Groundwater

Estimating River Conductance from Prior Information to Improve Surface–Subsurface Model Calibration

by Yohann Cousquer[1,2], Alexandre Pryet[3], Nicolas Flipo[4], Célestine Delbart[2,3,5], and Alain Dupuy[3]

Abstract

Most groundwater models simulate stream-aquifer interactions with a head-dependent flux boundary condition based on a river conductance (CRIV). CRIV is usually calibrated with other parameters by history matching. However, the inverse problem of groundwater models is often ill-posed and individual model parameters are likely to be poorly constrained. Ill-posedness can be addressed by Tikhonov regularization with prior knowledge on parameter values. The difficulty with a lumped parameter like CRIV, which cannot be measured in the field, is to find suitable initial and regularization values. Several formulations have been proposed for the estimation of CRIV from physical parameters. However, these methods are either too simple to provide a reliable estimate of CRIV, or too complex to be easily implemented by groundwater modelers. This paper addresses the issue with a flexible and operational tool based on a 2D numerical model in a local vertical cross section, where the river conductance is computed from selected geometric and hydrodynamic parameters. Contrary to other approaches, the grid size of the regional model and the anisotropy of the aquifer hydraulic conductivity are also taken into account. A global sensitivity analysis indicates the strong sensitivity of CRIV to these parameters. This enhancement for the prior estimation of CRIV is a step forward for the calibration and uncertainty analysis of surface-subsurface models. It is especially useful for modeling objectives that require CRIV to be well known such as conjunctive surface water-groundwater use.

Introduction

Numerical models are increasingly used to explore stream-aquifer interactions in a scope of water resources protection and management (Kalbus et al. 2006; Fleckenstein et al. 2010; Flipo et al. 2014). Owing to the continuity between these two entities, the development or the contamination of one is likely to affect the other (Sophocleous 2002). In such contexts, stream-aquifer flow needs to be carefully quantified.

In groundwater models, stream-aquifer flow can be considered with three kinds of boundary conditions: prescribed head (Dirichlet-type), head-dependent flux (Cauchy-type), and specified flux (Neumann-type). The last kind of boundary condition is rarely used to simulate streams. When a prescribed head is employed, the hydraulic head in the stream is imposed at the aquifer cells crossed by the stream. This kind of boundary condition is most often limited to the study of hyporheic flow at the local scale (Cardenas and Wilson 2007; Tonina and Buffington 2007; Cardenas 2009; Boano et al. 2011; Zlotnik et al. 2015) or in the case of coupled surface-subsurface models (Discacciati et al. 2002; Furman 2008; Sulis et al. 2010). However, the use of prescribed head boundary conditions for simulating streams is rare at the regional scale (Peyrard et al. 2008).

Stream to aquifer flow is usually parameterized with a river conductance (CRIV) using a head-dependent flux (Cauchy-type) boundary condition (e.g., Furman 2008; Ebel et al. 2009; Goderniaux et al. 2009; Flipo et al. 2014) such as implemented in the MODFLOW river package (McDonald and Harbaugh 1988; Furman 2008). The stream-aquifer exchange flow is calculated as the

[1]Corresponding author: Yohann Cousquer, EA 4592 Georessources & Environment, Bordeaux INP and Bordeaux Montaigne University, ENSEGID, 1 allée F.Daguin, 33607 Pessac cedex, France; +33(0) 5 56 84 69 56; yohann.cousquer@gmail.com

[2]Le LyRE, SUEZ Environnement, Domaine du Haut-Carré 43, rue Pierre Noailles, 33400 Talence, France.

[3]EA 4592 Georessources & Environment, Bordeaux INP and Univ. Bordeaux Montaigne, ENSEGID, 1 allée F. Daguin, 33607 Pessac cedex, France.

[4]Geosciences Department, MINES ParisTech, PSL Research University, 35 rue Saint-Honoré, 77305 Fontainebleau, France.

[5]Université François Rabelais de Tours, EA 6293 GéHCO, Parc de Grandmont, 37200 Tours, France.

Article Impact Statement: We present an efficient tool to estimate the river conductance from prior information on physical parameters.

Received May 2016, accepted November 2016.

doi: 10.1111/gwat.12492

product of CRIV by the head difference between the stream and the cell where the Cauchy-type boundary condition is applied:

$$Q_S = \text{CRIV} \times (H_s - H_c) \quad (1)$$

where Q_S [L^3/T] is the stream-aquifer flow, H_s [L] is the stream water level, H_c [L] is the hydraulic head at the center of the cell where the Cauchy-type boundary condition is applied. CRIV accounts for numerous processes and properties; it is a lumped parameter that cannot be measured on the field (McDonald and Harbaugh 1988; Rushton 2007; Ebel et al. 2009). As a consequence, the value of CRIV is commonly calibrated by history matching together with the other unknown hydraulic parameters (Engeler et al. 2011; Pryet et al. 2015).

Surface-subsurface models are affected by the quasi-systematic ill-posed nature of hydrogeological inverse problems, which is now wildly known (Carrera et al. 2005; Zhou et al. 2014). Ill-posedness may lead to non-uniqueness, non-existence, and non-steadiness of the inverse model solution (Zhou et al. 2014). An infinite number of parameter sets can equally well calibrate the model. In order to deal with the issue, several options have been proposed. Among them, Tikhonov regularization with prior information about model parameters has proven its efficiency (Tihonov 1963; Hunt et al. 2007). Calibration with Tikhonov regularization considers soft knowledge on model parameters in the calibration, so as obtain a well-posed problem (Doherty and Skahill 2006; Aster et al. 2005). In order to perform a calibration with Tikhonov regularization, there is a need for soft knowledge about model parameters. In general, soft knowledge comes from field measurements, literature or expert knowledge. For example, aquifer hydrodynamic properties, such as transmissivity and porosity, can be characterized from aquifer and permeability tests in the field or at the laboratory. However, as CRIV is a lumped parameter that encompasses many processes controlling stream-aquifer flow, it is challenging to estimate suitable initial and regularization values.

When Prickett and Lonnquist (1971) introduced the concept of river conductance, they considered a simplified conceptual model where stream-aquifer flow is controlled by the thickness and vertical hydraulic conductivity of streambed deposits. This widely used approach is described in the MODFLOW river package (McDonald and Harbaugh 1988) and reads as follows:

$$\text{CRIV} = \frac{K_r \times L \times W}{M} \quad (2)$$

where W [L] is the stream width, L [L] is the length of the river reach within the grid cell, M [L] is the streambed thickness, and K_r [L/T] is the hydraulic conductivity of the streambed. More parameterized methods have since been implemented in MODFLOW, as SFR1 and SFR2 (Prudic et al. 2004; Niswonger et al. 2005). These methods extend the original expression (McDonald and Harbaugh 1988), so as to include additional parameters such as the hydraulic gradient along the stream, and complex river cross sections.

These formulations based on the Prickett and Lonnquist (1971) model and used in the MODFLOW family of codes assume that all head losses occur in the streambed. Aquifer hydrodynamic properties and grid size are not taken into account. In fact, the value of CRIV depends on numerous additional parameters such as aquifer hydraulic conductivity and should also account for the effect of additional head losses due to converging/diverging flow that cannot be considered in a 2D horizontal model (Rushton 2007; Morel-Seytoux 2009). Moreover, the value of CRIV has been recently shown to differ by as much as 122% depending on the resolution of the model grid (Mehl and Hill 2010).

