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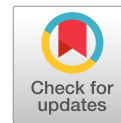
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Probability Density Functions in the Analysis of Hydraulic Conductivity Data

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Abstract: This paper reviews the role of probability density function (PDF) choice on: (1) the statistical characterization of hydraulic conductivity; and (2) the estimation of the local-scale effective hydraulic conductivity. The most widely used skewed PDFs, namely, the lognormal, gamma, and log-gamma PDFs are included in this study. It is shown that the gamma and log-gamma PDFs possess statistical features that render them competitive, if not advantageous, to the more commonly used and better-known lognormal PDF in: (1) the statistical description of hydraulic conductivity; and (2) the estimation of the effective hydraulic conductivity in local-scale groundwater flow. The effective hydraulic conductivity is the parameter relating the average specific discharge to the average hydraulic gradient. Several examples dealing with the statistical analysis of hydraulic conductivity and the estimation of the effective hydraulic conductivity are presented, including a sample of 201 slug-test measurements of hydraulic conductivity in the main clay aquitard underlying Mexico City.

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Introduction and Objectives

Hydraulic conductivity plays a fundamental role in the analysis of groundwater flow. This is best exemplified by the ubiquitous use of Darcy's law in the study of groundwater flow. Hydraulic conductivity was originally introduced as a deterministic, empirical, coefficient relating the groundwater specific discharge and the hydraulic gradient (Darcy 1856). Detailed measurements of hydraulic conductivity have shown that—even in apparently homogeneous formations—it commonly exhibits substantial spatial variability (Vargas and Ortega-Guerrero 2004). That trait renders it suitable for statistical, rather than deterministic, characterization, a fact realized in an early work by Freeze (1975). This realization was quickly followed by the rapid development of the field of stochastic groundwater hydrology (see, in this respect, the works by Bakr et al. 1978; Gutjahr et al. 1978; Gelhar and Axness 1983; Dagan 1989; Gelhar 1993), which enriched our understanding of flow and transport phenomena in porous media alongside with simultaneous advances made in numerical groundwater hydrology (see Willis and Yeh 1987; McDonald and Harbaugh 1988).

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The effective hydraulic conductivity is an important groundwater-flow parameter. This work focuses on effective hydraulic conductivity in local-scale groundwater flow. Groundwater flow is generally of a three-dimensional nature at the local scale. The flow system caused by a partially penetrating well is illustrative of a local-scale disturbance in hydraulic head. Other examples are given in Dagan (1989). Under certain simplifying conditions (see the section "Lognormal Hydraulic Conductivity and its Relation to Effective Hydraulic Conductivity in Small-Perturbations Approach"), the effective hydraulic conductivity is a parameter linking average groundwater specific discharge to average hydraulic gradient, and it has received a fair amount of attention in the stochastic groundwater literature (see Dagan 1989; Loáiciga et al. 1993, 1994, 1996). It is also useful in the calibration of three-dimensional groundwater flow models because it can serve as prior information in Bayesian and other parameter estimation approaches (Yeh 1986; Loáiciga and Marino 1987; Doherty et al. 1999).

This paper investigates the comparative advantages of probability density functions (PDFs) that are widely used in the statistical characterization of local-scale hydraulic conductivity and in the estimation of the effective hydraulic conductivity. The gamma and log-gamma PDFs, specifically, are proposed as sound alternatives to the more commonly used lognormal PDF in the statistical description of the hydraulic conductivity. Moreover, this work includes several examples dealing with the statistical analysis of hydraulic conductivity and the estimation of the effective hydraulic conductivity. One example relies on a sample of 201 slug-test measurements of hydraulic conductivity in the main clay aquitard underlying Mexico City.

