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Additional Information

# Joint identification of contaminant source and aquifer geometry in a sandbox experiment with the restart Ensemble Kalman filter

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## Abstract

Contaminant source identification is a key problem in handling groundwater pollution events. The ensemble Kalman filter (EnKF) is used for the spatiotemporal identification of a point contaminant source in a sandbox experiment, together with the identification of the position and length of a vertical plate inserted in the sandbox that modifies the geometry of the system. For the identification of the different parameters, observations in time of solute concentration are used, but not of piezometric head data since they were not available. A restart version of the EnKF is utilized because it is necessary to restart the forecast from time zero after each parameter update. The results show that the restart EnKF is capable of identifying both contaminant source information and aquifer-geometry-related parameters together with an uncertainty estimate of such identification.

*Keywords:* Inverse modeling; Observation error; Groundwater laboratory experiment; Stochastic hydrogeology

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## 1. Introduction

2 The problem of identifying a contaminant source in an aquifer using solute concentra-  
3 tion data has been the subject of attention for many years (e.g., Atmadja and Bagtzoglou,

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4 2001; Michalak and Kitanidis, 2004; Bagtzoglou and Atmadja, 2005; Sun et al., 2006, and  
5 references therein). Briefly, the proposed methods could be grouped into two categories:  
6 optimization approaches and probabilistic approaches. The main difference between the two  
7 approaches is that the optimization approaches cast the problem as a deterministic one in  
8 which parameters are found that minimize a given objective function, whereas the probabilis-  
9 tic approaches cast the problem in a stochastic framework and the parameters to estimate  
10 become random variables. In the first category, Gorelick et al. (1983) identified the ground-  
11 water pollution source information through an optimization model using linear programming  
12 and multiple regression; Wagner (1992) employed a non-linear maximum likelihood method  
13 to estimate source location and flux; Mahar and Datta (2000) used a nonlinear optimization  
14 model for estimating the magnitude, location and duration of groundwater pollution sources  
15 with binding equality constraints; Yeh et al. (2007) developed a hybrid approach, which  
16 combines simulated annealing, tabu search and a three-dimensional groundwater flow and  
17 solute transport model to solve the source identification problem; and Ayvaz (2010) utilized  
18 a harmony search-based simulation-optimization model to determine the source location and  
19 release histories by using an implicit solution procedure. In the second category, Bagtzoglou  
20 et al. (1992) applied a particle method to estimate, probabilistically, source location and  
21 spill-time history; Woodbury and Ulrych (1996) used a minimum relative entropy approach  
22 to recover the release and evolution histories of a groundwater contaminant plume in a one-  
23 dimensional system; Neupauer and Wilson (1999) employed a backward location model based  
24 on adjoint state method (BPM-ASM) to identify a contaminant source; Butera et al. (2013)  
25 utilized a simultaneous release function and source location identification (SRSI) method to  
26 identify the release history and source location of an injection in a groundwater aquifer; and  
27 Koch and Nowak (2016) derived and applied a Bayesian reverse-inverse methodology to infer  
28 source zone architectures and aquifer parameters.

29 The ensemble Kalman filter (EnKF), which could be included in the group of probabilistic  
30 approaches mentioned above, has recently addressed the problem of contaminant source

31 identification. The EnKF introduced by Evensen (2003) has gained much popularity in recent  
32 years for its efficiency in solving inverse problems in different fields such as oceanography,  
33 meteorology and hydrology (Houtekamer and Mitchell, 2001; Li et al., 2012a; Xu et al.,  
34 2013b). The advantages of the EnKF can be summarized as follows (Chen and Zhang, 2006;  
35 Zhou et al., 2011): computational efficiency when compared with other inverse approaches,  
36 easy integration with different forecast models, ability to account for model and observation  
37 errors, and easy uncertainty characterization since the final outcome is always an ensemble  
38 of realizations. In hydrogeology, the EnKF has been mainly applied for the identification of  
39 aquifer parameters such as hydraulic conductivity or porosity (Li et al., 2012b; Xu et al.,  
40 2013a; Zhou et al., 2014; Xu and Gómez-Hernández, 2015, 2016a). Recently, Xu and Gómez-  
41 Hernández (2016b) demonstrated the possibility to apply the EnKF for the identification of a  
42 contaminant source in a deterministic synthetic aquifer, and later Xu and Gómez-Hernández  
43 (2018) showed that the method can be also applied for the simultaneous identification of  
44 hydraulic conductivities and the parameters defining a contaminant source also in a synthetic  
45 aquifer.

46 All the works mentioned above were tested in synthetic cases. Only a few works can be  
47 found in the literature for laboratory or field cases. Woodbury et al. (1998) extended the  
48 minimum relative entropy (MRE) method to recover the release history of a contaminant and  
49 applied it to reconstruct the release history of a 1,4-dioxane plume observed at the Gloucester  
50 Landfill in Ontario, Canada. Michalak (2003); Michalak and Kitanidis (2004) employed a  
51 Bayesian inverse formulation to estimate the contaminant history of trichloroethylene (TCE)  
52 and perchloroethylene (PCE) in an aquifer at the Dover Air Force Base, Delaware, a site that  
53 had already been analyzed by Liu and Ball (1999) in the same context of source identifica-  
54 tion. Cupola et al. (2015b,a) compared the source location identification (SRSI) method to  
55 the backward probability model based on the adjoint state method (BPM-ASM) with data  
56 taken from a sandbox experiment. Zanini and Woodbury (2016) also used data from a sand-  
57 box experiment to apply an empirical Bayesian method combined with Akaike's Bayesian

58 Information Criterion (ABIC) to deduce the release history of a groundwater contaminant.

59 The main objective of this paper is to assess the performance of the restart EnKF (r-  
60 EnKF) for the identification of contaminant source parameters and aquifer geometry with  
61 data from a sandbox experiment. The source parameters of interest are the release location,  
62 release starting and ending times, and contaminant load, and regarding the geometry the  
63 method should try to retrieve the position and length of a plate that is inserted about the  
64 center of the sandbox and induces a deflection of the flowlines towards the bottom of the  
65 sandbox. The state information assimilated by the r-EnKF is limited to concentration data  
66 at a few observation points, since no piezometric head data were available.

67 The paper is organized as follows, first, the state equations and the fundamentals of the  
68 r-EnKF will be recalled, second, the sandbox characteristics are described together with the  
69 numerical model used to reproduce its behavior, third, the r-EnKF is tested with data from  
70 a synthetic experiment that mimics the sandbox experiment with the aim to verify if the r-  
71 EnKF is capable of identifying the kind of parameters sought, and four, the r-EnKF is applied  
72 with observation values taken from the sandbox experiment, the problems encountered are  
73 analyzed, alternative approaches are discussed and the final results presented. The paper  
74 ends with a summary and conclusions on the main findings.

