



Supplement of

A data-driven method coupling multiple physical constraints for correcting structural errors in groundwater contaminant transport models

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Introduction

This document provides supplementary information on the sensitivity analyses of constraint variances, predictions and evaluation metrics obtained using fixed weights, quantitative statistics of structural errors, and evaluations of predictive uncertainty for the two case studies.

The sensitivity analyses of the constraint variances (σ_c^2) for the two case studies are presented in Figures S1 and S2. Mass balance error rates under the multiple-constraint scenario with fixed weights are shown in Figures S3 and S4, while the corresponding DDM predictions and evaluation metrics are provided in Figures S5 and S6 and Tables S3 and S4, respectively. Evaluations of predictive uncertainty under the three scenarios with dynamic weights are shown in Tables S1 and S2. Quantitative statistics of structural errors and GPR prediction performance under the three scenarios with dynamic weights are shown in Tables S5 and S6.

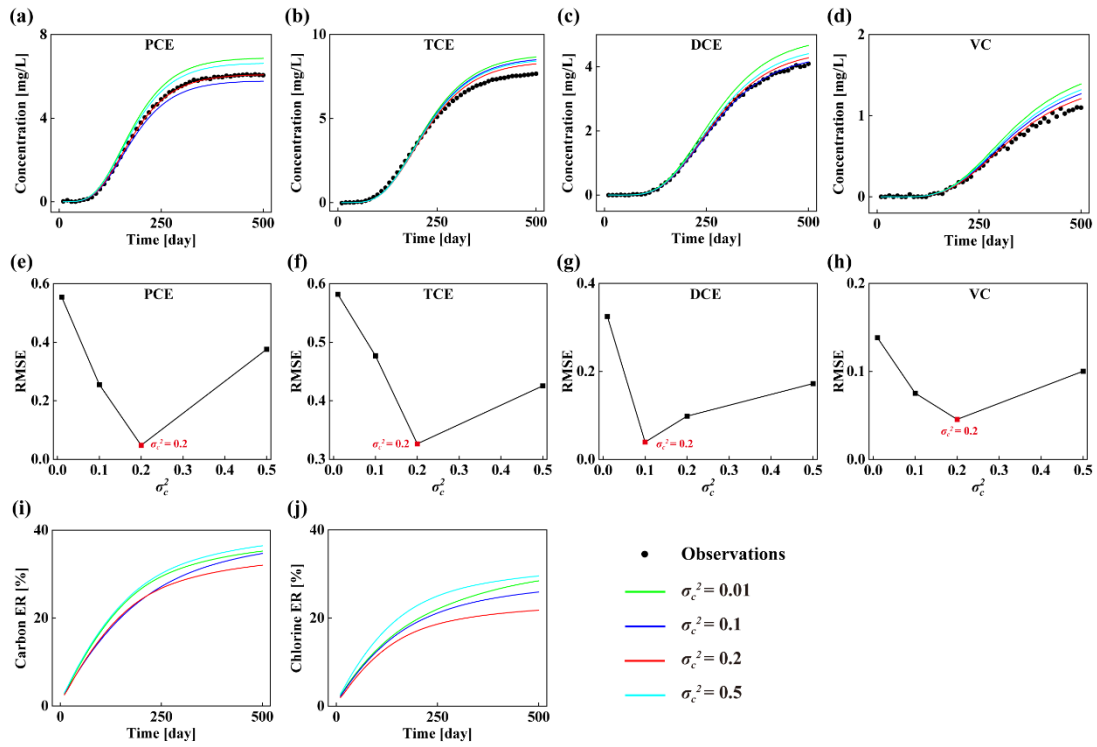


Figure S1. Predictions of synthetic groundwater PCE reactive transport simulation under different constraint variances (σ_c^2).