Properties of Lognormally Distributed Hydraulic Conductivity

The assumption of lognormal hydraulic conductivity has been widely adopted in stochastic groundwater hydrology. Research by

Freeze (1975) provided early impetus within the groundwater community for using the lognormal PDF as a statistical model to fit hydraulic conductivity data. Over time, the lognormal PDF has been accepted by many groundwater hydrologists as a general tenet for describing hydraulic conductivity data (see e.g., Dagan 1989, p. 160). Attractive features of the lognormal PDF in the modeling of hydraulic conductivity are: (1) it can fit positively skewed data (a common trait of hydraulic conductivity); (2) the parameters of the normally distributed log conductivity [symbolically $Y \sim N(\bar{Y}, \sigma_Y^2)$] are the mean \bar{Y} and the variance σ_Y^2 , which are easily estimable using the standard sample estimators for the mean and variance. Moreover, the quantiles of Y can be obtained straightforwardly from tabulated quantiles of the standard normal PDF $N(0, 1)$ or from ubiquitous statistical software. The lognormal PDF, on the other hand, cannot be used to model either skewed log conductivity—which, by definition of the lognormal PDF must be normally distributed, and, thus, symmetric—or negatively skewed hydraulic conductivity. Although the lognormal PDF allows positive lower bounds on hydraulic conductivity, it does not allow upper bounds on it. In contrast, the gamma PDF (reviewed in the section “Properties of Gamma-Distributed Hydraulic Conductivity”) or its extension, the log-gamma PDF (reviewed in the section “Extensions of Gamma PDF: Log-Gamma Distributed Hydraulic Conductivity”), can accomplish essentially anything that the lognormal PDF can, plus it allows lower or upper bounds on hydraulic conductivity. In addition, the gamma PDF is mathematically more tractable than the lognormal PDF in carrying out calculations of the effective hydraulic conductivity developed with a methodology that circumvents the small-perturbations assumption. The latter assumption requires that the variance of the log-hydraulic conductivity be much less than one (mathematically, $\sigma_Y^2 \ll 1$, in which Y denotes log-hydraulic conductivity; see the section “Lognormal Hydraulic Conductivity and its Relation to Effective Hydraulic Conductivity in Small-Perturbations Approach” for pertinent details).

Lognormal PDF

Let K and θ denote the hydraulic conductivity and its lower bound, respectively, and $Y = \ln(K - \theta)$ be the log-hydraulic conductivity (or, henceforth, log conductivity for simplicity). Evidently, $K = \exp(Y) + \theta$. The lognormal PDF, in its greatest generality, is given by the following formula:

$$f_K(s) = \frac{1}{(s - \theta)\sigma_Y\sqrt{2\pi}} \exp\left\{-\frac{1}{2}\left[\frac{\ln(s - \theta) - \bar{Y}}{\sigma_Y}\right]^2\right\} \quad s \geq \theta \quad (1)$$

in which the hydraulic conductivity's lower bound θ is, from, physical feasibility, nonnegative. Several important characteristics of the lognormally distributed hydraulic conductivity can be obtained from the PDF of K in Eq. (1), and from the fact that the log conductivity Y is normally distributed with mean \bar{Y} and variance σ_Y^2 or, symbolically, $Y \sim N(\bar{Y}, \sigma_Y^2)$. These are presented next.

Statistics of Lognormal PDF

The statistics of the lognormal PDF are as follows:

Expected value (mean, \bar{K})

$$\bar{K} = E(K) = E[e^Y] + \theta = e^{\bar{Y} + (\sigma_Y^2/2)} + \theta \quad (2)$$

Recall that when the lower bound $\theta=0$, the geometric mean of the hydraulic conductivity is defined by $K_G = \exp(\bar{Y})$. The geometric mean is widely used as an average or “effective” hydraulic conductivity in groundwater hydrology. An estimator of the geometric mean, denoted by \hat{K}_G , is formed from sample values of hydraulic conductivity $\hat{K}_1, \hat{K}_2, \dots, \hat{K}_n$ that are log transformed to $\hat{Y}_j = \ln(\hat{K}_j)$, $j=1, 2, \dots, n$. The arithmetic mean of the log conductivities is then $\bar{\hat{Y}} = (\hat{Y}_1 + \hat{Y}_2 + \dots + \hat{Y}_n)/n$, and the geometric mean is estimated by $\hat{K}_G = \exp(\bar{\hat{Y}})$ or by the alternative equation $\hat{K}_G = (\hat{K}_1 \cdot \hat{K}_2 \cdot \dots \cdot \hat{K}_n)^{1/n}$. Median ($K_{0.50}$)

$$K_{0.50} = e^{\bar{Y}} + \theta \quad (3)$$

Mode (the most likely value, K_M)

$$K_M = e^{\bar{Y} - \sigma_Y^2} + \theta \quad (4)$$

Eqs. (2)–(4) show that $K_M < K_{0.50} < \bar{K}$.