## 75 **2. Methodology**

### 76 *2.1. Groundwater Flow and Solute Transport Equation*

77 The sandbox will be modeled as a two-dimensional system in the  $XZ$  plane, where an  
78 inert contaminant spreads due to advection and dispersion under a steady-state flow. The  
79 dimension of the sandbox in the  $y$  direction is small enough to assume that the state variables  
80 are constant along any line for any given  $(x, z)$  value. The governing equations are:

$$\frac{\partial}{\partial x} \left( K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial h}{\partial z} \right) + w = 0 \quad (1)$$

$$\frac{\partial(\theta C)}{\partial t} = \nabla \cdot (\theta D \cdot \nabla C) - \nabla \cdot (\theta v C) - q_s C_s \quad (2)$$

81 where  $K_x$  and  $K_z$  are the principal components of the hydraulic conductivity tensor in the  $x$   
 82 and  $z$  spatial coordinates respectively [ $LT^{-1}$ ] which are assumed aligned with the coordinate  
 83 system of reference in the entire domain;  $h$  is the hydraulic head [ $L$ ];  $w$  represents distributed  
 84 sources or sinks [ $T^{-1}$ ];  $t$  is time [ $T$ ];  $\theta$  represents the porosity of the medium;  $C$  is dissolved  
 85 concentration [ $ML^{-3}$ ];  $\nabla \cdot$  is the divergence operator;  $\nabla$  is the gradient operator;  $D$  represents  
 86 the hydrodynamic dispersion coefficient tensor [ $L^2T^{-1}$ ];  $v$  is the flow velocity vector [ $LT^{-1}$ ]  
 87 derived from the solution of the flow model;  $q_s$  represents volumetric flow rate per unit  
 88 volume of aquifer associated with a fluid source or sink [ $T^{-1}$ ] and  $C_s$  is the concentration of  
 89 the source or sink [ $ML^{-3}$ ].

90 The flow equation is solved using MODFLOW (McDonald and Harbaugh, 1988), and the  
 91 transport equation is solved using MT3DS (Zheng and Wang, 1999).

## 92 2.2. The Ensemble Kalman Filter

93 The ensemble Kalman filter was first introduced by Evensen (2003) to circumvent the  
 94 difficulty of propagating covariances in time in the original and extended Kalman filter  
 95 formulations. The restart EnKF (r-EnKF) has proven its capacity for contaminant source  
 96 identification in synthetic cases (Xu and Gómez-Hernández, 2016b, 2018); now, we propose  
 97 to test the r-EnKF in a sandbox experiment. For this specific case, there will be eight  
 98 parameters to identify, six related to the contaminant source, and two related to aquifer  
 99 geometry. In the first group, they are the contaminant source location ( $X_s, Z_s$ ), the injection  
 100 concentration  $I_c$ , the injection rate  $I_r$ , plus the starting  $T_s$  and ending  $T_e$  release times. In  
 101 the second group, the algorithm will try to identify the position along the  $x$  direction  $X_b$   
 102 and the total depth  $Z_b$  of a vertical plate inserted about the center of the sandbox to deflect  
 103 the flowlines. The rest of the parameters defining the flow and transport conditions in the  
 104 sandbox are not subject to identification and are equal to their observed values as explained

105 in the description of the experiment in the next section. The r-EnKF is shortly described  
106 next.

107 In the ensemble Kalman filter with extended state vector, we deal with two types of  
108 variables, the system parameters subject of identification, of which there could be observa-  
109 tions or not, and the state of the system, of which there will be observations. The state  
110 is forecasted in time solving the corresponding state equations, with the latest parameter  
111 update, up to the specific time steps when observations are collected; these observations are  
112 assimilated by the filter and serve to update the parameters and the state of the system. In  
113 the restart filter, state variables are not updated, only system parameters are, because the  
114 system state forecast for the next observation time is restarted from time zero to make sure  
115 that the forecasted system state is fully coherent with the state equations, and, in our case,  
116 with the updated **contaminant source**. (In the original implementation of the filter, both  
117 state and parameters are updated, and the state system is forecasted from the last updated  
118 state values using the last updated parameters.) The r-EnKF is an iterative algorithm that  
119 cycles forecast and data assimilation (with the corresponding parameter update) until all  
120 observations have been accounted for. The implementation of the r-EnKF for the identi-  
121 fication of the eight parameters described above can be summarized as follows (**Evensen,**  
122 **2003; Xu and Gómez-Hernández, 2016b**):

123 1. Generate an initial ensemble of parameter values. An ensemble of  $N_e$  realizations  
124 of eight-tuples of the parameters to be identified is generated. Parameter values are  
125 drawn, independently, from uniform distributions defined between first-guess minimum  
126 and maximum values—there are no restrictions on these uniform distributions, their  
127 range can be wider or narrower than the one used in this paper, and they do not have  
128 to necessarily contain the “real” value, they are simply used to initialize the algorithm.  
129 We build  $N_e$  vectors  $S_i$  with the eight parameters for each realization:

$$S_i = [Xs_i, Zs_i, Xb_i, Zb_i, Ic_i, Ir_i, Ts_i, Te_i]^T \quad (3)$$

130 where  $i$  is the realization index and the superscript  $T$  stands for transpose.

- 131 2. Repeat for each system state observation time. Forecast the state. For each ensemble  
 132 member, forecast the system state, that is, the concentrations in the aquifer, for the  
 133  $t^{th}$  observation time using the values of the parameters from the last update (or the  
 134 initial parameters for the first observation time). In the original implementation of  
 135 the EnKF, the system state at the  $t^{th}$  observation time is forecasted based on the  
 136 concentrations at the  $(t-1)^{th}$  observation time and using the last updated parameters;  
 137 however, it is virtually impossible to account for an update of the source location or  
 138 the injection time unless the state equation is solved from time zero, thus the need to  
 139 restart the simulation from time zero (Xu and Gómez-Hernández, 2016b). The forecast  
 140 of concentrations is given by

$$C_i^f(t) = \psi [C_0, S_i^a(t-1)], \quad (4)$$

141 where the superscripts  $f$  and  $a$  refer to forecasted and updated values after assimilation,  
 142 respectively;  $\psi$  represents the numerical model that forecast, in time, concentrations,  
 143 on a grid with  $N_m$  nodes;  $C_i$  is an  $N_m \times 1$  column vector containing the forecasted  
 144 concentrations at all the discretization nodes of the numerical model for realization  
 145  $i$ ;  $S_i^a$  is the vector with the last updated parameters;  $C_0$  is the initial contaminant  
 146 concentration of the domain, which is the same for all realizations. The forecast of the  
 147 parameters is simply

$$S_i^f(t) = S_i^a(t-1). \quad (5)$$

- 148 3. Parameters update. First compute the parameter covariance through the ensemble of  
 149 forecasted realizations

$$P_S^f(t) = \frac{1}{N_e} \sum_{i=1}^{N_e} \left\{ \left[ S_i^f(t) - \overline{S_i^f(t)} \right] \left[ S_i^f(t) - \overline{S_i^f(t)} \right]^T \right\} \quad (6)$$



150 with

$$\overline{S_i^f(t)} = \frac{1}{N_e} \sum_{i=1}^{N_e} S_i^f(t), \quad (7)$$

151 where  $P_S^f$  is an  $8 \times 8$  matrix of parameter covariances and  $\overline{S_i^f(t)}$  is an  $8 \times 1$  column vector  
 152 of parameter averages. Then, compute the parameter-concentration cross-covariances  
 153 but only with the forecasted concentration values that fall at concentration observation  
 154 locations for time  $t$  (for the sake of simplicity, we will assume that observations are  
 155 taken coinciding with some of the numerical model nodes, if not, there will be a need to  
 156 provide a linear averaging procedure to estimate concentrations at observation locations  
 157 from model concentration forecasts)

$$P_{SC}^f(t) = \frac{1}{N_e} \sum_{i=1}^{N_e} \left\{ \left[ S_i^f(t) - \overline{S_i^f(t)} \right] \left[ C_i^f(t) - \overline{C_i^f(t)} \right]^T \right\} \quad (8)$$

