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4 **Hydraulic and transport parameter assessment using column infiltration experiments**

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25 ***Abstract***

26 In the present work, we study the quality of the statistical calibration of hydraulic and
27 transport soil properties using an infiltration experiment in which, over a given period, tracer-
28 contaminated water is injected into a laboratory column filled with a homogeneous soil. The
29 numerical model is based on the Richards' equation for solving water flow and the advection-
30 dispersion equation for solving solute transport. Several state variables (e.g., water content,
31 solute concentration, pressure head) are measured during the experiment. Statistical
32 calibration of the computer model is then carried out for different data sets and injection
33 scenarios with the DREAM_(ZS) Markov Chain Monte Carlo sampler. The results show that the
34 injection period has a significant effect on the quality of the estimation, in particular, the
35 posterior uncertainty range. The hydraulic and transport parameters of the investigated soil
36 can be estimated from the infiltration experiment using the concentration and cumulative
37 outflow, which are measured non-intrusively. A significant improvement of the identifiability
38 of the parameters is observed when the pressure data from measurements taken inside the
39 column are also considered in the inversion.

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41 **Keywords**

42 Infiltration experiment, Richards' equation, Statistical calibration, Markov Chain Monte
43 Carlo, Uncertainty ranges.

44



45 **1. Introduction**

46 The soil parameters that influence water flow and contaminant transport in unsaturated zones
47 are not generally known *a priori* and have to be estimated by fitting model responses to
48 observed data. Several studies have demonstrated that unsaturated soil hydraulic parameters
49 can be (more or less accurately) estimated from dynamic flow experiments (*e.g.*, Hopmans et
50 al., 2002; Vrugt et al., 2003a; Durner and Iden, 2011; Younes et al., 2013). Inoue et al. (2000)
51 showed that both hydraulic and transport parameters can be assessed by the combination of
52 flow and transport experiments. Indeed, the simultaneous estimation of hydraulic and
53 transport properties yields smaller estimation errors for model parameters than the sequential
54 inversion of hydraulic properties from the water content and/or pressure head followed by the
55 inversion of transport properties from concentration data (Misra and Parker, 1989).

56 In the present work, we consider the flow and the transport of an inert solute injected into a
57 laboratory column filled with a homogeneous sandy clay loam soil. The flow-transport model
58 is described by the Richards' equation (RE) for water flow and the advection dispersion
59 equation for solute transport. The Mualem-van Genuchten (MvG) models (Mualem 1976, van
60 Genuchten 1980) are chosen to describe the retention curve and to relate the hydraulic
61 conductivity of the unsaturated soil to the water content. The estimation of hydraulic and
62 transport parameters is performed in a Bayesian framework using the Markov Chain Monte
63 Carlo (MCMC) sampler (Vrugt and Bouten, 2002; Vrugt et al., 2008) for two injection
64 periods and different data measurement scenarios. Unlike classical parameter optimization
65 algorithms, the MCMC approach provides parameter joint probability distributions, which are
66 useful for the quality assessment of the estimation. Indeed, MCMC samples can be used to
67 summarize parameter uncertainties and to perform predictive uncertainty (Ades and Lu,
68 2003).



69 Soil parameters are usually investigated using multistep outflow experiments (e.g., Eching
 70 and Hopmans, 1993; Eching et al., 1994; van Dam et al., 1994) or continuously changing
 71 time-varying boundary conditions (Durner et al., 1999). Multistep outflow experiments are
 72 among the most popular laboratory methods (Hopmans et al., 2002). However, their
 73 application is limited by expensive measurement equipment (Nasta et al., 2011).

74 In this work, hydraulic soil parameters are investigated using an infiltration experiment in a
 75 1.2 m long laboratory column, which is the standard scale for these types of experiments. The
 76 column, which is initially hydrostatic and free of solute, is filled with a homogeneous sandy
 77 clay loam soil. Continuous flow and solute injection are performed during a time period T_{inj} at
 78 the top of the column and with a zero pressure head at the bottom. The unknown parameters
 79 for the water flow are k_s [LT^{-1}], the saturated hydraulic conductivity; θ_s [L^3L^{-3}], the
 80 saturated water content; θ_r [L^3L^{-3}], the residual water content; and α [L^{-1}] and n [–], the
 81 MvG shape parameters. The only unknown parameter of the tracer transport is the
 82 longitudinal dispersivity, a_L [L].

83 Several scenarios corresponding to different sets of measurements are investigated to address
 84 the following questions:

- 85 1) Can we obtain an appropriate estimation of all flow and transport parameters from the
 86 tracer-infiltration experiment, even though only moderately dry conditions are used?
- 87 2) What is the optimal set of measurements for the estimation of all the parameters? Can
 88 we use only non-intrusive measurements (cumulative outflow and concentration
 89 breakthrough curve) or are intrusive measurements required, such as the analysis of
 90 the pressure head and/or water content inside the column?
- 91 3) Does the duration of the injection period T_{inj} have an impact on the identification of
 92 the parameters?



93 Synthetic scenarios are considered in the sequel in which data from numerical simulations are
 94 manipulated to avoid the uncontrolled noise of experiments that could bias the conclusions.
 95 The paper is organized as follows. The mathematical models describing flow and transport in
 96 the unsaturated zone are detailed in section 2. Section 3 describes the MCMC Bayesian
 97 parameter estimation procedure used in the DREAM_(ZS) sampler. Section 4 presents the
 98 different investigated scenarios and discusses the results of the calibration in terms of mean
 99 parameter values and uncertainty ranges for each scenario. Conclusions are given in section 5.

100

101 **2. Unsaturated flow-transport model**

102 We consider a uniform soil profile in the column and an injection of a solute tracer such as
 103 bromide, as described in Mertens et al. (2009). The unsaturated water flow in the vertical soil
 104 column is modeled with the one-dimensional pressure head form of the RE:

$$105 \quad \begin{cases} \left(c(h) + S_s \frac{\theta}{\theta_s} \right) \frac{\partial h}{\partial t} = \frac{\partial q}{\partial z} \\ q = K(h) \left(\frac{\partial h}{\partial z} - 1 \right) \end{cases}, \quad (1)$$

106 where h [L] is the pressure head; q [LT⁻¹] is the Darcy velocity; z [L] is the depth, measured
 107 as positive in the downward direction; S_s (-) is the specific storage; θ and θ_s [L³.L⁻³] are the
 108 actual and saturated water contents, respectively; $c(h)$ [L⁻¹] is the specific moisture capacity;
 109 and $K(h)$ [L T⁻¹] is the hydraulic conductivity. The latter two parameters are both functions
 110 of the pressure head. In this study, the relations between the pressure head, conductivity and
 111 water content are described by the following standard models of Mualem (1972) and van
 112 Genuchten (1980):



$$S_e(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} = \begin{cases} \frac{1}{(1 + |\alpha h|^n)^m} & h < 0 \\ 1 & h \geq 0 \end{cases} \quad (2)$$

$$K(S_e) = K_s S_e^{1/2} \left[1 - (1 - S_e^{1/m})^m \right]^2,$$

where S_e (-) is the effective saturation, θ_r [$L^3 L^{-3}$] is the residual water content, K_s [$L T^{-1}$] is the saturated hydraulic conductivity, and $m = 1 - 1/n$, α [L^{-1}] and n (-) are the MvG shape parameters.

The tracer transport is governed by the following convection-dispersion equation:

$$\frac{\partial(\theta C)}{\partial t} + \frac{\partial(qC)}{\partial z} - \frac{\partial}{\partial z} \left(\theta D \frac{\partial C}{\partial z} \right) = 0, \quad (3)$$

where C [ML^{-3}] is the concentration of the tracer, D [$L^2 T^{-1}$] is the dispersion coefficient in which $D = a_l q + d_m$ and a_l [L] is the dispersivity coefficient of the soil and d_m [$L^2 T^{-1}$] is the molecular diffusion coefficient, which is set as $1.04 \cdot 10^{-4} \text{ cm}^2/\text{min}$.