Variance (σ_K^2)

$$\sigma_K^2 = e^{2\bar{Y} + \sigma_Y^2} \cdot (e^{\sigma_Y^2} - 1) \quad (5)$$

Coefficient of variation (C_{vK})

$$C_{vK} \equiv \frac{\sigma_K}{\bar{K}} = (e^{\sigma_Y^2} - 1)^{1/2} \quad (6)$$

Coefficient of skew (C_{sK})

$$C_{sK} \equiv \frac{E(K - \bar{K})^3}{\sigma_K^3} = \frac{(e^{3\sigma_Y^2} - 3e^{\sigma_Y^2} + 2)}{C_{vK}^3} \quad (7)$$

in which C_{vK} is given by Eq. (6). The C_{sK} in Eq. (7) is always positive.

Bias of the sample estimator of the geometric mean, $\hat{K}_G = \exp(\bar{\hat{Y}})$, for uncorrelated log-conductivity observations \hat{Y}_j , $j=1, 2, \dots, n$ (with lower bound $\theta=0$)

$$E[\hat{K}_G] = E[e^{\bar{\hat{Y}}}] = E\left(\exp\left[\frac{1}{n} \sum_{j=1}^n \hat{Y}_j\right]\right) = e^{\bar{Y} + (\sigma_Y^2/2n)} \neq e^{\bar{Y}} \quad (8)$$

Eq. (8) shows that the sample estimator of the geometric mean is biased. Yet, it is a consistent estimator of K_G

$$\lim_{n \rightarrow \infty} E[\hat{K}_G] = e^{\bar{Y}} = K_G \quad (9)$$

that is, the bias of the sample estimator vanishes for large sample size.

Bias of the sample estimator of the geometric mean, $\hat{K}_G = \exp(\bar{\hat{Y}})$, for correlated observations (with $\theta=0$, Loaiciga and Hudak 1989)

$$E(\hat{K}_G) = E(e^{\bar{Y}}) = E\left(\exp\frac{1}{n}\sum_{j=1}^n \hat{Y}_j\right) \\ = \exp\left[\bar{Y} + (1/2n^2)\sum_{i=1}^n \sum_{j=1}^n C_Y(r_{ij})\right] \neq e^{\bar{Y}} \quad (10)$$

in which $C_Y(r_{ij})$ denotes the correlation between the i th and j th log-conductivity observations, $i, j=1, 2, \dots, n$. It is evident in Eq. (10) that the sample estimator of the geometric mean is biased in the correlated case. Yet, it is consistent, that is, it converges to K_G as the sample size becomes very large, or $E[\hat{K}_G] \rightarrow \exp(\bar{Y}) \equiv K_G$ when $n \rightarrow \infty$.

Quantiles of K : for $0 < p < 1$, $P(K \leq K_p) = p$ defines the p th quantile (K_p) of the hydraulic conductivity. K_p is given by

$$K_p = \exp(\bar{Y} + z_p \sigma_Y) + \theta \quad (11)$$

In Eq. (11) z_p = p th quantile of the standard normal variate with zero mean and unit variance, which is readily obtained with ubiquitous software such as EXCEL, using the function $z_p = \text{normsin v}(p)$.

