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Developing a particle tracking surrogate model to improve inversion of ground water Surface water models

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ABSTRACT

The inverse problem of groundwater models is often ill-posed and model parameters are likely to be poorly constrained. Identifiability is improved if diverse data types are used for parameter estimation. However, some models, including detailed solute transport models, are further limited by prohibitive computation times. This often precludes the use of concentration data for parameter estimation, even if those data are available. In the case of surface water-groundwater (SW-GW) models, concentration data can provide SW-GW mixing ratios, which efficiently constrain the estimate of exchange flow, but are rarely used. We propose to reduce computational limits by simulating SW-GW exchange at a sink (well or drain) based on particle tracking under steady state flow conditions. Particle tracking is used to simulate advective transport. A comparison between the particle tracking surrogate model and an advective–dispersive model shows that dispersion can often be neglected when the mixing ratio is computed for a sink, allowing for use of the particle tracking surrogate model. The surrogate model was implemented to solve the inverse problem for a real SW-GW transport problem with heads and concentrations combined in a weighted hybrid objective function. The resulting inversion showed markedly reduced uncertainty in the transmissivity field compared to calibration on head data alone.

1. Introduction

Parameters involved in groundwater models are generally obtained by history-matching against hydraulic head data. However, this approach generally leads to ill-posed inverse problems (Anderman and Hill, 1997; Carrera et al., 2005). This is particularly the case for groundwater-surface water (GW-SW) models, where independent estimates of surface water in/outflow are most important for constraining surface water exchanges (Fleckenstein et al., 2010; Hunt et al., 2006; Sophocleous, 2002). The use of additional, diverse field observations can alleviate the ill-posedness (Zhou et al., 2014). However, successful examples of including solute concentration for parameter estimation are scarce (Christiansen et al., 1995; Hunt et al., 2006; Medina and Carrera, 1996; Pool et al., 2015).

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The computational burden of simulating advection and dispersion at the field scale is a primary barrier to the use of concentration data for GW-SW interaction investigations. Depending on the problem, a single simulation of advective–dispersive transport over periods of years to decades may require hours, even on modern computers (Hill and Tiedeman, 2006; Konikow, 2011). Several thousands of model runs are generally necessary to complete parameter estimation and uncertainty analysis (Anderson et al., 2015). This suggests that alternative approaches to simulate solute transport that reduce the computation effort could have significant advantages for modeling and understanding GW-SW processes.

Transport models fall into two general categories. In all cases, solution of the flow equation provides heads, water fluxes and flow directions. But, as discussed by Konikow (2011), transport modeling approaches are then based on either: i) modeling transport as advection dominated; or ii) solving the full advective–dispersive transport problem. Theoretically, measured concentrations can only be used to constrain the more complex models, which consider dispersion (Konikow, 2011). Only few cases that included

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concentration data for parameter estimation were based on advective-dispersion models (Christiansen et al., 1995; Fienen et al., 2009; Tonkin and Doherty, 2009).

All modeling efforts require trade-offs (Hill et al., 2016). One common example is that aquifer parameters may be considered to be homogeneous to allow for examination of other processes, such as GW-SW exchange. Thus, few studies have attempted to infer heterogeneous conductivity fields based on concentration data (Carniato et al., 2015). The goal of this study is to examine alternative modeling strategies to support such investigations.

Over the past decade, surrogate modeling has been used to reduce the computational requirements of some hydrogeological problems. Surrogate models are lower-fidelity models that adequately capture the most important features of the original complex model while reducing the computational cost (Razavi et al., 2012). Surrogates are used most often during parameter estimation or uncertainty analysis, which require numerous model runs. However, a candidate surrogate model should meet certain criteria (Burrows and Doherty, 2015): i) the surrogate model must compute the key outputs made by the complex model; ii) the output values of the surrogate model should be reasonably consistent with those of the original complex model; and iii) parameters used by both models must play similar roles. Our specific objective was to test whether particle tracking could act as a suitable surrogate for more computationally demanding advective–dispersive models, thereby allowing for the use of concentration data to constrain heterogeneous conductivity fields.

Particle-tracking techniques have been compared to advective–dispersive transport models such as MT3DMS. For example, Gusyev et al. (2014) found very similar simulated tritium concentrations based on particle-tracking (MODPATH – MODFLOW) and solute transport (MT3DMS – MODFLOW) models. Advective transport has also been used in SW-GW modeling to reproduce temperature observations (Brookfield et al., 2009; Engeler et al., 2011; Kurtz et al., 2014; Mouhri et al., 2013), lake plume elevation (Fienen et al., 2009; Hunt et al., 2006), advective front locations (Anderman and Hill, 1997; Hill and Tiedeman, 2006), travel time between a lake and a well (Pint et al., 2003) or to delineate the hyporheic zone (Kasahara and Wondzell, 2003; Storey et al., 2003). Particle tracking has already been used for parameter estimation (Pint et al., 2003; Hunt et al., 2006). However, particle tracking has never been used as a surrogate model for advective–dispersive transport to simulate SW-GW exchanges, nor has it been used with head and flow observations at production wells to constrain heterogeneous conductivity fields.

In this study, we do not use concentration data directly for calibration. Rather, we use simulated and inferred mixing ratios, which describe the fractional mixing of several end-member waters with different chemical compositions (Carrera et al., 2004, Rueedi et al., 2005). In this case, we examine the mixing of surface water (SW) and groundwater (GW). Mixing ratios are commonly inferred from concentrations measured in field-collected water samples. We proposed a method to use MODPATH results to define mixing ratios that can be compared with field-derived values. We first benchmark our MODPATH-based approach against results derived from MT3DMS advective-dispersion model results. Thereafter, we apply our particle tracking surrogate model to a case study and examine the benefits and limitations compared to calibration with head data alone.

