State-space first-order estimate of well catchment uncertainty

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Abstract Nonstationarity of groundwater flow and transport processes is relevant in well capture zone design and wellhead protection. We introduce a State-Space First-Order approach as an alternative to numerical Monte Carlo methods to quantify the uncertainty associated with well catchment prediction. The mean and covariance of system state variables (i.e. head, pore water velocity and particle trajectory) are approximated by a first-order Taylor's series with sensitivity coefficients estimated from the adjoint operator for a system of discrete equations (state-space equations). By employing numerical solution methods, it is possible to handle irregular geometry, varying boundary conditions, complicated sink/source terms and different covariance functions, all of which are important factors for real-world applications. Results obtained using the State-Space First-Order method compare favourably with those from Monte Carlo analysis and are considerably more efficient.

Keywords Monte Carlo method; nonstationarity; State-Space First-Order method; stochastic; well catchment

INTRODUCTION AND BACKGROUND INFORMATION

Of the aquifer properties that control the movement of water and conservative contaminants in the subsurface, hydraulic conductivity (or transmissivity) is generally the most important, as its spatial variability is considerably higher than that of other properties, such as porosity (Hoeksema & Kitanidis, 1984). During the last 20 years many stochastic theories have been developed to relate the statistical moments of hydraulic head, pore water velocity and other flow and mass transport quantities to those of transmissivity and mean flow characteristics (e.g. Zhang, 2002). Statistical nonstationarity of flow and mass transport processes may occur due to non-homogeneous statistics of medium properties, complex boundary configurations or source/sink terms (Osnes, 1995; Guadagnini & Neuman, 1999; Riva *et al*., 2001).

Nonstationary stochastic analysis provides a method for calculating the probability that a given location in the aquifer contributes water to a pumping well. The problem has usually been studied (Guadagnini & Franzetti, 1999; van Leeuwen *et al.*, 2000; Feyen *et al.*, 2003) with a Monte Carlo framework, to determine how uncertainty in hydraulic parameters, mainly transmissivity, propagates to well capture/catchment location. Limitations of the Monte Carlo method have been discussed in the literature (e.g. Ballio & Guadagnini, 2004). In particular, it can be computationally very

demanding when conditioning transmissivity realizations on state variable measurements, such as hydraulic head, pore water velocity or travel time (Bakr & Butler, 2004), as this requires solutions of the inverse flow problem (e.g. McLaughlin & Townley, 1996). As an alternative approach, Kunstmann & Kinzelbach (2000) used a first-order second moment method to compute well capture zones and their associated uncertainty on the basis of an Eulerian framework. Stauffer *et al*. (2002) subsequently used a first-order approximation to investigate uncertainty in two-dimensional, steady-state well catchment boundaries in random transmissivity fields. They locally scaled the stationary covariance derived by Rubin (1990) to account for nonstationary velocity covariances that result from pumping. More recently, Lu & Zhang (2003) presented a moment equation approach to derive time-dependent mean capture zones and their associated uncertainties.

Here we use an alternative, first-order approximated, numerical approach for nonstationary stochastic analysis of well capture zones, which is based on a Taylor's series approximation of the discrete system of equations and is often termed the vector space-state/adjoint state approach (Zhang, 2002). Our focus here is on the nonstationarity due to a pumping well. We start from the work of Bakr & Butler (2005), where the original partial differential equation is first discretized on a specified grid using finite elements and the resulting system of equations, the so-called space-time equation, is used to derive statistical moments of the flow and mass transport quantities. As will be shown later, the main task of this approach is to determine flow and transport sensitivity coefficients.

STOCHASTIC WELL CATCHMENT DETERMINATION USING FIRST-ORDER TAYLOR'S SERIES APPROXIMATION

Forward modelling

A forward operator, which takes the form of a partial differential equation, is used to predict the response of groundwater systems to initial and boundary conditions and hydraulic parameters. Here, the flow equation and Darcy's law are solved numerically using the Galerkin (central) finite element method. This leads to a system of linear equations that can be stated as:

$$\mathbf{g}(\mathbf{s},\boldsymbol{\rho}) = 0 \tag{1}$$

where $\mathbf{s}$ is a vector of nodal values of state variables (i.e. head and pore water velocity), and $\boldsymbol{\rho}$ is a vector of nodal natural log transmissivity values. Throughout this paper we use bold small letters to indicate vectors and bold capital letters to indicate matrices, and regular fonts to indicate scalars. We consider transmissivity as the only uncertain parameter.

