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Technical note: Quantification of flow field variability using intrinsic random function theory

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Abstract. Much of the stochastic analysis of flow field variability in heterogeneous aquifers in the literature assumes that the parameters in the associated stochastic flow equation are weakly (second order) stationary. On this basis, the spectral representation approach can then be used to quantify the variability of the flow fields given known covariance functions of the input parameters. However, the condition of second-order stationarity is rarely encountered in nature and is difficult to verify using the limited experimental data available. The purpose (or novelty) of this work, therefore, is to develop a new framework for modeling the variability of the flow fields that generalizes the stochastic theory that applies to stationary second-order random input parameters to intrinsic (nonstationary) random input parameters. In this work, the log hydraulic conductivity and log aquifer thickness are assumed to be intrinsic random functions for flow through heterogeneous confined aquifers of variable thickness. On this basis, semivariograms of depth-averaged hydraulic head and integrated specific discharge fields are developed to characterize the variability of flow fields. The application of the proposed stochastic theory to the case where the variability of a random input parameter can be characterized by a linear semivariogram model is provided.

1 Introduction

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Much of the literature on solving the stochastic groundwater flow problem assumes that the covariance functions of the random input parameters in the corresponding stochastic differential equation for groundwater flow can be characterized by spatial covariance functions. Based on these known covariance functions of parameters, the variability of flow fields in heterogeneous aquifers can then be represented by the covariances of hydraulic head and specific discharge using the spectral representation approach (e.g., Dagan, 1989; Gelhar, 1993; Zhang, 2002; Rubin, 2003). It is important to recognize that the approach is built on the assumption that the random processes of the input parameters are second order stationary, so they can be represented by a covariance function. The question arises: can the statistics of the flow field be determined if it is not possible to identify the covariance function of the input parameter from the available data or if the covariance functions of the parameter do not exist?

In many practical applications, the experimental variance of a random variable (function) sampled from a field increases with the size of the field (e.g., Desbarats and Bachu, 1994; Molz et al., 2004; Dell'Oca et al., 2020). This means that the data have an almost unlimited scattering capacity and cannot be properly described by ascribing a finite a priori variance to them. This implies that the second-order stationarity hypothesis does not appear to be suitable and that the approach assuming spatial variation of input parameters characterized by a spatial covariance function in the treatment of stochastic models of groundwater flow is not appropriate.

But even if there is no finite a priori variance, the spatial increments of a random function may still have a finite variance. Note that the random function that obeys the intrinsic hypothesis (Matheron, 1965, 1971), i.e., the assumption that the increments of the random function are weakly stationary, is called the intrinsic (nonstationary) random function. In this case, the variability of a nonstationary random function can be characterized by its semivariogram. This implies that it might be possible to determine the characteristics of the random flow fields based on the known semivariogram of the random input parameter from the field data for the case of a nonstationary process of the input parameter. It is clear that the intrinsic hypothesis is weaker than the second-order stationarity hypothesis.

According to Yaglom (1987) and Christakos (1992), an intrinsic function and its semivariogram admit a spectral representation. From these spectral representations, the associated stochastic groundwater flow equation can be solved in the wavenumber domain. Therefore, a spectral relationship between the wavenumber spectra of the input parameter fluctuations and the spectra of the output fluctuations can be obtained based on the solution of the stochastic

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equation. This means that, given intrinsic semivariograms of the input parameters, the variability of the flow fields can be characterized by the semivariograms of the hydraulic head and the specific discharge fields using the spectral representation approach. In other words, it is possible to establish stochastic theories to characterize the variability of the flow fields without considering the hypothesis of second-order stationarity for the random input parameters, which is the goal of this study.

This work develops a general stochastic framework for quantifying the variability of flow fields by semivariograms of depth-averaged hydraulic head and integrated specific discharge for essentially horizontal steady groundwater flow through a heterogeneous confined aquifer of variable thickness. It is assumed that the random input parameters appearing in the associated stochastic differential equation, such as the log hydraulic conductivity and the log thickness of the confined aquifer, are intrinsic random functions and therefore nonstationarity in the depth-averaged head and integrated discharge. This work shows how to develop a stochastic modeling framework for quantifying the variability of the flow fields given semivariograms of the random input parameters, which, to our knowledge, has not been presented in the literature before. An application of the proposed stochastic theories to the case where the variability of a random input parameter can be characterized by a linear

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semivariogram model is given.

2 Statement of the problem

In many practical situations, a variable measured on small samples over very short distances may exhibit very large variations over those distances. To get around this phenomenon, a variable is often measured as an average over a given volume or area rather than at a point. This means that in reality the field data are never collected at a single point, but always include support with finite dimensions, so that the semivariogram over the sample support can no longer be considered a point semivariogram (the theoretical semivariogram). Note that the theoretical semivariogram $\gamma(\boldsymbol{h})$ defined at point $\boldsymbol{x}$ associated with a pointwise support can be defined as

$$\gamma(\xi)=\frac{1}{2}Var[Z(\boldsymbol{x}+\xi)-Z(\boldsymbol{x})], \tag{1}$$

In Eq. (1), $Z(\boldsymbol{x})$ is a random function.

It can be shown that the semivariogram of an intrinsic random function within a volume $\mathcal{V}$ is related to the point-theoretical semivariogram by the formula (e.g., Matheron, 1971; Journel and Huijbregts, 1978):

$$\gamma_{\mathcal{V}}(\xi)=\frac{1}{\mathcal{V}^2}\int_{\mathcal{V}}d\boldsymbol{x}\int_{\mathcal{V}}\gamma(\xi+\boldsymbol{x}-\boldsymbol{x}')d\boldsymbol{x}'-\frac{1}{\mathcal{V}^2}\int_{\mathcal{V}}d\boldsymbol{x}\int_{\mathcal{V}}\gamma(\boldsymbol{x}-\boldsymbol{x}')d\boldsymbol{x}', \tag{2}$$

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where $\gamma_{\forall}(\boldsymbol{x})$ is the transformed semivariogram and $\gamma(\boldsymbol{x})$ is the theoretical semivariogram defined in Eq. (1). Matheron (1971) points out that Eq. (2) holds for any intrinsic random function, even if the covariance function does not exist.