2. A proxy-model for Advective-dispersive transport

2.1. Approach

To test our proposed proxy modeling approach, we simulate SW-GW mixing in a pumping well under steady-state flow conditions. The value of the mixing ratio may range between 0 (GW only) to 1 (SW only). For the sake of simplicity, we assume that mass transport is non-reactive. The approach is based on using backward tracking to determine the origins of a set of particles disseminated around a sink point of interest (well or drain). The method is based on the assumption that particle velocity and concentrations can be used to define the mass flux coming from a flow tube (Atteia, 2011). The procedure to compute the mixing ratio (β) at a given sink point can be detailed as follows:

1. The flow field is computed for steady state conditions with the flow model.
2. A large number of particles (>=1000) are disseminated around the sink point of interest.
3. Backward particle tracking is conducted from the sink point back to the origin of flow (stream and boundary condition).
4. The mixing ratio at the sink point, β, is then calculated from the fraction of the particles that originate in the stream or at a boundary.

The procedure for the computation of the concentration associated with each particle, β_i, depends on the type of the source point (Fig. 1). When a particle originates from an external boundary condition (prescribed head or flow) the particle concentration as it reaches the sink simply corresponds to the mixing ratio of GW ($\beta_i = 0$) (Fig. 1, A). In contrast, a particle originating from an aquifer cell in interaction with a stream is not necessarily entirely SW ($\beta_i = 1$). Rather, these particles will be a mix of stream water and GW (Fig. 1B). Determination of the average β_i value for particles originating passing through these cells requires consideration of the balance of flow into the cell from the stream and from neighboring aquifer cells (Fig. 2). Defining water originating from the neighboring cells to have a mixing ratio of 0 (pure GW), the mixing ratio of water leaving the cell, β_r, can be obtained as follows:

$$\beta_r = \frac{Q_s}{\sum_{i=1} Q_i} \tag{1}$$

where Q_S is the flow from the stream to the aquifer cell in interaction with the stream and $\sum_{i=1} Q_i$ is the sum of all inputs to this cell ($Q_S + Q_B + Q_L$ see Fig. 2), where Q_B is the flow from back and front sides of the cell, Q_L is the flow from the left and right side of the cell longitudinal to the stream. for the case depicted in Fig. 2). Note that β_r will only be greater than zero for losing reaches ($Q_S > 0$).

The value of the mixing ratio, β, at the sink point (step 4) is obtained from the mean of the respective particle mixing ratios, β_i, weighted by particle velocities, v_i:

$$\beta = \frac{\sum_{i=1} (v_i \times \beta_i)}{\sum_{i=1} v_i} \tag{2}$$

2.2. Validation: a synthetic case

2.2.1. Model setting

The major assumption underlying the use of a particle tracking surrogate model is that dispersion can be neglected for the mixing ratios of the sink points. A synthetic 2D case is considered to test this assumption. We consider a production well in an unconfined aquifer in interaction with a stream (Fig. 3). The domain (100 × 150 m) is discretized with a fine 2D regular mesh (1 × 1 m cells), which thus satisfies the criteria on the grid Peclet number to avoid numerical dispersion with a finite difference scheme ($P_e < 1$), even for a dispersivity of 1 m (Zheng and Wang, 1999). Lateral boundary conditions are fixed head (FH): 10 m to the left and 9.5 m to the right. No flow is imposed at the upper and lower domain bound-

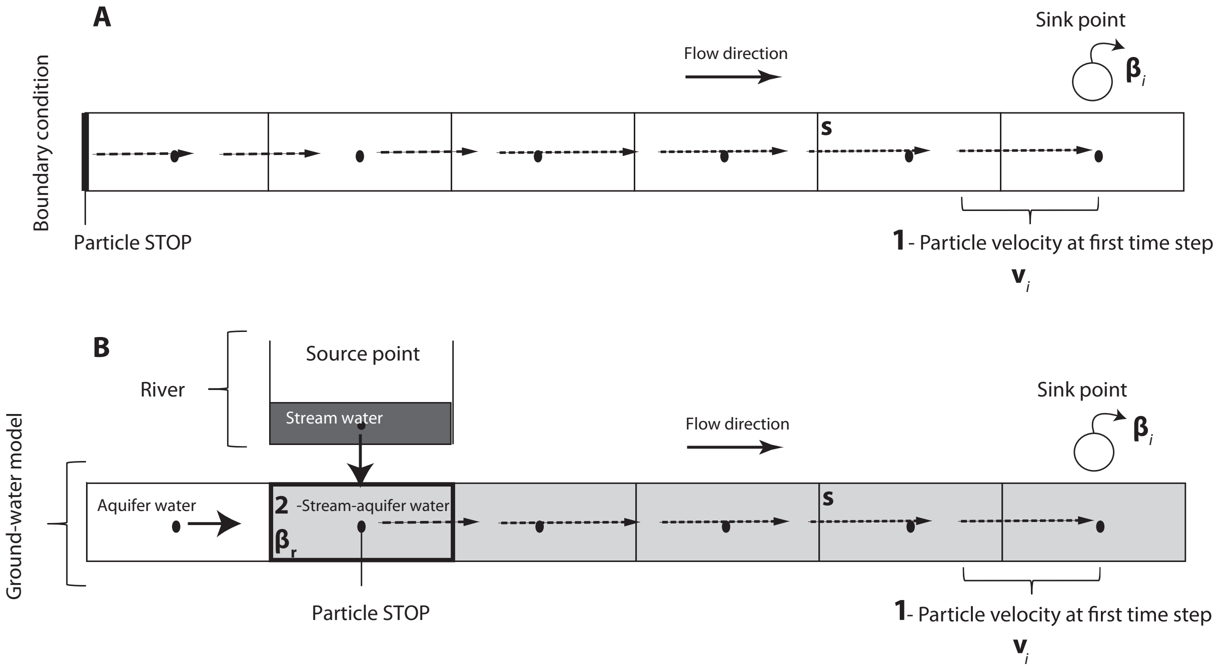

Fig. 1. Procedure for computing the mixing ratio, β_i, depending on the location of a particle's source: A) When the particle originates from an external boundary condition, $\beta_i = 0$ (GW only). B) If it originates from a stream, the particle account for a mix between GW and SW, $\beta_i = \beta_r$.