The initial conditions are as follows: a hydrostatic pressure distribution with zero pressure head at the bottom of the column ($z = L$) and a solute concentration of zero inside the whole column. An infiltration with a flux q_{inj} of contaminated water with a concentration C_{inj} is then applied at the upper boundary condition ($z = 0$) during a period T_{inj} . Hence, the boundary conditions at the top of the column can be expressed as:

$$\text{for } 0 < t \leq T_{inj} \quad \begin{cases} K \left(\frac{\partial h}{\partial z} - 1 \right) = q_{inj} \\ \theta D \frac{\partial C}{\partial z} + qC = q_{inj} C_{inj} \end{cases} \quad \text{for } t > T_{inj} \quad \begin{cases} K \left(\frac{\partial h}{\partial z} - 1 \right) = 0 \\ C_{inj} = 0 \end{cases} \quad (4)$$

A zero pressure head is maintained at the lower boundary ($z = L$) of the column and a zero concentration gradient is used as the lower boundary condition for the solute transport.



$$(h)_{z=l} = 0 \quad \left(\frac{\partial C}{\partial z} \right)_{z=l} = 0 \quad (5)$$

In the sequel, the infiltration rate and the injected solute concentration are $q_{inj} = 0.015$ cm/min and $C_{inj} = 1$ g/cm³, respectively. The system (1)-(3) is solved using the finite volume method for both flow and transport spatial discretization. A uniform mesh of 600 cells is employed. Temporal discretization is performed with the high-order method of lines (MOL) (e.g., Miller et al., 1998; Tocci et al., 1997; Fahs et al., 2009). Error checking, robustness, order selection and adaptive time step features, available in sophisticated solvers, are applied to the time integration of partial differential equations in the MOL (Tocci et al., 1997). The MOL has been successfully used to solve RE in many studies (e.g., Farthing et al., 2003; Miller et al., 2006; Li et al., 2007; Fahs et al., 2009).

The unknown parameters for the water flow are k_s , θ_s , θ_r and the MvG shape parameters α and n . The only unknown parameter of the tracer transport is the longitudinal dispersivity a_L . Hence, the total vector of parameters is $\xi = (k_s, \theta_s, \theta_r, \alpha, n, a_L)$. A reference solution is generated using the following parameter values (corresponding to a sandy clay loam soil): $k_s = 50$ cm/day, $\theta_s = 0.43$, $\theta_r = 0.09$, $\alpha = 0.04$ cm⁻¹, $n = 1.4$ and $a_L = 0.2$ cm. Four types of observations are deduced from the results of the simulation, which include the following: the pressure head and water content near the surface (5 cm below the top of the column) as well as the cumulative outflow and the breakthrough concentration at the output of the column. The vector of observations y_{mes} is formed by the four data series, which are independently corrupted with a normally distributed noise using the following standard deviations: $\sigma_h = 1$ cm for the pressure head, $\sigma_\theta = 0.02$ for the water content, $\sigma_Q = 0.1$ cm for the cumulative outflow and $\sigma_C = 0.01$ g/cm³ for the exit concentration.



152 3. Bayesian parameter estimation

153 The flow-transport model is used to analyze the effects of different measurement sets on
 154 parameter identification. For this purpose, we adopt a Bayesian approach that involves the
 155 parameter joint posterior distribution (Vrugt et al., 2008). The latter is assessed with the
 156 DREAM_(ZS) MCMC sampler (Laloy and Vrugt, 2012). This software generates random
 157 sequences of parameter sets that asymptotically converge toward the target joint posterior
 158 distribution (Gelman et al., 1997). Thus, if the number of runs is sufficiently high, the
 159 generated samples can be used to estimate the statistical measures of the posterior
 160 distribution, such as the mean and variance among other measures.

161 The Bayes theorem states that the probability density function of the model parameters
 162 conditioned onto data can be expressed as:

$$163 \quad p(\xi | y_{mes}) \propto p(y_{mes} | \xi) p(\xi), \quad (6)$$

164 where $p(\xi | y_{mes})$ is the likelihood function measuring how well the model fits the
 165 observations y_{mes} , and $p(\xi)$ is the prior assumption of the parameter before the observations
 166 are made. In this work, a Gaussian distribution defines the likelihood function because the
 167 observations are simulated and corrupted with Gaussian errors. In addition, independent
 168 uniform priors are considered. Hence, the parameter posterior distribution is expressed as:

$$169 \quad p(\xi / y_{mes}) \propto \exp \left(-\frac{SS_h(\xi)}{2\sigma_h^2} - \frac{SS_\theta(\xi)}{2\sigma_\theta^2} - \frac{SS_Q(\xi)}{2\sigma_Q^2} - \frac{SS_C(\xi)}{2\sigma_C^2} \right), \quad (7)$$

170 where $SS_h(\xi)$, $SS_\theta(\xi)$, $SS_Q(\xi)$ and $SS_C(\xi)$ are the sums of the squared differences
 171 between the observed and modeled data of the pressure head, water content, cumulative
 172 outflow and output concentration, respectively. For instance, $SS_h(\xi) = \sum_{k=1}^{Nh} (h_{mes}^{(k)} - h_{mod}^{(k)}(\xi))^2$,



173 which includes the observed and predicted pressure heads $h_{mes}^{(k)}$ and $h_{mod}^{(k)}$ at time t_k and the
 174 number of pressure head observations Nh .
 175 Bayesian parameter estimation is performed hereafter with the DREAM_(ZS) software (Laloy
 176 and Vrugt, 2012), which is an efficient MCMC sampler. DREAM_(ZS) computes multiple sub-
 177 chains in parallel to thoroughly explore the parameter space. Archives of the states of the sub-
 178 chains are also stored and used to allow a strong reduction of the "burn-in" period in which
 179 the sampler generates individuals with poor performances. Taking the last 25% of individuals
 180 of the MCMC (when the chains have converged) yields multiple sets of parameters, ξ , that
 181 adequately fit the model onto observations. These sets are then used to estimate the updated
 182 parameter distributions, the pairwise parameter correlations and the uncertainty of the model
 183 predictions. As suggested in Vrugt et al. (2003b), the posterior distribution becomes
 184 stationary if the Gelman and Ruban (1992) criterion is ≤ 1.2 .

185 **4. Results and discussion**

186 In this section, the identifiability of the parameters is investigated for different scenarios of
 187 measurement sets and for two periods of injections. In all cases, the MCMC sampler was run
 188 with 3 simultaneous chains for a total number of 50000 runs. Depending on the scenario, the
 189 MCMC required between 5000 and 20000 model runs to reach convergence. The last 25% of
 190 the runs that adequately fit the model onto observations are used to estimate the updated
 191 probability density function (pdf).

193 **4.1. Reference solution and data measurements**

194 The reference solutions obtained from solving the flow-transport problems (1)-(3) using the
 195 parameters given above are shown in Fig. 1 to 6. The pressure head at 5 cm, at the top of the
 196 column (Fig. 1), increases quickly from its initial hydrostatic negative value (approximately -



115 cm) and reaches a plateau (-1.75 cm) during the injection period. After the injection is finished, it progressively decreases due to the drainage caused by the gravity effect. A similar behavior is observed for the water content at the same location (Fig. 2), where the value of the plateau is close to the saturation value. The cumulative outflow (Fig. 3) starts to increase at approximately 1000 min after the beginning of the injection. It shows an almost linear behavior until 5500 min. It then slowly increases with an asymptotic behavior due to the natural drainage after the end of the injection. Fig. 4 displays the water saturation as a function of the pressure head. It is worth noting that only a few parts of this curve are described during the infiltration experiment. Indeed, only moderate dry conditions are established because the minimum pressure head reached in the column is -120 cm, which corresponds to the initial pressure head near the top of the column.