158 with

$$\overline{C_i^f(t)} = \frac{1}{N_e} \sum_{i=1}^{N_e} C_i^f(t), \quad (9)$$

159 where  $P_{SC}^f$  is an  $8 \times N_o$  matrix of parameter-concentration cross-covariances, with  $N_o$   
 160 being the number of nodes of the numerical model at which observations are taken at  
 161 time step  $t$ , and  $\overline{C_i^f(t)}$  is an  $N_o \times 1$  column vector of average concentrations. Next,  
 162 compute the  $8 \times N_o$  Kalman gain matrix  $K(t)$  as

$$K(t) = P_S^f(t) [P_{SC}^f(t) + R(t)]^{-1} \quad (10)$$

163 where  $R(t)$  is an  $N_o \times N_o$  **diagonal** observation error covariance matrix (**implying**  
 164 **that there is no correlation between observation errors**) and proceed to update  
 165 the parameter values, realization by realization by

$$S_i^a(t) = S_i^f(t) + K(t) \left[ d_i(t) - C_{io}^f(t) \right], \quad (11)$$

166 where  $d_i(t)$  is an  $N_o \times 1$  vector of observed concentrations (including observation errors  
167 with covariance given by  $R(t)$ ) and  $C_{io}^f(t)$  is an  $N_o \times 1$  vector of forecasted concentra-  
168 tions.

169 4. Go back to step 2 and repeat the whole process until all observations are assimilated.

### 170 3. Experimental Case

#### 171 3.1. Description of the experiment

172 A single point pollution experiment was performed in a sandbox using sodium fluorescein  
173 as tracer. The sandbox is built in plexiglass and has external dimensions of 120 cm  $\times$  14  
174 cm  $\times$  70 cm as sketched in Fig. 1. The internal volume of 96 cm  $\times$  10 cm  $\times$  70 cm is  
175 filled with constant-diameter spherical glass beads. There are two reservoirs at the edges of  
176 the box imposing constant water levels of 60.7 cm and 53.6 m upstream and downstream,  
177 respectively. An injector was set up at the upstream part of the sandbox at the location  
178 indicated by a red square in the figure, and a plastic plate was vertically inserted inside  
179 the glass beads in the middle of the sandbox, whose position and length is also shown in  
180 the figure. The experimental equipment was placed in a dark box and a digital camera was  
181 used to capture, every 5 s, the fluorescein luminosity within the rectangular zone of 85 cm  
182 by 44 cm marked with a ticked rectangle in Fig. 1. The pictures were then processed and  
183 the fluorescein luminosity transformed into concentrations after a calibration procedure, as  
184 described by Citarella et al. (2015). In this case, eight different fluorescein concentrations  
185 ( $C = 0; 2.5; 5; 10; 20; 25; 30; 35$  mg/l) were used to calibrate and generate the luminosity-  
186 concentration curves in each picture pixel. The total experiment time lasted 1965 s, the  
187 injection started at time 120 s and finished at time 1000 s. During the experiment, the rate  
188 and concentration of the injection were also recorded.

189 It is very important to note that there are no piezometric head observations. The design  
190 of the tank did not allow for those observations. Had there been piezometric head data, they

191 could have been assimilated in the filter and, without doubt, would have helped in improving  
192 the identification (as shown by Xu and Gómez-Hernández (2018)).

### 193 *3.2. Numerical Model*

194 Since the thickness of the sandbox along the  $y$  axis is relatively small, we can assume  
195 that the variability of piezometric heads and concentration along this direction is negligible.  
196 Therefore, a two-dimensional groundwater flow and transport model in the  $XZ$  plane is  
197 built. The upstream and downstream vertical boundaries are set as constant prescribed  
198 piezometric head values, and the bottom boundary is impermeable while the top boundary  
199 is the phreatic surface. The model corresponds to the yellowish area in Fig. 1, where  
200 the coordinates of the four model corners are given. The tank is filled with homogeneous  
201 spherical glass beads with a conductivity of 0.58 cm/s and a porosity of 0.37. The vertical  
202 plastic plate was inserted at a distance of 52 cm from the left boundary and its length is of  
203 42 cm. It is modeled as an impermeable barrier, which will deflect the flowlines towards the  
204 bottom of the sandbox. The sandbox is discretized into 96 columns, one row, and 70 layers;  
205 the size of each cell is  $(\Delta x, \Delta y, \Delta z) = (1, 10, 1)$  cm. The total simulation time is 1800 s and  
206 is discretized into 90 uniform time steps. Citarella et al. (2015) evaluated the longitudinal  
207 and transverse dispersivities of the spherical beads, resulting in values of 0.16 cm and 0.048  
208 cm, respectively. The flow and transport parameters are collected in Table 1.

209 The release happens at coordinates (18.5 cm, 30.5 cm), with a concentration of 20 mg/l  
210 and an injection rate of 0.95 cm<sup>3</sup>/s. To start the ensemble Kalman filter 800 8-tuples of  
211 the source and plate parameters are generated from uniform distributions (not centered at  
212 the true values). The true values of the parameters to identify and the suspect range of the  
213 uniform distributions used to generate the initial ensemble are collected in Table 2.

## 214 4. Application

215 The objective of this work is to demonstrate the capacity of the r-EnKF for the identifi-  
216 cation of contaminant source information, including contaminant source location  $(X_s, Z_s)$ ,  
217 injection information  $(I_c, I_r)$  and release time  $(T_s, T_e)$  together with the position and length  
218 of the vertical plate  $(X_b, Z_b)$ , using concentration observations collected in a laboratory ex-  
219 periment. As a prior test, we analyze a synthetic case, in which the concentration data are  
220 generated by the numerical model of the sandbox, therefore removing any modeling error  
221 since the forward model used to forecast by the r-EnKF will coincide with the model used to  
222 generate the observations. In the next section, we will redo the analysis using the laboratory  
223 data, we will analyze the problems found and propose some solutions.

### 224 4.1. Synthetic Sandbox Test

225 In this case, we design two scenarios  $(S1, S2)$  with different number of observation wells  
226 to evaluate the performance of the r-EnKF: scenario  $S1$  with 20 observation wells, and  
227 scenario  $S2$  with 24 observation wells containing 4 additional wells (#21, #22, #23, #24)  
228 located at the four corners of the suspect release area (see Fig. 1). **The rationale for the**  
229 **second scenario is that, after analyzing the first scenario, we felt that additional**  
230 **information about the plume evolution was needed, and thus we decided to**  
231 **add four wells around the suspect release zone. Such an addition will, indeed,**  
232 **improve the characterization.** In both scenarios, model error is neglected and we assume  
233 that observation errors are uncorrelated with mean zero, and standard deviation of 0.1 mg/l.