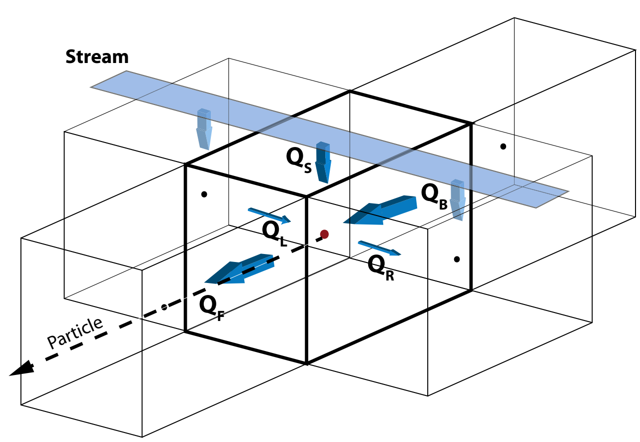

Fig. 2. Aquifer cell exchanging with a stream in a 2D horizontal flow model where Q_s is the flux from the stream, Q_B and Q_F are the flux from back and front sides of the cell, Q_L and Q_R are the fluxes from the left and right side of the cell longitudinal to the stream.

aries. The stream is simulated with a head-dependent flux (Cauchy-type) boundary condition, with a head of 9 m and a conductance of 0.01 $m^2\,s^{-1}$. These boundary conditions have been adjusted to achieve some mixing of SW and GW in the stream cells (see cross-section in Fig. 3). The hydraulic conductivity is homogeneous over the model with a value of 3×10^{-4} m s^{-1}. Aquifer thickness is set to 30 m. Transmissivity is assumed to be independent of water level fluctuations (MODFLOW parameter laycon = 0), Which corresponds to the Boussineq assumption. Simulations have been conducted for flow rates in the sink point ranging from 0 to 600 $m^3\,h^{-1}$. The wells are considered as fully penetrating.

The stream water concentration is arbitrarily fixed to 1, while fixed head boundary conditions yield water with concentration 0. The SW-GW mixing ratio in the production well is simulated with the advective–dispersive transport model MT3DMS and the particle tracking code (MODPATH). Steady state flow conditions are simulated with MODFLOW using the PCG solver. Models (MODFLOW – MODPATH – MT3DMS) are pre- and post processed using the Python wrapper FloPy (Bakker et al., 2016) and Qgridder (Pryet et al., 2015) on the Qgis platform (QGIS, 2012). Particle tracking with MODPATH is performed with a set of 1 000 particles disseminated around the production well, at 0.5 m from it. Exchange flow with the stream is simulated with the weak source option set to 2, which stops particles in cells with a weak source such as a stream in losing condition. The IFACE parameter, used to associate a flow term with a grid cell face (Pollock, 1994) is set to 6, to be consistent with recommendation of Abrams et al. (2012) for surface water weak sinks. The weak sink option is set to 1, which allows particles to pass through cells with weak sinks such as a stream in gaining conditions. MT3DMS simulations are performed with HMOC solvers, which is a hybrid of MOC and MMOC scheme (Zheng and Wang, 1999), with a longitudinal dispersion set to 1 m. The same simulations are also performed for a longitudinal dispersion set to 10 and 100 m to determine the impact of dispersion on the simulated mixing ratio in a pumping well. Transverse dispersion is set to 10% of the longitudinal dispersion.

2.2.2. Synthetic case results

Mixing ratios in the pumping well simulated with MODPATH and MT3DMS are compared in Fig. 4. Both models yield very similar results (Fig. 4A). Below a pumping rate of 100 $m^3\,h^{-1}$, the head in the well is above the head of the stream so that well water has a mixing ratio of 0. Above this pumping rate, a mix of stream water and water originating from the right fixed-head boundary conditions supplies the well. The agreement between mixing ratios computed with MT3DMS and MODPATH validates the proposed approach in terms of particle count, weighting of each particle by its velocity and computing the mixing ratios of stream particles (β_i). Results obtained with a longitudinal dispersion of 10 m and 100 m reveal interesting features (Fig. 4). In Fig. 4B) the same simulation as A) is performed for MODPATH that does not take into account dispersion. When longitudinal dispersion reaches excessively large values (100 m), β decreases, but remains similar (the error on β is 6%). This can be compared to the uncertainty on mixing ratio associated with measurement error, which generally

