Modeling groundwater velocity uncertainty in nonstationary composite porous media

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Received 12 September 2005; received in revised form 13 January 2006; accepted 13 January 2006

Summary Despite the intensive research over the past decades in the field of stochastic subsurface hydrology, our ability to analyze and model heterogeneous groundwater systems remains limited. Most existing theories are either too restrictive to handle practical complexity or too expensive to be applied to realistic problem sizes. In this paper we present approximate, closed-form equations that allow modeling 2D nonstationary flows in statistically inhomogeneous aquifers, including composite aquifers containing multiple zones characterized by different statistical models. The composite representation has the effect of decreasing the variance of deviations from the mean, relaxing the limitation of the small-perturbation assumption. The simple formulas are illustrated with a number of examples and compared with a corresponding first-order nonstationary numerical analysis and Monte Carlo simulation. The results show that, despite the gross simplifications, the closed-form equations are robust and able to capture complex variance dynamics, reproducing surprisingly well the first-order numerical solutions and the Monte Carlo simulation even in highly nonstationary, variable situations.

KEYWORDS Stochastic modeling; Spectral method; Perturbation method; Heterogeneity; Uncertainty modeling; Composite porous media; Monte Carlo simulation

1. Introduction Probabilistic theories of subsurface flow and transport have had a significant impact on the way we think about uncertainty and heterogeneity. However, they have not had much impact on the way that predictions are generated and reported in practical groundwater modeling studies [39]. One major reason for this significant gap lies in that most existing stochastic theories require that the aquifer of interest must be statistically homogeneous, the hydraulic gradient statistically uniform, and the deviation from the uniform mean small (e.g., [19,31]).

It is becoming increasingly clear that if stochastic modeling is to become a viable practical tool, it must be made much more general and flexible. Specifically, a stochastic model must be able to easily incorporate site-specific aquifer structure before it can be routinely applied in practice. It must allow modeling flexible zonations, layering, and general trending as most real-world aquifers exhibit not only “random” variability but also systematic “structural” variations and the statistics characterizing aquifer heterogeneity can
vary (e.g., from region to region and layer to layer) in response to systematic changes in the distribution of aquifer materials. The research by Graham and McLaughlin [5], Li and McLaughlin [13], and Neuman and Orr [20] represents first steps in this direction. Loaiciga et al. [16], Gelhar [4], Li and McLaughlin [14], Rubin [25], Indelman and Rubin [9], Indelman and Zlotnik [10], and Ni and Li [21] later investigated flows in heterogeneous trending media and presented explicit, analytical solutions in illustration of the effect of nonstationarity. More recently, Winter and Tartakovsky [32], Lu and Zhang [17], Rubin [26], and Guadagnini et al. [7] derived closed-form solutions in flow in special composite media that consist of multiple zones with nonstationary fluctuation statistics. These illustrative solutions provided useful insight into how large-scale nonuniformity and zonations interact with small-scale heterogeneity, although they must be generalized before they can actually be used in practice.

There are a number of numerical approaches that can be used to analyze statistically nonuniform flow and transport in more general, statistically inhomogeneous aquifers. These include, for example, Monte Carlo methods (e.g., [28,29,20,15]) and perturbation techniques, such as the moment equation methods (e.g., [5,38,33,17,34,37]) and the so-called first-order second-moment methods based on Taylor’s expansions (e.g., [30,35,2]). All of these methods, however, are computationally demanding when applied to flow and transport problems of realistic size, mostly because they all require solving large numbers of partial differential equations on very fine spatial discretizations in order to predict the impact of the small-scale heterogeneous dynamics (e.g., [5,4,11,12]).

In this paper we present a general, approximate methodology for modeling two-dimensional groundwater systems in complex, composite media. In particular, we apply the popular spectral technique [4] to derive a set of closed-form formulas for predicting nonstationary velocity variances in aquifers that consist of complex zones characterized by different statistical models. These formulas provide nonstationary predictive capabilities of a stochastic numerical model while retaining the convenience of analytical solutions. We demonstrate the effectiveness of the simple closed-form formulas using a number of examples involving complex material zonations and nonstationary conductivity statistics.