Several alternatives for the estimation of the CRIV have been proposed, either based on analytical or numerical methods (Anderson 2003a, 2003b, 2005; Rushton 2007; Morel-Seytoux 2009; Mehl and Hill 2010; Morel-Seytoux et al. 2014).

In line with Anderson (2003a, 2003b), Morel-Seytoux (2009) proposes a formulation which takes into consideration flow convergence/divergence at the vicinity of the stream with the complex potential theory. This method is extended to more complex partially penetrating stream geometries in Morel-Seytoux et al. (2014). However, the presence of streambed deposits and the dependence of CRIV on grid size are not taken into account. Although its importance has been highlighted by Nield et al. (1994), the importance of the anisotropy of aquifer hydraulic conductivity is not considered.

As an alternative, Rushton (2007) proposes to estimate CRIV with a 2D vertical numerical model. The 2D fine-grid model represents one single cell of the regional model centered over the stream. The river conductance is then inferred from the regression between stream-aquifer flow, on one hand, and the head difference between the aquifer cell and the stream on the other. This work points out the predominant influence of aquifer horizontal hydraulic conductivity compared with vertical streambed hydraulic conductivity for certain configurations. Rushton (2007) explains that for a relatively thin streambed (0.2 m) with a hydraulic conductivity of 0.05 m/d, less than a third of head losses occur in the streambed, the rest is due to convergent/divergent fluxes in the aquifer at the stream vicinity. However, this method does not account for anisotropy and grid size.

This work first details an extension of the numerical approach developed by Rushton (2007) for the estimation of CRIV. Numerous parameters often neglected so far are considered. The use of the method is illustrated with a synthetic application, where the value of CRIV is estimated and provided with a confidence interval. A parametric study is then conducted to describe the respective effects and sensitivities of CRIV to controlling parameters. The advantages and limitations of the methodology are then discussed.

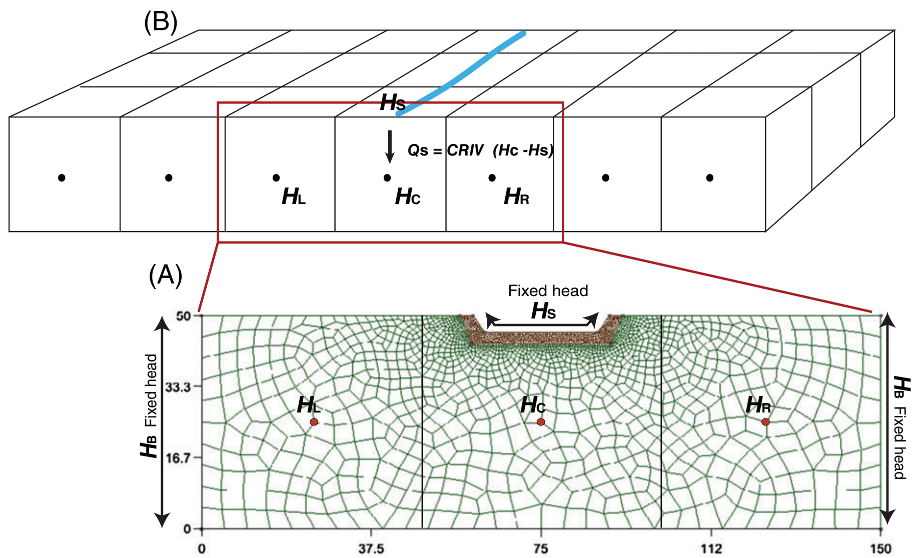

Figure 1. The local 2D vertical finite element model transverse to the river (forefront, A) is used for the estimation of the CRIV controlling the Cauchy boundary condition in the regional 2D horizontal finite difference model (background, B).

The Approach

The approach proposed in this work consists in computing the CRIV used in a 2D horizontal large-scale finite difference model from a 2D vertical local scale model transverse to the stream (Figure 1). Although a longitudinal component may sometimes be observed (Woessner 2000), aquifer flow is assumed to be strictly perpendicular to the stream. In addition, boundary conditions are imposed so that the stream and the aquifer remain hydraulically connected. Transient flow and disconnection are beyond the scope of this study, more information on the subject can be found in Brunner et al. (2009a, 2009b), Brunner et al. (2010), Rivière et al. (2014). The vertical model is run several times, with the same geometry using different head differences between the stream and the aquifer. After these executions of the vertical model, CRIV is obtained by linear regression between the stream-aquifer flow and the head difference between the stream and the aquifer cell where the Cauchy boundary condition is applied (Figure 2).

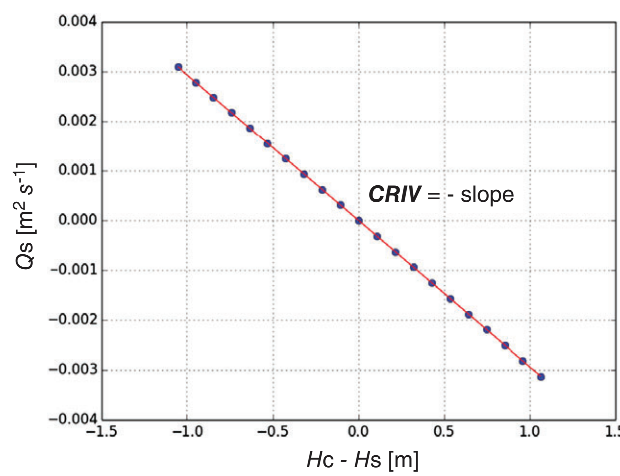

Figure 2. The value of CRIV can be inferred by linear regression of stream aquifer flow per unit river length, Q_s [L^2/T] against the difference in hydraulic head between the aquifer cell (H_c) and the stream (H_s). Q_s is an output of the vertical model. The effect of grid size is taken into account through H_c, computed with Equation 6.

The 2D Vertical Fine-Grid Model

The 2D vertical local scale cross section model covers the extent of three cells of the horizontal model in a direction transverse to the stream (Figure 1). A fixed head boundary condition, H_S, is imposed to the nodes located at the stream-aquifer boundary. The presented method considers symmetric head conditions. A fixed head, H_B, is applied at both sides of the model lateral boundaries (Figure 1).

Other boundaries of the local model are impermeable. The flow equation is solved with the variable saturation, finite element code SUTRA (Voss 1984). This model was chosen because it can simulate an unconfined aquifer in a vertical plan. Furthermore, it is compatible with unstructured grids, which provide flexible refinement possibilities and a good representation of stream bottom geometry. The model grid is composed of quadrilateral elements generated with Gmsh depending on selected model geometry (Geuzaine and Remacle 2009).

Vertical Model Extent and Horizontal Grid Size Cell

In this study, we consider that CRIV accounts for all head losses due to converging/diverging flows in the vicinity of the stream. As a consequence, the grid cell of the horizontal model where a Cauchy-type boundary condition is applied should be large enough to include all the converging/diverging flows associated with the stream. For these reasons, the distance away from the stream where groundwater flow is horizontal, X_{far}, must be estimated. In other words, X_{far} corresponds to the distance from the stream where the Dupuit-Forchheimer approximation is valid. A "characteristic leakage length" λ [L] can be used to approximate X_{far}, as 95% of converging/diverging flows are included in 3λ from surface water shore (Haitjema et al. 2001; Hunt et al. 2003; Haitjema 2006). Here, X_{far} can be easily inferred from the vertical model in the configuration where X_{far} is the largest, i.e., with the maximum head gradient between the stream and the aquifer. We will assume that X_{far} is reached when the ratio between the vertical and the horizontal components of groundwater flow is less than 5%. Assuming the stream to be located at the center of the cell in the horizontal model where a Cauchy-type boundary condition is applied, this cell should be at least as large as $2\,X_{\text{far}}$. The computation of X_{far} is a preliminary step to the calculation of CRIV, as it constrains the grid resolution of river cells in the large-scale horizontal model.