Solving (1) provides an estimation of nodal values of state variables, in particular pore water velocity. These can then be used in a solution of the advective mass transport problem by particle tracking. For example, Euler's method can be employed to delineate a well catchment starting from the generated stagnation point, such that:

$$y^{i+1} = y^{i} + \frac{u_y^i}{u_x^i}\Delta x \tag{2}$$

Here, y^i and y^{i+1} are the well catchment location at steps i and $i + 1$, respectively; Δx is the tracking step in the x-direction; u_x^i and u_y^i are the pore water velocities in the x- and y-direction at step i. We start tracking from a point which is located within a circle of small radius centred at the well's stagnation point (x_s,y_s). Note that, we can similarly track a well catchment in the y-direction assuming a uniformly spaced grid with a step Δy, such that:

$$x^{i+1} = x^i + \frac{u_x^i}{u_y^i}\Delta y \tag{3}$$

In practise, applications (2) and (3) are used interchangeably to avoid very small values of u_x^i or u_y^i causing singularities and truncation errors.

First-order Taylor's series approximation

The first-order Taylor's series approximation (Dettinger & Wilson, 1981) is an approach used to propagate uncertainties in model parameters (independent variables) to its state (dependent) variables. Using (1), **s** can be stated as a function of ρ, **s**(ρ), such that its Taylor's series expansion is given by:

$$\mathbf{s}(\rho) = \mathbf{s}(\bar{\rho}) + \frac{d\mathbf{s}(\bar{\rho})}{d\rho} + \frac{1}{2}\frac{d^2\mathbf{s}(\bar{\rho})}{d\rho^2}(\rho - \bar{\rho})^2 + \cdots \tag{4}$$

where $\bar{\rho}$ is a vector of the mean values of ρ. Taking the expected value of (4) and ignoring the second and higher-order terms, leads to the following expression:

$$E[\mathbf{s}(\rho)] = \bar{\mathbf{s}}(\rho) = \mathbf{s}(\bar{\rho}); \qquad E[\rho - \bar{\rho}] = 0 \tag{5}$$

which is a typical linearized solution. The covariance of **s**, $\mathbf{C}_s$, is obtained by a similar procedure as:

$$\mathbf{C}_s = \frac{ds(\bar{\rho})}{d\rho}\mathbf{C}_\rho\left(\frac{ds(\bar{\rho})}{d\rho}\right)^T \tag{6}$$

No assumption have been made about the statistical properties of ρ. It is also clear from (6) that the main computational task in calculating the state variable covariance is the calculation of the sensitivity coefficients of **s** with respect to ρ.

Stochastic capture zone design using first-order Taylor's series approximation

In this study we use back tracking from the well stagnation point to determine the effects of uncertainty on well catchment. The mean and variance of the catchment boundary location can be estimated by applying the Taylor's series approximations, (5) and (6), to the forward model (equations (1) to (3)). In (5) and (6), the state variable **s** denotes well catchment location x^{i+1}, y^{i+1}. In this case the derivatives of y^{i+1}

and x^{i+1} are obtained by differentiating (2) and (3) with respect to ρ, such that:

$$\frac{dy^{i+1}}{d\boldsymbol{\rho}} = \frac{dy^{i}}{d\boldsymbol{\rho}} + \left(\frac{du_y^i}{d\boldsymbol{\rho}} \frac{1}{u_x^i} - \frac{du_x^i}{d\boldsymbol{\rho}} \frac{u_y^i}{\left(u_x^i\right)^2} \right) \Delta x \tag{7}$$

and:

$$\frac{dx^{i+1}}{d\boldsymbol{\rho}} = \frac{dx^{i}}{d\boldsymbol{\rho}} + \left(\frac{du_x^i}{d\boldsymbol{\rho}} \frac{1}{u_y^i} - \frac{du_y^i}{d\boldsymbol{\rho}} \frac{u_x^i}{\left(u_y^i\right)^2} \right) \Delta y \tag{8}$$

Derivatives of u_x^i are given by:

$$\frac{du_x^i}{d\boldsymbol{\rho}} = \frac{\partial u_x^i}{\partial \boldsymbol{\rho}} + \frac{\partial u_x^i}{\partial x^i} \frac{\partial x^i}{\partial \boldsymbol{\rho}} + \frac{\partial u_x^i}{\partial y^i} \frac{\partial y^i}{\partial \boldsymbol{\rho}} \tag{9}$$

The derivative of u_y^i with respect to ρ can be obtained in a similar manner.