234 Figure 2 and 3 show the time evolution of the ensemble mean and the ensemble variance,  
235 respectively, of the updated state parameters for the two scenarios. Figure 4 shows the  
236 evolution in time of the boxplots computed from the 800 ensemble members. **After time**  
237 **step 60, the convergence rate of the means and variances of the parameters**  
238 **are less than 1% and 5%, respectively, all the parameters get close to the final**  
239 **estimation and become stable. Notice also the sudden drop of the variance at a**

240 **given time step for most of the parameters. This drop is related to the activation**  
241 **of new observation wells as time progresses, what implies that the amount of**  
242 **information assimilated by the filter does not vary continuously in time, but**  
243 **rather it increases stepwise, with steps occurring when new wells observe, for**  
244 **the first time, the arrival of the solute plume.** We can distinguish between the  
245 parameters that are perfectly identified by an ensemble mean equal to the true value, and  
246 practically zero variance, and those that are approximated closely but which are not exact  
247 and present some residual uncertainty. In the first group, there are the position parameters  
248 for the plate,  $Xb$  and  $Zb$ , plus the vertical location of the release source  $Zs$ , independently  
249 of whether 20 or 24 data are used during the assimilation steps; in the second group are  
250 the remaining parameters, which become more precise (mean closer to the true value) and  
251 less uncertain (smaller variability) for  $S2$  than for  $S1$ . The horizontal source location  $Xs$   
252 is less sensitive to the concentration data, and only when the four additional data points  
253 in the corners of the suspect release location are added the algorithm is able to provide a  
254 good estimate for this parameter; similar comment can be made about the beginning  $Ts$   
255 and end  $Te$  times of the release. The injection concentration  $Ic$  and injection rate  $Ir$  are  
256 well identified by their median values, with smallest uncertainty for  $S2$ . These results are  
257 consistent with the sensitivity of concentrations at the observation locations to changes in  
258 the parameter values: concentration distributions are most sensitive to the position of the  
259 plate, which affects the flow field, and the vertical release location, which affects the main  
260 trajectory of the contaminant plume, but are less sensitive to the other parameters, for which  
261 variations within the identified uncertainty ranges induce concentration changes of the same  
262 order of magnitude as the observation errors. Also notice that the horizontal coordinate  
263 of the release and the starting and ending release times are correlated for the purpose of  
264 identifying their values (a displacement of the horizontal coordinate of the release could  
265 be compensated with a displacement of its starting time), what also explains their larger  
266 uncertainties.

267 These results prove that the r-EnKF could work for the identification of a contaminant  
268 source and of some parameters defining the geometry of the aquifer. The next step is to test  
269 the algorithm under more realistic conditions using observations obtained from a laboratory  
270 experiment.

#### 271 *4.2. Laboratory Sandbox Test*

272 The sandbox experiment was carried out as described previously. Figure 5 shows a  
273 picture of the fluorescein plume at the 48th time step (840 s since the beginning of the  
274 release) already transformed into concentration values and the position of the observation  
275 points. The deflection of the flowlines induced by the vertical plate is clearly seen. Notice  
276 that only a few observation piezometers will actually detect the plume breakthrough. Before  
277 testing the r-EnKF, we performed a simulation of the concentration evolution using the  
278 known release parameters and compared the predictions with the observed data. Figure  
279 6 shows a comparison between observed and numerically predicted concentrations at five  
280 observation locations (wells #7, #9, #10, #13, #22) through which the plume passes. As  
281 can be seen, the reproduction is very good for the closest well #22, and it deteriorates with  
282 the distance from the source, but not dramatically, except for well #9. For this well, the  
283 beginning and ending times of the breakthrough curve are the same for predictions and  
284 observations, but the mismatch in concentrations indicates either some error in the model  
285 parameters or faulty observations. The predicted breakthrough curve in the farthest well,  
286 though, is quite close to the observed one. In the application that follows we will analyze  
287 different observation error distributions in an attempt to identify the source parameters by  
288 the r-EnKF.

289 We have run the r-EnKF with three different magnitudes of the observation error, which  
290 will be referred to as  $R1$ ,  $R2$ , and  $R3$ . In all three cases, the error mean is zero and its  
291 standard deviation is 0.5 mg/l for  $R1$ , 1.0 mg/l for  $R2$ , and 3.0 mg/l for  $R3$ . **We must**  
292 **notice that in previous experiments, Cupola et al. (2015a) report an observation**

293 **error with a standard deviation around 1 mg/l.**

294 The hydraulic conductivity value of the beads, which is considered homogeneous in each  
295 realization, is considered uncertain and drawn from a Gaussian distribution with a mean of  
296 0.58 cm/s and a standard deviation of 0.05 cm/s. **We have decided to introduce some**  
297 **uncertainty on the beads hydraulic conductivity as a surrogate to model error.**  
298 **The choice of a Gaussian distribution centered at the calibrated conductivity**  
299 **value was arbitrary, any other distribution could have been used. Considering**  
300 **that the differences in the results between including or not such an uncertainty**  
301 **are minimal (and not reported here), we believe that the choice of the specific**  
302 **distribution has little effect in the final outcome.**

303 Fig. 7 shows the boxplots of the updated parameters at different time steps for the three  
304 scenarios *R1*, *R2*, and *R3*. The results are not as good as for the synthetic case, for which the  
305 observed concentrations were generated with the same numerical model used for the forecast  
306 step in the Kalman filter. The first thing to note is that for scenario *R1*, the use of a small  
307 observation error makes the r-EnKF to seek for source parameter values that can be far  
308 from the true ones in order to produce concentrations that are close to the observed values,  
309 and, particularly, the injection concentration and injection rate do not seem to converge to  
310 a stable value after 90 time steps. The other parameters do reach a stable median, not as  
311 close to the true values as for the synthetic case but close enough except for the horizontal  
312 position of the vertical plate.

313 When the observation error is increased (scenario *R2*), the two main findings are that the  
314 two injection parameters now seem to reach a stable estimate (albeit with large uncertainty)  
315 with a median close to the true value, and that all parameters have a wider uncertainty range.  
316 The median estimate of the initial and ending release times is also closer to the true ones  
317 than in *R1*. The horizontal position of the vertical plate continues to be underestimated, as  
318 well as the length of the plate.

319 When the observation error is increased even more (scenario *R3*) the main effect is that

320 the final estimates have wide uncertainty estimates, and for some of the parameters it seems  
321 as if the concentration observations do not bring any added value since the boxplot width  
322 remains unaltered through the assimilation steps. The estimates of the parameters by their  
323 median is comparable to the results in *R2*, but their uncertainty is larger.

324 The predicted concentrations at three observation wells that were not used during the  
325 assimilation step computed using the initial 8-tuples of parameters, and using the 8-tuples  
326 obtained at the end of the three scenarios are shown in Figure 8. The figure shows the  
327 true concentrations in the sandbox as a dotted blue line, each one of the 800 predicted  
328 concentration breakthrough curves computed with the 8-tuples of the ensemble, along with  
329 their median, as a red line, and their 90% confidence interval, as dashed lines. It can be  
330 observed that, prior to assimilation (top row), concentration predictions were very scattered,  
331 and that after the assimilation (bottom three rows, one for each scenario) the breakthrough  
332 curves change substantially (compare, for instance, the median curves). For scenario *R1*, the  
333 scatter of prediction curves is the smallest but recall that these wells were not used during  
334 the assimilation, the updated parameters were biased because the algorithm tried to fit the  
335 observed concentrations too closely and as a result, at the control wells, the prediction of  
336 the true curves by the ensemble median is also biased, up to the point that the true curves  
337 are outside the 90% confidence interval. For scenarios *R2* and *R3* the median curves for the  
338 three wells have a smaller bias than for *R1*, and the main difference between *R2* and *R3* is  
339 the same as for parameter prediction, the uncertainty is the widest for *R3*. The true curve  
340 is in both cases within the 90% confidence interval of the predictions.