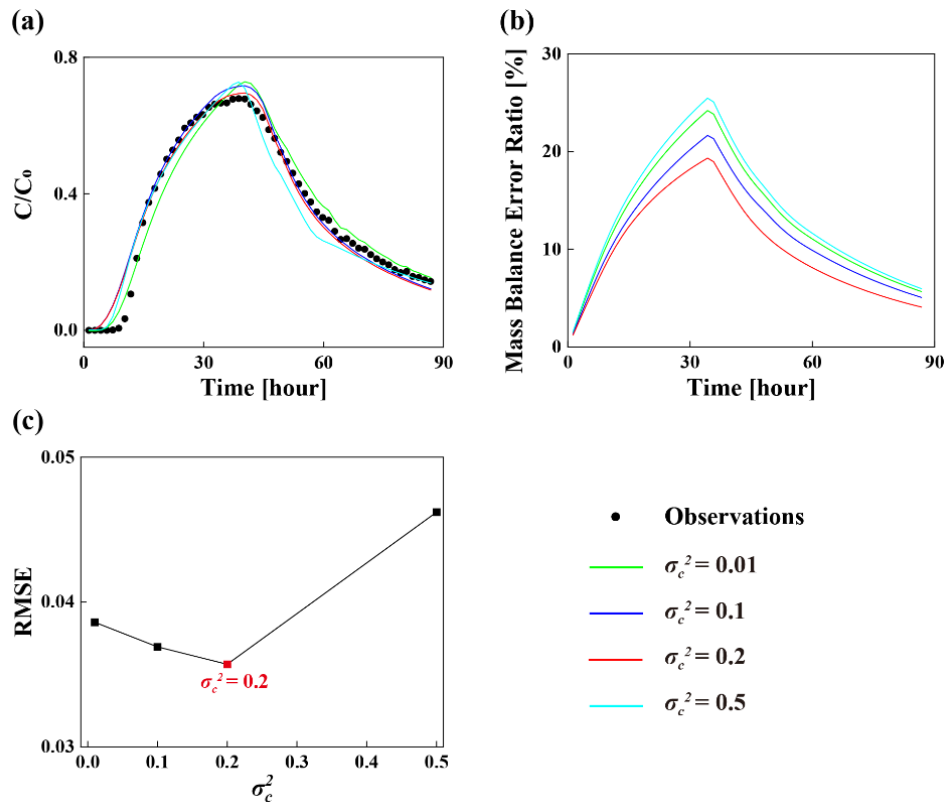


Figure S2. Predictions of sand column Cd-phosphate cotransport simulation under different constraint variances.

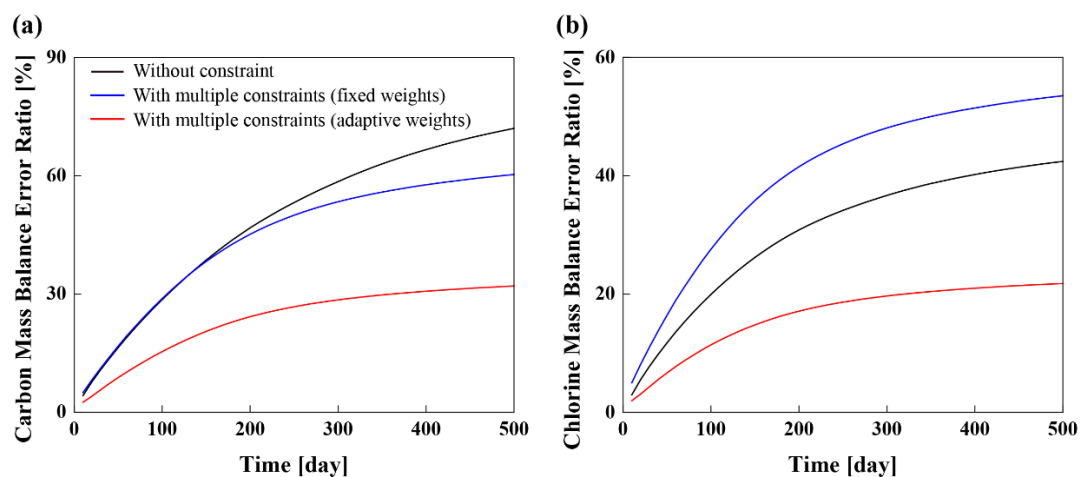


Figure S3. Variation in the carbon/chlorine mass balance error rate for the synthetic groundwater PCE reactive transport model under the multiple-constraint scenario with fixed weights.