This work presents a stochastic analysis of flow through heterogeneous confined aquifers of variable thickness (see Appendix A). The variability of the flow results from the variation of the random input parameters, such as the log hudraulic conductivity and the log thickness of the confined aquifer. In this work, the log conductivity and log aquifer thickness are considered as spatially intrinsic random functions whose semivariogram can be represented by Eq. (2). In addition, the variation of depth-averaged hydraulic head and integrated specific discharge can be described by the perturbation equations (A3) and (A4), respectively. The spectral representation approach is used to develop the semivariograms of depth-averaged hydraulic head and vertically integrated specific discharge to quantify the variability of the flow fields.

3 Theoretical developments of semivariograms of flow fields

Given the assumption that f and β in Eq. (A3) satisfy the intrinsic hypothesis, the intrinsic random functions f and β each admit a spectral representation of the form (Yaglom, 1987;

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Christakos, 1992),

$$f(x_1,x_2)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\exp[i(w_1x_1+w_2x_2)]-1}{i\sqrt{w_1^2+w_2^2}}dZ_{Sf}(w_1,w_2)\,, \tag{3a}$$

$$\beta(x_1,x_2)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\exp[i(w_1x_1+w_2x_2)]-1}{i\sqrt{w_1^2+w_2^2}}dZ_{S\beta}(w_1,w_2)\,, \tag{3b}$$

where the w_i are the components of the wavenumber vector $\boldsymbol{w}$ (= (w_1,w_2)) and $Sf(w_1,w_2)$ and $S\beta(w_1,w_2)$ are stationary spatial random processes with uncorrelated complex Fourier increments $dZ_{Sf}(w_1,w_2)$ and $dZ_{S\beta}(w_1,w_2)$, respectively. Due to the property of the linearity of the driving forces in Eq. (A3), the depth-averaged head perturbation can alternatively be decomposed into two parts as

$$h(x_1,x_2)=h_f(x_1,x_2)+h_\beta(x_1,x_2)\,, \tag{4a}$$

where h_f represents the head fluctuation in response to the change in log hydraulic conductivity, while h_β represents the head fluctuation in response to the change in log thickness of the aquifer. Without any restrictions, each component of the depth-averaged head perturbation in Eq. (4a) can be expressed by Fourier-Stieltjes representations (Priestley, 1965) as follows:

$$h_f(x_1,x_2)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Lambda_f(x_1,x_2;w_1,w_2)dZ_{Sf}(w_1,w_2)\,, \tag{4b}$$

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$$h_\beta(x_1,x_2)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Lambda_\beta(x_1,x_2;w_1,w_2)\,dZ_{S\beta}(w_1,w_2)\,. \tag{4c}$$

In Eqs. (4b) and (4c), Λ_f and Λ_β are referred to as oscillatory functions (Priestley, 1965).

Introducing Eqs. (3)-(4) into Eq. (A3), the solution of Eq. (A3) is

$$h_f(x_1,x_2)=J\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{w_1}{(w_1^2+w_2^2)^{3/2}}\left\{1-\exp[i(w_1x_1+w_2x_2)]+i(w_1x_1+w_2x_2)\right\}dZ_{Sf}(w_1,w_2)\,, \tag{5a}$$

$$h_\beta(x_1,x_2)=2J\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{w_1}{(w_1^2+w_2^2)^{3/2}}\left\{1-\exp[i(w_1x_1+w_2x_2)]+i(w_1x_1+w_2x_2)\right\}dZ_{S\beta}(w_1,w_2)\,. \tag{5b}$$

That is,

$$h(x_1,x_2)=J\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{w_1}{(w_1^2+w_2^2)^{3/2}}\left\{1-\exp[i(w_1x_1+w_2x_2)]+i(w_1x_1+w_2x_2)\right\}dZ_{Sf}(w_1,w_2)$$

$$+2J\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{w_1}{(w_1^2+w_2^2)^{3/2}}\left\{1-\exp[i(w_1x_1+w_2x_2)]+i(w_1x_1+w_2x_2)\right\}dZ_{S\beta}(w_1,w_2)\,. \tag{5c}$$

The details of the development of this solution are given in Appendix B.

Furthermore, making use of the spectral representation Eq. (3) and Eq. (5) in Eq. (A4), the perturbation for the integrated specific discharge in the direction of x_1 (mean flow) is given by

$$q_1(x_1,x_2)=q_{f_1}(x_1,x_2)+q_{\beta_1}(x_1,x_2)\,, \tag{6a}$$

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where

$$q_{f_1}(x_1,x_2)=e^{F+B}J\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\exp[i(w_1x_1+w_2x_2)]-1}{i\sqrt{w_1^2+w_2^2}}\left(1-\frac{w_1^2}{w^2}\right)dZ_{Sf}(w_1,w_2)\,, \tag{6b}$$

$$q_{\beta_1}(x_1,x_2)=e^{F+B}J\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\exp[i(w_1x_1+w_2x_2)]-1}{i\sqrt{w_1^2+w_2^2}}\left(1-2\frac{w_1^2}{w^2}\right)dZ_{S\beta}(w_1,w_2)\,. \tag{6c}$$

The semivariograms of depth-averaged head can now be calculated using Eq. (5) in Eq. (1)

$$\gamma_h(\boldsymbol{x},\boldsymbol{y})=\gamma_{h_f}(\boldsymbol{x},\boldsymbol{y})+\gamma_{h_\beta}(\boldsymbol{x},\boldsymbol{y})\,, \tag{7a}$$

where $\boldsymbol{x}=(x_1,x_2)$, $\boldsymbol{y}=(y_1,y_2)$, and

$$\gamma_{h_f}(\boldsymbol{x},\boldsymbol{y})=\Xi_1(\boldsymbol{x}-\boldsymbol{y})+r_1\Xi_2(\boldsymbol{x},\boldsymbol{y})+r_2\Xi_3(\boldsymbol{x},\boldsymbol{y})\,, \tag{7b}$$

$$\gamma_{h_\beta}(\boldsymbol{x},\boldsymbol{y})=4\left[\Omega_1(\boldsymbol{x}-\boldsymbol{y})+r_1\Omega_2(\boldsymbol{x},\boldsymbol{y})+r_2\Omega_3(\boldsymbol{x},\boldsymbol{y})\right], \tag{7c}$$

$r_1 = x_1$-y_1, $r_2 = x_2$-y_2. The expressions for Ξ_1-Ξ_3 and Ω_1-Ω_3 in Eq. (7) are given in the Appendix C. Note that the random process of the spectral representation according to Eq. (5) and the semivariogram according to Eq. (7) is called an intrinsic random function of order 1 (Matheron, 1973).