2. Problem formulation

We can make our presentation and discussion more specific by considering a relatively simple problem: steady-state simulation of hydraulic heads and groundwater velocities in a saturated region. Here we assume that the region is composed of multiple subregions containing systematically different materials characterized by different statistical models. We further assume that fluctuation in each subregion is locally isotropic and statistically uniform but their statistics can vary from region to region and the means trends vary more smoothly than the fluctuations. In practice, the trend can be estimated from a sample conductivity function by applying a low-pass or moving window filter [24].

Model-based groundwater velocity predictions form the basis for travel time, capture zone, wellhead protection, and solute transport analyses. Uncertainties in these velocities can be substantial if the hydraulic conductivity is heterogeneous, even when the piezometric head is smooth. In practical groundwater modeling applications it is important to have some feeling for the magnitude of velocity uncertainty.

The random log conductivity fluctuation is approximately related to the fluctuations in piezometric head and Darcy velocity by the following first-order, mean-removed flow equations:

\[
\frac{\partial^2 h^i}{\partial x_i \partial x_j} + \mu_i(x) \frac{\partial h^i}{\partial x_i} = J_i(x) \frac{\partial f}{\partial x_i}, \quad x \in D, \tag{1}
\]

\[
u_i' = K_i(x) \left[ J_i(x) f - \frac{\partial h^i}{\partial x_i} \right] \quad x \in D, \tag{2}
\]

where \(J_i(x) = -\partial h^i/\partial x_i\) is the deterministic mean head gradient, \(\mu_i(x) = \partial f/\partial x_i\) is the mean log conductivity gradient, and \(K_i(x)\) is the geometric mean conductivity. Both \(\mu_i, K_i\) are in general spatially variable and may be discontinuous across internal subregion boundaries. These equations are written in Cartesian coordinates, with the vector location symbolized by \(x\) and summation implied over repeated indices. The point values of the log hydraulic conductivity fluctuation \(f(x)\), head fluctuation \(h(x)\), and Darcy velocity fluctuation \(u_i(x), i = 1, 2, 3\), are defined throughout the domain \(D\). A homogeneous condition is defined on the specified head boundary \(\Gamma_D\) and the specified flux boundary \(\Gamma_N\). Note that we consider \(f\) is solely the source of uncertainty applied in the aquifer system and is locally (within an individual subregion) stationary and globally (across different regions) nonstationary.

3. Spectral solution in composite media

Spectral methods offer a particularly convenient way to derive groundwater velocity statistics from linearized fluctuation equations such as (1) and (2) [1,4,13–15,11,12]. Invoking the spectral representation in each subregion for the locally stationary log conductivity perturbation gives

\[
f'(x) = \int_{-\infty}^{\infty} \exp(i k x) dZ_l(k, x), \tag{3}
\]

where \(i = (-1)^{1/2}\), \(k_i\) is component \(i\) of the wave number \(k\), and \(dZ_l(k, x)\) is the random Fourier increment of \(f'(x)\), evaluated at \(k\). The \(x\) dependence in the spectral amplitude reflects the fact that it is in general globally nonstationary and can vary from region to region. The Fourier representation can be viewed as the continuous version of a Fourier series expansion of \(f(x)\). The random Fourier increment at a particular wave number is analogous to the random amplitude of one of the terms in the Fourier integral. Stationary Fourier increments within each region satisfy the following orthogonality property [23,4]:

\[
\]
where the asterisk superscript represents the complex conjugate, \(\delta(k)\) is the Dirac delta function, and \(\psi_f(k,x)\) is the spectral density function of the log hydraulic conductivity.

Papoulis [22] shows that the output (e.g., \(h', u'\)) of linear transformations such as (1) and (2) are stationary only if the input (e.g., \(f\)) is stationary and the transformations are spatially invariant. In the problem of interest here, spatial invariance implies that the fluctuations Eqs. (1) and (2) should have constant coefficients with the boundaries sufficiently distant having no effect on velocity fluctuations in the region of interest. Such spatial invariance requirement is clearly not met because, for heterogeneous composite media, the coefficients \(\mu(x)\) and \(J_i(x)\) may both vary with \(x\) (e.g., [5,16,27,20,8,14,32,7]).