341 At this point, it seems that an observation error with a standard deviation of 1 mg/l  
342 was the most consistent with our observations and model. **As mentioned above, this**  
343 **conclusion fits the findings by (Cupola et al., 2015b).** Yet, we were concerned with  
344 the big discrepancy between predictions and observations at well #9, so we decided to rerun  
345 scenario *R2* without using the data from this well. The results for this scenario, called *R2b*,  
346 are shown in Figure 9. When comparing this figure to the middle two rows in Figure 7 we



347 can notice that there is some overall improvement in the estimation of the true parameters  
348 —particularly for the position parameters— by the median values of the ensemble without  
349 a significant change on their uncertainty. This improvement reinforces our suspicion that  
350 there could have been some problems in the data collection at well #9.

351 We also considered that there could be a problem with the tightness of the vertical plate  
352 after its insertion in the sandbox. **The plate was supposed to represent a perfectly**  
353 **impermeable barrier, and no evidence of the contrary was observed during the**  
354 **experiments, yet the contact between the plate and sandbox walls could have**  
355 **had some small gaps, making the plate slightly permeable.** Therefore, we decided  
356 to rerun scenario *R2* but assuming that the plate is slightly permeable, more precisely, with  
357 a conductivity of two orders of magnitude smaller than the beads, **this value was chosen**  
358 **arbitrarily low since nothing was actually observed in the laboratory.** The results  
359 for the new scenario, referred to as *R2c* are shown in Figure 10. (Note that well #9 was kept  
360 in this scenario.) The main difference of this run is that the estimate of the size of the vertical  
361 plate by the median of the ensemble jumps from 40.5 cm to 44.2 cm (true value is 42.0 cm)  
362 indicating that possibly the plate conductivity used in this scenario was too large and, as  
363 a consequence, the algorithm enlarges the plate to reproduce the observed concentrations.  
364 **This result, while does not serve to justify that the tightness of the plate explains**  
365 **the numerical model misfit, shows the impact that such permeability would have**  
366 **in the estimation of the remaining parameters defining the plate.**

367 We can conclude that the r-EnKF can be applied to a more realistic case of a homogeneous  
368 aquifer in a sandbox for the identification of a contaminant source and some geometry  
369 parameters. A proper evaluation of the observation errors is paramount, since attempting  
370 to match too closely the data may result in biased estimates of the parameters.

## 371 5. Summary and Conclusion

372 The main purpose of this paper was to test whether the restart ensemble Kalman filter,  
373 which had been successfully applied in synthetic experiments, could be applied to a more  
374 realistic case based on a sandbox experiment. The test focuses on the identification of the  
375 parameters defining a finite-pulse point injection of a solute, together with the position of a  
376 vertical plate that modifies the initial rectangular geometry of the sandbox.

377 As a preliminary step, we tested the r-EnKF in a synthetic case mimicking the sandbox.  
378 Under these very controlled conditions, the algorithm performs well, as expected. The main  
379 difference with previous synthetic analyses is that no piezometric head data were used during  
380 the assimilation step of the filter.

381 Then, the r-EnKF is tested using the data coming from the laboratory experiment. In this  
382 case, the observations were not generated by a computer code nor we knew the observation  
383 error magnitude. The analysis of the results show that using a too small observation error  
384 variance results in more or less precise but biased estimates, both for the parameters subject  
385 to identification and for the concentrations at control locations. When a larger observation  
386 error (with a standard deviation of 1 mg/l) is introduced, estimates and predictions improve,  
387 although with larger uncertainty. And finally, when the observation error is large, the results  
388 worsen considerably. The removal of a suspicious observation well, the concentration of which  
389 is always underestimated by our forecast model, improves the results, indicating that the  
390 measurements from such well may need to be reconsidered. The changes observed after  
391 making the vertical plate slightly permeable do not appear to justify the hypothesis that the  
392 plate leaks.

393 The r-EnKF appears as a good algorithm for source identification in aquifers, yet it still  
394 needs further tests in closer-to-reality conditions. Currently, the sandbox has been replaced  
395 with a heterogeneous distribution of glass beads, and the challenge is to test the method in  
396 this new sandbox.

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Table 1: Parameters of the groundwater flow and transport model

Hydr. conduct., $K$	0.58 cm/s
Porosity, $\phi$	0.37
Long. disp., $\alpha_L$	0.16 cm
Transv. disp., $\alpha_T$	0.048 cm

Table 2: Source and geometry parameters. True values and suspect ranges for the generation of the initial ensemble of realizations

Parameter	Actual Value	Suspect Range
$X_s$ (cm) - $x$ -coordinate of source	18.5	16 – 25
$Z_s$ (cm) - $z$ -coordinate of source	30.5	23 – 32
$X_b$ (cm) - $x$ -coordinate of plate	52.5	50 – 59
$Z_b$ (cm) - plate length	42.5	35 – 43
$I_r$ (cm <sup>3</sup> /s) - injection rate	0.95	0.6 – 1.1
$I_c$ (mg/l) - injection load	20	5 – 24
$T_s$ (s) - starting release time	120	80 – 260
$T_e$ (s) - ending release time	1000	960 – 1140

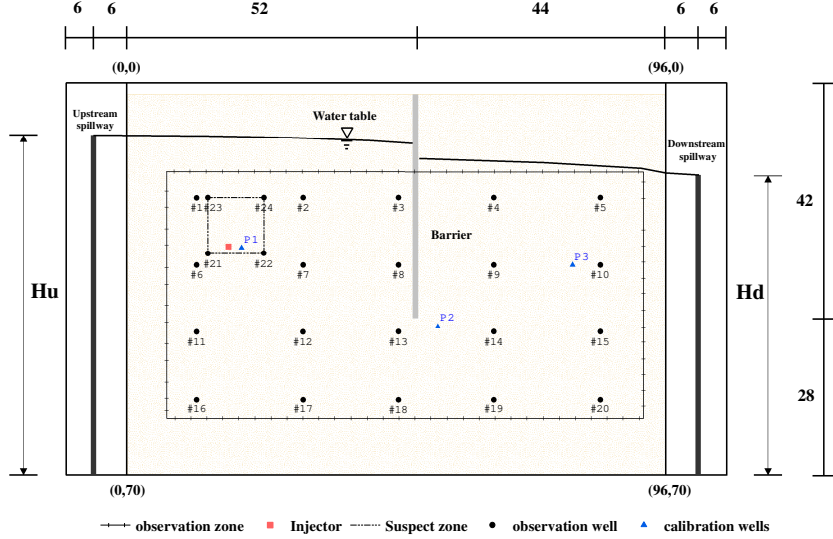


Figure 1: Sketch of the experimental device with indication of the upstream ( $H_u$ ) and downstream ( $H_d$ ) constant head boundaries. The ticked rectangle corresponds to the area captured by the camera in which concentrations will be monitored. Red dot is the release location. Dashed line around red dot indicates the release suspect location. Dimensions are in cm. Coordinates of the four corners of the flow and transport models are also shown.