Similarly, the application of Eq. (6) in Eq. (1) yields the semivariogram of the integrated specific discharge in the mean flow direction of the form

$$\gamma_q(\boldsymbol{x},\boldsymbol{y})=\gamma_{q_f}(\boldsymbol{x}-\boldsymbol{y})+\gamma_{q_\beta}(\boldsymbol{x}-\boldsymbol{y})\,, \tag{8a}$$

where

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$$\gamma_{q_f}(\boldsymbol{x}-\boldsymbol{y}) = e^{2(F+B)} J \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{1-\cos(w_1 r_1)\cos(w_2 r_2)}{w_1^2+w_2^2}\left(1-\frac{w_1^2}{w_1^2+w_2^2}\right)^2 S_{Sf}(w_1,w_2)\,dw_1 dw_2\,, \quad (8b)$$

$$\gamma_{q_\beta}(\boldsymbol{x}-\boldsymbol{y}) = e^{2(F+B)} J \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{1-\cos(w_1 r_1)\cos(w_2 r_2)}{w_1^2+w_2^2}\left(1-2\frac{w_1^2}{w_1^2+w_2^2}\right)^2 S_{S\beta}(w_1,w_2)\,dw_1 dw_2\,. \quad (8c)$$

From Eqs. (6) and (8), it can be seen that the random process for the integrated discharge in the mean flow direction is an intrinsic random process (or an intrinsic random function of order 0, Matheron, 1973).

To evaluate Eqs. (7) and (8), which are used to quantify the variability of flow fields, the spectral density functions S_{Sf} and $S_{S\beta}$ must be determined. It can be shown that when the intrinsic random function has a spectral representation as in Eq. (3), the semivariograms of the intrinsic functions f and β are related to the covariance functions of the stationary processes Sf and $S\beta$ by

$$\frac{\partial^2}{\partial r_1^2}\gamma_f(\boldsymbol{x}-\boldsymbol{y}) + \frac{\partial^2}{\partial r_2^2}\gamma_f(\boldsymbol{x}-\boldsymbol{y}) = C_f(\boldsymbol{x}-\boldsymbol{y}), \quad (9a)$$

$$\frac{\partial^2}{\partial r_1^2}\gamma_\beta(\boldsymbol{x}-\boldsymbol{y}) + \frac{\partial^2}{\partial r_2^2}\gamma_\beta(\boldsymbol{x}-\boldsymbol{y}) = C_\beta(\boldsymbol{x}-\boldsymbol{y}), \quad (9b)$$

where γ_f and γ_β are semivariograms of f and β functions, respectively, and C_f and C_β are covariance functions of Sf and $S\beta$ processes, respectively. The spectral density functions of the fluctuations of f and β are then obtained by the inverse Fourier transform of C_f and C_β, respectively, i.e.,

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$$S_{Sf}(w_1, w_2) = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp[w_1\xi_1 + w_2\xi_2] C_f(\xi_1, \xi_2) d\xi_1 d\xi_2 \,, \tag{10a}$$

$$S_{S\beta}(w_1, w_2) = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp[w_1\xi_1 + w_2\xi_2] C_\beta(\xi_1, \xi_2) d\xi_1 d\xi_2 \,. \tag{10b}$$

Equations (7) and (8), together with Eqs. (2), (9), and (10), provide the necessary framework for quantifying the variability of the flow fields. The results can be obtained for specific input parameter models. This line of research will be pursued in the next section.

4 Application

4.1 The linear intrinsic semivariogram

If a volume $\mathcal{V}$ is taken as a straight segment of length L and the point-theoretical semivariogram of an input parameter in Eq. (2) is considered to be described by a linear model (e.g., Journel and Huijbregts, 1978; Bardossy, 1997; Usowicz and Lipiec, 2021), i.e.,

$$\gamma(\xi) = \alpha|\xi| \,, \tag{11}$$

then the transformed semivariogram in Eq. (2) can be written as

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$$\gamma_L(\xi) = \frac{\alpha}{L^2}\int_L dx \int_L \left|\xi + x - x'\right| dx' - \frac{\alpha}{L^2}\int_L dx \int_L \left|x - x'\right| dx' . \tag{12}$$

Note that the semivariogram of a second order stationary random function is necessarily bounded, while the semivariogram of an intrinsic random function is not. The integration of Eq. (12) can be performed using the Cauchy algorithm (e.g., Matheron, 1971)

$$\gamma_L(\xi) = \frac{\alpha}{L^2}\int_{-L}^{L} (L - |x|)\left|\xi + x\right| dx - \frac{\alpha}{L^2}\int_{-L}^{L} (L - |x|)\left|x\right| dx$$

$$= \alpha\left(|\xi| - \frac{L}{3}\right) \qquad |\xi| \geq L. \tag{13}$$

The details of this development are given in Appendix D. This result agrees with that of Journel and Huijbregts (1978) obtained by a different integrating approach. Note that γ_L in Eq. (13) reaches -L/3 when ξ approaches zero, and that this negative value is called the "pseudo-negative nugget effect" (Journel and Huijbregts, 1978) due to regularization.

In this study, it is assumed that the variograms of the input parameters depend only on the magnitude of the distance between the two points and not on its direction. The spatial variability of the input parameters (such as the log conductivity and log thickness of the aquifer) can be characterized by the following semivariograms

$$\gamma_{L_f}(\xi_1, \xi_2) = \alpha_f\left(|\xi| - \frac{L}{3}\right) \qquad |\xi| \geq L, \tag{14a}$$

$$\gamma_{L_\beta}(\xi_1, \xi_2) = \alpha_\beta\left(|\xi| - \frac{L}{3}\right) \qquad |\xi| \geq L, \tag{14b}$$

which represent the extension of Eq. (13) to two dimensions. In Eq. (14), $|\xi|$ =

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$(\xi_1^2+\xi_2^2)^{1/2}$.