The Determination of the River Conductance

Stream-aquifer flow is computed with the vertical model for a set of values of head-gradient between the stream and the aquifer. To this effect, different values of H_{B} are imposed at the lateral boundaries of the local model while the stream level, H_{S}, remains fixed (Figure 1). Interactions between the different parts of the model are managed with a Python script: (1) the user defines the input variables listed in Table 1, consisting of hydrodynamic properties and geometric settings (Figure 3); (2) Gmsh software is run to build the grid with the user-defined geometry; (3) SUTRA input files are generated from grid coordinates and hydrodynamic parameters (e.g., Table 1); (4) the following steps (4a) and (4b) are repeated for different values of stream-aquifer head difference: (a) SUTRA is run (b) SUTRA output files are post-processed so as to extract stream-aquifer flow; eventually, (5) the unit length river conductance coefficient (CRIV_{u}) is inferred by linear regression between

Table 1
Geometric and Hydrodynamics Parameters Used in the Illustrative Case

Parameter	Value	Unit	GSA range
Aquifer thickness (ct)	30	[m]	—
Horizontal model cell width (cw)	100	[m]	[15, 200]
River width (w)	10	[m]	[5, 10]
River depth (d)	1	[m]	[1, 5]
Bank angle (a)	90	[°]	[90, 100]
Riverbed thickness (m)	0	[m]	[1, 10]
Aquifer horizontal hydraulic conductivity (K_{h})	10^{-3}	[m s^{-1}]	[1e−5, 1e−1]
Riverbed vertical hydraulic conductivity (K_{vb})	—	[m s^{-1}]	[1e−5, 1e−1]
Anisotropy ($anis$)	0.1	[−]	[1e−3, 1]

Notes: The second column provides the most probable value for each parameter; the fourth is the chosen range to perform the probabilistic sampling for the Global Sensitivity Analysis.

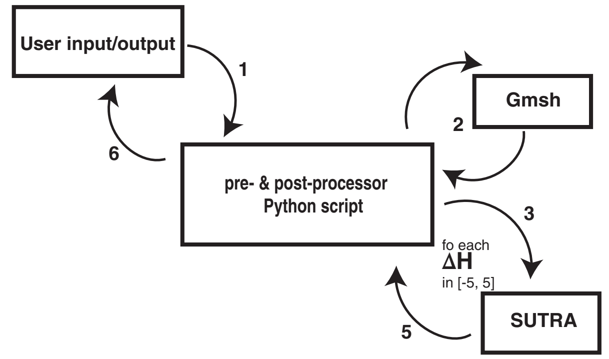

Figure 3. Schematic representation of the Python script used for the computation of the river conductance with the vertical model. The program Gmsh builds the mesh and the numerical code SUTRA solves the Richard's equation.

the computed stream-aquifer flow and the head difference between the stream and the aquifer ($H_{\text{C}} - H_{\text{S}}$) (Figure 2). Given the linearity between the stream-aquifer flow and the head difference between the stream and the connected aquifer (Figure 2), the linear regression of step (5) may be reduced to a simple ratio considering only two distinct head differences. However, considering multiple head differences (approximately 10) is a quality check, which makes the method more robust to potential model failures.

The obtained CRIV_{u} [L/T] accounts for stream-aquifer flow per unit river length. CRIV_{u} should therefore be multiplied by the length of the stream reach within the grid cell (L) to obtain CRIV [L^2/T] as used in MODFLOW.

Grid-Size Dependence of Cauchy Boundary Conditions

One of the difficulties of this approach is to obtain the value of H_{c} in the vertical model, which corresponds to the head at the center of the middle cell in the horizontal model (Figure 4). Because of divergent/convergent fluxes, H_{c} cannot be obtained from the vertical model at its corresponding location. In contrast, finite-element mesh nodes at the centers of adjacent cells (L and R, Figure 4) are located far enough from the stream for vertical flow to be negligible so that H_{L} and H_{R} can be directly inferred from the vertical model. To address the issue, a relation between H_{L}, H_{R}, and H_{C} can be established from the diffusivity equation in finite difference expressed in steady conditions for the central cell of the horizontal model (Figure 4). The flow from the left and right cells to the middle cell is deduced from Darcy's law:

$$Q_{\text{L}} = T_{\text{L-C}} \times (H_{\text{L}} - H_{\text{C}}) \times \frac{1}{cw} \times \text{L} \tag{3}$$

$$Q_{\text{R}} = T_{\text{R-C}} \times (H_{\text{R}} - H_{\text{C}}) \times \frac{1}{cw} \times \text{L} \tag{4}$$

where $Q_{(\text{L/R})}$ [L^2/T] is the flow between right/left cells and center cell, $H_{(\text{L/R})}$ [L] is the hydraulic head at the centroid of the right/left cell, H_{C} [L] is the hydraulic head at the centroid of center cell; cw [L] is the width of the cells.

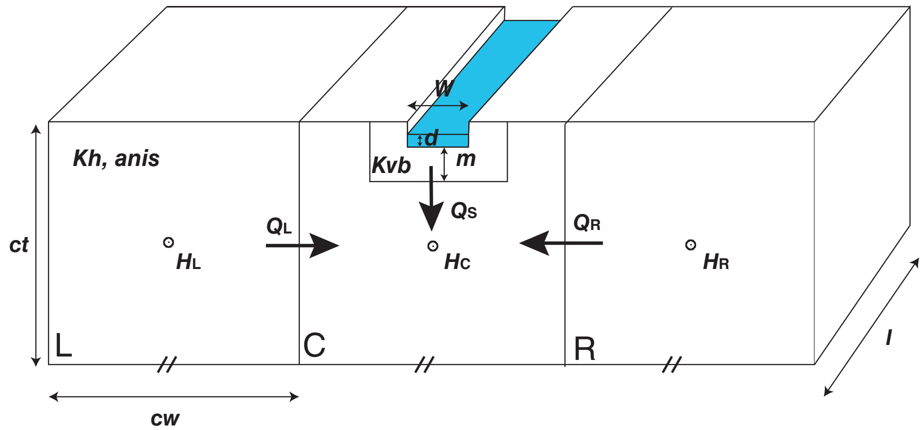

Figure 4. Idealized cross section of an aquifer in interaction with a stream over three cells of the horizontal regional model, which corresponds to the extent of the vertical model. H_{L}, H_{C}, and H_{R} are the hydraulic heads at the center of the left, middle, and right cell of the horizontal model, respectively. See Table 1 for further parameter definitions.

$T_{(\mathrm{L/R})\text{-}\mathrm{C}}$ [L^2/T] is the equivalent transmissivity between the right/left cell and the middle cell.