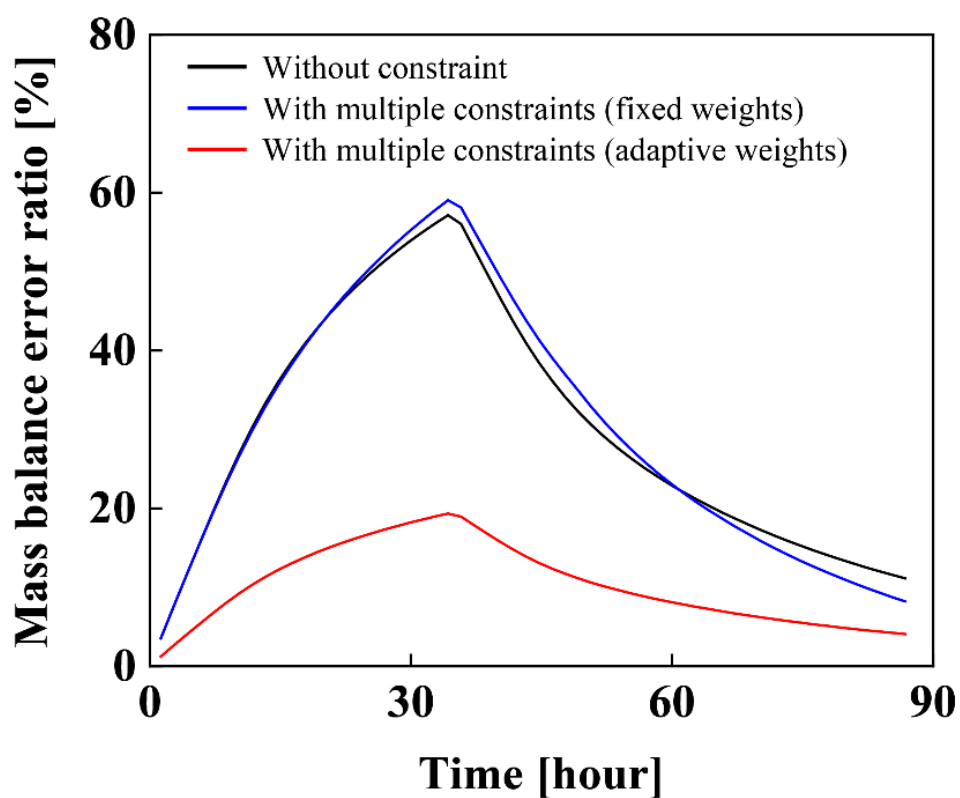


Figure S4. Variation in the cadmium mass balance error rate for the sand column Cd-phosphate cotransport model under the multiple-constraint scenario with fixed weights.