The breakthrough concentration curve (Fig. 5) shows a sharp front, which starts shortly after 3000 min. If the injection of both water and contaminant are stopped once the solute reaches the output, i.e., after an injection period of 3000 min, the breakthrough curve exhibits a smoother progression (Fig. 6).

The observed data, which are used as conditioning information for model calibration, are also shown in Fig. 1 to 6. Fig. 2 shows that the water content is more affected by the perturbation of data than by the pressure head and cumulative outflow because (i) we mimic the relative importance of the measurement errors of the water content due to time-domain-reflectometry probes and (ii) the weak variation of the water content during the infiltration experiment. The perturbation of the breakthrough curve is relatively small because output concentrations can be accurately measured. The perturbations of the pressure head and cumulative outflow seem weak because of the large variation of these variables during the experiment.

220



221 **4.2. Results of the parameter estimation**

222 The uncertainty model parameters are assumed to be distributed uniformly over the ranges
 223 reported in Table 1. This table also lists the reference values used to generate data
 224 observations before perturbation. Seven scenarios, corresponding to different sets of
 225 measurements for the estimation of the soil parameters, are considered (Table 2).

226 The MCMC results of the seven studied scenarios are given in Figs. 8 to 13. The "on-
 227 diagonal" plots in these figures display the inferred parameter distributions, whereas the "off-
 228 diagonal" plots represent the pairwise correlations in the MCMC sample. If the drawings are
 229 independent, non-sloping scatterplots should be observed. However, if a good value of a
 230 given parameter is conditioned by the value of another parameter, then their pairwise
 231 scatterplot should show a narrow sloping stripe. To facilitate the comparison between the
 232 different scenarios, Fig. 14 to 19 show the mean and the 95% confidence intervals of the final
 233 MCMC sample that adequately fit the model onto observations for each scenario, and Table 3
 234 summarizes the pairwise parameter correlations.

235 Fig. 7 shows the inferred distributions of the parameters identified with the MCMC sampler
 236 using only the pressure and cumulative outflow measurements (scenario 1). The parameters
 237 k_s , α and n are well estimated; their prior intervals of variation are strongly narrowed and
 238 they essentially show bell-shaped posterior distributions. Parameter k_s is strongly correlated
 239 to α (0.94) and n (-0.97). Because the water retention relationship depends on the difference
 240 between θ_s and θ_r , these parameters are strongly correlated (0.96) and cannot be identified.

241 The dispersivity coefficient a_l has not been identified.

242 The MCMC results (Fig. 8) show that θ_r strongly correlates to k_s (-0.94) and n (0.98) when
 243 water content measurements are added into the model (scenario 2). The parameter k_s remains
 244 strongly related to α (0.94) and n (-0.98). Although the water content data are subject to



245 relatively high measurement errors, a good estimation is obtained for θ_s and θ_r . The
 246 parameters k_s , α and n are estimated with the same accuracy as for the first scenario.
 247 When the concentration measurements are also considered (scenario 3), the results depicted in
 248 Fig. 9 show very significant correlations between k_s and θ_r (-0.94), k_s and α (0.91), k_s and
 249 n (-0.97) and n and θ_r (0.99). The posterior uncertainty ranges of k_s , α , n and θ_r are
 250 similar to the previous scenarios. Those of θ_s and a_l are strongly reduced, leading to a good
 251 identification of these parameters when using C measurements (Fig. 15 and 19). A better
 252 estimate of the saturated water content is expected because advective transport is a function of
 253 this variable.
 254 The measurements of the water content are not considered in the inversion procedure of
 255 scenario 4. This scenario leads to the same quality of the estimation for the parameters k_s , θ_r ,
 256 α and n (Fig. 14, 16, 17, 18) and similar correlations between the parameters as in the
 257 previous scenario. This result shows that the intrusive water content measurements, which are
 258 subject to more measurement errors than the output concentration, are not required if the
 259 output concentration is measured. Compared with the results of scenario 2, it can be
 260 concluded that better parameter estimations are obtained using h , Q and C data than using
 261 h , Q and θ data, especially for θ_s . Therefore, using C instead of θ measurements in
 262 combination with h and Q measurements allows the estimation of a_l and leads to a better
 263 estimate of θ_s .
 264 The pressure head, cumulative outflow and concentration measurements are used in the
 265 estimation procedure of scenario 5, but the injection period is now reduced to $T_{inj} = 3000$ min .
 266 The obtained results (Fig. 11) show the same correlations between the parameters as for
 267 $T_{inj} = 5000$ min . For the parameters k_s , θ_s , θ_r , α and n , almost the same mean estimates are



268 obtained as for scenario 4. However, the parameters are better identified (Fig. 14 to 18).
 269 Indeed, the uncertainty of these parameters is smaller because the credible interval is reduced
 270 by a factor of 25% for k_s , 8% for θ_s , 26% for θ_r , 10% for α and 25% for n when compared
 271 to the results obtained for $T_{inj} = 5000 \text{ min}$. The parameter a_l is also estimated much better
 272 than in the previous scenario. Its mean value approaches the reference solution and the
 273 posterior uncertainty range is reduced by approximately 75% (Fig. 19).
 274 The pressure head measurements are removed in scenario 6 and only non-intrusive
 275 measurements (Q and C data) are used with an injection period of $T_{inj} = 5000 \text{ min}$. The
 276 results depicted in Fig. 12 show high correlations only between k_s and n (-0.95) and θ_r and
 277 n (0.95). Compared with the results of scenario 4, which also considers the pressure data, k_s
 278 is poorly estimated (the mean value is less close to the reference value and the credible
 279 interval is 27% larger). The mean estimated values for θ_r and n also degraded (less close to
 280 the reference solution), although their confidence intervals are similar to those of scenario 4
 281 (Fig. 16, 18). The estimated mean value of parameter α is similar to that in scenario 4.
 282 However, its uncertainty is much larger because the credible interval is 77% larger (Fig. 19).
 283 The parameters θ_s and a_l are estimated as well in scenario 4 (in terms of mean estimated
 284 value and credible interval).
 285 The last scenario (scenario 7) is similar to the previous one, but the injection period is reduced
 286 to $T_{inj} = 3000 \text{ min}$. The results depicted in Fig. 13 show similar correlations between the
 287 parameters as for $T_{inj} = 5000 \text{ min}$. However, a significant improvement is observed for the
 288 mean estimated values, which approach the reference solution for k_s , θ_r , n and a_l (Fig. 14,
 289 16, 18, 19). The uncertainties of k_s , α and a_l are also reduced by approximately 40%, 15%
 290 and 70%, respectively. The parameter θ_s is estimated as well in scenario 6.



291 5. Conclusions

292 In this work, hydraulic and transport soil parameters have been estimated using an infiltration
 293 experiment performed in a laboratory column filled with sandy clay loam soil, which was
 294 subjected to continuous flow and solute injection over a period T_{inj} . Parameter estimation was
 295 performed for different scenarios of data measurements in a Bayesian framework using the
 296 DREAM_(zs) MCMC sampler (Laloy and Vrugt, 2012).

297

298 The results reveal the following conclusions:

- 299 1. All hydraulic and transport parameters can be appropriately estimated from the
 300 described infiltration experiment. However, the accuracy differs and depends on the
 301 type of measurement and the duration of the injection T_{inj} , even if the water content
 302 remains close to saturated conditions.
- 303 2. The use of concentration measurements at the column outflow, in addition to
 304 traditional measured variables (water content, pressure head and cumulative outflow),
 305 reduces the correlation between the hydraulic parameters and their uncertainties,
 306 especially that of the saturated water content.
- 307 3. The saturated hydraulic conductivity is estimated with the same order of accuracy,
 308 independent of the observed variables.
- 309 4. The estimation of the dispersivity is sensitive to the injection duration.
- 310 5. A better identifiability of the soil parameters is obtained using C instead of θ
 311 measurements, in combination with h and Q data.
- 312 6. Using only non-intrusive measurements (cumulative outflow and output
 313 concentration) allows the satisfactory estimation of all parameters. The uncertainty of
 314 the parameters significantly decreases when the injection of water and solute is
 315 maintained for a limited period.



