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A multi-chain surrogate-assisted hybrid optimization framework for joint identification of groundwater contaminant sources and hydrogeological parameters

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Table S1. Actual values of the source location and its release fluxes in Case 1.

Contaminant Source	**Release fluxes (kg/day)**				
(SI, SJ)	S_1P_1	S_1P_2	S_1P_3	S_1P_4	S_1P_5
S_1 (5, 9)	21.4	52.2	13.5	40.7	22.9

Table S2. Actual values of the source locations and their release fluxes in Case 2.

Source Location	**Release fluxes of stress periods (kg/day)**				
(SI, SJ)	SP_1	SP_2	SP_3	SP_4	SP_5
S_1 (4, 9)	21.1	52.2	13.1	40.5	21.9
S_2 (6, 6)	14.3	5.1	29.6	14.2	39.7
S_3 (5, 12)	32.2	25.2	6.8	18.7	23.2

Table S3. Actual values of the source locations and their release fluxes in Case 3.

Source Location	**Release fluxes of stress periods (kg/day)**				
(SI, SJ)	SP_1	SP_2	SP_3	SP_4	SP_5
S_1 (17, 46)	72.2	45.1	31.7	20.4	15.7
S_2 (19, 51)	21.3	64.9	43.2	35.2	27.6
S_3 (24, 57)	13.7	16.9	60.5	35.7	31.8

Table S4. Tuned hyperparameters and candidate grids of the four surrogate models.

Surrogate	Tuned hyperparameters	Candidate grid
KRG	Kernel k; Regression r; Length-scale l;	$k \in \{Gaussian, Cubic, Exponential\}$; $r \in \{Constant, Linear, Quadratic\}$; $l \in \{10^{-3}, 10^{-2}, 10^{-1}, 10^{-3}, 1, 10^{1}, 10^{2}, 10^{3}\}$;
GP	Kernel k; v (Matérn only); α (RQ only); Length-scale θ	$k \in \{Gaussian, Matérn, Rational\ Quadratic\ (RQ)\}$; $v \in \{0.5, 1.5, 2.5\}$; $\theta \in \{10^{-3}, 10^{-2}, 10^{-1}, 1, 10^{1}, 10^{2}, 10^{3}\}$; $\alpha \in \{0.1, 0.3, 1, 3, 10\}$;
SVR	Kernel k; γ; C; d_{poly}(Polynomial only)	$k \in \{Gaussian, Polynomial\}$; $r \in \{10^{-3}, 10^{-2}, 10^{-1}, 10^{-3}, 1, 10^{1}, 10^{2}, 10^{3}\}$; $C \in \{10^{-2}, 10^{-1}, 10^{-3}, 1, 10^{1}, 10^{2}, 10^{3}, 10^{4}\}$; $d_{poly} \in \{1, 2, 3, 4\}$;
RBF	Kernel k; Shape parameter ϵ	$k \in \{Linear, Thin\ Plate\ Spline\ (TPS), Cubic, Multiquadric\ (MQ), Gaussian\}$; $\epsilon \in \{10^{-3}, 10^{-2}, 10^{-1}, 10^{-3}, 1, 10^{1}, 10^{2}, 10^{3}\}$;

Table S5. Comparison of identified values under different noise levels for Case 1. The values in parentheses denote the relative error (%).

Parameters	Actual value	Identified values under varying noise levels			
		0%	0.5%	1%	2%
H_1	42.7	42.3 (0.9%)	42.9 (0.5%)	43.1 (1.0%)	41.9 (1.9%)
H_2	35.3	35.1 (0.5%)	35.5 (0.6%)	35.7 (1.1%)	34.6 (2.0%)
K	18.1	18.3 (1.1%)	18.5 (2.2%)	18.7 (3.3%)	18.4 (1.6%)
SI_1	5	5 (0%)	5 (0%)	5 (0%)	5 (0%)
SJ_1	9	9 (0%)	9 (0%)	9 (0%)	9 (0%)
S_1P_1	21.4	20.7 (3.3%)	21.7 (1.4%)	22.9 (7.0%)	20.3 (5.1%)
S_1P_2	52.2	51.7 (1.0%)	52.9 (1.3%)	52.5 (0.6%)	54.7 (4.8%)
S_1P_3	13.5	13.1 (3.0%)	12.4 (8.1%)	11.6 (14.1%)	12.1 (10.4%)
S_1P_4	40.7	41.6 (2.2%)	41.6 (2.2%)	40.4 (0.7%)	41.7 (2.5%)
S_1P_5	22.9	23.8 (3.9%)	21.2 (7.4%)	23.4 (2.2%)	22.3 (2.6%)

Table S6. Comparison of identified values under different noise levels for Case 2. The values in parentheses denote the relative error (%).

