.11
Backward scattering probability (p_b)	0.71
Side scattering probability (p_s)	0.045
SFM parameter *a*	0.87
SFM parameter *b*	0.66
Corrected scattering albedo (ω_{corr})	0.75