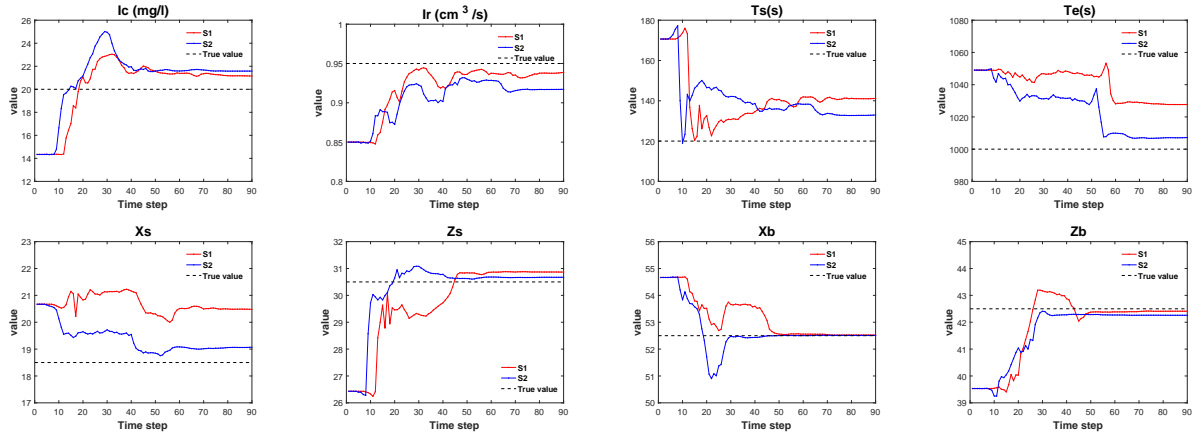


Figure 2: Time evolution of the ensemble mean of the 8 updated parameters, contaminant source location ( $X_s$ ,  $Z_s$ ), plate position ( $X_b$ ,  $Z_b$ ), injection information ( $I_c$ ,  $I_r$ ) and release time interval ( $T_s$ ,  $T_e$ ) for scenarios  $S_1$  and  $S_2$

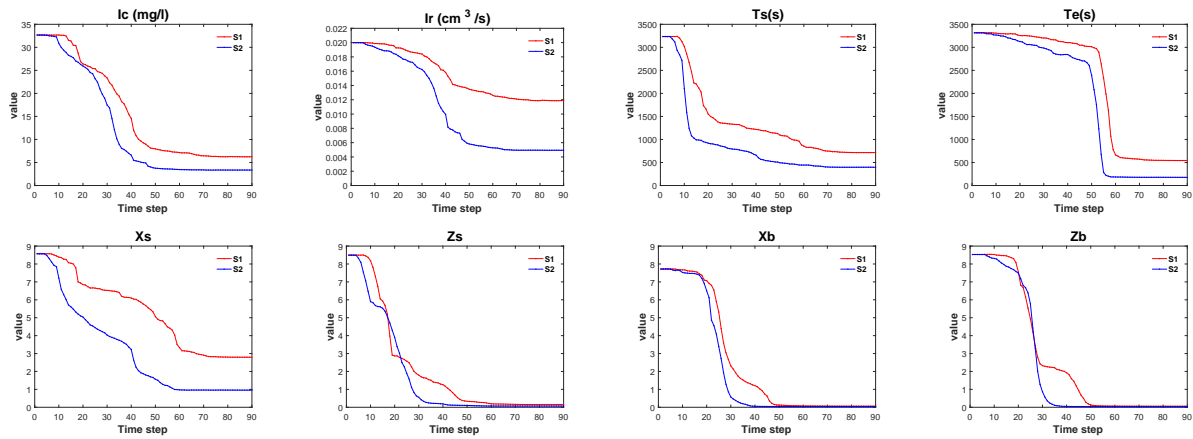


Figure 3: Time step evolution of the ensemble variance for the same parameters and scenarios as in the previous figure.

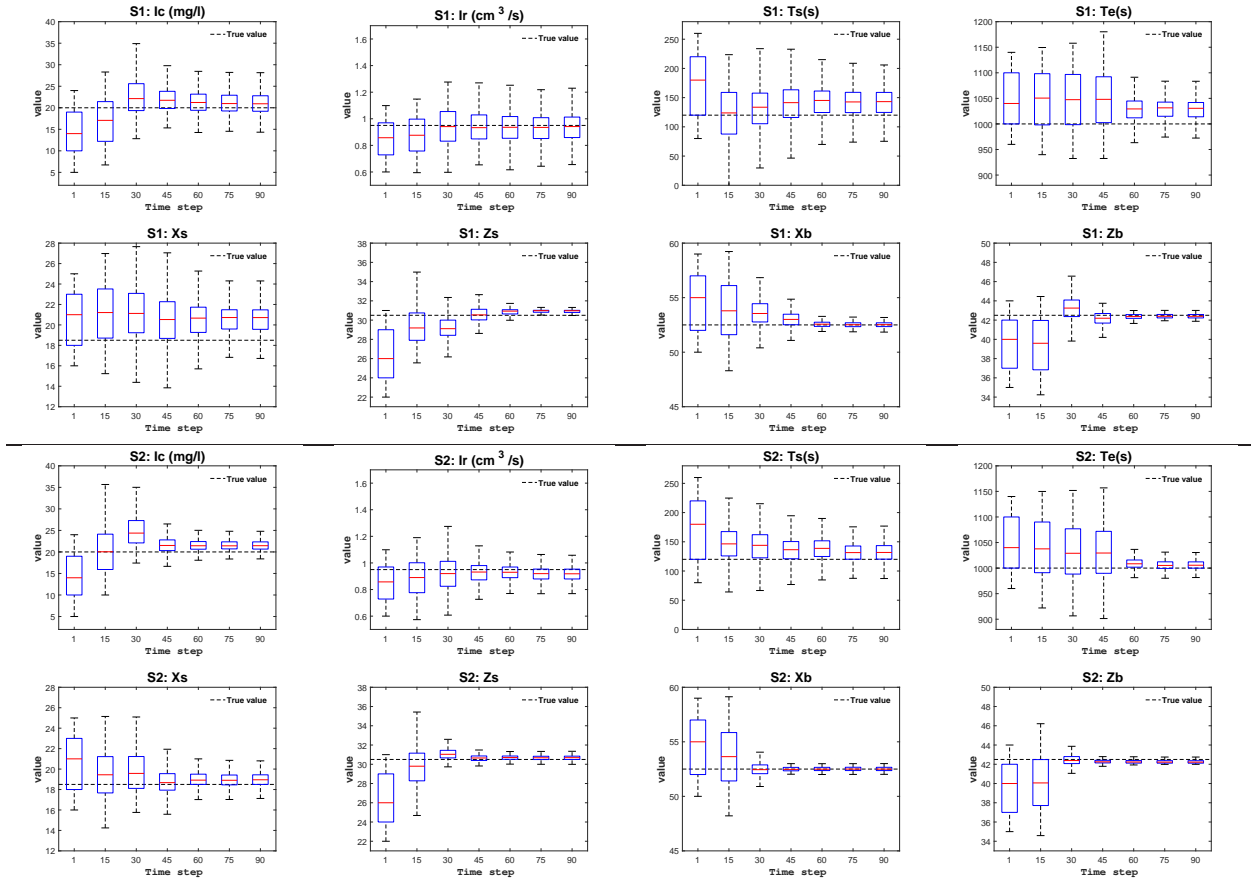


Figure 4: Boxplot of the 8 updated parameters at different time steps (1, 15, 30, 45, 60, 75, 90) for scenarios S1 and S2