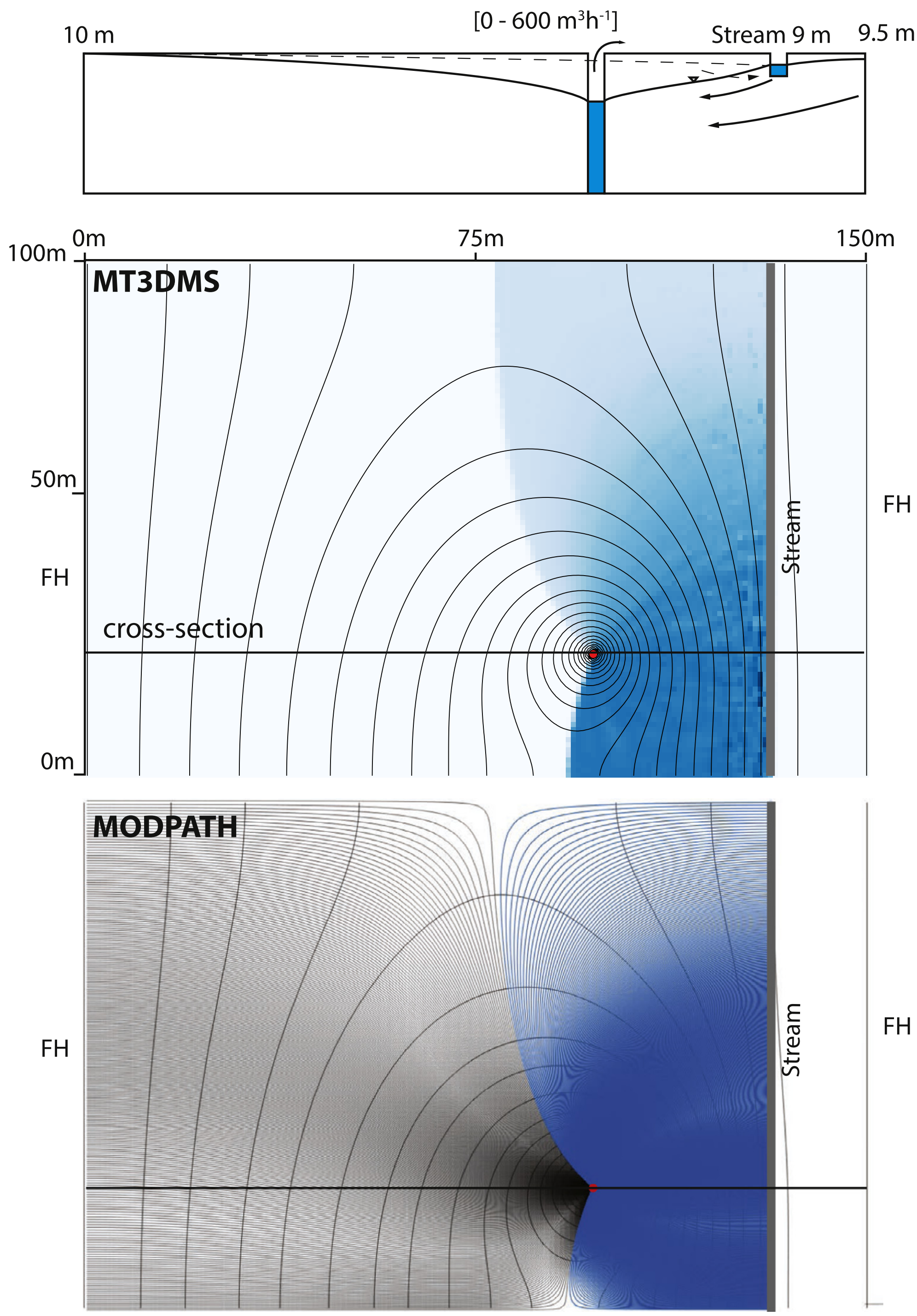

Fig. 3. MT3DMS and MODPATH simulations show mixing between surface water and groundwater, a cross-section describes model settings.

range between 8 and 20% (Rueedi et al., 2005). For the presented test case, even with an excessively large longitudinal dispersion value of 100 m, the error of the surrogate model remains small with respect to the expected measurement error.

3. Application

3.1. Study site

A particle tracking surrogate for transport model is applied to a study of a well field, which supplies about 20% of the fresh water to the urban area of Bordeaux (France) (Fig. 5). A stream crosses the well field, so that stream-aquifer interactions are of strategic interest. The stream flows over Plio-quaternary sandy materials, overlying an Oligocene limestone aquifer. These two geological formations are hydraulically connected, with similar hydraulic conductivity, and therefore considered herein as a single heterogeneous aquifer (Canik, 1968).

Groundwater is abstracted with two pumping wells and a 500 m long drainage gallery equipped with a pump. The mean hydraulic conductivity is on the order of $5{\cdot}10^{-4}$ m s^{-1}. The thickness of the aquifer varies between 40 and 60 m. The structure of the aquifer is highly heterogeneous, with some structures

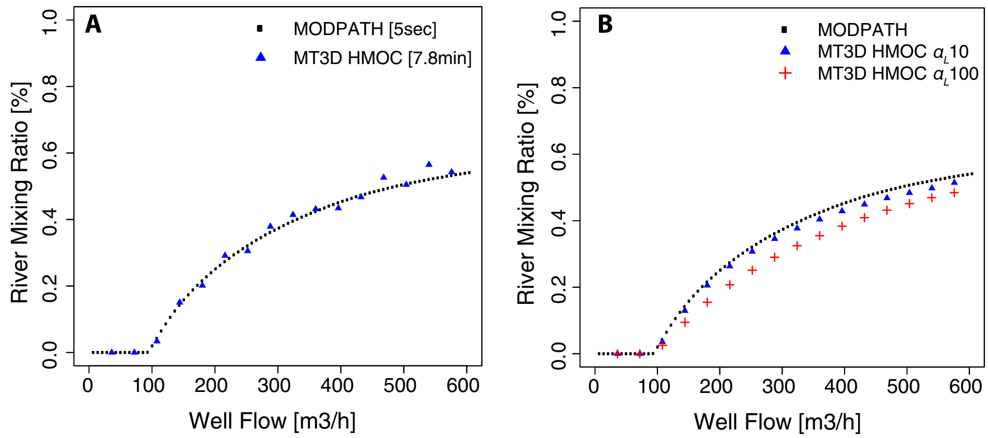

Fig. 4. Evolution of the SW-GW mixing ratio (β) in the production well as function of well discharge. A) With low dispersion (1 m), the accuracy of the surrogate model is shown with a great reduction in computation time. B) With lateral dispersion α_L of 10 m and 100 m ($\alpha_T = 0.1 \times \alpha_T$) or MT3MS simulations, simulated β is still acceptable for the MODPATH surrogate model.