The covariance functions of Sf and $S\beta$ processes are determined from substituting Eq. (14) into Eq. (9), respectively,

$$C_f(\xi_1,\xi_2)=\frac{\partial^2}{\partial\xi_1^2}\gamma_{L_f}(\xi_1,\xi_2)+\frac{\partial^2}{\partial\xi_2^2}\gamma_{L_f}(\xi_1,\xi_2)=\frac{\alpha_f}{\sqrt{\xi_1^2+\xi_2^2}}, \tag{15a}$$

$$C_\beta(\xi_1,\xi_2)=\frac{\partial^2}{\partial\xi_1^2}\gamma_{L_\beta}(\xi_1,\xi_2)+\frac{\partial^2}{\partial\xi_2^2}\gamma_{L_\beta}(\xi_1,\xi_2)=\frac{\alpha_\beta}{\sqrt{\xi_1^2+\xi_2^2}}. \tag{15b}$$

From Eqs. (10) and (15), the corresponding spectral density functions of f and β are obtained, respectively, as follows:

$$S_{Sf}(w_1,w_2)=\frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\exp[w_1\xi_1+w_2\xi_2]\frac{\alpha_f}{\sqrt{\xi_1^2+\xi_2^2}}d\xi_1 d\xi_2=\frac{\alpha_f}{2\pi}\frac{1}{\sqrt{w_1^2+w_2^2}}, \tag{16a}$$

$$S_{S\beta}(w_1,w_2)=\frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\exp[w_1\xi_1+w_2\xi_2]\frac{\alpha_\beta}{\sqrt{\xi_1^2+\xi_2^2}}d\xi_1 d\xi_2=\frac{\alpha_\beta}{2\pi}\frac{1}{\sqrt{w_1^2+w_2^2}}. \tag{16b}$$

The semivariogram of depth-averaged hydraulic head used to quantify the variability of the head field can then be obtained by substituting Eq. (16) into Eq. (7) and integrating over the wavenumber range. Note that the first term on the right-hand side of Eq. (7b) or Eq. (7c), $\Xi_1(\boldsymbol{x}\text{-}\boldsymbol{y})$ or $4\Omega_1(\boldsymbol{x}\text{-}\boldsymbol{y})$, is called the generalized covariance function by Matheron (1973). Figure 1 shows the numerical integration result for the generalized covariance function of depth-averaged hydraulic head Ξ_1, i.e., the component of γ_{h_f} that reflects the effect of variation in hydraulic conductivity fields,

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using Eq. (16a) in Eq. (C1). The unbounded increase in the generalized covariance function Ξ_1 with separation distance suggests that there is no finite depth-averaged head variance. This implies that the variation in depth-averaged hydraulic head does not satisfy the second-order stationarity hypothesis. Quantifying the variability in depth-averaged head using the assumption of second-order stationarity for the input parameter can lead to a significant underestimation of head variability for the case of intrinsic random log-conductivity fields. It can also be shown that similar conclusions can be drawn from the term $4\Omega_1(\boldsymbol{x}\text{-}\boldsymbol{y})$ in Eq. (7c), the component of γ_{h_β} reflecting the effect of variation in the log-aquifer thickness fields, for the case of intrinsic random log-aquifer thickness fields.

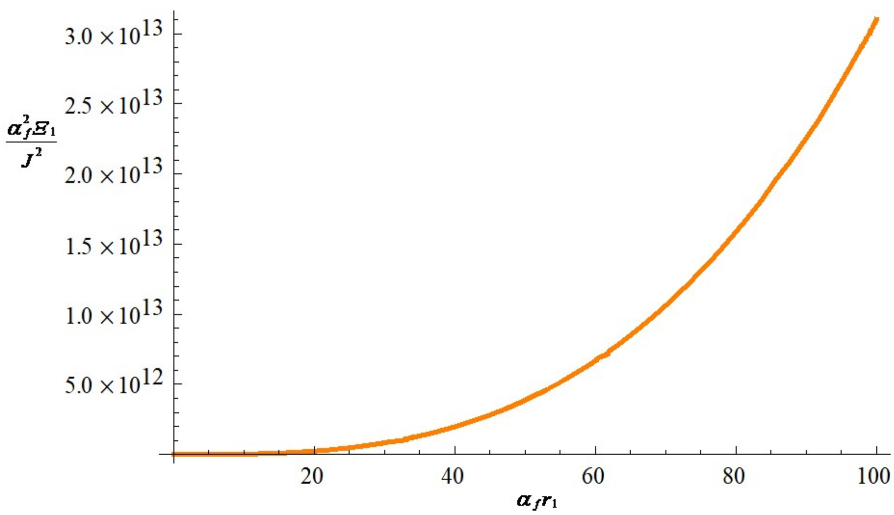

Figure 1. The generalized covariance function of depth-averaged hydraulic head (the component of γ_{h_f} that reflects the effect of variation in the log hydraulic conductivity fields) as a function of separation distance in the mean flow direction, where $r_1 = x_1\text{-}y_1$.

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Figure 2 depicts the behavior of the generalized covariance function Ξ_1 as a function of parameter α_f for a given separation distance r_1. A larger α_f increases the variability of the log conductivity fields, resulting in a larger Ξ_1 and thus a larger semivariogram γ_{h_f}. It can also be shown that the larger the parameter α_β, the larger the variability of the generalized covariance function $4\Omega_1$. It can therefore be concluded that the variability of the depth-averaged hydraulic head caused by the variation of the log hydraulic conductivity and log aquifer thickness is larger for larger parameters α_f and α_β.