316

317 This last point has practical applications for designing simple experimental setups dedicated
318 to the estimation of hydrodynamic and transport parameters for unsaturated flow in soils. The
319 setup has to be appropriately equipped to measure the cumulative water outflow (e.g.,
320 weighing machine) and the solute breakthrough at the column outflow (e.g., flow through
321 electrical conductivity). The injection should be stopped as soon as the solute concentration
322 reaches the outflow. The accuracy of the estimation of θ_r , α and n can be improved by
323 adding pressure measurements inside the column, close to the injection.

324

325 **Acknowledgments**

326 The authors are grateful to the French National Research Agency, which funded this work
327 through the program AAP Blanc - SIMI 6 project RESAIN (n° ANR-12-BS06-0010-02).

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444 **List of table captions**

445

446 Table 1. Prior lower and upper bounds of the uncertainty parameters and reference values.

447

448 Table 2. Measurement sets and injection periods for the different scenarios. The pressure head
449 h and the water content θ are measured at 5 cm from the top of the column. The cumulative
450 outflow Q and the concentration C are measured at the exit of the column.

451

452 Table 3. Summary of the pairwise parameter correlations.

453



454

Parameters	Lower bounds	Upper bounds	Reference values
k_s [cm min ⁻¹]	0.025	0.1	0.0347
θ_s [-]	0.3	0.5	0.43
θ_r [-]	0.05	0.2	0.09
α [cm ⁻¹]	0.01	0.3	0.04
n [-]	1.2	5	1.4
a_l [cm]	0.05	0.6	0.2

455

456 Table 1. Prior lower and upper bounds of the uncertainty parameters and reference values.

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460

Scenario	Measured variables				injection period	
	h	θ	Q	C	$T_{inj} = 5000$ min	$T_{inj} = 3000$ min
1	v		v		v	
2	v	v	v		v	
3	v	v	v	v	v	
4	v		v	v	v	
5	v		v	v		v
6			v	v	v	
7			v	v		v

461

462 Table 2. Measurement sets and injection periods for the different scenarios. The pressure head
 463 h and the water content θ are measured at 5 cm from the top of the column. The cumulative
 464 outflow Q and the concentration C are measured at the exit of the column.

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Scenario				
1	(k_s, n)	(k_s, α)		(θ_r, θ_s)
2	(k_s, n)	(k_s, α)	(k_s, θ_r)	(θ_r, n)
3	(k_s, n)	(k_s, α)	(k_s, θ_r)	(θ_r, n)
4	(k_s, n)	(k_s, α)	(k_s, θ_r)	(θ_r, n)
5	(k_s, n)	(k_s, α)	(k_s, θ_r)	(θ_r, n)
6	(k_s, n)			(θ_r, n)
7	(k_s, n)			(θ_r, n)

471 Table 3. Summary of the pairwise parameter correlations.

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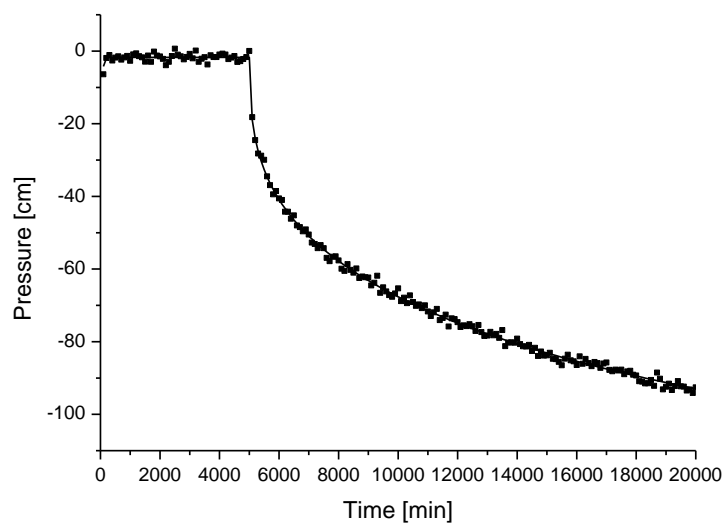


474 **List of figure captions**

- 475 Fig. 1. Reference pressure head at 5 cm from the soil surface. Solid lines represent model
 476 outputs and dots represent the sets of perturbed data serving as conditioning information for
 477 model calibration.
- 478 Fig. 2. Reference water content at 5 cm from the soil surface [see Fig. 1 caption].
- 479 Fig. 3. Reference cumulative outflow [see Fig. 1 caption].
- 480 Fig. 4. Reference retention curve for the infiltration experiment [see Fig. 1 caption].
- 481 Fig. 5. Reference breakthrough output concentration for $T_{inj} = 5000$. [see Fig. 1 caption].
- 482 Fig. 6. Reference breakthrough output concentration for $T_{inj} = 3000$ min. [see Fig. 1 caption].
- 483 Fig. 7. MCMC solutions for the transport scenario 1. The diagonal plots represent the inferred
 484 posterior probability distribution of the model parameters. The off-diagonal scatterplots
 485 represent the pairwise correlations in the MCMC drawing.
- 486 Fig. 8. MCMC solutions for transport scenario 2 [see Fig. 7 caption].
- 487 Fig. 9. MCMC solutions for transport scenario 3 [see Fig. 7 caption].
- 488 Fig. 10. MCMC solutions for transport scenario 4 [see Fig. 7 caption].
- 489 Fig. 11. MCMC solutions for transport scenario 5 [see Fig. 7 caption].
- 490 Fig. 12. MCMC solutions for transport scenario 6 [see Fig. 7 caption].
- 491 Fig. 13. MCMC solutions for transport scenario 7 [see Fig. 7 caption].
- 492 Fig. 14. Posterior mean values and 95% confidence intervals of the saturated hydraulic
 493 conductivity for the different scenarios.
- 494 Fig. 15. Posterior mean values and 95% confidence intervals of the saturated water content for
 495 the different scenarios.
- 496 Fig. 16. Posterior mean values and 95% confidence intervals of the residual water content for
 497 the different scenarios.
- 498 Fig. 17. Posterior mean values and 95% confidence intervals of the shape parameter α for the
 499 different scenarios.
- 500 Fig. 18. Posterior mean values and 95% confidence intervals of the shape parameter n for the
 501 different scenarios.
- 502 Fig. 19. Posterior mean values and 95% confidence intervals of dispersivity for the different
 503 scenarios.
- 504



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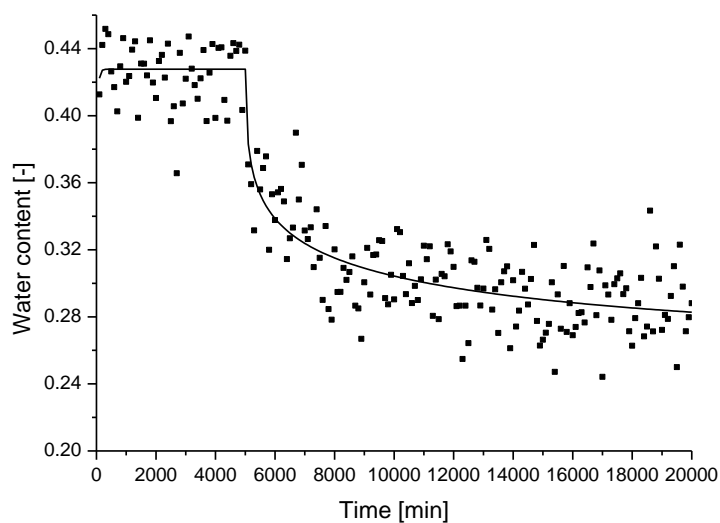
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Fig. 1. Reference pressure head at 5 cm from the soil surface. Solid lines represent model outputs and dots represent the sets of perturbed data serving as conditioning information for model calibration.