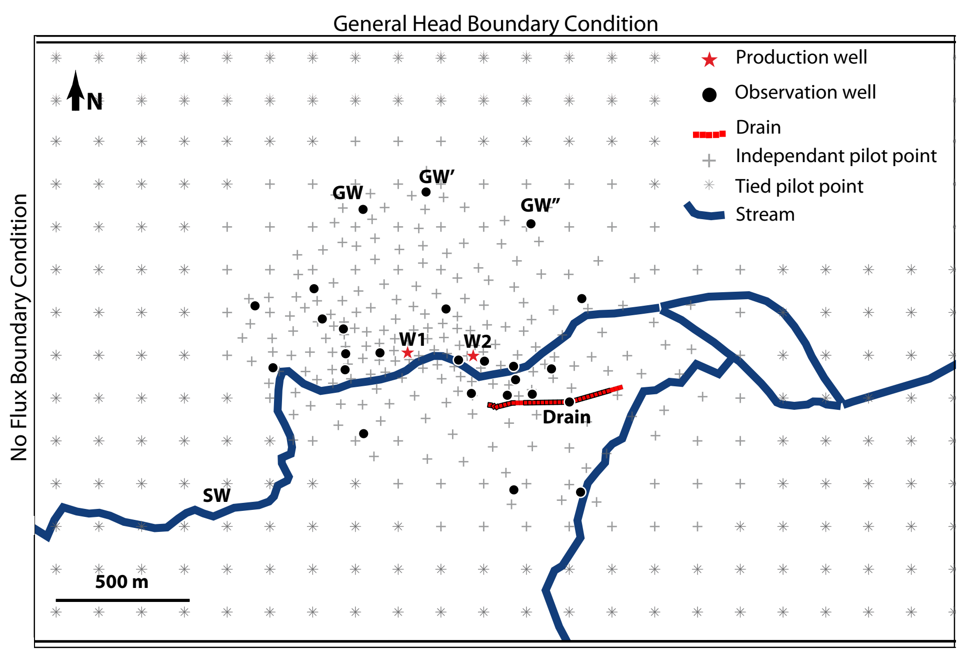

Fig. 5. Study plan with locations of production and observation wells. The parameterization of hydraulic conductivity and storage has been conducted with pilot points. They are "independant" (each pilot point form an adjustable parameter) at the center of the study area and "tied" (all of tied pilot points constitute a single adjustable parameter) in the outer portion of model domain.

highlighted by field observations and geophysical surveys (Cousquer, 2017). The width of the stream varies between 10 and 15 m, with a depth of about 1 m depending on the hydraulic regime of the stream.

3.2. Field measurements

Flow and transport observations have been collected in the field. Concentration measurements at the production wells and drain are interpreted as a mixture of surface water and groundwater. The chemical composition of surface water is based on water samples collected in the stream; the groundwater end-member is based on water samples collected from a well sufficiently distant from the stream to avoid mixing. The mixing model is based on the concentrations Ca^{2+} and HCO_3^-. Ion concentrations at production wells and gallery are reported by orthogonal projection on the mixing line that links the two end-members (Carrera et al., 2004; Rueedi et al., 2005). Ion concentration is then obtained after field water sampling on October 10th, 2015, and analyzed by a DIONEX IC Columns for Ca^{2+} and titration for HCO_3^-.

Estimates of mixing ratios may be affected by two kinds of uncertainties: (i) on the location of end-members and (ii) measured concentrations of Ca^{2+} and HCO_3^- for the point of interest. The error on the end-member compositions has been estimated by the standard deviation between concentrations of ions Ca^{2+} and HCO_3^- in points estimated to be likely end-members. Three piezometers have been selected to be likely groundwater end-members and stream water was sampled at three locations. The error on production well ions concentration is based on reported analytical method errors. An uncertainty of about 8% (Fig. 6) was found through error propagation on the orthogonal projection equation (Hughes and Hase, 2010). Wells W1 and W2 and the drain have 10%, 30% and 90% stream water, respectively, which are very contrasting values given their proximity to the stream. This can be explained by the high heterogeneity of the aquifer that can lead to preferential flow paths. Pressure was monitored in all of the wells shown in Fig. 5.

3.3. Model development

Two models have been developed for parameter estimation. Both models are based on the same spatial extents but they differ in temporal discretization and in their underlying equations. Both models are based on the assumption of a head-independent transmissivity (Boussinesq assumption) and consider 2D horizontal flow only (Dupuit-Forchheimer assumption). The validity of this latter hypothesis was verified with the criteria provided by Haitjema (2016). The first model simulates transient flow with MODFLOW-2005 (McDonald and Harbaugh, 1988). It aims to reproduce observed water levels in the observations wells (Fig. 5) over a period of 700 days. Stream level, drain level, recharge and wells discharge are time varying boundary conditions and were set according to field observations. The second model is the surrogate model for flow and advective transport under steady state flow conditions. This model is based on MODFLOW-2005 and MODPATH with the methodology described and tested in the previous section. The results of the second model will be compared with simulated values from a third model based on the advective–dispersive transport code MT3DMS with a longitudinal dispersion of 1 m. This third model is not used for parameter estimation process; rather, it is only used to assess the validity of the surrogate model by comparing the values of mixing ratios obtained with the surrogate model with those obtained with the advection–dispersion model.