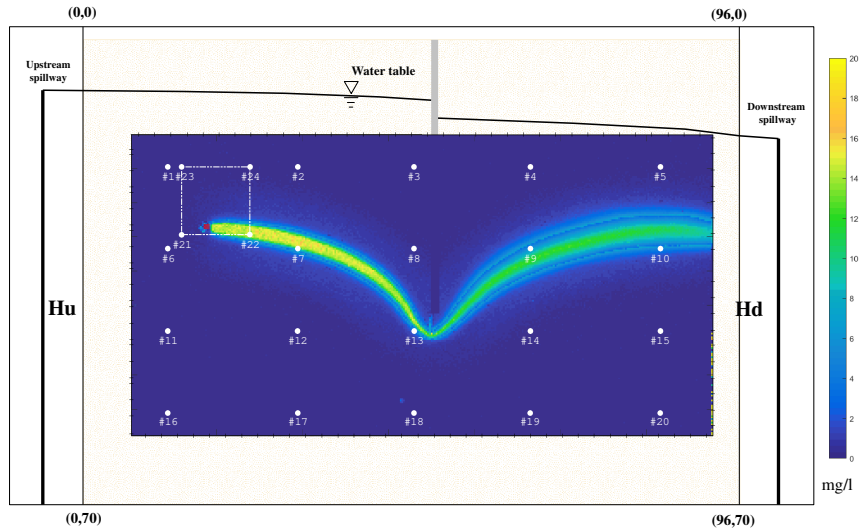


Figure 5: Fluorescein concentration field in the sandbox at the 48th time step. The area shown corresponds to the observation zone indicated in Fig. 1. The dash line shows the suspect zone for the injection and the white dots indicate the observation wells.

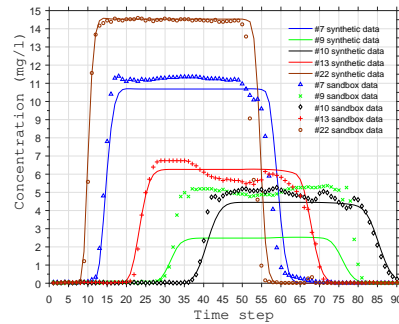


Figure 6: Fluorescein observed breakthrough curves at the observation wells located inside the plume and the curves computed from the numerical model

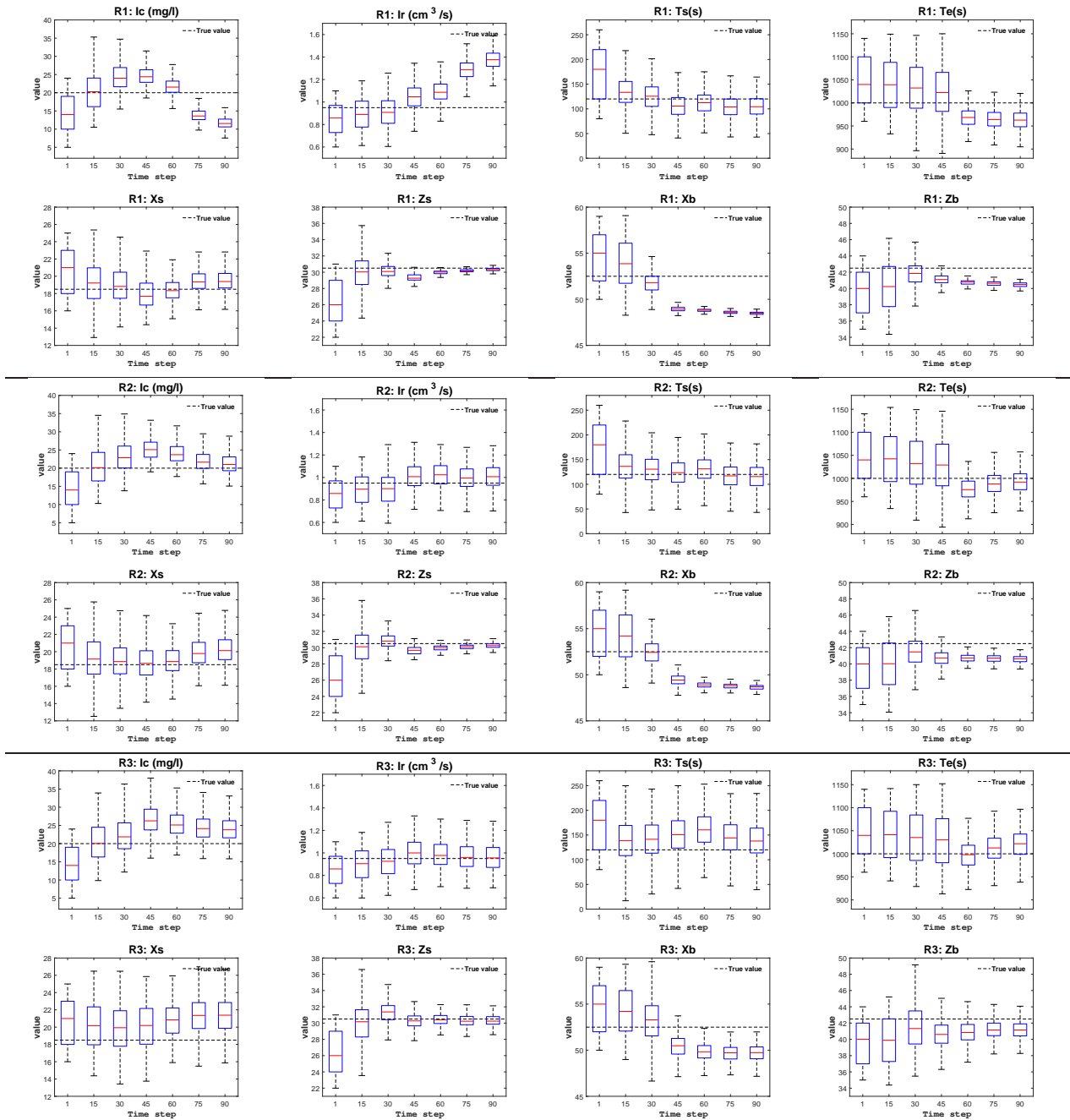


Figure 7: Boxplot of of the 8 updated parameters at time steps 1, 15, 30, 45, 60, 75 and 90 for scenarios  $R1$ ,  $R2$  and  $R3$