Lognormal Hydraulic Conductivity and Its Relation to Effective Hydraulic Conductivity in Small-Perturbations Approach

This section reviews the centrality of the lognormal PDF in the small-perturbations approach to deriving the effective hydraulic conductivity. The stochastic analysis of groundwater flow assumes that the log conductivity $Y = \ln(K) \sim N(\bar{Y}, \sigma_Y^2)$, with $\sigma_Y^2 \ll 1$ (see, e.g., Matheron 1967; Bakr et al. 1978; or Gutjahr et al. 1978, for pioneering papers in this field). The lower bound of hydraulic conductivity is $\theta = 0$ in this approach. The log conductivity is written as the sum of a constant mean \bar{Y} and a zero-mean residual y , that is, $Y = \bar{Y} + y$, and has (stationary) covariance $C_Y(r)$. Evidently, $K = \exp(\bar{Y} + y) = K_G \exp(y)$, in which $\exp(y)$ can be replaced by a Taylor-series expansion about $y=0$. The specific discharge q_u in the direction u (where u can equal any of the principal directions x , y , or z) can be written as follows (letting the hydraulic head $\phi = H + \varphi$, where H and φ = mean hydraulic head and zero-mean head residual, respectively)

$$q_u = -K \frac{\partial \phi}{\partial u} = -K_G e^y \frac{\partial \phi}{\partial u} \\ = -K_G \left(1 + y + \frac{y^2}{2!} + \frac{y^3}{3!} + \frac{y^4}{4!} + \dots\right) \left(\frac{\partial H}{\partial u} + \frac{\partial \varphi}{\partial u}\right) \quad (12)$$

The expected values of odd powers of the residual y (i.e., y , y^3 , etc.) in the Taylor series of Eq. (12) are zero. The expected values of even powers y^2 , y^4 , y^6 , ..., are of order σ_Y^2 , σ_Y^4 , σ_Y^6 , ..., respectively. Considering that $\sigma_Y^2 \ll 1$, by assumption, it is evident that terms containing y^n , where $n > 2$, are negligible compared with σ_Y^2 and can be dropped from the series. Using this simplification, the expected value of both sides of Eq. (12) produces the following result (letting $J_u = \partial H / \partial u$ denote the average hydraulic gradient in the direction u)

$$\bar{q}_u \approx -K_G \cdot \left(1 + \frac{\sigma_Y^2}{2}\right) J_u - K_G \cdot E\left(y \frac{\partial \varphi}{\partial u}\right) \quad u = x, y, z \quad (13)$$

in which the cross moment, $E[(y^2/2)(\partial \varphi / \partial u)]$, was neglected in the right-hand side term of Eq. (13) because it is of order σ_Y^3 .

Several authors (see, e.g., Gutjahr et al. 1978; Dagan 1989; Loaiciga et al. 1996) have simplified Eq. (13) assuming: (1) constant average hydraulic gradient J_u , and (2) axisymmetric and anisotropic log-conductivity covariance functions. In these covariance functions the separation vector $r = r_1 - r_2$ is resolved in terms of components r_h and r_z on the horizontal and vertical planes, respectively, and the axis of symmetry is parallel to the vertical direction. Specifically, let I_{Yh} and I_{Yz} be the horizontal (in the x, y plane) and vertical correlation scales of the log conductivity, respectively, and ρ_Y be the log-conductivity correlation function. As before, σ_Y^2 denotes the variance of the log conductivity. An axisymmetric (anisotropic) covariance is of the form $C_Y(r) = \sigma_Y^2 \rho_Y(r)$, $r = [(r_h/I_{Yh})^2 + (r_z/I_{Yz})^2]^{1/2}$. The simplified Eq. (13) takes the following form, in which the effective hydraulic conductivity (\tilde{K}_{eu}) is a coefficient relating the average specific discharge and the average hydraulic gradient

$$\bar{q}_u \cong -\tilde{K}_{eu} \cdot J_u \quad u = x, y, z \quad (14)$$

The horizontal and vertical effective hydraulic conductivities (\tilde{K}_{eh} and \tilde{K}_{ez} , respectively) are as follows:

$$\tilde{K}_{eh} = K_G \cdot \left[1 + \sigma_Y^2 \left(\frac{1}{2} - \frac{\tau}{2}\right)\right] \quad (15)$$