Assuming that the component of groundwater flow longitudinal to the stream is negligible, the equation of mass conservation in steady state expressed for the middle cell reads as follows:

$$Q_{\mathrm{L}} + Q_{\mathrm{R}} + Q_{\mathrm{S}} = 0 \tag{5}$$

where Q_{S} is the flow from the stream to the middle cell. Combining Equations 3, 4, and 5 we obtain:

$$H_{\mathrm{C}} = \frac{1}{2}\left(\frac{Q_S \times cw}{T \times L} + H_{\mathrm{L}} - H_{\mathrm{R}}\right) \tag{6}$$

where the values of Q_{s}, H_{L} and H_{R} are provided by the vertical model, and T is the aquifer transmissivity, assumed to be homogeneous and independent of hydraulic head over the three cells of interest ($T_{\mathrm{L\text{-}C}} = T_{\mathrm{R\text{-}C}}$). H_{L} and H_{R} are taken at a single node in the centroid of L and R cells of the vertical model. Using this latter expression of H_{c} for the regression of Q_{S} against ($H_{\mathrm{C}} - H_{\mathrm{S}}$), we consider the dependence of the horizontal grid-size, cw, for the calculation of the river conductance.

Applications of the Methodology

As to illustrate the interest of the approach, we consider a 2D horizontal large-scale groundwater model where the simulated aquifer interacts with a stream. The characteristics of the aquifer and the stream are chosen to correspond to a classical context (Table 1). The value of CRIV used in the large-scale horizontal model will be eventually adjusted by calibration together with other model parameters, but this is out of the scope of this study. However, when the accurate quantification of stream-aquifer flow is essential, initial and regularization values should be carefully chosen for the calibration of CRIV. In addition, the probabilistic distribution of CRIV prior to calibration is also useful for post-calibration uncertainty analysis.

Estimation of the River Conductance from Expected Parameter Values

The most probable parameter values for this synthetic case (Table 1) are set in the Python script, which generates the finite-element grid and runs the model for various head differences between the stream and the aquifer. X_{far} is first calculated with the tool so as to take into account the grid size. With an X_{far} of about 50 m, the river cell size in the horizontal model should be set to 100 m. With these parameter values for this synthetic case, $\mathrm{CRIV_u}$ is estimated at 6.69×10^{-5} m/s with a computation time shorter than a minute. Multiplied by the length of the reach within the grid cell of the model (100 m), the value of CRIV is 6.69×10^{-3} m^2/s. This value can be used as initial and regularization values for the calibration of the horizontal model (see e.g., Hunt et al. 2007).

Prior Probabilistic Distribution of the River Conductance

The probabilistic CRIV distribution can also be obtained with the presented tool by random sampling from the prior statistical distributions of input parameters. We assumed a normal distribution for geometric parameters and log-normal distribution for hydrodynamic parameters (Table 1, Figure 5). CRIV is then computed for each of the parameter sets. The resulting CRIV distribution (Figure 5) is an essential element to perform parameter and predictive uncertainty analysis (see e.g., Gallagher and Doherty 2007).

Sensitivity of the River Conductance to Hydrodynamic and Geometric Parameters

The effect of the parameters considered in this study over CRIV is first illustrated with parameter variations, taken one by one, from the reference configuration of the stream described in Table 1. This parametric analysis

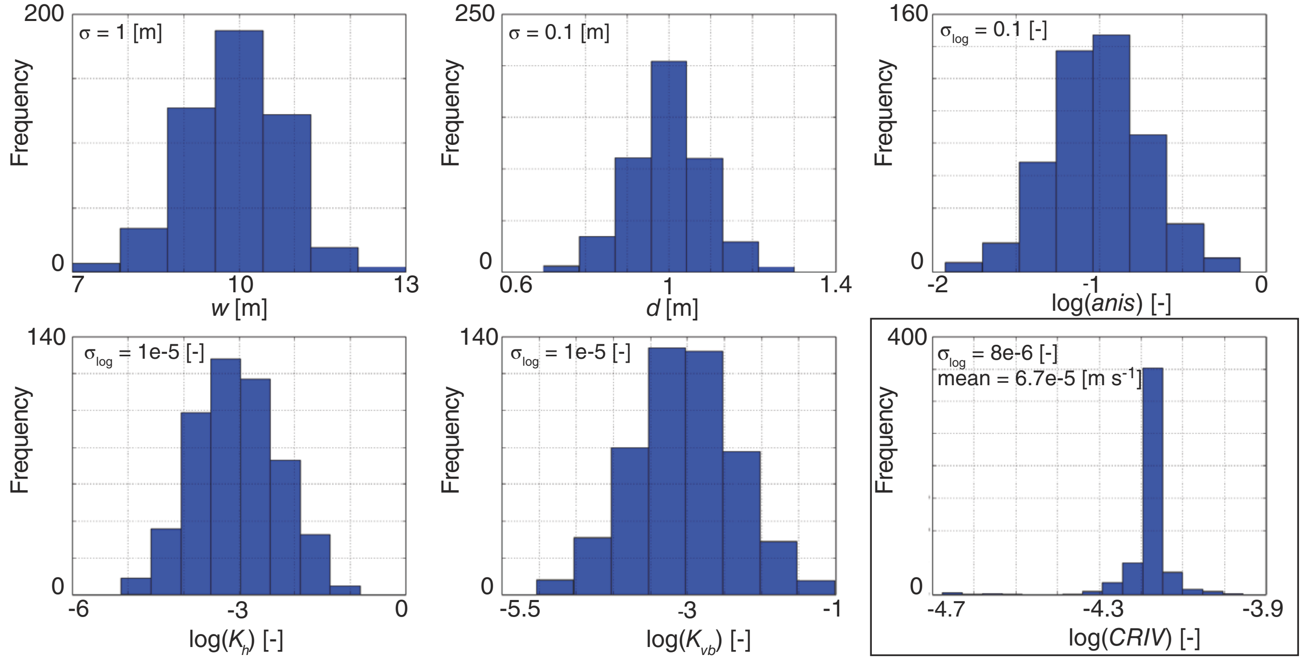

Figure 5. The probabilistic distribution of CRIV (bottom right) is obtained with the presented tool from the distributions of input parameters.

is useful to describe how each parameter may impact CRIV in a regular stream-aquifer configuration. A global sensitivity analysis is thereafter performed to rank the sensitivities of CRIV to its parameters over a wide range of realistic parameter values.

Parametric Analysis

CRIV values have been calculated for a range of likely values of aquifer hydraulic conductivity (K_h) and anisotropy (*anis*), horizontal grid size (*cw*), and streambed vertical hydraulic conductivity (K_{vb}) (Figure 6). When they are fixed, parameters are kept to the reference values from the synthetic case study (Table 1).

Several studies solely base the estimation of CRIV on K_h (Rushton 2007; Pryet et al. 2015). This approach is validated here, because K_h is one of the most important controlling factors of the stream aquifer exchanges for this case (Figure 6A). A modification by one order of magnitude of K_h produces a modification by one order of magnitude of CRIV.

The influence of *anis* (Figure 6B) (which stands for K_v/K_h where K_v is the vertical hydraulic conductivity of the aquifer [L/T]) is explained by the occurrence of vertical flow in the vicinity of the stream. A high value of anisotropy impedes the occurrence of converging/diverging flow and reduces stream-aquifer flow. An increase by one order of magnitude of *anis* (from 1 and 0.1) leads to an increase of CRIV by a factor approaching 30. Modelers often choose a rather arbitrary value of 0.1 for *anis* (Doppler et al. 2007; Derx et al. 2010; Engeler et al. 2011) following Chen (2000). Our results highlight that an inappropriate value of anisotropy may imply a large error on stream-aquifer flow estimates.