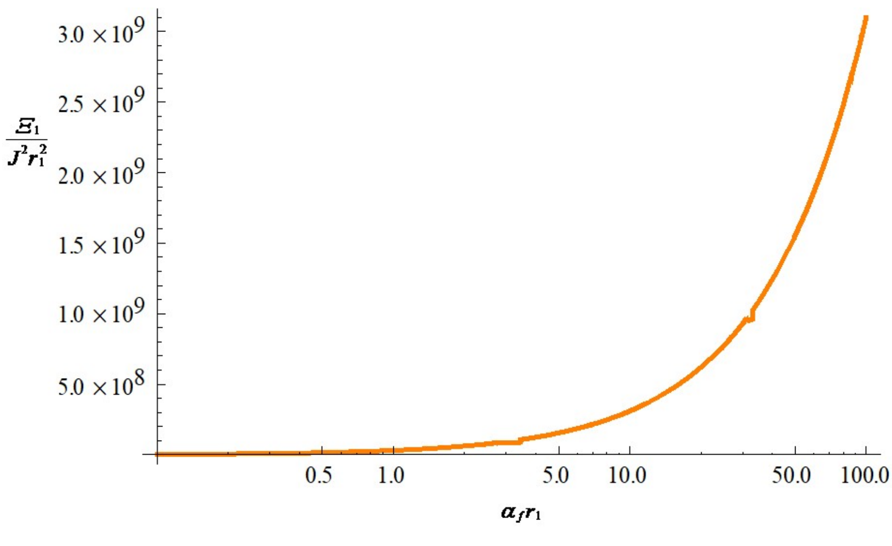

Figure 2. The generalized covariance function of depth-averaged hydraulic head (the component of γ_{h_f} that reflects the effect of variation in the log hydraulic conductivity fields) as a function of parameter α_f in the mean flow direction, where $r_1 = x_1\text{-}y_1$.

The numerical integration results for the components of the semivariogram of the integrated specific discharge in the mean flow direction, γ_{q_f} and $\gamma_{q\,\beta}$, obtained by

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substituting Eq. (16) into Eq. (8), are shown in Figs. (3a) and (3b). The unlimited increase of the integrated discharge semivariogram with the separation distance shown in Fig. 3 indicates that the variation of the integrated discharge process is nonstationary. This is the result of the nonstationary process of the depth-averaged hydraulic head caused by the intrinsic random log-conductivity and log-aquifer thickness fields. The figure also shows that there is an increase in the semivariogram of the integrated specific discharge in the mean flow direction with parameters α_f and α_β for a given separation distance. Larger α_f and α_β cause greater variability in the depth-averaged pressure fields and thus greater variability in the integrated specific discharge fields.

4.2 The exponential semivariogram

It is important to note that the stationary variables always satisfy the intrinsic hypothesis, while the opposite is not always true, since the intrinsic variable can be nonstationary. The stochastic theory developed here to quantify the variability of the flow fields remains valid for any second order stationary random variable. For example, if the point theoretic semivariogram of an input parameter is chosen as

$$\gamma(\xi) = \mu\left(1 - \exp\left[-\frac{|\xi|}{\lambda}\right]\right), \tag{17}$$

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the transformed semivariogram over a segment of length L can then be calculated using Eq. (2) and the Cauchy algorithm (e.g., Matheron, 1971) as follows:

$$\gamma_L(\xi) = \frac{\mu}{L^2}\int_{-L}^{L}(L-|x|)(1-\exp[-\frac{|\xi+x|}{\lambda}])dx - \frac{\mu}{L^2}\int_{-L}^{L}(L-|x|)(1-\exp[-\frac{|x|}{\lambda}])dx\,, \tag{18}$$

This results in

$$\gamma_L(\xi) = \mu\frac{\lambda^2}{L^2}\{2\exp[-\frac{|\xi|}{\lambda}]-\exp[-\frac{|\xi|+L}{\lambda}]-\exp[-\frac{|\xi|-L}{\lambda}]+2(-1+\exp[-\frac{L}{\lambda}]+\frac{L}{\lambda})\} \quad |\xi|\ge L. \tag{19}$$

For the development of Eq. (19), the reader is referred to Appendix E.

Extending Eq. (19) to two dimensions and substituting it into Eq. (9), the covariance functions of the random input parameters (f and β) can then be expressed, respectively, as

$$C_f(\xi_1,\xi_2) = \mu_f\frac{(\exp[\frac{L}{\lambda_f}]-1)^2}{L^2}\frac{\lambda_f-\sqrt{\xi_1^2+\xi_2^2}}{\sqrt{\xi_1^2+\xi_2^2}}\exp[-\frac{\sqrt{\xi_1^2+\xi_2^2}+L}{\lambda_f}], \tag{20a}$$

$$C_\beta(\xi_1,\xi_2) = \mu_\beta\frac{(\exp[\frac{L}{\lambda_\beta}]-1)^2}{L^2}\frac{\lambda_\beta-\sqrt{\xi_1^2+\xi_2^2}}{\sqrt{\xi_1^2+\xi_2^2}}\exp[-\frac{\sqrt{\xi_1^2+\xi_2^2}+L}{\lambda_\beta}]. \tag{20b}$$

Using Eq. (20) in Eq. (10), it follows that the spectral density functions of the fluctuations of f and β each have the form

$$S_{ff}(w_1,w_2) = \frac{\mu_f}{2\pi}\frac{(\exp[\frac{L}{\lambda_f}]-1)^2}{(\frac{L}{\lambda_f})^2}\frac{\lambda_f^2(w_1^2+w_2^2)}{[1+\lambda_f^2(w_1^2+w_2^2)]^2}, \tag{21a}$$

$$S_{\beta\beta}(w_1,w_2) = \frac{\mu_\beta}{2\pi}\frac{(\exp[\frac{L}{\lambda_\beta}]-1)^2}{(\frac{L}{\lambda_\beta})^2}\frac{\lambda_\beta^2(w_1^2+w_2^2)}{[1+\lambda_\beta^2(w_1^2+w_2^2)]^2}. \tag{21b}$$

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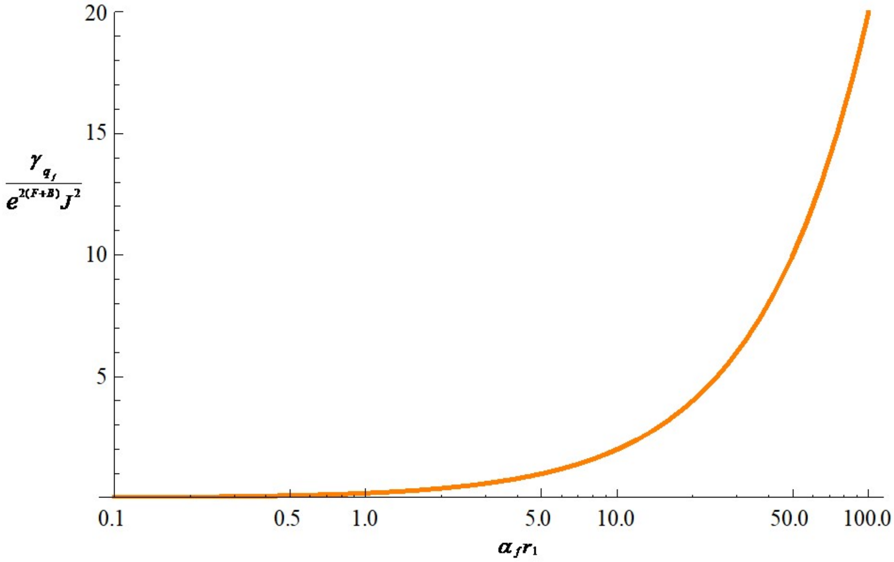
(a)