$$\tilde{K}_{ez} = K_G \cdot \left[1 + \sigma_Y^2 \left(\tau - \frac{1}{2}\right)\right] \quad (16)$$

in which the factor τ is defined by

$$\tau = \frac{\xi^2}{1 - \xi^2} \left[\frac{1}{\xi \sqrt{1 - \xi^2}} \tan^{-1} \left(\sqrt{\frac{1}{\xi^2} - 1} \right) - 1 \right] \quad (17)$$

where $\xi = I_{Yz}/I_{Yh}$ = ratio of log-conductivity correlation scales. The inverse tangent function is expressed in radians in Eq. (17). In the isotropic case, i.e., $\xi = 1$, $\tau = 2/3$, and, therefore

$$\tilde{K}_{eh} = \tilde{K}_{ez} = \tilde{K}_e = K_G \cdot \left(1 + \frac{\sigma_Y^2}{6}\right) \quad (\text{isotropic case}) \quad (18)$$

The results presented in this section—which apply to lognormally distributed hydraulic conductivity with $\sigma_Y^2 \ll 1$, among other assumptions—indicate that the effective hydraulic conductivity can be expressed by the generic equation

$$\tilde{K}_{eu} = K_G \cdot [1 + O(\sigma_Y^2)] \quad (19)$$

in which O in Eq. (19) denotes a quantity of order σ_Y^2 . Eq. (19) shows that the effective hydraulic conductivity converges to the geometric mean K_G as $\sigma_Y^2 \rightarrow 0$. This lends theoretical—yet conditional—support to the use of the geometric mean of the hydraulic conductivity as an effective parameter in local-scale groundwater models.

While the asymptotic convergence of the effective conductivity to the geometric mean of the hydraulic conductivity is laudable, the review presented in this section shows that the use of the geometric mean as an effective groundwater parameter is applicable under the restrictive condition $\sigma_Y^2 \ll 1$ when the hydraulic conductivity is lognormally distributed. The following sections show that neither the small-perturbations assumption nor lognor-

mality are necessary in either the statistical characterization of hydraulic conductivity or in the derivation of the effective hydraulic conductivity.

Properties of Gamma-Distributed Hydraulic Conductivity

Loaiciga (2004) proposed the gamma PDF as an alternative to the lognormal PDF in an analysis of stochastic groundwater flow and solute transport. In its greater generality, the PDF of gamma-distributed hydraulic conductivity is

$$g_K(s) = \frac{\left(\frac{s-\theta}{\beta}\right)^\alpha |s-\theta|^{-1} e^{-(s-\theta/\beta)}}{\Gamma(\alpha)},$$

$$s \geq \theta \text{ if } \beta > 0, \quad s \leq \theta \text{ if } \beta < 0 \quad (20)$$

in which α and β =shape and scale parameters, respectively, and $\alpha > 0$; θ =lower bound of the hydraulic conductivity when $\beta > 0$, and an upper bound when $\beta < 0$; Γ denotes the gamma function

$$\Gamma(\alpha) = \int_0^\infty e^{-v} v^{\alpha-1} dv \quad (21)$$

The gamma function is widely tabulated and programmed in commercial software (EXCEL, MATLAB, MATHEMATICA, for example). It is noteworthy that when $\alpha=1$ and $\beta > 0$ the gamma PDF in Eq. (20) becomes the exponential PDF with parameter $1/\beta$. The exponential PDF has been used in modeling hydraulic conductivity (Gardner 1958; Philip 1969).

The domain of the gamma PDF is $[-\infty, \theta]$ when $\beta < 0$, which contains negative numbers and, thus, violates the non-negativity of the hydraulic conductivity. The next subsection presents a summary of the properties of the gamma PDF for positive or negative scale parameter β . This sets the stage for the study of the log-gamma PDF, which features positive or negative scale parameter and is defined over nonnegative domains.