The influence of the grid size of the horizontal model, *cw*, is also important (Figure 6C). CRIV decreases by a factor of 25 when the grids cell size increases from 10 to 110 m.

The influence of K_{vb} is highly nonlinear (Figure 6D). As long as K_{vb} is greater than K_h, K_{vb} has no influence on CRIV. In contrast, when K_{vb} is lower than K_h, CRIV decreases with K_{vb}. We recall that in this study, CRIV is calculated for values of the K_{vb}/K_h ratio that remain characteristic of a connection between the stream and the aquifer (Brunner et al. 2009a, 2009b).

In the range of likely values for hydrogeological model parameters, the most important controlling factors of CRIV, in this case, are, in decreasing order of importance (Figure 5): K_h, which can change CRIV by six orders of magnitude (1) K_{vb} by four orders of magnitude, (2) *cw* by three orders of magnitude, (3) *anis* by two orders of magnitude. However a variation by one order of magnitude in *anis* or *cw* has more impact on CRIV than K_h and K_{vb}.

This parametric analysis is relevant to graphically illustrate how each parameter affects CRIV. However, this method is very dependent on the choice of reference parameter values and does not quantify the effect of joint parameter variations. Those issues can be addressed with a global sensitivity analysis.

Global Sensitivity Analysis of CRIV

The importance of the parameters used to compute CRIV is discussed here through a global sensitivity analysis (GSA). Compared with the sensitivity analysis based on the local derivative (see e.g., Hill and Tiedeman 2006), the GSA can be applied to nonlinear models,

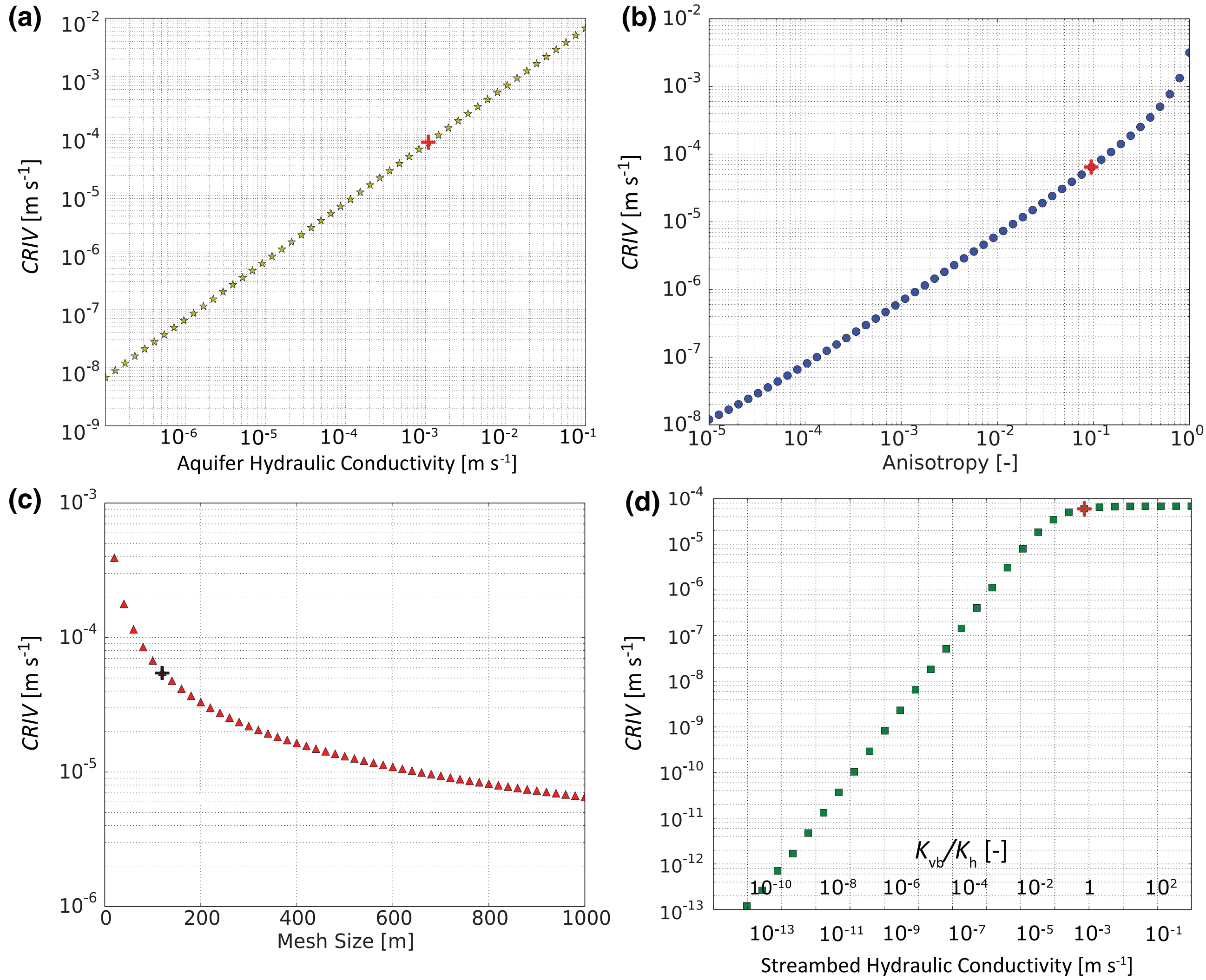

Figure 6. Dependence of $\mathrm{CRIV_u}$ per unit river length to model parameters values. (a) Streambed hydraulic conductivity (K_{vb}). (b) Aquifer anisotropy (*anis*). (c) Horizontal grid size (*cw*). (d) Aquifer hydraulic conductivity (K_h). Cross marks indicate reference parameter values (Table 1).

and provides more robust information on the effect of respective parameters to a model output, here CRIV. Over the large variety of GSA methods, the variance-based sensitivity indicator (Sobol) is largely used (Sobol et al. 2001; Saltelli et al. 2004; Welter et al. 2015). Sobol method is based on the analysis of model output values obtained from a large range of parameters sets sampled from probabilistic distributions (Saltelli et al. 2004). This is applicable to nonlinear models. The sensitivity of each parameter is described by the first order sensitivity index, which is the contribution of a single model parameter to the model output variance (Sobol et al. 2001):

$$S_i = \frac{V_i}{V_{\mathrm{tot}}} \qquad (7)$$

where V_i is the variance of CRIV attributed to the i-th parameter and V_{tot} is the variance of model output CRIV.

Parameter lower and upper bounds are provided in Table 1. About 15,000 CRIV values have been computed with a uniform distribution of parameter sets obtained with the Saltelli sampler (Saltelli et al. 2004) from the SALib (2015) Python script.

The influence of hydrodynamic parameters prevails over geometric parameters (Figure 7). Results highlight the strong influence of hydrodynamics parameters K_{vb}, K_h, and *anis*. Taken together they account for 30% of the total CRIV variance, as they respectively explain 14%, 10%, and 6% of the CRIV variance. Geometric parameters such as stream depth and bank angle have a small effect. Taken together, they account for approximately 2% of the CRIV variance. However the grid cell size (*cw*) has more influence on CRIV with 4.5% of the CRIV variance as well as the riverbed thickness (*m*) with 7% of the CRIV variance. In total, 43.5% of the total CRIV variance is explained by parameters taken alone, the remaining 56.5% is explained by the interactions between parameters.