The model domain is centered on the well field and extends over ca. 12 km^2 (4.5 km × 2.6 km) (Fig. 6). Model boundary conditions were set in accordance with regional groundwater heads and flow directions (Cabaret, 2011). North and south boundary conditions are head-dependent flux boundary conditions (GHB). East and West boundary conditions are no flux. Both models are discretized on a 10 m × 10 m grid, with a total of 117 448 cells. The stream is simulated with head-dependent flux boundary conditions (Cauchy-type) (Cousquer et al., 2017) with the MODFLOW RIV package. The drain (gallery) is also simulated with head-dependent flux boundary conditions with the MODFLOW DRN package. Wells are represented by sink terms in corresponding aquifer cells. Groundwater recharge is calculated with a reservoir model (Ledoux et al., 1984) from climate data. Soil condition are fairly homogeneous over the area of interest (Cousquer, 2017), therefore a uniform recharge has been applied to the entire model area.

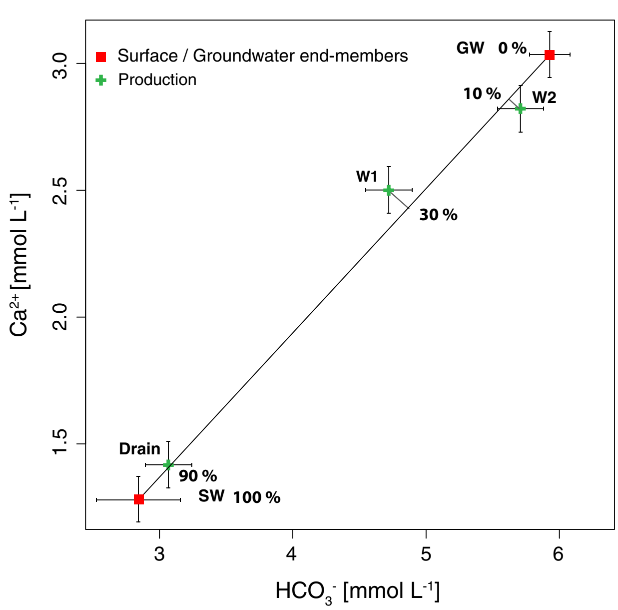

Fig. 6. Mixing ratio β Ca2+/HCO$_3^-$ of water sample and mixing model between the two end-members surface-water (GW, $\beta = 0$) and groundwater (SW, $\beta = 1$).

3.4. Parameter estimation and uncertainty analysis

3.4.1. Parameter estimation

Parameter estimation was conducted to minimize the residual between observed and simulated groundwater heads, discharge rates at the drainage gallery, and mixing ratios at the production wells and the drain. Both transient and steady state models are used for parameter estimation as described in Fig. 7.

Fields of hydraulic conductivity and porosity have been parameterized with a set of 250 adjustable pilot points (de Marsily et al., 1984) with an extension of pilot point value to grid cells by kriging with an exponential viariogram, with a range of 250 m a sill of 1 and a nugget of 0.1 following the recommendations of Doherty et al. (2011). Parameter estimation has been conducted with the Gauss Levemberg Marqart Algorithm (GLMA), a non-linear Newton method for parameter estimation, implemented in PEST++ (Welter et al., 2012). A hybrid regularization Tikhonov-TSVD has also been conducted to stabilize the solution (Fienen et al., 2009). The algorithm is based on the minimization of an objective function representing the weighted mean square error between model outcome values and measured values. In the presented test case, three data types are considered in the objective function: water levels, wells discharge rates and mixing ratios. It is preferred that each data type is equally well represented in the objective function (Anderson et al., 2015). Furthermore, for a given data type, each observation location should be equally well presented. To satisfy these two requirements, observations are weighted in the objective function as follows:

$$\phi = \sum_{l=1}^{L}\sum_{k=1}^{K_l}\sum_{i=1}^{N_{k,l}}(\omega_{k,l} \times r_{k,l}^2) \tag{3}$$

where L is the number of data types (heads, discharge rates, concentrations), K_l is the number of observation points for the l-th data type, and $N_{k,l}$ is the number of observation records for the k-th observation point of the l-th data type ($N_{k,l} = 1$ when considering steady state values). The weighing factor of each observation is defined as follows:

$$\omega_{k,l} = \sqrt{\frac{1}{N_{k,l} \times K_l \times \sigma_{k,l}^2}} \tag{4}$$

where $\sigma_{k,l}$ is the standard deviation of the variable of interest. Every observation of each station inside each data type is well balanced in the pre-calibration objective function (Table 1).

A total of 38 000 model runs were required for parameter estimation, which were run in parallel on a 20-core CPU. This required 2.75 days with the surrogate model, and would have required more than a month if a classical advective–dispersive model had been used. With the calibrated parameter set, the simulated values showed a reasonably good adjustment with observed values, with RMSE errors of: 0.19 m for heads in the observations wells; a RMSE of 11.7 m^3 h^{-1} for flow in the drainage gallery; and 11% for mixing ratios at the 3 production wells. Parameter values estimated based on the surrogate and MT3DMS are very close (Table 2), supporting the use of the surrogate model.