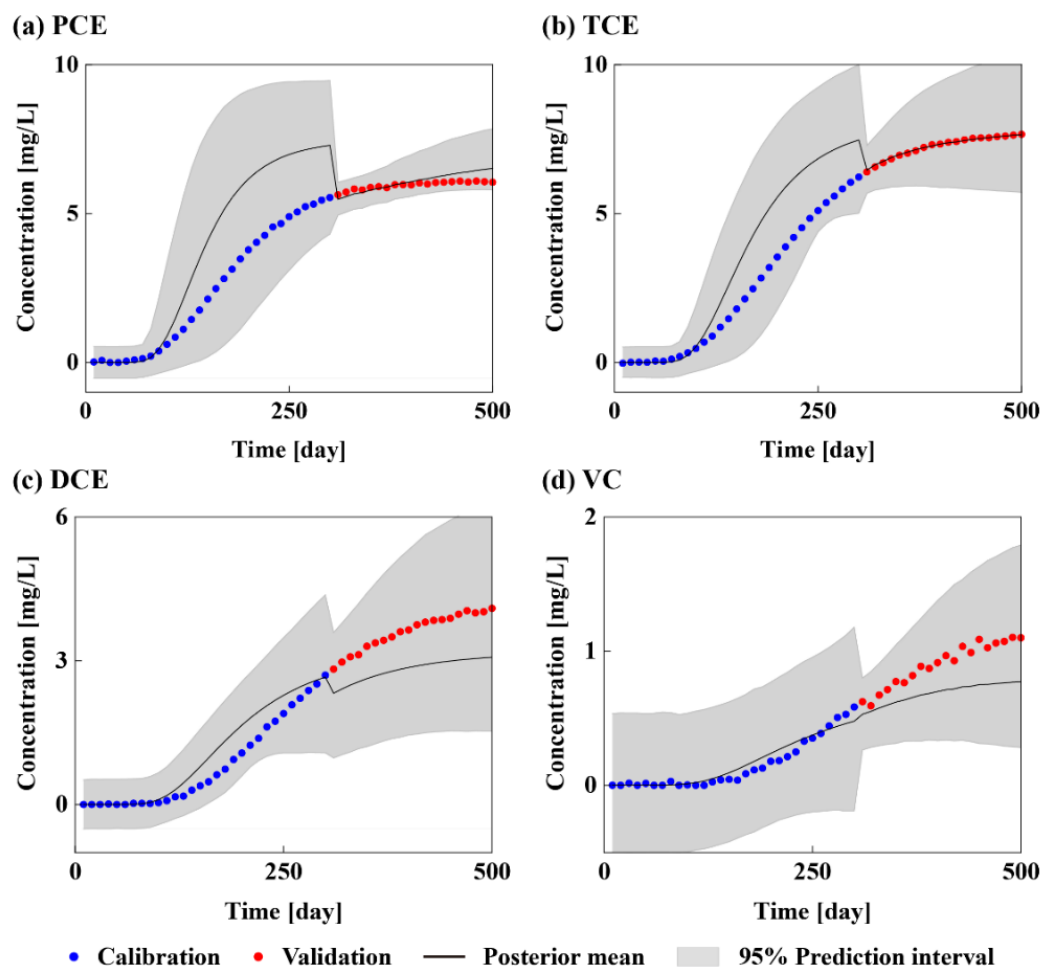


Figure S5. DDM predictions of chlorinated ethenes concentrations under the multiple-constraint scenario with fixed weights.

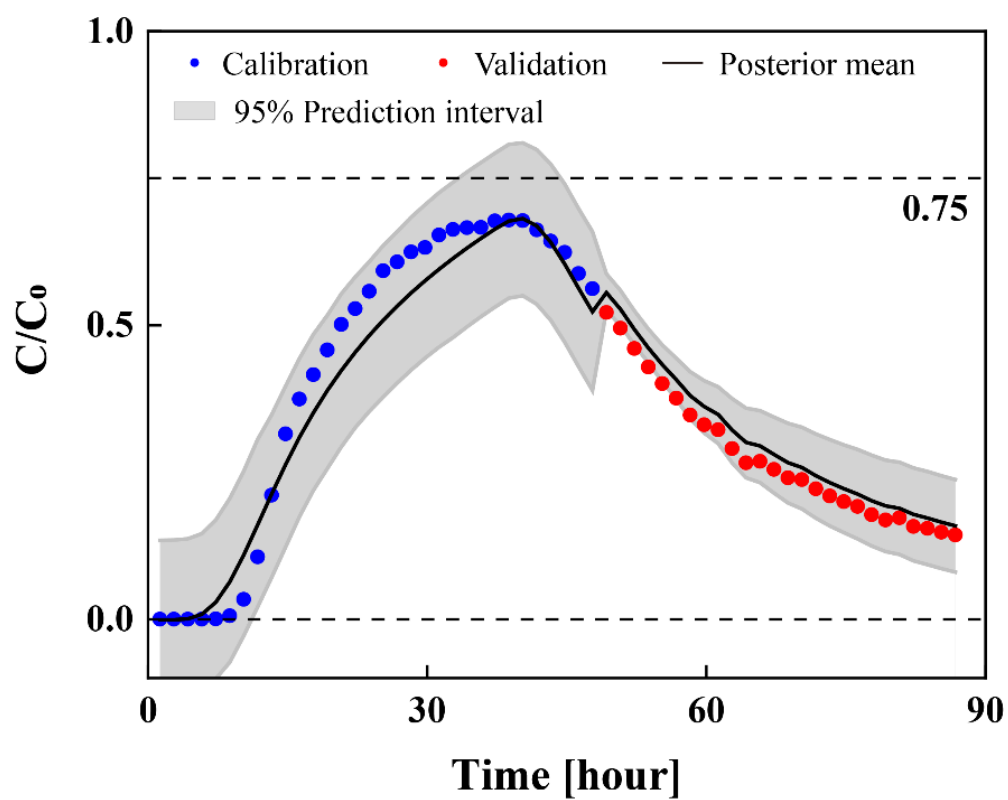


Figure S6. DDM predictions of cadmium concentration under the multiple-constraint scenario with fixed weights.