(b)

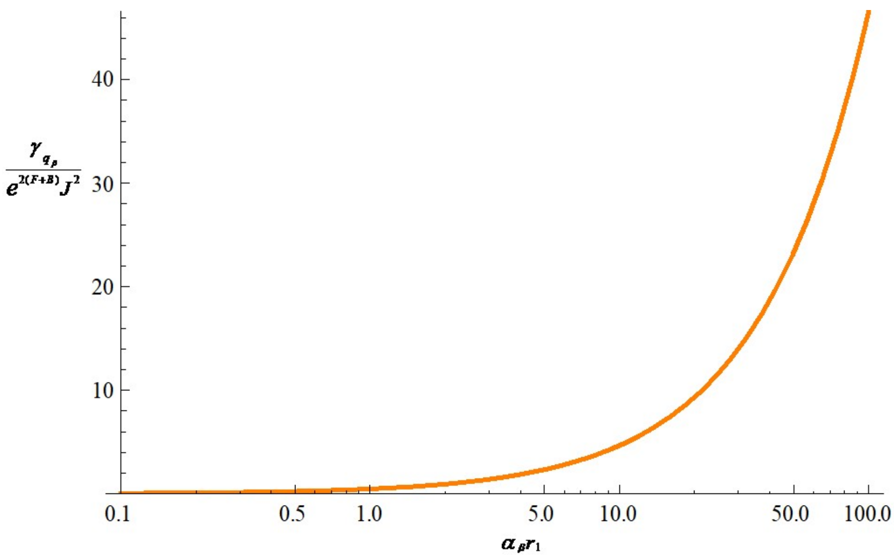


Figure 3. The components of the semivariogram of the integrated specific discharge in the mean flow direction, (a) γ_{q_f}, reflecting the effect of variation in the log hydraulic conductivity fields, and (b) γ_{q_β}, reflecting the effect of variation in the log aquifer thickness fields, as a function of parameters α_f and α_β and separation distance.

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Finally, substituting Eq. (21) into Eqs. (7) and (8), the semivariograms of depth-averaged head and the semivariogram of integrated specific discharge in the mean flow direction can now be evaluated.

The practical advantage of using the general stochastic modeling framework developed here with the intrinsic hypothesis is a wider range of possible semivariogram models compared to the cases with second-order stationarity. The condition of second-order stationarity is rarely encountered in nature (e.g., Wu and Hu, 2004) and is difficult to verify using the limited experimental data available. It is under these conditions that the presented stochastic approach has the greatest utility of quantification of the flow field variability.

5 Conclusions

In this work, a general stochastic methodology is developed for quantifying the variability of flow fields in heterogeneous confined aquifers of variable thickness. The stochastic theories developed here, namely the semivariograms of depth-averaged hydraulic head and integrated specific discharge used to characterize flow field variability, can address the effects of nonstationarity due to variations in parameters and output. The proposed stochastic theories generalize existing stochastic theory, which applies to second order stationary random input parameters, to nonstationary random input parameters. Stationarity in the spatial variation of soil properties is very rarely encountered in nature. The stochastic theories developed here improve the quantification of flow field variability in natural confined aquifers.

The results show that the introduction of intrinsic random input parameters leads to a nonstationary process of depth-averaged hydraulic head fluctuations (an intrinsic random function of order 1) and a nonstationary process of integrated specific discharge fluctuations (an intrinsic random function of order 0). Application of the stochastic theories developed here to the case where the variability of a random input parameter can be characterized by a linear semivariogram model shows that larger parameters α_f and α_β increase the variability of the depth-averaged head and thus the variability of the integrated discharge in the mean flow direction.

Appendix A: A steady flow through a heterogeneous confined aquifer of variable thickness

According to Chang et al. (2021), an essentially horizontal, steady groundwater flow through a heterogeneous confined aquifer of variable thickness can be represented as follows:

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$$\frac{\partial^2}{\partial x_i^2}\tilde{h}(x_1,x_2)+[\frac{\partial}{\partial x_i}\ln K(x_1,x_2)+2\frac{\partial}{\partial x_i}\ln b(x_1,x_2)]\frac{\partial}{\partial x_i}\tilde{h}(x_1,x_2)=0 \qquad i=1,2, \tag{A1}$$

which is the vertically integrated form of the continuity equation. In Eq. (A1), $\tilde{h}(x_1,x_2)$ is the depth-averaged hydraulic head, $K(x_1,x_2)$ is the hydraulic conductivity and $b(x_1,x_2)$ is the aquifer's thickness. From Eq. (A1), it can be seen that the variations in hydraulic conductivity and aquifer thickness that occur affect the depth-averaged hydraulic head. If the log conductivity and log thickness in Eq. (A1) are treated as stochastic (random) variables, Eq. (A1) can be considered as a stochastic partial differential equation with a stochastic output $\tilde{h}$.

Similarly, integrating the equation for specific discharge along the x_3-axis and applying Leibniz's rule leads to the vertically integrated specific discharge in the x_i direction as follows:

$$Q_{x_i}(x_1,x_2)=-K(x_1,x_2)b(x_1,x_2)\frac{\partial}{\partial x_i}\tilde{h}(x_1,x_2) \tag{A2}$$

Under the influence of a uniform mean hydraulic gradient, the perturbation equations for the depth-average hydraulic head and integrated specific discharge associated with Eqs. (A1) and (A2) are given, respectively, by

$$\frac{\partial^2}{\partial x_i^2}h(x_1,x_2)=J[\frac{\partial}{\partial x_1}f(x_1,x_2)+2\frac{\partial}{\partial x_1}\beta(x_1,x_2)] \qquad i=1,2, \tag{A3}$$

$$q_i(x_1,x_2)=e^{F+B}J\{[f(x_1,x_2)+\beta(x_1,x_2)]\delta_{1i}-\frac{\partial}{\partial x_i}h(x_1,x_2)\} \qquad i=1,2. \tag{A4}$$

In Eqs. (A3) and (A4), h and q_i are the fluctuations of depth-average head and integrated discharge, respectively, J is the constant mean hydraulic gradient, F and B

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are the mean log conductivity and mean aquifer thickness, respectively, and f and β are the fluctuations of log conductivity and log aquifer thickness, respectively. A detailed development of Eqs. (A3) and (A4) can be found in Chang et al. (2021).