Like many investigators [1,18,4], here we seek approximate solutions to (1) and (2). Taking advantage of the scale disparity between the fluctuation process and the mean process, we further assume that the input log-conductivity, the dependent head, and velocity output fluctuation be stationary in a local sense (away from the immediate proximity of boundaries), so that they also have an approximate spectral representation defined in terms of a location-dependent spectral amplitude

\[
h'(x) = \int_{-\infty}^{\infty} \exp(ikx) d\psi_h(k,x);
\]

\[
u'(x) = \int_{-\infty}^{\infty} \exp(ikx) d\psi_u(k,x),
\]

This local homogeneity assumption implies that we regard \(\mu(x)\) and \(J_i(x)\) in (1) and (2) as varying slowly in space relative to the characteristic scale of the fluctuation, that is, that they do not change significantly over distance corresponding to the correlation scale of \(h\). Note that \(\mu_i^{-1}\) will be a typical length scale for change in the mean gradient, so that the notion of local statistical homogeneity will be meaningful when the product of \(\mu_i\) and the correlation scale is small relative to 1 [4]. By using the local spectral representations (5) in (1), the spectral amplitude for head in two-dimensional problems is

\[
d\psi_h(k,x) = -\frac{-1}{k^2 - ik_0} d\psi_f(k,x), \quad k_0 = k_x^1 + k_y^2.
\]

Substituting (5) and (6) in (2), we obtain the following spectral amplitude of Darcy velocity:

\[
d\psi_u(k,x) = K_g(x) J_i(x) \left( \delta_{ij} - \frac{k_j k_i}{k^2 - ik_k \mu_j(x)} \right) d\psi_f(k,x),
\]

where \(\delta_{ij}\) is the Kronecker delta function. Now, if the \(x_1\) coordinate is selected to be aligned with the local mean hydraulic gradient \((J_i(x) = J(x), J_1(x) = 0)\), then the velocity spectral density functions in each material zone becomes

\[
\psi_{s_u}(k,x) = K_g^2(x) J_i^2(x) \left( \frac{1}{k^2 - ik_0 \mu_j(x)} \right) \left( \frac{1}{k^2 + ik_0 \mu_j(x)} \right) \psi_f(k,x).
\]

Integrating in the wave number domain, one obtains the following integral expression for evaluating the velocity variance:

\[
\sigma_u^2(x) = C_u(\mu) \sigma_v^2(x) \psi_{s_u}(k)^2 \psi_f(k,x),
\]

where

\[
C_u(\mu) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left( \frac{1}{k^2 - ik_0 \mu_j(x)} \right) \frac{1}{k^2 + ik_0 \mu_i(x)} \psi_f(k,x) d\psi_f(k,x).
\]

Note \(\psi_f\) is dimensionless spectral density function, \(s_{ff} = \psi_f/\psi_f^2\). The symbols \(\sigma_{u_h}^2\) and \(\sigma_{u_v}^2\) represent respectively the longitudinal and transverse velocity variances.

### 3.1. Approximate spectral method

To obtain explicit results, one must in general evaluate the associated double integrals numerically. In most cases, these evaluations can be quite difficult. Most prior research focuses on some very special cases for which (10) can be reduced to a form that allows exact, closed-form integration [3,4,36,26]. In this paper, we evaluate (10) approximately under more general conditions. Our approximate solution is based on the following observations:

- Trends in conductivity influence the variance dynamics through \(C_u(\mu)\) and \(K_g(x)J_i(x)\) (see (9)).
- It is the evaluation of \(C_u\) for a general, multi-dimensional trend distribution \(\mu_i(x)\) that is difficult. More specifically, it is the presence of the \(\mu_i^{-1}\) term in (10) that makes the integration analytically intractable.
- It is, however, predominantly \(K_g(x)J_i(x)\) that controls the nonstationary variance dynamics.
- For most trending situations, change in the mean log conductivity over the characteristic length of small-scale heterogeneity (a correlation scale \(\lambda\)) is small (or \(\mu_i^{-1} \lambda^2 \ll 1\)) since the mean conductivity is expected to be much smoother than the fluctuation [4].