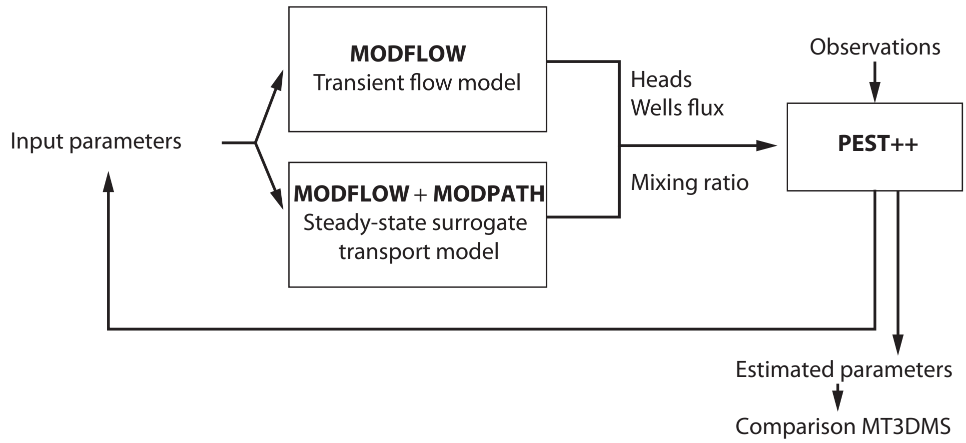

Fig. 7. Parameter estimation approach: two models are executed with the same input parameters; model outputs are compared with observations using PEST++ to estimate input parameters that minimize the objective function.

The calibrated hydraulic conductivity field of the flow-only model is rather homogeneous except for the areas around production well W1 and around the drain. However, the hydraulic conductivity field based on head and mixing ratio data is more heterogeneous, with corridors of high hydraulic conductivity between the production wells and gallery. These preferential flow paths were necessary to reproduce the observed mixing ratios, while head data contained no information to constrain them.

3.4.2. Uncertainty of hydraulic conductivity using null-space Monte-Carlo analysis

The solution obtained with the GLMA is not unique. A Null-Space Monte Carlo (NSMC) analysis was performed to quantify the uncertainty of the parameter values. The same analysis was conducted for both the flow model only and with the surrogate transport model. The NSMC procedure has been performed following Tonkin and Doherty (2009). A series of 100 parameter sets following a log-normal law has been stochastically generated from the previously obtained calibrated model. Then, each parameter has been projected into the parameter null-space. Parameter sets that did not sufficiently reproduce observations have been recalibrated. 82 parameter sets that provided an adequate calibration were eventually selected. The uncertainty of the hydraulic conductivity is shown in Fig. 7. The fields were obtained by kriging the standard deviation of the log value of the hydraulic conductivity at the pilot points. These values were obtained from the standard deviation of the 82 selected NSMC parameter sets.

Table 1
Quantitative details on the parameter estimation.

Adjustable parameter	Number	
GHB conductance [$m^2\ s^{-1}$]	2	
Recharge parameters [–]	2	
River conductance [$m^2\ s^{-1}$]	1	
Drain conductance [$m^2\ s^{-1}$]	1	
Hydraulic conductivity (pilot points) [$m^2\ s^{-1}$]	250	
Observations	Number	Measurement error
Heads [m]	25 × 700 days	0.01 [m]
Wells/drain discharge [$m^2\ s^{-1}$]	3 × 700 days	10 [$m^3\ h^{-1}$]
Mixing ratio [%]	3	10%
Objective function model 1 (head + flux)	Initial Objectif function	Final Objectif function
Head group	0.430	0.009
Flux group	0.250	0.006
Total	0.680	0.015
Objective function model 2 (head + flux)	Initial Objectif function	Final Objectif function
Head group	0.430	0.012
Flux group	0.250	0.005
Mixing ratio group	0.420	0.010
Total	1.100	0.026
Objective function model 2 (head + flux)	RMSE	
Head	0.19 m	
Flux	11.7 $m^3\ h^{-1}$	
Mixing ratio	11%	

Table 2
Observed value of β and simulated value obtained with the surrogate model after calibration and with MT3D for validation.

Observation point	Simulated β MODPATH [%]	Validated β MT3D [%]
Drain	92	90
W2	13	12
W1	49	51

When considering the flow model only (Fig. 8a), uncertainty is more homogeneous than with the use of the surrogate model (Fig. 8c). Uncertainty is relatively limited around W1, W2 and drain on both models (Fig. 8b and d), this can be explained by the use of well water levels and drain fluxes in the calibration target for both models that leads to decreased uncertainty. However, using the surrogate transport model (Fig. 8b) these zones with low uncertainty are more extended and the global uncertainty on the conductivity field decreases. There is also a correlation between relatively high conductivity and low uncertainty. These preferential flow paths bring water to production wells to reproduce well/drain discharge and mixing ratio observations. This clearly indicates that the inversion made use of information contained in the transport data to find potentially important features of the conductivity field.

4. Discussion

The presented case study illustrates that the use of a surrogate model can improve hydrogeologic interpretations with a considerable reduction of the computational burden. Importantly, parametric uncertainty is markedly reduced in the areas of the hydrologically important structures.

The purpose of the surrogate model based on particle tracking is not to replace original advective-dispersion models such as MT3DMS, but to reduce the computational cost associated with