Appendix B: Derivation of Eq. (5)

Since equation (A3) is linear, it can alternatively be divided into two parts as follows:

$$\frac{\partial^2}{\partial x_1^2} h_f(x_1, x_2) + \frac{\partial^2}{\partial x_2^2} h_f(x_1, x_2) = J \frac{\partial}{\partial x_1} f(x_1, x_2)\,, \tag{B1a}$$

$$\frac{\partial^2}{\partial x_1^2} h_\beta(x_1, x_2) + \frac{\partial^2}{\partial x_2^2} h_\beta(x_1, x_2) = 2J \frac{\partial}{\partial x_1} \beta(x_1, x_2)\,. \tag{B1b}$$

Applying Eqs. (3a) and (4b) into Eq. (B1a), it follows that

$$\frac{\partial^2}{\partial x_1^2} \Lambda_f(x_1, x_2; w_1, w_2) + \frac{\partial^2}{\partial x_2^2} \Lambda_f(x_1, x_2; w_1, w_2) = J \frac{w_1}{\sqrt{w_1^2 + w_2^2}} \exp[i(w_1 x_1 + w_2 x_2)]\,, \tag{B2}$$

which is known as Poisson's equation and has a particular solution in the form

$$\Lambda_f(x_1, x_2; w_1, w_2) = J \frac{w_1}{\sqrt{w_1^2 + w_2^2}} \frac{1 - \exp[i(w_1 x_1 + w_2 x_2)] + i(w_1 x_1 + w_2 x_2)}{w_1^2 + w_2^2}\,. \tag{B3}$$

Similarly, using Eqs. (3b) and (4c), Eq. (B1b) can be written as follows:

$$\frac{\partial^2}{\partial x_1^2} \Lambda_\beta(x_1, x_2; w_1, w_2) + \frac{\partial^2}{\partial x_2^2} \Lambda_\beta(x_1, x_2; w_1, w_2) = 2J \frac{w_1}{\sqrt{w_1^2 + w_2^2}} \exp[i(w_1 x_1 + w_2 x_2)]\,, \tag{B4}$$

and accordingly,

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$$\Lambda_{\beta}(x_1,x_2;w_1,w_2)=2J\frac{w_1}{\sqrt{w_1^2+w_2^2}}\frac{1-\exp[i(w_1x_1+w_2x_2)]+i(w_1x_1+w_2x_2)}{w_1^2+w_2^2}. \tag{B5}$$

Finally, substituting Eqs. (B4) and (B5) into Eq. (4), Eq. (5) is obtained.

Appendix C: Expressions for the functions in Eq. (7)

$$\Xi_1(\boldsymbol{x}-\boldsymbol{y})=J^2\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{w_1^2}{(w_1^2+w_2^2)^3}\left[1-\cos(w_1r_1)\cos(w_2r_2)+\frac{1}{2}(w_1^2r_1^2+w_2^2r_2^2)\right]S_{Sf}(w_1,w_2)dw_1dw_2, \tag{C1}$$

$$\Xi_2(\boldsymbol{x},\boldsymbol{y})=J^2\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{w_1^3}{(w_1^2+w_2^2)^3}\left[-\sin(w_1x_1)\cos(w_2x_2)+\sin(w_1y_1)\cos(w_2y_2)\right]S_{Sf}(w_1,w_2)dw_1dw_2, \tag{C2}$$

$$\Xi_3(\boldsymbol{x},\boldsymbol{y})=J^2\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{w_1^2w_2}{(w_1^2+w_2^2)^3}\left[-\cos(w_1x_1)\sin(w_2x_2)+\cos(w_1y_1)\sin(w_2y_2)\right]S_{Sf}(w_1,w_2)dw_1dw_2, \tag{C3}$$

$$\Omega_1(\boldsymbol{x}-\boldsymbol{y})=J^2\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{w_1^2}{(w_1^2+w_2^2)^3}\left[1-\cos(w_1r_1)\cos(w_2r_2)+\frac{1}{2}(w_1^2r_1^2+w_2^2r_2^2)\right]S_{S\beta}(w_1,w_2)dw_1dw_2, \tag{C4}$$

$$\Omega_2(\boldsymbol{x},\boldsymbol{y})=J^2\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{w_1^3}{(w_1^2+w_2^2)^3}\left[-\sin(w_1x_1)\cos(w_2x_2)+\sin(w_1y_1)\cos(w_2y_2)\right]S_{S\beta}(w_1,w_2)dw_1dw_2, \tag{C5}$$

$$\Omega_3(\boldsymbol{x},\boldsymbol{y})=J^2\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{w_1^2w_2}{(w_1^2+w_2^2)^3}\left[-\cos(w_1x_1)\sin(w_2x_2)+\cos(w_1y_1)\sin(w_2y_2)\right]S_{S\beta}(w_1,w_2)dw_1dw_2, \tag{C6}$$

$r_1 = x_1$-y_1, $r_2 = x_2$-y_2, and S_{Sf} and $S_{S\beta}$ are the spectral density functions of the stationary processes of Sf and $S\beta$, respectively.