Table S1. Evaluation of predictive uncertainty for the synthetic groundwater PCE reactive transport model under the three scenarios.

Constraints	Calibration/ Validation	Species	Coverage rate of 95% PI	Average width of 95% PI
Without physical constraint	Calibration	PCE	100.00%	4.8549
		TCE	100.00%	3.3433
		DCE	100.00%	1.7583
		VC	100.00%	0.8372
	Validation	PCE	100.00%	4.6832
		TCE	100.00%	4.8017
		DCE	100.00%	3.3493
		VC	100.00%	1.0976
With single physical constraint	Calibration	PCE	100.00%	4.0288
		TCE	100.00%	2.2447
		DCE	100.00%	0.6820
		VC	100.00%	0.2225
	Validation	PCE	100.00%	4.1261
		TCE	100.00%	3.7011
		DCE	100.00%	3.0829
		VC	100.00%	1.0726
With multiple physical constraints	Calibration	PCE	100.00%	1.1897
		TCE	100.00%	1.1904
		DCE	100.00%	1.1828
		VC	100.00%	1.0828
	Validation	PCE	100.00%	1.2039
		TCE	100.00%	1.2668
		DCE	100.00%	1.2304
		VC	100.00%	1.0867

Table S2. Evaluation of predictive uncertainty for the sand column Cd-phosphate cotransport model under the three scenarios.

Constraints	Calibration/ Validation	Coverage rate of 95% PI	Average width of 95% PI
Without physical constraint	Calibration	100.00%	0.4517
	Validation	92.31%	0.2395
With single physical constraint	Calibration	100.00%	0.3839
	Validation	100.00%	0.2332
With multiple physical constraints	Calibration	87.50%	0.1260
	Validation	100.00%	0.1195

Table S3. Evaluation of predictions for the synthetic groundwater PCE reactive transport model under the multiple-constraint scenario with fixed weights.

Constraints	Calibration/ Validation	Species	NSE	MAE	RMSE
With multiple physical constraints (fixed weights)	Calibration	PCE	0.3562	1.3212	1.6362
		TCE	0.6518	1.0199	1.2937
		DCE	0.8649	0.2452	0.3297
		VC	0.9274	0.0381	0.0492
	Validation	PCE	-2.1390	0.1848	0.2252
		TCE	0.9921	0.0253	0.0328
		DCE	-3.5710	0.7924	0.8078
		VC	-1.0849	0.2150	0.2324

Table S4. Evaluation of predictions for the sand column Cd-phosphate cotransport model under the multiple-constraint scenario with fixed weights.

Constraints	Calibration/ Validation	NSE	MAE	RMSE
With multiple physical constraints (fixed weights)	Calibration	0.9112	0.0408	0.0499
	Validation	0.9028	0.0258	0.0265

Table S5. Quantitative statistics of structural errors and GPR prediction performance for the synthetic groundwater PCE reactive transport simulation under the three scenarios.

Constraints	Species	GPR prediction error (RMSE)	Mean of structural error	Standard deviation of structural error	Range of structural error
Without physical constraint	PCE	0.6653	-1.1629	0.5854	2.2019
	TCE	0.7688	0.0967	0.8372	2.4760
	DCE	0.3763	0.4085	0.5429	1.5274
	VC	0.1118	0.1455	0.1675	0.4985
With single physical constraint	PCE	0.3538	-0.9716	0.3812	1.4644
	TCE	0.3326	-0.0809	0.5454	1.6375
	DCE	0.2832	0.2941	0.4461	1.2877
	VC	0.0502	0.0992	0.1201	0.3857
With multiple physical constraints	PCE	0.1567	0.0744	0.1774	0.7876
	TCE	0.1444	0.2350	0.2224	0.8359
	DCE	0.0738	0.1262	0.1536	0.5336
	VC	0.0242	0.0248	0.0387	0.1399

Table S6. Quantitative statistics of structural errors and GPR prediction performance for the sand column Cd-phosphate cotransport simulation under the three scenarios.

Constraints	GPR prediction error (RMSE)	Mean of structural error	Standard deviation of structural error	Range of structural error
Without physical constraint	0.0984	-0.0050	0.1061	0.4113
With single physical constraint	0.0426	-0.0010	0.0485	0.2104
With multiple physical constraints	0.0396	-0.0021	0.0380	0.1677