To enable variance modeling under general, complex conditions, we propose approximating \(C_u(\mu)\) via the following Taylor’s expansion-based expression:

\[
C_u(\mu) = C_u(0) + \frac{\partial C_u(0)}{\partial \mu_j} \mu_j + \ldots \approx C_u(0),
\]

Essentially we suggest that the small, but hard-to-evaluate contribution to variance nonstationarity from \(C_u\) be ignored relative to the much more important contribution from \(K_g(x)J_i(x)\). This assumption may seem quite crude but proves to be highly effective and makes general, approximate variance modeling in nonstationary media possible. Previous studies investigating the effects of trending are all based on full integration of (9) and (10) or full solution of (1) that is intractable unless the trends are assumed to be of special forms [9]. These highly restrictive assumptions severely limit the practical utilities of the results.
Substituting (11) into (9), we obtain

\[
\sigma_{u_i}^2(x) = \sigma_j^2(x) K_i^2(x) J_i^2(x) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left( 1 - \frac{k_i k_j}{k^2} \right) \psi_i(k, x) \, dk_1 \, dk_2. \tag{12}
\]

Eq. (12) can be easily integrated in the polar coordinate system. For the statistically isotropic case, the result is the following simple, explicit expressions, independent of the specific form of the \( \ln K \) spectrum:

\[
\sigma_{u_i}^2(x) = 0.375 \sigma_j^2(x) K_i^2(x) J_i^2(x), \tag{13}
\]

\[
\sigma_{u_i}^2(x) = 0.125 \sigma_j^2(x) K_i^2(x) J_i^2(x). \tag{14}
\]

Note these expressions are of the same form as those derived by many previous researchers (e.g., [3, 4, 6, 7]) for statistically uniform flow, except that \( K_i \) and \( J_i \) are now allowed to vary over space as a function of the trending and correlation scale.

To systematically test the effectiveness, robustness, and generality of the closed-form solutions, we consider a range of nonstationary, composite media configurations, and use different statistical models to represent the small-scale heterogeneity. Our first example considers a relatively simple situation in which the overall domain of interest contains two embedded, rectangular areas of distinctly different materials. Our second example is patterned after a real situation involving more complex zonations of irregular shapes delineated based on a map of surficial deposits. Our third example considers fan-shaped deposits of water-transported material (alluvium) that forms at the base of fractured mountain blocks where there is a marked break in slope. The alluvial fan is coarse-grained and very permeable at the mouth and becomes gradually finer-grained towards the edge as it meets with a large surface water body.

In all three examples, the overall conductivity distributions are strongly nonstationary both in the mean and fluctuation. The mean conductivity varies within the zones (Example 3) and between them (Examples 1–3) and these large-scale nonstationarities are represented as deterministic trends. The fluctuation statistics in each zone are characterized by an independent statistical model with a zone-dependent variance and correlation scale. It is our opinion that if a methodology is able to predict the groundwater velocity uncertainty in such different composite media configurations, it should be able to handle perhaps most situations that can be realistically represented using field data in real-world groundwater modeling.

Table 1 presents detailed information defining the aquifer parameters, boundary conditions, and other inputs used in the three examples. Figure 1a–c present realizations of the conductivity distributions along the domain center line for Example 1–3, respectively. Figure 2a–c illustrate the distributions of the mean conductivity, prescribed stresses, and corresponding steady-state mean head. The strong trends and irregular zonations in the mean log hydraulic conductivities yield nonuniform flow patterns which in turn cause strong nonstationarity in the velocity variances.