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Appendix D: Derivation of Eq. (13)

The condition for Eq. (13) that the absolute value of ξ is greater than or equal to L ($|\xi| \geq L$) means that $\xi \geq L$ or $\xi \leq$ -L. For $\xi \geq L$, the integrand of the integral Eq. (13) can be expressed as

$$\gamma_L(\xi) = \frac{\alpha}{L^2}\int_{-L}^{0}(L+x)(|\xi|+x)dx + \frac{\alpha}{L^2}\int_{0}^{L}(L-x)(|\xi|+x)dx - \frac{\alpha}{L^2}\int_{-L}^{0}(L+|x|)(-x)dx - \frac{\alpha}{L^2}\int_{0}^{L}(L-x)xdx$$

$$= \alpha(|\xi| - \frac{L}{3}). \quad \text{(D1)}$$

For $\xi \leq$ -L, the integrand of the integral Eq. (13) can be expressed as

$$\gamma_L(\xi) = \frac{\alpha}{L^2}\int_{-L}^{0}(L+x)(|\xi|-x)dx + \frac{\alpha}{L^2}\int_{0}^{L}(L-x)(|\xi|-x)dx - \frac{\alpha}{L^2}\int_{-L}^{0}(L+|x|)(-x)dx - \frac{\alpha}{L^2}\int_{0}^{L}(L-x)xdx$$

$$= \alpha(|\xi| - \frac{L}{3}). \quad \text{(D2)}$$

Appendix E: Derivation of Eq. (19)

Analogous to Eq. (13), the integral of Eq. (18) under the condition $|\xi| \geq L$ can be evaluated separately as the integration of Eq. (18) under the condition $\xi \geq L$ and that under the condition $\xi \leq$ -L.

For $\xi \geq L$,

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$$\gamma_L(\xi) = \frac{\mu}{L^2}\int_{-L}^{0}(L+x)(1-\exp[-\frac{|\xi|+x}{\lambda}])dx + \frac{\mu}{L^2}\int_{0}^{L}(L-x)(1-\exp[-\frac{|\xi|+x}{\lambda}])dx$$

$$-\frac{\mu}{L^2}\int_{-L}^{0}(L+x)(1-\exp[\frac{x}{\lambda}])dx - \frac{\mu}{L^2}\int_{0}^{L}(L-x)(1-\exp[-\frac{x}{\lambda}])dx$$

$$=\mu\frac{\lambda^2}{L^2}\{2\exp[-\frac{|\xi|}{\lambda}]-\exp[-\frac{|\xi|+L}{\lambda}]-\exp[-\frac{|\xi|-L}{\lambda}]+2(-1+\exp[-\frac{L}{\lambda}]+\frac{L}{\lambda})\}. \qquad \text{(E1)}$$

For $\xi \le$ -L,

$$\gamma_L(\xi) = \frac{\mu}{L^2}\int_{-L}^{0}(L+x)(1-\exp[-\frac{|\xi|-x}{\lambda}])dx + \frac{\mu}{L^2}\int_{0}^{L}(L-x)(1-\exp[-\frac{|\xi|-x}{\lambda}])dx$$

$$-\frac{\mu}{L^2}\int_{-L}^{0}(L+x)(1-\exp[\frac{x}{\lambda}])dx - \frac{\mu}{L^2}\int_{0}^{L}(L-x)(1-\exp[-\frac{x}{\lambda}])dx$$

$$=\frac{\mu^2}{L^2}\{2\exp[-\frac{|\xi|}{\lambda}]-\exp[-\frac{|\xi|+L}{\lambda}]-\exp[-\frac{|\xi|-L}{\lambda}]+2(-1+\exp[-\frac{L}{\lambda}]+\frac{L}{\lambda})\}. \qquad \text{(E2)}$$

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Author contributions. C-MC: Conceptualization, Methodology, Formal analysis, Writing - original draft preparation, Writing - review & editing.
C-FN: Conceptualization, Methodology, Formal analysis, Writing - original draft preparation, Writing - review & editing, Supervision, Funding acquisition.
C-PL: Conceptualization, Methodology, Formal analysis, Writing - original draft preparation, Writing - review & editing.
I-HL: Conceptualization, Methodology, Formal analysis, Writing - original draft preparation, Writing - review & editing.

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References

Bardossy, A.: Introduction to Geostatistics, Institute of Hydraulic Engineering, University of Stuttgart, 1997.

Chang, C-M, Ni, C-F, Li, W-C, Lin, C-P, and Lee, I-H: Stochastic analysis of the variability of groundwater flow fields in heterogeneous confined aquifers of variable thickness, Stoch. Environ. Res. Risk Assess., https://doi.org/10.1007/s00477-021-02125-7, 2021.

Christakos, G.: Random Field Models in Earth Sciences, Academic, San Diego, 1992.

Dagan, G.: Flow and Transport in Porous Formations, Springer, New York, 1989.

Dell'Oca, A., Guadagnini, A., and Riva, M.: Interpretation of multi-scale permeability data through an information theory perspective, Hydrol. Earth Syst. Sci., 24, 3097-3109, 2020.

https://doi.org/10.5194/hess-2023-161
Preprint. Discussion started: 1 August 2023

Hydrology and Earth System Sciences
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Gelhar, L.W.: Stochastic Subsurface Hydrology, Prentice Hall, Englewood Cliffs, New Jersey.

Journel, A. G. and Huijbregts, C. J.: Mining Geostatistics, Academic Press, New York, 1978.

Matheron, G.: Les variables regionalisees et leur estimation, Masson, Paris, 1965.

Matheron, G.: The theory of regionalized variables and its applications, Les Cahiers du Centre de Morphologie Mathematique in Fontainebleu, Paris, 1971.

Molz, F. J., Rajaram, H., and Lu, S. L.: Stochastic fractal-based models of heterogeneity in subsurface hydrology: Origins, applications, limitations, and future research questions, Rev. Geophys., 42, RG1002, 2004.

Priestley, M. B.: Evolutionary spectra and non-stationary processes, J. R. Stat. Soc. Ser. B., 27(2), 204-237, 1965.

Rubin, Y.: Applied Stochastic Hydrogeology, Oxford University Press, New York, 2003.

Usowicz, B. and Lipiec, J.: Spatial variability of saturated hydraulic conductivity and its links with other soil properties at the regional scale, Sci. Rep., 11, 1-12, 2021.

Wu, J. and Hu, B.: Stochastic study of solute flux in nonstationary flow field conditioning on measured data, Developments in Water Science, 55(1), 705-716, 2004.

https://doi.org/10.5194/hess-2023-161
Preprint. Discussion started: 1 August 2023

Yaglom, A. M.: Correlation Theory of Stationary and Related Random Functions, Vol. I: Basic Results, Springer Series in Statistics, Springer, New York, 1987.

Zhang, D.: Stochastic Methods for Flow in Porous Media: Coping with Uncertainties, Academic Press, San Diego, 2002.