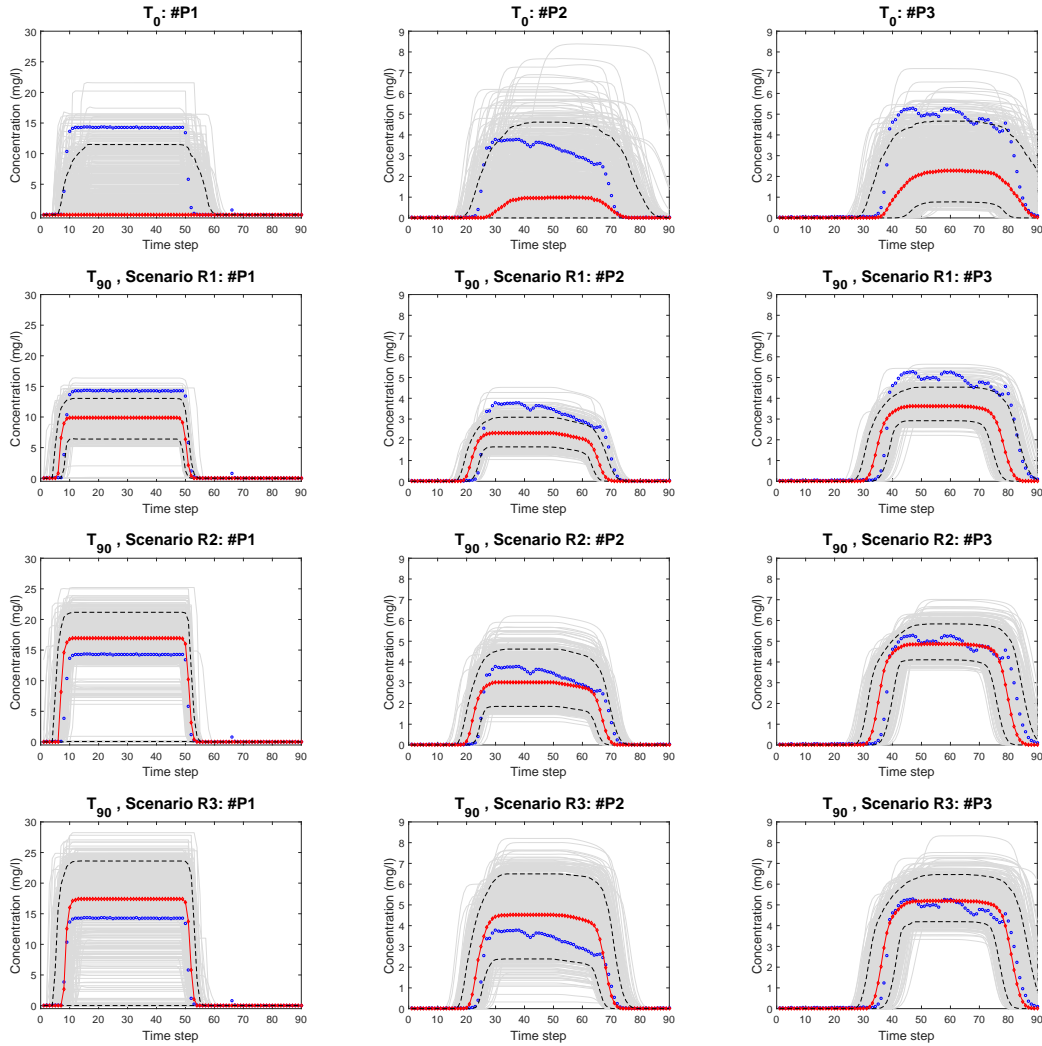


Figure 8: Breakthrough curves at control wells. The blue dots correspond to the curves in the sandbox experiment. The thin gray lines are the curves for all 800 realizations; they are summarized by their median (red diamond lines) and their 5 and 95 percentiles (black dash lines).

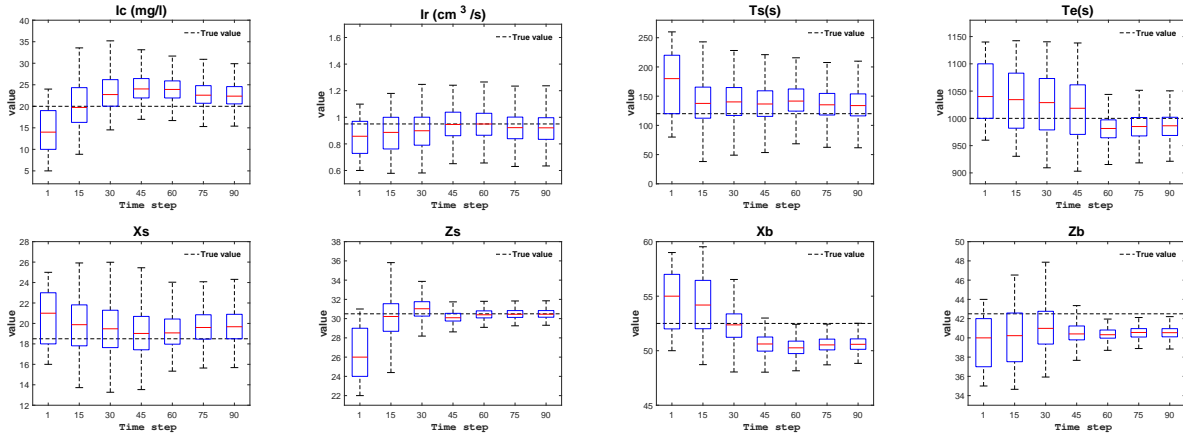


Figure 9: Boxplot of the 8 updated parameters in scenario *R2b* at different time steps (1, 15, 30, 45, 60, 75, 90)

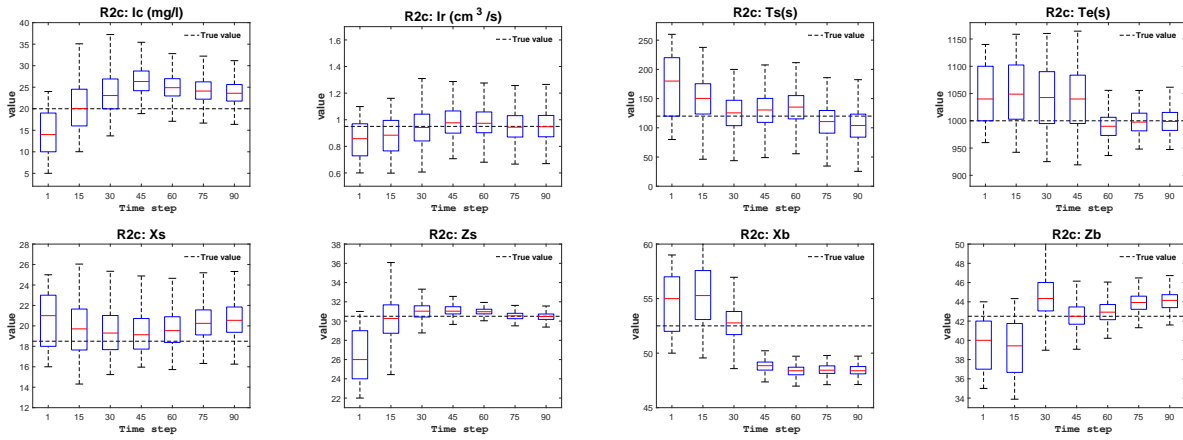


Figure 10: Boxplot of the 8 updated parameters in scenario *R2c* at different time steps (1, 15, 30, 45, 60, 75, 90)