NUMERICAL EXAMPLE

We will demonstrate our methodology for a synthetic problem. We consider a two-dimensional rectangular domain in a saturated heterogeneous porous material. The flow domain has dimensions of 18 × 8 [L] with a pre-specified head boundary condition at east 10 [L] and west 11.0 [L], and no-flux boundary at the north and south. The domain is uniformly discretized using finite elements of size (Δx_g = 0.2 [L], Δy_g = 0.2 [L]). Effective porosity is assumed to be constant and equal to 0.25 [L^0]. The natural logarithm of the local transmissivity is characterized by its mean, ($\bar{\rho}$) = 0.0 (i.e. the geometric mean of the transmissivity is 1.0 [L^2 T^{-1}]), variance (σ^2) = 0.1, correlation length (λ) = 1.0 [L], and an exponential covariance ($\mathbf{C}_\rho$). A pumping well is located at (x_w = 9 [L], y_w = 4 [L]) with a pumping rate of Q = 5.0 [L^3 T^{-1}]. Figure 1 depicts the problem set-up.

The well catchment is obtained by: (a) tracking in the *y*-direction to estimate the associated catchment variable (x_i) from the stagnation point (x_s, y_s) to the well location

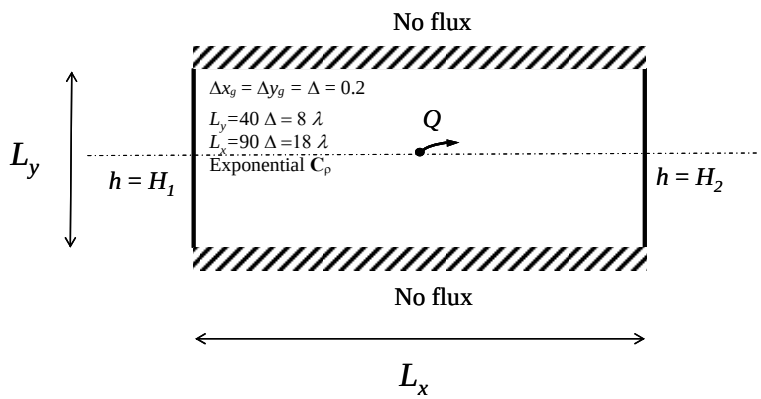

Fig. 1 Problem setup.

x_w, and then (b) tracking in the x-direction until the boundary is reached. Such a procedure reduces the effect of singularities and/or high truncation errors due to small values of u_x^i in the vicinity of the well. A comparison between the Monte Carlo (MC) and the State-Space First-Order (SSFO) methods to estimate variance of the well catchment in the x- and y-direction shows excellent results. Figure 2 shows the variance of x (left) and y (right) in the y- and x-direction, respectively, as computed by the MC and the SSFO methods. Here, we use 500 MC realizations to obtain the well catchment statistics.

