Supplementary material to

From waste to resource: Computing-based optimization of used water filter for sustainable industrial effluent treatment

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Table S1. *Complete results from five independent runs of each LLM using the same six experimental observations and an identical standardised prompt for empirical response surface equation generation*

LLMs	Gemini 2.5 Flash with Extended Thinking					DeepSeek-R1 with Deep Think					GPT-5.6 Sol - High reasoning				
	Run 1	Run 2	Run 3	Run 4	Run 5	Run 1	Run 2	Run 3	Run 4	Run 5	Run 1	Run 2	Run 3	Run 4	Run 5
RMSE	11.64	11.64	14.88	11.64	11.64	11.64	11.64	0.00	0.00	11.64	11.64	11.64	11.64	11.64	11.64
MAE	8.15	8.15	13.32	8.15	8.15	8.15	8.15	0.00	0.00	8.15	8.15	8.15	8.15	8.15	8.15
R^2	0.7752	0.7752	0.6327	0.7752	0.7752	0.7752	0.7752	1.0000	1.0000	0.7752	0.7752	0.7752	0.7752	0.7752	0.7752
Estimated COD removal, %															
ID-1	76.15	76.15	81.32	76.15	76.15	76.15	76.15	68.00	68.00	76.15	76.15	76.15	76.15	76.15	76.15
ID-2	70.25	70.25	80.16	70.25	70.25	70.25	70.25	92.00	92.00	70.25	70.25	70.25	70.25	70.25	70.25
ID-3	59.31	59.31	69.64	59.31	59.31	59.31	59.31	43.00	43.00	59.31	59.31	59.31	59.31	59.31	59.31
ID-4	22.28	22.28	20.56	22.28	22.28	22.28	22.28	25.00	25.00	22.28	22.28	22.28	22.28	22.28	22.28
ID-5	89.00	89.00	77.16	89.00	89.00	89.00	89.00	89.00	89.00	89.00	89.00	89.00	89.00	89.00	89.00
ID-6	80.00	80.00	68.16	80.00	80.00	80.00	80.00	80.00	80.00	80.00	80.00	80.00	80.00	80.00	80.00
Estimated optimum operating condition															
V / L	1.0	1.0	1.2	1.0	1.0	1.0	1.0	1.35	1.35	1.0	1.0	1.0	1.0	1.0	1.0
Q / mL min^{-1}	200	200	480	200	200	200	200	480	480	200	200	200	200	200	200
COD removal, %	94.9	94.9	82.66	94.9	94.9	94.9	94.9	96.5	96.58	94.9	94.9	94.9	94.9	94.9	94.9

Gemini 2.5 Flash with Extended Thinking	Run 1	$Y = 111.6205+13.4273V-10.0909V^2-0118091Q+0.00089034Q^2$
	Run 2	$Y = 111.6205+13.4273V-10.0909V^2-0118091Q+0.00089034Q^2$
	Run 3	$Y = 45.4691+44.4307\ V-18.7030\ V^2+0.0450\ Q-0.000046875\ Q^2$
	Run 4	$Y = 111.6205+13.4273V-10.0909V^2-0118091Q+0.00089034Q^2$
	Run 5	$Y = 111.6205+13.4273V-10.0909V^2-0118091Q+0.00089034Q^2$
DeepSeek-R1 with Deep Think	Run 1	$Y = 111.62+13.43V-10.09V^2-0.1181Q+8.903\times10^{-5}\ Q^2$
	Run 2	$Y = 111.62+13.43V-10.09V^2-0.1181Q+8.903\times10^{-5}\ Q^2$
	Run 3	$Y = -508.125+1060.8333V-594.5V^2+99.6667V^3+0.045Q-0.000046875Q^2$
	Run 4	$Y = -508.125+1060.8333V-594.5V^2+99.6667V^3+0.045Q-0.000046875Q^2$
	Run 5	$Y = 111.62+13.43V-10.09V^2-0.1181Q+8.903\times10^{-5}\ Q^2$
GPT-5.6 Sol – High reasoning	Run 1	$Y = 111.6205+13.4273V-10.0909V^2-0.118091Q+8.90341\times10^{-5}\ Q^2$
	Run 2	$Y = 111.6205+13.4273V-10.0909V^2-0.118091Q+8.90341\times10^{-5}\ Q^2$
	Run 3	$Y = 111.6205+13.4273V-10.0909V^2-0.118091Q+8.90341\times10^{-5}\ Q^2$
	Run 4	$Y = 111.6205+13.4273V-10.0909V^2-0.118091Q+8.90341\times10^{-5}\ Q^2$
	Run 5	$Y = 111.6205+13.4273V-10.0909V^2-0.118091Q+8.90341\times10^{-5}\ Q^2$

The repeated-run analysis revealed different levels of consistency among the three LLMs. GPT-5.6 Sol produced identical outputs across all five independent runs, including the estimated COD removal values, goodness-of-fit and error metrics, and suggested optimum operating conditions. Gemini 2.5 Flash showed high consistency, with four of the five runs generating identical results, while one run produced a different empirical equation and corresponding estimates. Greater run-to-run variability was observed for DeepSeek-R1, where three runs generated similar results, whereas two runs produced equations that exactly fitted the six experimental observations (R^2 = 1.0). These results indicate that LLM-generated empirical equations may exhibit run-to-run variability despite identical input data and prompting conditions, although the extent of variation differed among the tested LLMs.

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