To compute the velocity variances and demonstrate their accuracy, we follow the following three step procedure. First, we solve the mean deterministic groundwater flow equation without accounting for the small-scale heterogeneity. We then use the computed head to evaluate the mean hydraulic gradient and substitute it into (13) and (14) to obtain the local variance values. Finally, we compare the closed-form solutions with the corresponding numerical solutions obtained from the first-order nonstationary spectral method [13,14,11,12] and Monte Carlo simulation (based on 10,000 realizations). The nonstationary spectral method is based on a generalized, nonstationary spectral representation theorem and solves numerically the full version of the linearized perturbation equation. Without having to make the “local stationarity” assumption and dropping the secondary terms (in the head perturbation equation), the nonstationary spectral approach allows accommodating exactly boundary conditions, spatially variable mean gradients, and other sources of nonstationarity [13–15,11,12].

### Table 1 Parameter definitions for three examples

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Example 1</th>
<th>Example 2</th>
<th>Example 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\ln K) correlation structure</td>
<td>Exponential/hole</td>
<td>Exponential/hole</td>
<td>Exponential/hole</td>
</tr>
<tr>
<td>(\ln K) variance</td>
<td>0.5, 1.0, and 2.0</td>
<td>0.5, 0.8, 1.0, and 1.5</td>
<td>1.0 and 2.0</td>
</tr>
<tr>
<td>(\ln K) correlation scale (\xi) (m)</td>
<td>0.5, 1.0, and 2.0</td>
<td>0.5, 0.8, 1.0, and 1.5</td>
<td>5.0 and 10.0</td>
</tr>
<tr>
<td>Mean conductivity (K_g) (m/day)</td>
<td>5, 25, and 125</td>
<td>5, 25, 50, and 100</td>
<td>2.0 and kriged field</td>
</tr>
<tr>
<td>Domain length (m)</td>
<td>80 \times 80</td>
<td>160 \times 160</td>
<td>2000 \times 1500</td>
</tr>
<tr>
<td>Grid number (ASM and NSM)</td>
<td>81 \times 81</td>
<td>161 \times 161</td>
<td>251 \times 186</td>
</tr>
<tr>
<td>Grid number (MCS)</td>
<td>256 \times 256</td>
<td>512 \times 512</td>
<td>1024 \times 768</td>
</tr>
<tr>
<td>Global recharge (m/day)</td>
<td>No recharge</td>
<td>No recharge</td>
<td>0.002</td>
</tr>
<tr>
<td>West boundary condition</td>
<td>Const. Head 100 m</td>
<td>Const. Head 100 m</td>
<td>No flow</td>
</tr>
<tr>
<td>East boundary condition</td>
<td>Const. Head 99.2 m</td>
<td>Const. Head 98.4 m</td>
<td>No flow</td>
</tr>
<tr>
<td>North boundary condition</td>
<td>No flow</td>
<td>No flow</td>
<td>No flow</td>
</tr>
<tr>
<td>South boundary condition</td>
<td>No flow</td>
<td>No flow</td>
<td>No flow</td>
</tr>
</tbody>
</table>

ASM: approximate spectral method; NSM: nonstationary spectral method; MCS: Monte Carlo simulation.
5. Results and discussion

Figures 3–5 present the comparative results for all three examples. Figure 3 presents contour maps showing the complex, nonuniform distributions of the predicted velocity standard deviations. The results are obtained using the approximate spectral method (left column), the numerical nonstationary spectral method (middle column), and the Monte Carlo simulation (right column) based on the simple exponential covariance model. Figure 4 shows the same results in a profile along the domain centerline. The results clearly show that, despite the simplifications and the strong multi-dimensional medium nonstationarities, the simple first-order, nonstationary spectral solutions and allow capturing both the spatial structure (see Fig. 3) and the magnitude (see Fig. 4) of the highly nonstationary, complex uncertainty distributions. The closed-form predictions of the velocity uncertainty also match very well with those obtained from the Monte Carlo simulation for three examples.