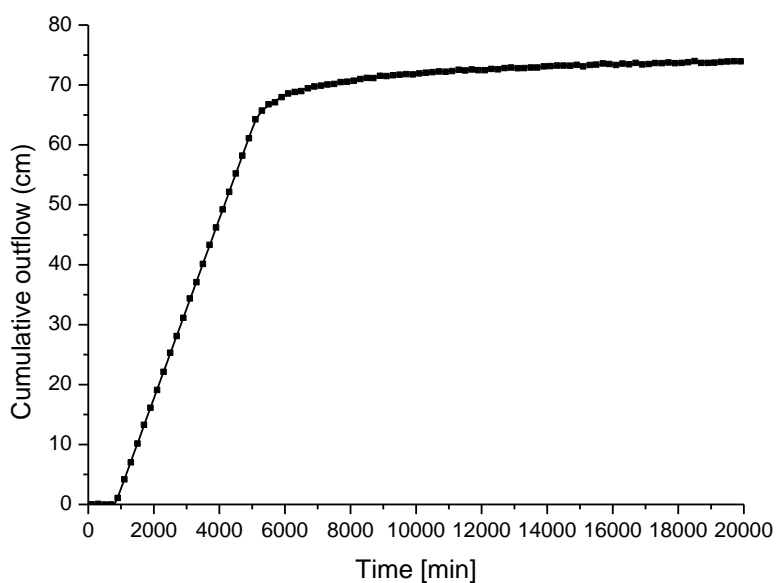


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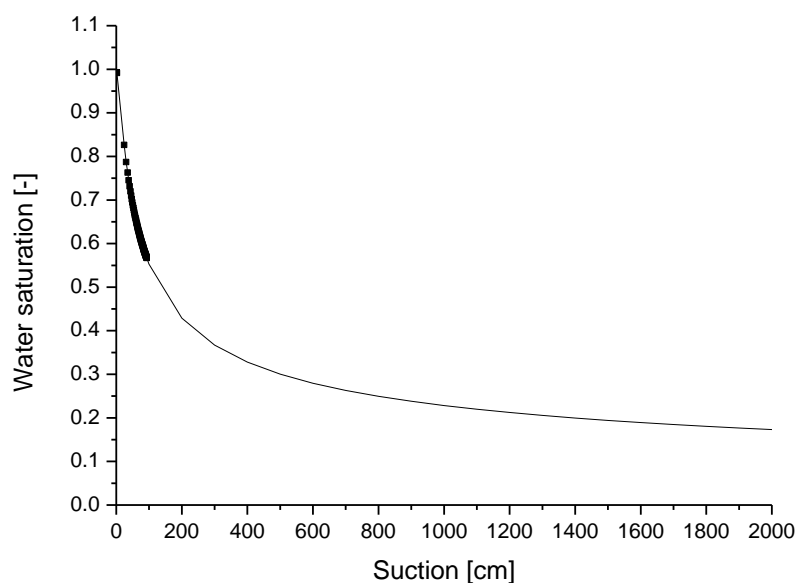
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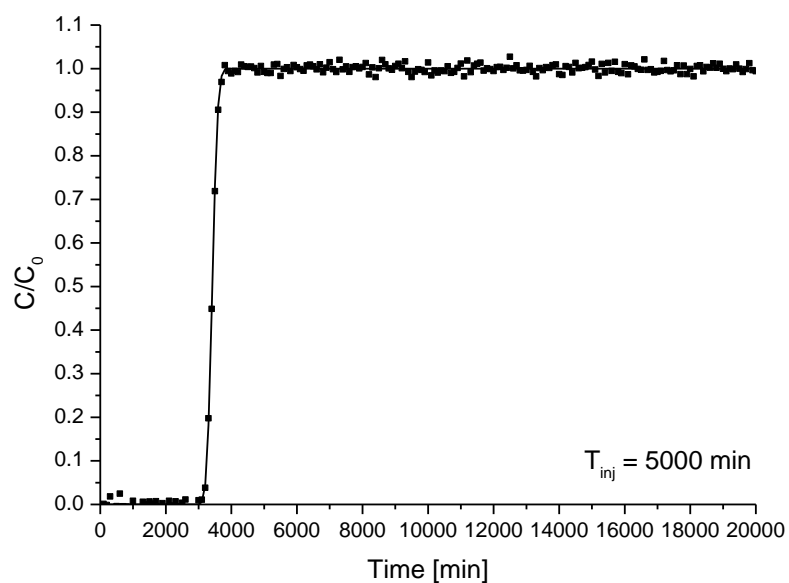
Fig. 2. Reference water content at 5 cm from the soil surface [see Fig. 1 caption].



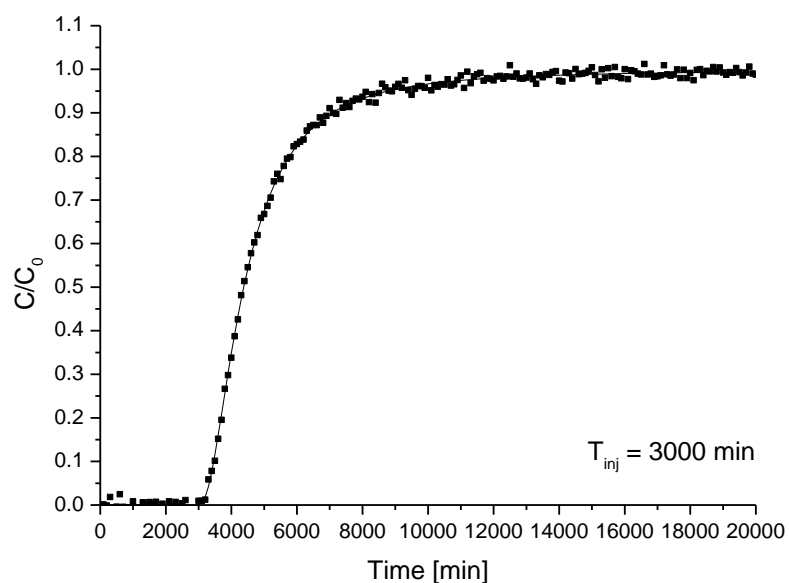
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 514 Fig. 3. Reference cumulative outflow [see Fig. 1 caption].