Results of the GSA confirm the observations made with the parametric analysis. K_h, K_{vb}, and *anis* are the major controlling factors; *cw* and *m* are strong controlling factors. While K_h and K_{vb} are generally taken into

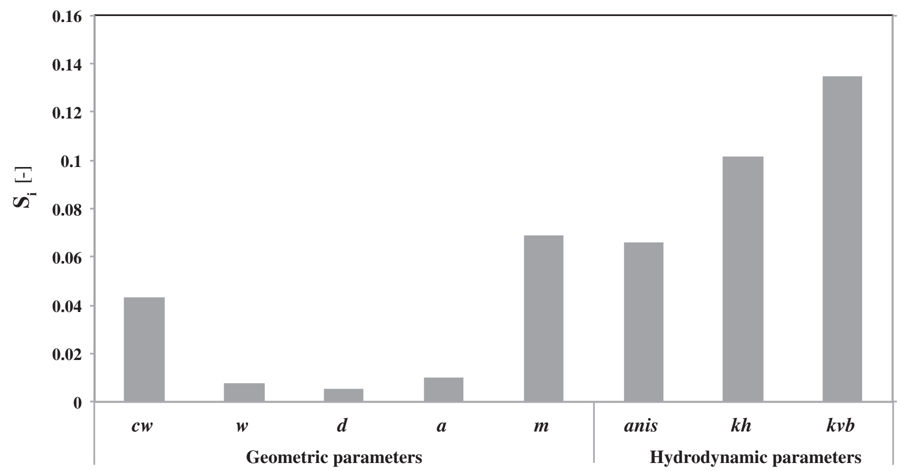

Figure 7. Global sensitivity analysis (GSA) of the CRIV coefficient to model parameters where S_i is the first order sensitivity index. The main controlling factors of CRIV are K_{vb}, K_{h}, *anis* and m and in a lesser extent cw. The parameter ranges are presented in Table 1.

account for the estimation of CRIV, the importance of *anis* and *cw* is often disregarded. Our results highlight that neglecting the importance of these parameters may induce an error by multiple orders of magnitude on the value of CRIV.

Discussion

The proposed method aims at constraining the value of CRIV from a local vertical model given hydrodynamic and geometric parameters. These parameters correspond to physical properties potentially measurable in the field or at the laboratory. Geometric parameters such as stream width, depth and bank angle, aquifer, and streambed thicknesses can be easily obtained from direct measurements, geological logs, or geophysical methods (Cardenas and Markowski 2010). The spatial variability of these parameters can also be investigated based on local hydrogeophysical measurements (Mouhri et al. 2013). Hydrodynamic properties of the aquifer and the streambed can be characterized from pumping and permeability tests in the field or at the laboratory (Chen 2000). The measurement of hydraulic heads at different depths near a stream can provide estimates of the anisotropy of hydraulic conductivity (Kalbus et al. 2006). However, it should be acknowledged that obtaining reliable and representative estimates for each of the hydrodynamics parameters is challenging.

As demonstrated by numerous authors (Gaffield et al. 1998; Levy et al. 2011; Gianni et al. 2016), the use of a temporally and spatially constant value for CRIV is questionable and can be affected by biological clogging in the riverbed (Newcomer et al. 2016). However, it is so far considered as constant in regional models. For the spatial aspect, the user can split the stream network in interaction with the simulated aquifer into a limited number of reaches sharing common features (aquifer properties, stream geometry, ...) and estimate a value of CRIV for each of the respective reaches.

The accuracy of CRIV estimates obtained with the proposed method depends on the uncertainty of the parameters of the local scale vertical model, as shown by the probabilistic CRIV distribution (Figure 5). A calibration step is generally needed where the value of CRIV estimated with the presented approach is used as initial and regularization values. Calibration by history matching is usually conducted against observations of stream flow and groundwater level fluctuations (Engeler et al. 2011; Pryet et al. 2015). However, obtaining an initial value from prior information can be critical. Pryet et al. (2015) based their initial estimates on the relation between CRIV and horizontal hydraulic conductivity developed by Rushton (2007). Our method improves this approach by including in the prior estimate of CRIV numerous parameters often neglected. Obtaining objective initial and regularization values of CRIV from the approach presented in this paper is a significant improvement to the uniformed and evaluated calibration of CRIV. Moreover, our method takes into consideration the effect of grid-size, providing an upscaling procedure for the estimation of CRIV from the local scale to the watershed scale ($\sim$10 to $\sim$1000 km^2) (Mehl and Hill 2010; Flipo et al. 2014). Given these elements, the method described in this study is likely to improve simulation of stream-aquifer interactions, especially at the scale of watersheds (Flipo et al. 2012).

The method presented in this study has been developed with the assumption of symmetric settings with a straight stream located at the center of a horizontal model cell. The precision of CRIV estimated with this approach may therefore become questionable when the configuration of interest strongly deviates from this simplified model, such as very winding stream with important meanders within a single horizontal model cell. Such configurations may require a 3D local model for the estimate of CRIV. However, the gain of precision with such a more complex approach is likely to be small with respect to the irreducible uncertainty attributed to the estimates of controlling parameters, in particular aquifer and riverbed hydraulic properties. The value of CRIV obtained with the presented approach should be considered as a first, but objective estimate that can subsequently be adjusted by calibration.

The Software

As to simplify the tedious task of considering multiple configurations, a flexible Python script has been developed and is provided as supplementary materials to this article. It can be used to estimate a value of CRIV from a single parameter set, or to obtain the probabilistic distribution of CRIV given the probabilistic distributions of input parameters. The code is available here: https://github.com/rivtools/criv.

Conclusion

A method has been described to compute the value of CRIV with a vertical fine-grid cross-sectional model transverse to the stream. This model is applicable to a wide range of stream characteristics, aquifer properties, and grid resolutions. The value of CRIV can now be estimated from physical parameters that can be measured in the field. Parameters, neglected so far are now taken into account: (1) the anisotropy of aquifer hydraulic conductivity, and (2) the size of river cells in the regional model grid. The global sensitivity analysis highlighted the importance of these parameters and justifies their consideration. The estimate of CRIV from prior information can constitute initial and regularization values for the calibration of a surface-subsurface model. This is crucial when the inverse problem is ill-posed, which is often the case. The approach also provides the probabilistic distribution of CRIV given input parameter probabilistic distributions, which is essential for post-calibration uncertainty analysis.

Acknowledgments

This work was conducted in the frame of the Mhyqadeau project supported by Suez Environnement (LyRE) and the French Aquitaine regional council. The authors are very grateful to Dr Randal J. Hunt and two anonymous reviewers for their valuable comments for improving this manuscript. We also thank Clotilde Thompson for her help in improving English language.

Authors' Note: The authors do not have any conflicts of interest to report.

Appendix

Stream to aquifer flow obtained from the 2D cross-sectional numerical model are validated with two analytical solutions describing stream to aquifer flow with simplified geometries. Similar stream-aquifer designs have been chosen for each validation cases. Firstly an analytical formulation given by Morel-Seytoux (2009) from complex potential theory approach is used. In this case, the stream is represented by a point source without the effect of a streambed deposit and the stream-aquifer flow is given by:

$$Q_S = 2 \times \mathrm{KL}\left\{\frac{1}{\left(\frac{0.5\ \times e_B}{B_{\mathrm{rect}}}\right)+\left(\frac{B_{\mathrm{rect}}+\Delta x}{\bar{e}}\right)}\right\} \times \left(H_s - H_{r/l}\right) \quad \text{(A1)}$$

where L [L] is the length of the stream reach, K [L/T] is the aquifer hydraulic conductivity assumed to be isotropic, e_B [L] is the aquifer depth below the bottom of the reach cross section, B_{rect} [L] is the width of the stream, and $\bar{e}$ [L] is the average aquifer thickness. Δx [L] is the distance from the riverbank to the centroids of adjacent cell $H_{r/l}$ [L].