Figure 5 presents similar comparisons between the closed-form and numerical solutions based on an alternative lnK covariance model—the hole exponential covariance model. Although the hole-type model looks similar to the simple exponential model in the physical space domain, it is very different in the frequency domain at low wave numbers. Gelhar [4] suggested that a hole-exponential model may represent the field data better than the simple exponential model. The results show that the closed-form solutions based on this hole model also match very well for all three examples with the corresponding numerical perturbation and Monte Carlo solutions.
The surprisingly robust performance of the closed-form solutions for various highly nonstationary situations involving different media zonations, mean conductivity distributions, flow and uncertainty patterns, boundary conditions, and conductivity covariance models suggests that the seemingly crude simplifying assumptions and empirical observations made in deriving the analytical formulas are highly effective. These simple assumptions can indeed capture the dominant factors controlling the spatial uncertainty distributions and make it possible to model velocity uncertainty in complex, nonstationary groundwater systems. The closed-form formulas do introduce errors near media interfaces as they make no explicit use of boundary conditions. The solutions become inaccurate near the zone discontinuities, especially at the prescribed head boundaries (see Figs. 3–5). However, these errors are limited to approximately within 2 or 3 log-conductivity correlation scales of the discontinuities. The inaccurate regions are considered localized since for stochastic modeling to apply the domain size must be much larger than the size of heterogeneity. We feel these errors are especially easy to accept considering what we gain from the simplifying assumptions—the enormous flexibility and efficiency in our ability to model complex, composite systems.

It should also be pointed out that our ability to model composite media has the effect of decreasing significantly the variance of deviations from the mean. This is why our first-order solutions match so well with the Monte Carlo simulations even under highly variable conditions. Large-scale changes in log conductivity that increase the variance around a constant mean are now treated as nonstationarities (e.g., trends) since the method does not require that the log conductivity mean be constant. Therefore, the small-perturbation assumption becomes much less limiting an assumption as in other stationarity-based perturbation methods.

The method’s requirement that all uncertainty must ultimately be related to stationary random fluctuations in each medium component (zone) may still seem to be a significant limitation. In reality, this requirement reflects a very important tacit assumption of stochastic groundwater hydrology. To be specific, suppose we wish to know how predicted velocity uncertainty is affected by spatial variations in hydraulic conductivity. A number of probabilistic methods, including the one described here may be used to infer the (possibly nonstationary) ensemble statistics of velocity from the ensemble statistics of hydraulic conductivity. In order to apply any stochastic methods to practical problems, we need to obtain zone specific estimates of the conductivity statistics which form the basis for our stochastic analysis.

In practice, these statistics are typically derived from a limited number of field measurements available in a zone. In
In most situations, the only type of parameter nonstationarity that we can hope to infer from field data is a large-scale trend in the local mean (both within the zones or between them). The closed-form formulas can accommodate such trends since they require that the mean removed parameter within a zone be stationary. This suggests that the method's requirement that uncertainty be related to stationary random parameters within a zone is really not a practical lim-
Figure 3 (continued)

Figure 4 Centerline profile of the predicted velocity standard deviations using the closed-form formulas, numerical spectral method, and Monte Carlo simulation based on the simple exponential covariance model: (a) Example 1, (b) Example 2, (c) Example 3.
We need to do this any way if we want our composite media analysis to rely on data gathered in the field.

6. Conclusions

In this paper we have developed and demonstrated closed-form formulas to predict velocity variances for two-dimensional flow in complex composite media. Three examples were used to illustrate the approximate methodology. The results reveal that, despite the gross simplifications, the analytical expressions are highly effective and robust and reproduce surprisingly well the solutions of corresponding first-order and Monte Carlo predictions. The results also show how the nonuniform log conductivity structure changes significantly the spatial distributions of the velocity variances.

In summary, the approximate spectral method makes it possible to model the velocity uncertainty in complex composite media. The analysis represents a step closer to our ultimate goal to include a systematic uncertainty analysis as a part of routine groundwater modeling. We are currently in the process of extending the approximate methodology to model velocity variances and velocity covariances for general unsteady flow in confined/unconfined and anisotropic aquifers in the presence of a variety of complex sources and sinks (e.g., streams, lakes, recharge, and wells).

References


Figure 5 Centerline profile of the predicted velocity standard deviations using the closed-form formulas, numerical spectral method, and Monte Carlo simulation based on a hole-type covariance model: (a) Example 1, (b) Example 2, (c) Example 3.