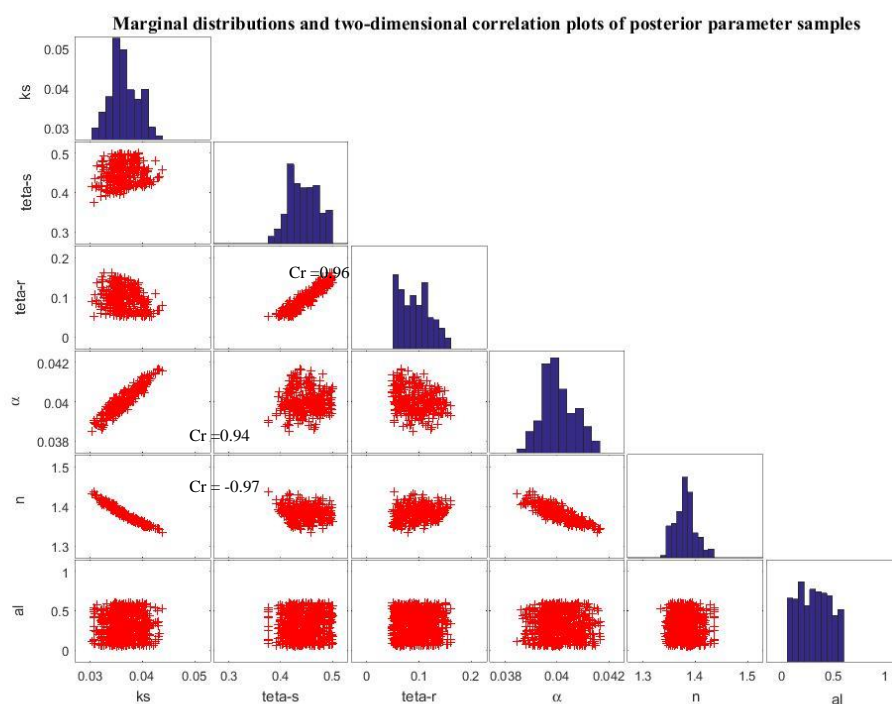
515
 516 Fig. 4. Reference retention curve for the infiltration experiment [see Fig. 1 caption].
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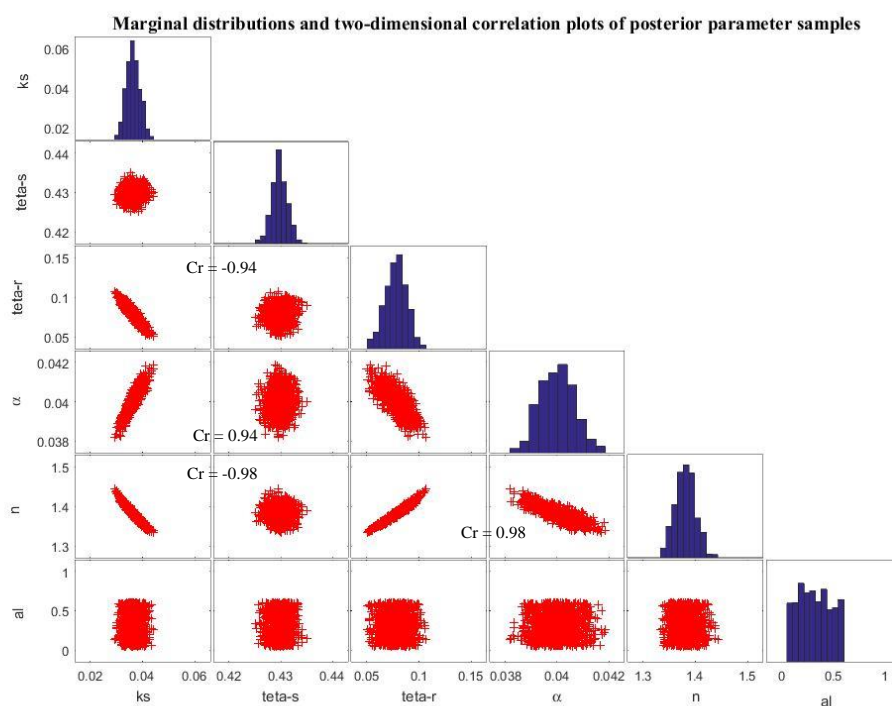
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 519 Fig. 5. Reference breakthrough output concentration for $T_{inj}=5000$. [see Fig. 1 caption].



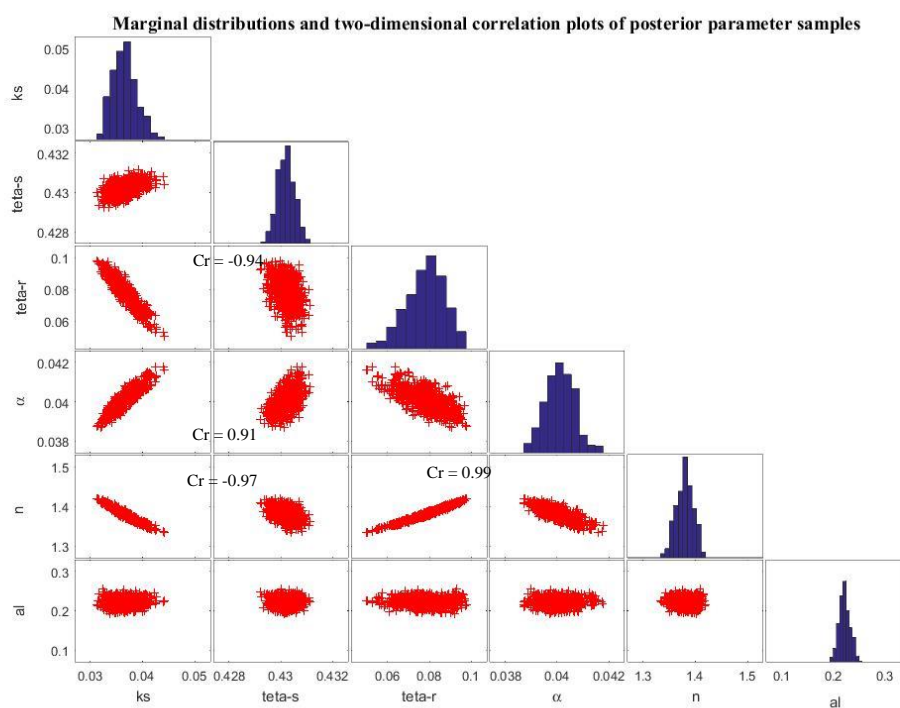
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 521 Fig. 6. Reference breakthrough output concentration for $T_{inj}=3000$ min. [see Fig. 1 caption].
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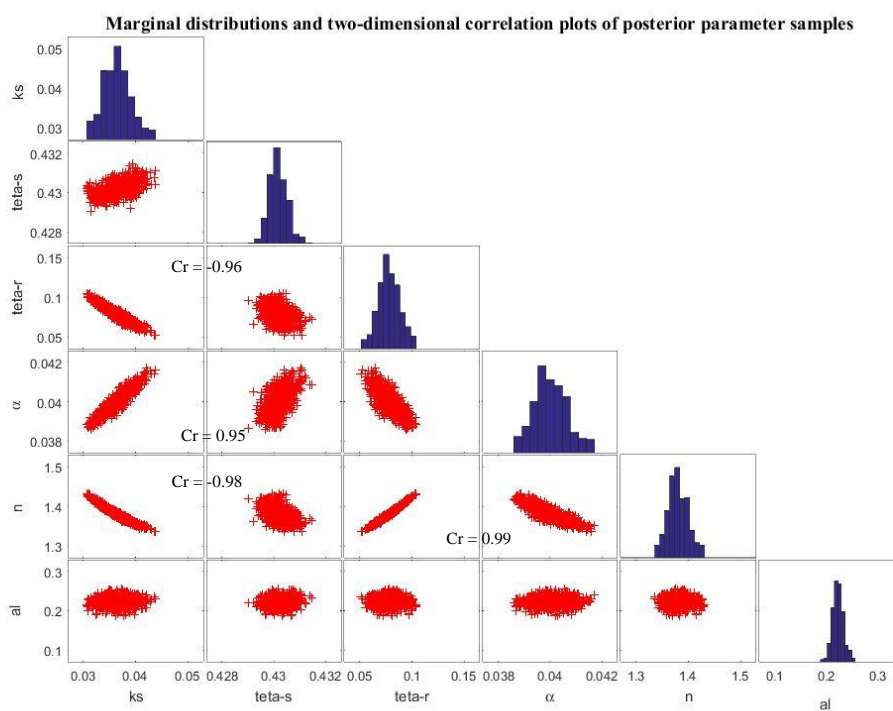
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 2 Fig. 7. MCMC solutions for the transport scenario 1. The diagonal plots represent the inferred posterior probability distribution of the model
 3 parameters. The off-diagonal scatterplots represent the pairwise correlations in the MCMC drawing.