Another approach, proposed by Herbert (1970), considers a small circular stream channel in comparison to the saturated thickness of the aquifer e_B. The flow from the aquifer to the stream is assumed to be radial. Then, adapting the Thiem equation:

$$Q_S = \pi \mathrm{LK}\frac{H_s - H_c}{\ln\left(\frac{0.5\times e_B}{r_s}\right)} \quad \text{(A2)}$$

where r_s [L] is the effective stream radius. When the stream channel has a trapezoidal cross section, an effective stream radius must be used. For a channel width of 10 m and a water depth of 1.0 m, the effective radius of the stream is 5.0 m (Rushton 2007).

The values of Q_S [L^3/T] obtained with these two analytical solutions are compared to the output of the local numerical model with parameters presented in Table 2. Stream-aquifer flow obtained from the three methods is nearly identical and validates the vertical numerical model used in the present approach

Table A1
Parameters of Analytical Solutions Used for the Validation of the Local Numerical Model

Parameters	Morel-Seytoux (2009)	Herbert (1970)	Presented method
e_B [m]	28	28	28
B_{rect} [m]	5	—	5
X_{far} [m]	95	—	—
e [m]	30.5	—	30.5
$H_S - H_c$ [m]	—	0.56	0.56
ΔH [m]	5	—	—
r_s [m]	—	5	—
K [m/s]	10^{-3}	10^{-3}	10^{-3}
Q [m^2/s]	1.65E−03	1.71E−03	1.75E−03
Difference	6.4%	2.4%	—

References

Anderson, E.I. 2003a. An analytic solution representing groundwater-surface water interaction. *Water Resources Research* 39, no. 3: 1071.

Anderson, E.I. 2003b. The effective resistance to vertical flow in Dupuit models. *Advances in Water Resources* 26, no. 5: 513–523.

Anderson, E.I. 2005. Modeling groundwater-surface water interactions using the Dupuit approximation. *Advances in Water Resources* 28, no. 4: 315–327.

Aster, R., B. Borchers, and C. Thurber. 2005. *Parameter Estimation and Inverse Problems*. Burlington, Vermont: Elsevier Academic Press.

Boano, F., R. Revelli, and L. Ridolfi. 2011. Water and solute exchange through flat streambeds induced by large turbulent eddies. *Journal of Hydrology* 402, no. 3: 290–296.

Brunner, P., P.G. Cook, and C.T. Simmons. 2009a. Hydrogeologic controls on disconnection between surface water and groundwater. *Water Resources Research* 45, no. 1: 1422.

Brunner, P., P.G. Cook, and C.T. Simmons. 2009b. Hydrogeologic controls on disconnection between surface water and groundwater. *Water Resources Research* 45, no. 1.

Cardenas, M.B. 2009. Stream-aquifer interactions and hyporheic exchange in gaining and losing sinuous streams. *Water Resources Research* 45, no. 6: 6429.

Cardenas, M.B., and M.S. Markowski. 2010. Geoelectrical imaging of hyporheic exchange and mixing of river water and groundwater in a large regulated river. *Environmental Science & Technology* 45, no. 4: 1407–1411.

Cardenas, M.B., and J.L. Wilson. 2007. Exchange across a sediment—water interface with ambient groundwater discharge. *Journal of Hydrology* 346, no. 3: 69–80.

Carrera, J., A. Alcolea, A. Medina, J. Hidalgo, and L.J. Slooten. 2005. Inverse problem in hydrogeology. *Hydrogeology Journal* 13, no. 1: 206–222.

Chen, X. 2000. Measurement of streambed hydraulic conductivity and its anisotropy. *Environmental Geology* 39, no. 12: 1317–1324.

Derx, J., A. Blaschke, and G. Bloschl. 2010. Three-dimensional flow patterns at the river—aquifer interface—a case study at the Danube. *Advances in Water Resources* 33, no. 11: 1375–1387.

Discacciati, M., E. Miglio, and A. Quarteroni. 2002. Mathematical and numerical models for coupling surface and groundwater flows. *Applied Numerical Mathematics* 43, no. 1: 57–74.

Doherty, J., and B.E. Skahill. 2006. An advanced regularization methodology for use in watershed model calibration. *Journal of Hydrology* 327, no. 3: 564–577.

Doppler, T., H.-J.H. Franssen, H.-P. Kaiser, U. Kuhlman, and F. Stauffer. 2007. Field evidence of a dynamic leakage coefficient for modelling river—aquifer interactions. *Journal of Hydrology* 347, no. 1: 177–187.

Ebel, B.A., B.B. Mirus, C.S. Heppner, J.E. VanderKwaak, and K. Loague. 2009. First-order exchange coefficient coupling for simulating surface water-groundwater interactions: Parameter sensitivity and consistency with a physics-based approach. *Hydrological Processes* 23, no. 13: 1949–1959.

Engeler, I., H.H. Franssen, R. Muller, and F. Stauffer. 2011. The importance of coupled modelling of variably saturated groundwater flow-heat transport for assessing river—aquifer interactions. *Journal of Hydrology* 397, no. 3: 295–305.

Fleckenstein, J.H., S. Krause, D.M. Hannah, and F. Boano. 2010. Groundwater-surface water interactions: New methods and models to improve understanding of processes and dynamics. *Advances in Water Resources* 33: 1291–1295.

Flipo, N., C. Monteil, M. Poulin, C. Fouquet, and M. Krimissa. 2012. Hybrid fitting of a hydrosystem model: Long-term insight into the Beauce aquifer functioning (France). *Water Resources Research* 48, no. 5: 5509.

Flipo, N., A. Mouhri, B. Labarthe, S. Biancamaria, A. Rivière, and P. Weill. 2014. Continental hydrosystem modelling: the concept of nested stream—aquifer interfaces. *Hydrology and Earth System Sciences* 18, no. 8: 3121–3149.

Furman, A. 2008. Modeling coupled surface-subsurface flow processes: A review. *Vadose Zone Journal* 7, no. 2: 741–756.

Gaffield, S.J., K. Bradbury, and K.W. Potter. 1998. Hydrologic assessment of the Kickapoo Watershed, southwestern Wisconsin, Madison, Wisconsin: Wisconsin Geological and Natural History Survey.

Gallagher, M., and J. Doherty. 2007. Parameter estimation and uncertainty analysis for a watershed model. *Environmental Modelling & Software* 22, no. 7: 1000–1020.

Geuzaine, C., and J.-F. Remacle. 2009. Gmsh: A 3-D finite element mesh generator with built-in pre-and post-processing facilities. *International Journal for Numerical Methods in Engineering* 79, no. 11: 1309–1331.

Gianni, G., J. Richon, P. Perrochet, A. Vogel, and P. Brunner. 2016. Rapid identification of transience in streambed conductance by inversion of a flood-wave response. *Water Resources Research* 52, no. 4: 2647–2658.

