Supplementary

Joint characterization of heterogeneous conductivity fields and pumping well attributes through iterative ensemble smoother with a reduced-order modeling strategy for solute transport

Chuan-An Xia[1], Jiayun Li[2*], Bill X. Hu[3], Alberto Guadagnini[4,5], Monica Riva[4*]

[1]Zijin School of Geology and Mining, Fuzhou University, Fuzhou, China

[2]Fujian Provincial Key Lab of Coastal Basin Environment, Fujian Polytechnic Normal University, Fuqing, China

[3]School of Water Conservancy & Environment, University of Jinan, Jinan, China

[4]Dipartimento di Ingegneria Civile e Ambientale, Politecnico di Milano, Milano, Italy

[5]Sonny Astani Department of Civil and Environmental Engineering, Viterbi School of Engineering, Los Angeles, California 90089-2531, USA

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Corresponding author: Jiayun Li; Monica Riva

Email: lijy@fpnu.edu.cn; monica.riva@polimi.it

Table S1 Values of Kullback-Leibler Divergence (KLD) between the sample probability density functions of heads at the three reference points (i.e., I, II, and III) at the final outer iteration through iES_FSM (h_{FSM}) and iES_ROM (h_{ROM}) with n = 5 (TC1), 10 (TC2), 20 (TC4), and 30 (TC6).

KLD(h_{ROM}||h_{FSM}), KLD(h_{FSM}||h_{ROM})	I	II	III
TC1	2.63, 1.70	3.40, 1.90	2.25, 1.66
TC2	2.01, 1.08	2.15, 1.10	1.21, 1.04
TC4	1.48, 1.35	1.56, 1.31	1.07, 1.01
TC6	1.27, 1.49	1.23, 1.34	0.79, 1.02

Table S2 Values of Kullback-Leibler Divergence (KLD) between the sample probability density functions of solute concentrations at the three reference points (i.e., I, II, and III) at the final outer iteration through iES_FSM (c_{FSM}) and iES_ROM (c_{ROM}) with n = 5 (TC1), 10 (TC2), 20 (TC4), and 30 (TC6).

KLD(c_{ROM}‖c_{FSM}), KLD(c_{FSM}‖c_{ROM})	I	II	III
TC1	0.32, 0.82	1.86, 1.92	1.25, 1.25
TC2	0.41, 0.34	1.42, 1.17	0.37, 0.71
TC4	0.28, 0.33	0.85, 1.14	0.24, 0.59
TC6	0.30, 0.32	0.93, 1.11	0.11, 0.43

Table S3 Values of Kullback-Leibler Divergence (KLD) between the sample probability density functions of x_{1,q_s} (x_{2,q_s}, or $\ln q_s$) obtained through iES_FSM ($p_{j\text{FSM}}$, j = x_{1,q_s}, x_{2,q_s}, and $\ln q_s$) and iES_ROM ($p_{j\text{ROM}}$) with n = 30, considering N_m = 9, 18, and 55 (corresponding to TCs 18, 19, and 6, respectively).

KLD($p_{j\text{ROM}}\|p_{j\text{FSM}}$), KLD($p_{j\text{FSM}}\|p_{j\text{ROM}}$)	$j = x_{1,q_s}$	$j = x_{2,q_s}$	$j = \ln q_s$
TC18	4.54, 5.51	4.68, 5.36	7.30, 7.80
TC19	2.02, 1.86	3.18, 3.67	7.21, 7.04
TC6	1.43, 0.78	3.49, 3.34	5.98, 6.70