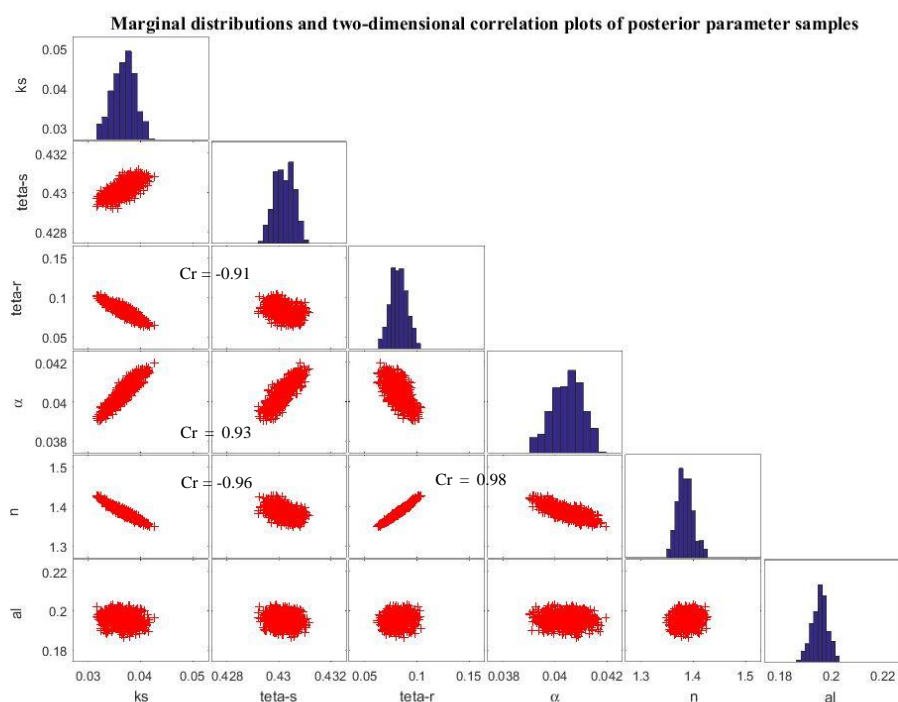
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 2 Fig. 8. MCMC solutions for transport scenario 2 [see Fig. 7 caption].



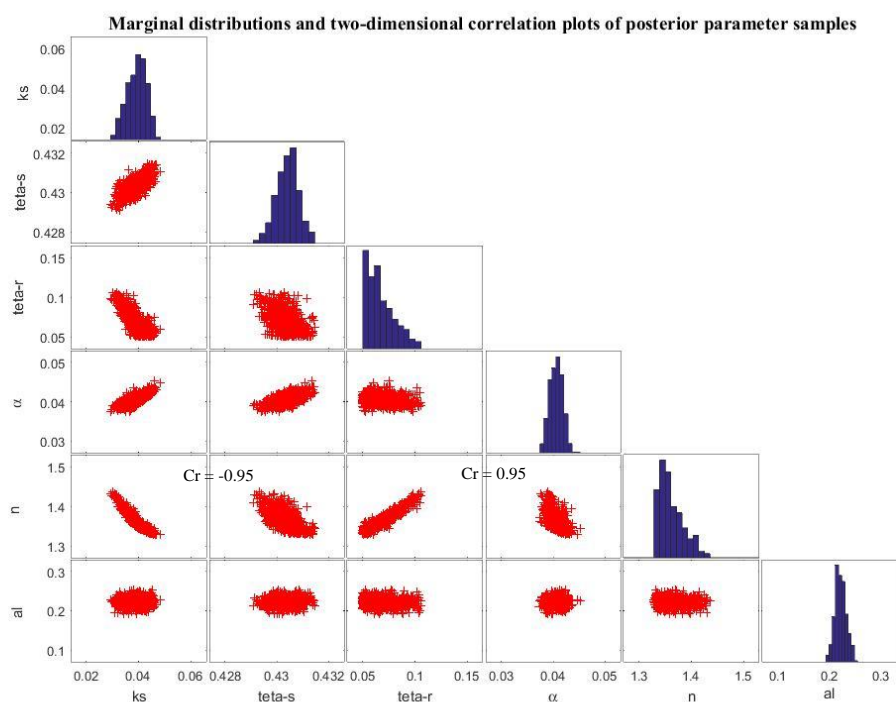
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 2 Fig. 9. MCMC solutions for transport scenario 3 [see Fig. 7 caption].



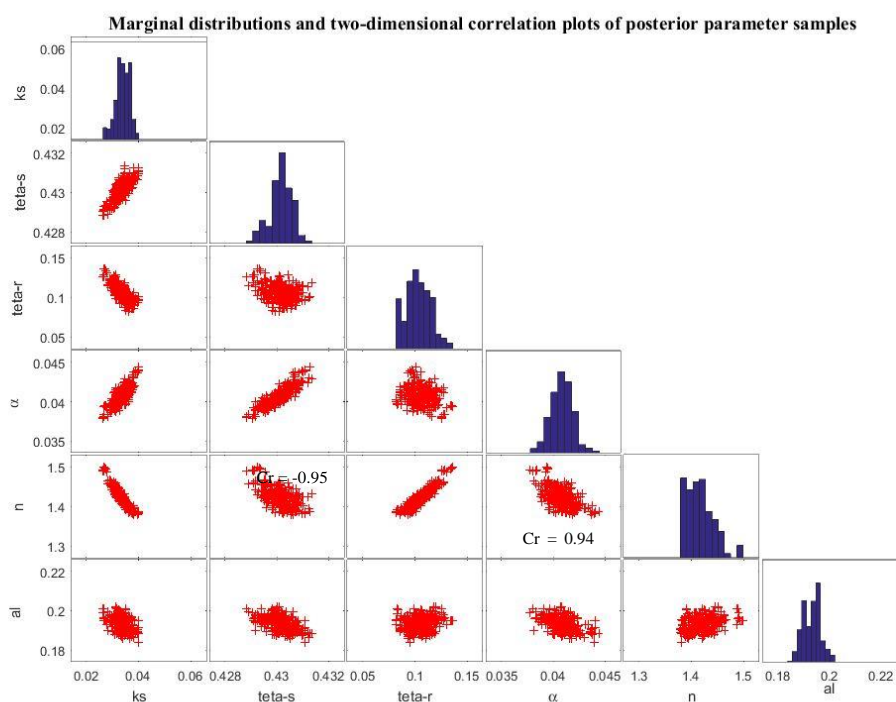
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 2 Fig. 10. MCMC solutions for transport scenario 4 [see Fig. 7 caption].



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 2 Fig. 11. MCMC solutions for transport scenario 5 [see Fig. 7 caption].



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 2 Fig. 12. MCMC solutions for transport scenario 6 [see Fig. 7 caption].



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 2 Fig. 13. MCMC solutions for transport scenario 7 [see Fig. 7 caption].

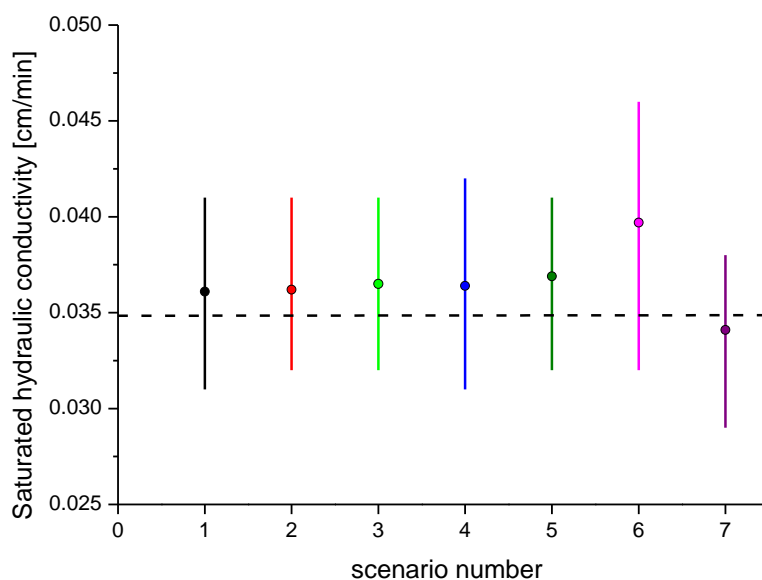


Fig. 14. Posterior mean values and 95% confidence intervals of the saturated hydraulic conductivity for the different scenarios.