Goderniaux, P., S. Brouyère, H.J. Fowler, S. Blenkinsop, R. Therrien, P. Orban, and A. Dassargues. 2009. Large scale surface–subsurface hydrological model to assess climate change impacts on groundwater reserves. *Journal of Hydrology* 373, no. 1: 122–138.

Haitjema, H. 2006. The role of hand calculations in ground water flow modeling. *Ground Water* 44, no. 6: 786–791.

Haitjema, H., V. Kelson, and W. Lange. 2001. Selecting modflow cell sizes for accurate flow fields. *Groundwater* 39, no. 6: 931–938.

Herbert, R. 1970. Modelling partially penetrating rivers on aquifer models. *Groundwater* 8, no. 2: 29–36.

Hill, M.C., and C.R. Tiedeman. 2006. *Effective Groundwater Model Calibration: With Analysis of Data, Sensitivities, Predictions, and Uncertainty*. John Wiley & Sons.

Hunt, R.J., H.M. Haitjema, J.T. Krohelski, and D.T. Feinstein. 2003. Simulating ground water-lake interactions: approaches and insights. *Ground Water* 41, no. 2: 227–237.

Hunt, R.J., J. Doherty, and M.J. Tonkin. 2007. Are models too simple? Arguments for increased parameterization. *Ground Water* 45, no. 3: 254–262.

Kalbus, E., F. Reinstorf, and M. Schirmer. 2006. Measuring methods for groundwater—surface water interactions: A review. *Hydrology and Earth System Sciences Discussions* 10, no. 6: 873–887.

Levy, J., M.D. Birck, S. Mutiti, K.C. Kilroy, B. Windeler, O. Idris, and L.N. Allen. 2011. The impact of storm events on a riverbed system and its hydraulic conductivity at a site of induced infiltration. *Journal of environmental management* 92, no. 8: 1960–1971.

McDonald, M.G., and Harbaugh, A.W. 1988. A modular three-dimensional finite-difference ground-water flow model. Technical report, Reston, Virginia: USGS.

Mehl, S., and M.C. Hill. 2010. Grid-size dependence of Cauchy boundary conditions used to simulate stream—aquifer interactions. *Advances in Water Resources* 33, no. 4: 430–442.

Morel-Seytoux, H.J. 2009. The turning factor in the estimation of stream-aquifer seepage. *Groundwater* 47, no. 2: 205–212.

Morel-Seytoux, H.J., S. Mehl, and K. Morgado. 2014. Factors influencing the stream-aquifer flow exchange coefficient. *Groundwater* 52, no. 5: 775–781.

Mouhri, A., N. Flipo, F. Réjiba, C. De Fouquet, L. Bodet, B. Kurtulus, G. Tallec, V. Durand, A. Jost, P. Ansart, et al. 2013. Designing a multi-scale sampling system of stream-aquifer interfaces in a sedimentary basin. *Journal of Hydrology* 504: 194–206.

Newcomer, M.E., S.S. Hubbard, J.H. Fleckenstein, U. Maier, C. Schmidt, M. Thullner, C. Ulrich, N. Flipo, and Y. Rubin. 2016. Simulating bioclogging effects on dynamic riverbed permeability and infiltration. *Water Resources Research* 52, no. 4: 2883–2900.

Nield, S.P., L.R. Townley, and A.D. Barr. 1994. A framework for quantitative analysis of surface water-groundwater interaction: Flow geometry in a vertical section. *Water Resources Research* 30, no. 8: 2461–2475.

Niswonger, R.G., and D.E. Prudic. 2005. *Documentation of the streamflow-routing (SFR2) package to include unsaturated flow beneath streams–A modification to SFR1. U.S. Department of the Interior*. Reston, Virginia: U.S. Geological Survey.

Peyrard, D., S. Sauvage, P. Vervier, J.-M. Sanchez-Perez, and M. Quintard. 2008. A coupled vertically integrated model to describe lateral exchanges between surface and subsurface in large alluvial floodplains with a fully penetrating river. *Hydrological Processes* 22, no. 21: 4257–4273.

Prickett, T.A., and C.G. Lonnquist. 1971. Selected digital computer techniques for groundwater resource evaluation. Technical report, Urbana, Illinois*:* Illinois Water Survey Bulletin.

Prudic, D.E., L.F. Konikow, and E.R. Banta. 2004. A new streamflowrouting (sfr1) package to simulate stream-aquifer interaction with modflow-2000. Technical report. Reston, Virginia: USGS.

Pryet, A., B. Labarthe, F. Saleh, M. Akopian, and N. Flipo. 2015. Reporting of stream-aquifer flow distribution at the regional scale with a distributed process-based model. *Water Resources Management* 29, no. 1: 139–159.

Rivière, A., J. Goncalves, A. Jost, and M. Font. 2014. Experimental and nu- merical assessment of transient stream-aquifer exchange during disconnection. *Journal of Hydrology* 517: 574–583.

Rushton, K. 2007. Representation in regional models of saturated river—aquifer interaction for gaining/losing rivers. *Journal of Hydrology* 334, no. 1: 262–281.

SALib. 2015. Sensitivity Analysis Library in Python (Numpy). https://github.com/SALib/SALib.

Saltelli, A., S. Tarantola, F. Campolongo, and M. Ratto. 2004. *Sensitivity analysis in practice: a guide to assessing scientific models*. John Wiley & Sons.

Sobol, I.M. 2001. Global sensitivity indices for nonlinear mathematical models and their monte carlo estimates. *Mathematics and Computers in Simulation* 55, no. 1: 271–280.

Sophocleous, M. 2002. Interactions between groundwater and surface water: the state of the science. *Hydrogeology Journal* 10, no. 1: 52–67.

Sulis, M., S.B. Meyerhoff, C. Paniconi, R.M. Maxwell, M. Putti, and S.J. Kollet. 2010. A comparison of two physics-based numerical models for simulating surface water—groundwater interactions. *Advances in Water Resources* 33, no. 4: 456–467.

Tihonov, A.N. 1963. Solution of incorrectly formulated problems and the regularization method. *Soviet Mathematics Doklady* 4: 1035–1038.

Tonina, D., and J.M. Buffington. 2007. Hyporheic exchange in gravel bed rivers with pool-riffle morphology: Laboratory experiments and three-dimensional modeling. *Water Resources Research* 43, no. 1: W01421.

Voss, C.I. 1984. SUTRA (Saturated-Unsaturated Transport). A finite-element simulation model for saturated-unsaturated, fluid-density-dependent ground-water flow with energy transport or chemically-reactive single-species solute transport (no. USGS/WRI/84-4369). Reston, Virginia: Geological Survey Water Resources Division.

Welter, D.E., White, J.T., Hunt, R.J., and Doherty, J.E. 2015. Approaches in highly parameterized inversionest++ version 3, a parameter estimation and uncertainty analysis software suite optimized for large environmental models. Technical report. Reston, Virginia: USGS.

Woessner, W.W. 2000. Stream and fluvial plain ground water interactions: Rescaling hydrogeologic thought. *Ground Water* 38, no. 3: 423–429.

Zhou, H., J.J. Gómez-Hernández, and L. Li. 2014. Inverse methods in hydrogeology: Evolution and recent trends. *Advances in Water Resources* 63: 22–37.

Zlotnik, V.A., D. Toundykov, and M.B. Cardenas. 2015. An analytical approach for flow analysis in aquifers with spatially varying top boundary. *Groundwater* 53, no. 2: 335–341.