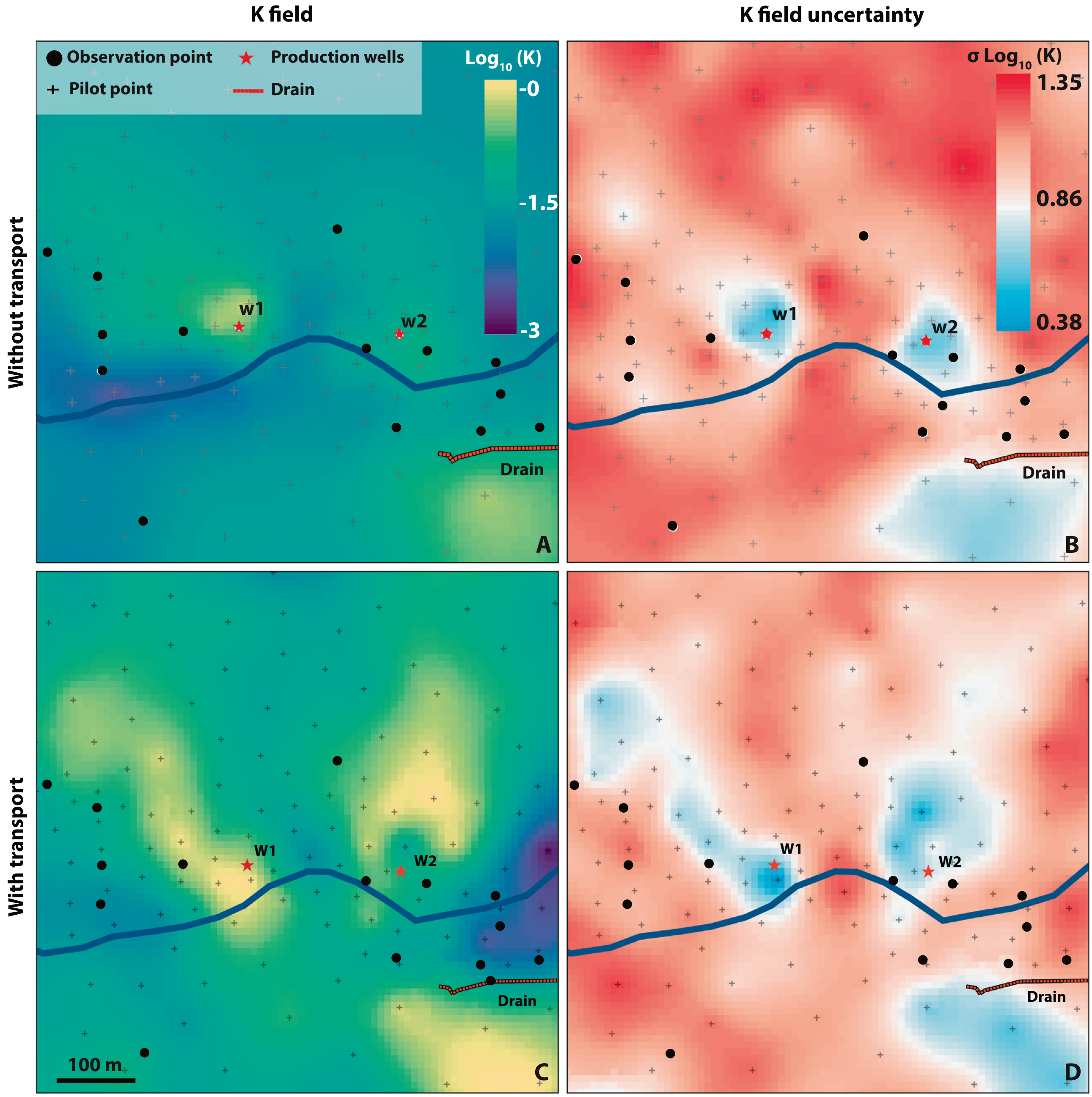

Fig. 8. Comparison between hydraulic conductivity field and standard deviation log the hydraulic conductivity at pilot point of NSMC sets. Uncertainty of hydraulic.

operations that require a large number of model calls such as parameter calibration, optimization, uncertainty and sensitivity analysis. The synthetic model analysis (Section 2.2) suggests that the effects of dispersion may be limited to sites with relatively high dispersivities. The presented methodology has been developed for non-reactive transport. It could, however, be extended to consider degradation based on transient times, as it is often used for the computation of groundwater age based on particle tracking (Eberts et al., 2012). The method is described for a stream simulated with a head-dependent flux (Cauchy-type) boundary condition. However, it could also be used with other kind of boundary conditions (fixed head and fixed flux).

The principal limitation of the proposed method is related to the effects of dispersion, especially under transient conditions. If the hydrochemical dynamics are not steady-state, a succession of steady-state periods representative of each system variation may be considered (Haitjema, 2006). But, future research should examine the suitability of the particle tracking surrogate model approach for transient flow conditions and for more complex boundary conditions (Faybishenko et al., 1995; Grubb, 1993).

The presented surrogate model has only been described and validated with 2D models. We have not identified any limitation for the extension of the presented methodology to 3D models. However, some experiments should be conducted on the weak sinks modeling, especially the stream (Abrams et al., 2012; Starn et al., 2012) and the vertical distribution of particles around partially penetrating wells.

While there may be many conditions for which the proposed surrogate model is not suitable, there are many real-world applications that are primarily focused on contaminant transport of a pumping well in the vicinity of a stream (Derx et al., 2010; Doppler et al., 2007; Engeler et al., 2011; Kurtz et al., 2014). These applications alone warrant consideration of the use of the surrogate model and mixing ratios to reduce parameter uncertainty and improve the reliability of predictions while avoiding excessive computational demands.

5. Conclusion

The proposed surrogate model has proven to be efficient for the simulation of SW-GW mixing ratios at sink points (wells or drains) during steady state flow for non-reactive species. Very short computation times of the surrogate transport model make possible the execution many thousands of model runs in a reasonable amount of time. The introduction of SW-GW mixing ratio data in the parameter estimation process markedly reduced the uncertainty on the field of hydraulic conductivity and identified potentially important hydrogeologic structures. Although the method is not universally applicable, it may be useful for a variety of cases of strategic importance. In particular, surrogate models may improve our ability to manage drinking water supply wells in the vicinity of surface water bodies. These benefits may include both improved hydrogeological characterization and improved parameter estimation, with more quantitative uncertainty analyses, to support decision-making under uncertainty.

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