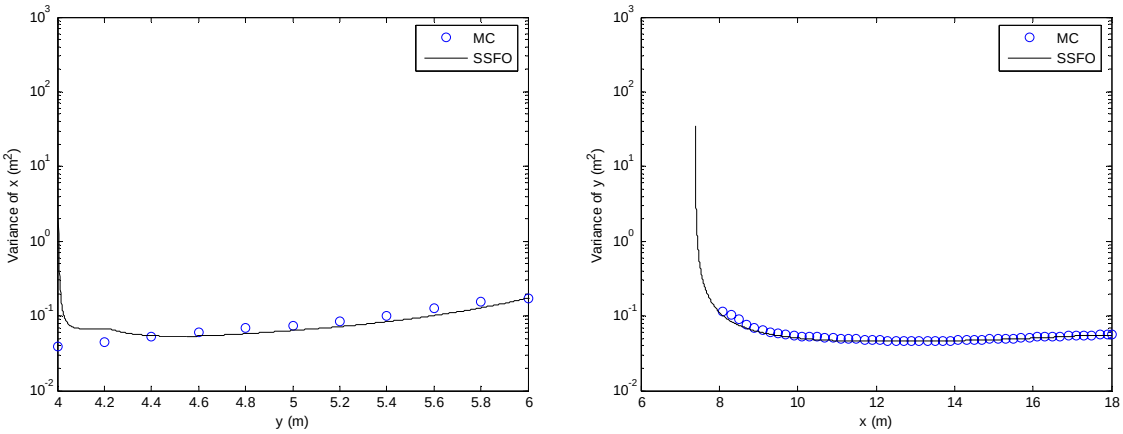

Fig. 2 Variance of x (left) and y (right) in y- and x-direction, respectively.

The SSFO method can then be used to estimate the 95% confidence interval of the well catchment. Figure 3 provides a comparison with the MC method and shows excellent agreement between the two solutions. The curves in Fig. 3 were obtained on the assumption that the well catchment is normally distributed and the confidence interval is obtained by adding and subtracting $1.96\sigma_y$ (or σ_x) to the mean well catchment.

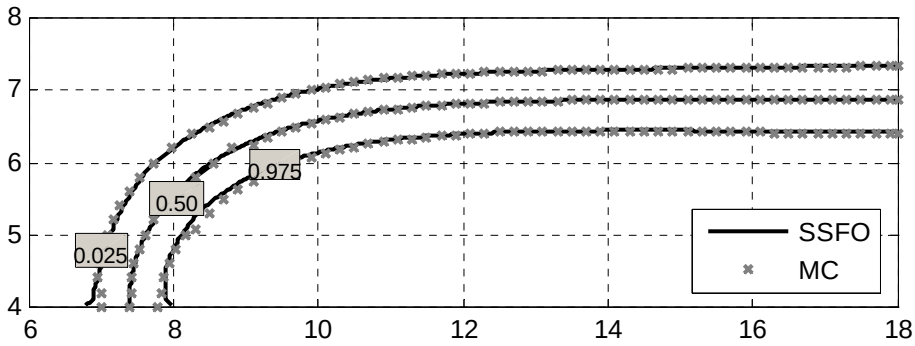

Fig. 3 The 95% confidence interval of the well catchment.

A final point to mention here is the efficiency of the SSFO method as compared to the MC analysis. For the example solved here, the MC analysis required 500 calls to the iterative solver to obtain the head fields, 1000 calls to the iterative solver to obtain the pore water velocities in *x*- and *y*-direction and 500 calls to the tracking routine. Whereas, the SSFO analysis required one forward run that requires one call to the iterative solver for the flow problem and two calls for the solving Darcy's law. It also required 2 × 153 calls to the iterative solver to obtain the sensitivity coefficients of the pore water velocities at 153 nodes with respect to ρ, and just one call to the tracking routine. So, in general, the SSFO method is less CPU demanding than the MC method.

CONCLUSIONS

In this study, the State-Space First-Order (SSFO) method to estimate a well catchment confidence interval is presented and its potential demonstrated via a synthetic example. The main computational demands for the method are in estimating the sensitivity coefficients of the well catchment with respect to the uncertain parameter (i.e. the transmissivity, ρ, in this study). These coefficients, in turn, require the sensitivities of head and pore water velocity with respect ρ to be determined. The method adopts a discrete approach where the governing differential equations are first discretized and then used to estimate sensitivity coefficients by means of the adjoint method. To overcome difficulties related to the singularity at the well stagnation point, we perturb the location of the well stagnation point perpendicular to the natural flow direction (*x*-direction in this study). Also, to overcome truncation errors due to small pore water velocity in the *x*-direction close to the well, we perform tracking along different directions, depending on the current position along the mean catchment within the flow field.

A comparison between the results of the SSFO and the MC methods showed that the two methods produce comparable results either for the simulated mean, variance, or confidence interval of the well catchment. The SSFO method is therefore proposed as an attractive alternative for stochastic well catchment analysis, as it requires less CPU time than the MC method (in this case 16 hours and 26 hours respectively, representing a 40% reduction). Although the example presented here is for an unconditional case, it is expected that CPU time savings for conditional cases will be much higher.

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