Parameters	Actual value	Identified values under varying noise levels			
		0%	0.5%	1%	2%
H_1	42.7	42.3 (1.2%)	43.4 (1.6%)	43.1 (0.7%)	41.9 (1.9%)
H_2	35.3	35.1 (0.8%)	34.2 (3.1%)	35.7 (1.7%)	34.6 (1.7%)
K	18.1	18.3 (1.1%)	18.5 (2.2%)	18.7 (3.3%)	18.4 (1.6%)
SI_1	4	4 (0.0%)	4 (0.0%)	4 (0.0%)	4 (0.0%)
SJ_1	9	9 (0.0%)	9 (0.0%)	9 (0.0%)	9 (0.0%)
S_1P_1	21.1	20.7 (1.90%)	21.5 (1.9%)	22.0 (4.3%)	20.2 (4.3%)
S_1P_2	52.2	50.2 (3.83%)	55.1 (5.6%)	53.9 (3.3%)	50.1 (4.0%)
S_1P_3	13.1	12.6 (3.81%)	13.7 (4.6%)	12.3 (6.1%)	13.6 (3.8%)
S_1P_4	40.5	38.8 (4.20%)	42.9 (5.9%)	38.4 (5.2%)	38.5 (4.9%)
S_1P_5	21.9	20.8 (5.0%)	23.8 (8.7%)	22.5 (2.7%)	20.4 (6.9%)
SI_2	6	6 (0.0%)	6 (0.0%)	6 (0.0%)	6 (0.0%)
SJ_2	6	6 (0.0%)	6 (0.0%)	6 (0.0%)	6 (0.0%)
S_2P_1	14.3	13.8 (3.49%)	14.9 (4.2%)	14.9 (4.2%)	13.6 (4.9%)
S_2P_2	5.1	4.5 (11.76%)	5.8 (13.7%)	5.8 (13.7%)	5.7 (11.8%)
S_2P_3	29.6	29.0 (2.0%)	28.6 (3.4%)	30.5 (3.0%)	30.5 (3.0%)
S_2P_4	14.2	12.7 (10.6%)	12.5 (12.0%)	16.1 (13.4%)	15.7 (10.6%)
S_2P_5	39.7	38.5 (3.0%)	40.5 (2.0%)	41.7 (5.0%)	38.4 (3.3%)
SI_3	5	5 (0.0%)	5 (0.0%)	5 (0.0%)	5 (0.0%)
SJ_3	12	12 (0.0%)	12 (0.0%)	12 (0.0%)	12 (0.0%)
S_3P_1	32.2	30.2 (6.2%)	34.6 (7.5%)	29.8 (7.5%)	35.1 (9.0%)
S_3P_2	25.2	24 (4.8%)	24.5 (2.8%)	22.8 (9.5%)	25.8 (2.4%)
S_3P_3	6.8	5.8 (14.7%)	7.3 (7.4%)	6.4 (5.9%)	6.2 (8.8%)
S_3P_4	18.7	16.9 (9.6%)	17.1 (8.6%)	16.9 (9.6%)	22.1 (18.2%)
S_3P_5	23.2	22.8 (1.7%)	22.4 (3.5%)	24.1 (3.9%)	24.5 (5.6%)

Table S7. Comparison of identified values under different noise levels for Case 3. The values in parentheses denote the relative error (%).

Parameters	Actual value	Identified values under varying noise levels			
		0%	0.5%	1%	2%
K_1	22.9	22.5 (1.7%)	22.3 (2.6%)	23.4 (2.2%)	22.5 (1.7%)
K_2	16.8	17.6 (4.7%)	16.5 (1.8%)	15.7 (6.5%)	17.8 (5.9%)
K_3	12.2	12.6 (3.3%)	13.3 (9.0%)	11.1 (9.4%)	12.7 (4.5%)
K_4	27.8	28.9 (3.9%)	26.4 (5.1%)	28.4 (2.2%)	27.3 (1.7%)
SI_1	17	17 (0.0%)	17 (0.0%)	17 (0.0%)	17 (0.0%)
SJ_1	46	46 (0.0%)	46 (0.0%)	46 (0.0%)	46 (0.0%)
S_1P_1	72.2	70.4 (2.5%)	73.8 (2.2%)	69.9 (3.2%)	74.2 (2.8%)
S_1P_2	45.1	44.1 (2.2%)	46.6 (3.3%)	47.1 (4.4%)	47.9 (6.2%)
S_1P_3	31.7	29.4 (7.3%)	28.9 (8.8%)	34.1 (7.6%)	33.8 (6.6%)
S_1P_4	20.4	18.8 (7.8%)	22.1 (8.3%)	22.4 (9.8%)	17.8 (12.7%)
S_1P_5	15.7	14.0 (10.8%)	17.6 (12.1%)	13.8 (12.1%)	17.3 (10.2%)
SI_2	19	19 (0.0%)	19 (0.0%)	19 (0.0%)	19 (0.0%)
SJ_2	51	51 (0.0%)	51 (0.0%)	51 (0.0%)	51 (0.0%)
S_2P_1	21.3	19.4 (8.9%)	18.9 (11.3%)	22.7 (6.6%)	23.6 (10.8%)
S_2P_2	64.9	61.4 (5.4%)	67.9 (4.6%)	67.9 (4.6%)	62.7 (3.4%)
S_2P_3	43.2	40.2 (6.9%)	41.1 (4.8%)	46.2 (6.9%)	46.8 (8.3%)
S_2P_4	35.2	33.4 (5.1%)	36.9 (4.8%)	33.2 (5.7%)	33.6 (4.5%)
S_2P_5	27.6	25.6 (7.2%)	25.3 (8.3%)	29.6 (7.2%)	25.9 (6.2%)
SI_3	24	24 (0.0%)	24 (0.0%)	24 (0.0%)	24 (0.0%)
SJ_3	57	57 (0.0%)	57 (0.0%)	57 (0.0%)	57 (0.0%)
S_3P_1	13.7	12.4 (9.5%)	12.5 (8.8%)	14.8 (8.0%)	12.1 (11.7%)
S_3P_2	16.9	16.0 (5.3%)	15.8 (6.5%)	18.2 (7.7%)	15.4 (8.9%)
S_3P_3	60.5	63.2 (4.5%)	57.8 (4.5%)	63.2 (4.5%)	57.8 (4.5%)
S_3P_4	35.7	35.2 (1.4%)	34.5 (3.4%)	33.9 (5.0%)	34.1 (4.1%)
S_3P_5	31.8	31.6 (0.6%)	32.2 (1.3%)	30.9 (2.8%)	30.5 (4.6%)