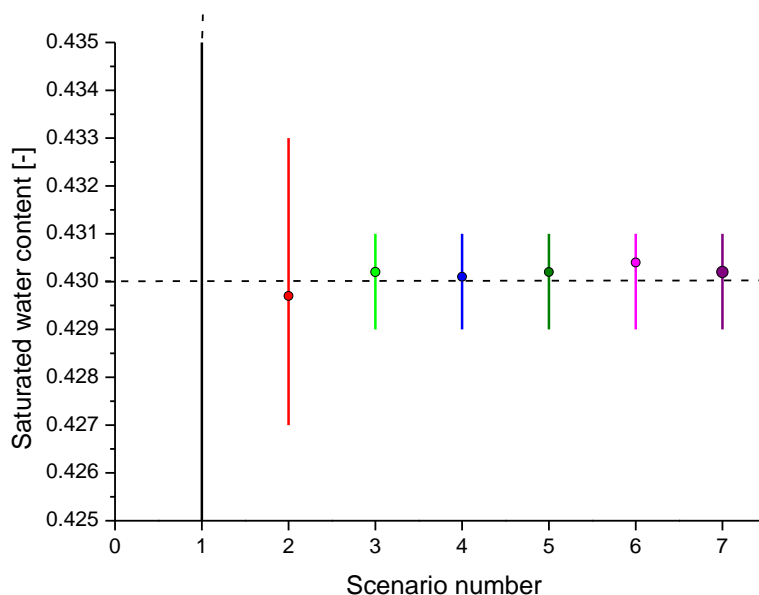


Fig. 15. Posterior mean values and 95% confidence intervals of the saturated water content for the different scenarios.

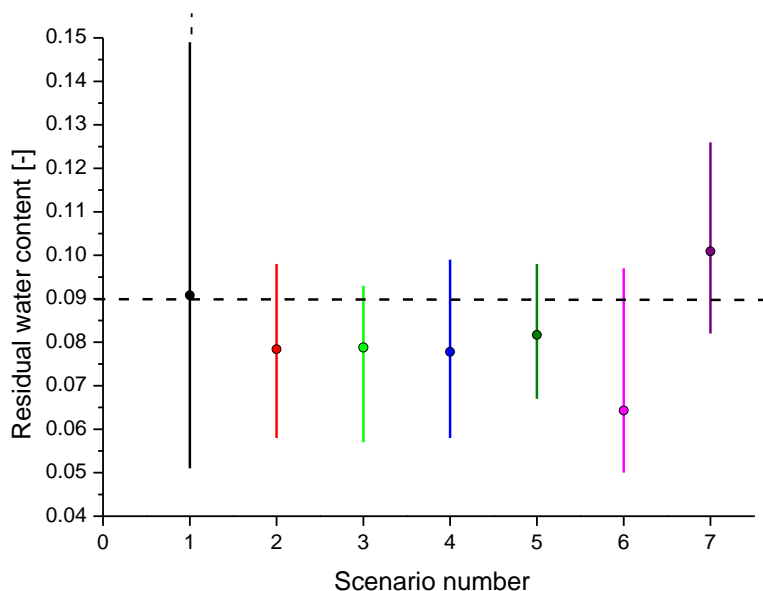


Fig. 16. Posterior mean values and 95% confidence intervals of the residual water content for the different scenarios.

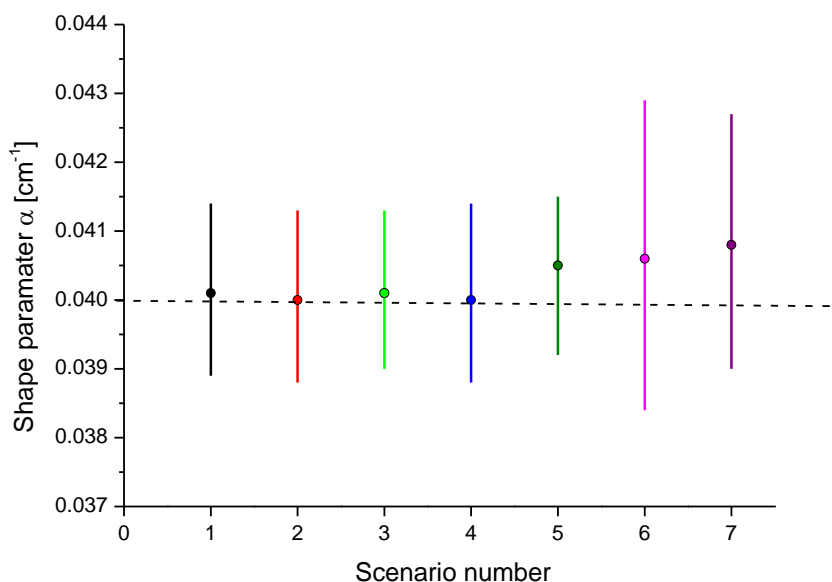


Fig. 17. Posterior mean values and 95% confidence intervals of the shape parameter α for the different scenarios.

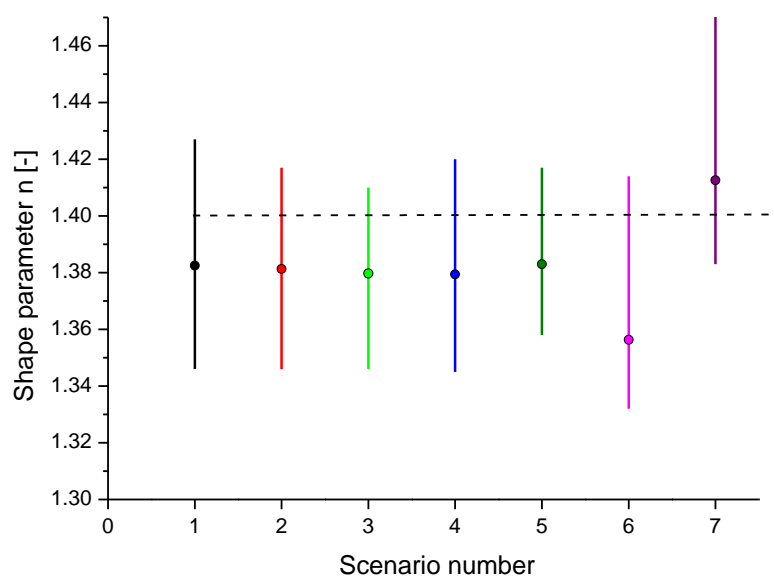


Fig. 18. Posterior mean values and 95% confidence intervals of the shape parameter n for the different scenarios.

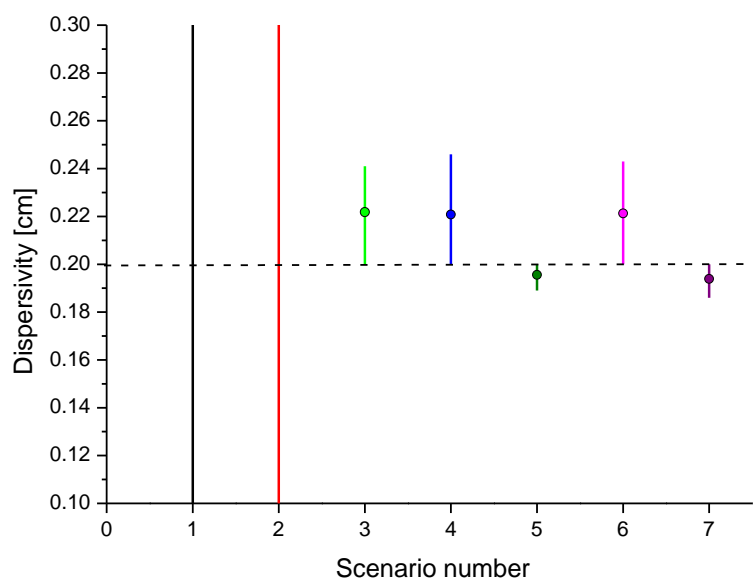


Fig. 19. Posterior mean values and 95% confidence intervals of dispersivity for the different scenarios.