Statistics of Gamma PDF

The following properties for gamma-distributed hydraulic conductivity are derivable from the PDF Eq. (20):

Expected value (mean)

$$\bar{K} = \alpha\beta + \theta \quad (22)$$

Median

$$K_{0.50} = \psi_{0.50}\beta + \theta \quad (23)$$

in which $\psi_{0.50}$ must be obtained from the integral equation

$$\frac{1}{\Gamma(\alpha)} \int_0^{\psi_{0.50}} e^{-v} v^{\alpha-1} dv = \frac{1}{2} \quad (24)$$

The integral on the left-hand side of Eq. (24) is called the incomplete gamma function $\gamma(\alpha, \psi_{0.50})$ [see, e.g., Gradshteyn and Ryzhik 1994, Eq. 8.350.1], so that Eq. (24) can be shortened to

$$\frac{1}{\Gamma(\alpha)} \gamma(\alpha, \psi_{0.50}) = \frac{1}{2} \quad (25)$$

The left-hand side of Eq. (25) can be evaluated using the GAMMAINV (probability, alpha, beta) function in the software EXCEL, with probability=1/2, alpha= α , and beta=1, which re-

turns the value of $\psi_{0.50}$. Mode, when $\alpha > 1$

$$K_M = (\alpha - 1) \cdot \beta + \theta \quad (26)$$

and it is equal to θ when $0 < \alpha \leq 1$.

Variance

$$\sigma_K^2 = \alpha\beta^2 \quad (27)$$

Coefficient of variation

$$C_{vK} = \frac{|\alpha^{1/2}\beta|}{|\alpha\beta + \theta|} \quad (28)$$

Coefficient of skew

$$C_{sK} = \frac{2\alpha\beta^3}{\sigma_K^3} \quad (29)$$

in which the sign of the skew is determined by that of the shape parameter β . $C_{sK} > 0$ when $\beta > 0$, in which case the PDF is positively skewed with lower bound θ . $C_{sK} < 0$ when $\beta < 0$, in which case the PDF is negatively skewed with upper bound θ .

Moment estimators of the α , β , and θ parameters are deducible from Eqs. (22)–(29). They are

$$\alpha = \frac{4}{C_{sK}^2} \quad (30)$$

$$\beta = \frac{\sigma_K C_{sK}}{2} \quad (31)$$

$$\theta = \bar{K} - \frac{2\sigma_K}{C_{sK}} \quad (32)$$

in which \bar{K} , σ_K , and C_{sK} are replaced in Eqs. (30)–(32) by the standard sample estimators of the mean, variance, and coefficient of skewness of the hydraulic conductivity, respectively. Quantiles: for $0 < p < 1$, $P(K \leq K_p) = p$ defines the p th quantile. In particular, $K_{0.50}$ equals the median. In general, K_p is given by the following equation:

$$K_p = \bar{K} + \left(\frac{\psi_q C_{sK}}{2} - \frac{2}{C_{sK}} \right) \sigma_K \quad (33)$$

in which ψ_q must be obtained from the following integral equation ($0 < p < 1$):

$$\frac{1}{\Gamma(\alpha)} \int_0^{\psi_q} e^{-v} v^{\alpha-1} dv = p \quad \text{if } C_{sK} > 0 \text{ (i.e., } \beta > 0) \quad (34)$$

in which $\alpha = 4/C_{sK}^2$ or from

$$\frac{1}{\Gamma(\alpha)} \int_0^{\psi_q} e^{-v} v^{\alpha-1} dv = 1 - p \quad \text{if } C_{sK} < 0 \text{ (i.e., } \beta < 0) \quad (35)$$

in which $\alpha = 4/C_{sK}^2$. Eqs. (30)–(35) are sufficient to characterize the gamma-distributed hydraulic conductivity. All the special functions used in the previous equations are available in commercial software and their calculation is expeditious. In particular, the left-hand side of Eqs. (34) and (35) can be evaluated using the GAMMAINV (probability, alpha, beta) function in the software EXCEL, with probability $q=p$ (if $C_{sK} > 0$) or $1-p$ (if $C_{sK} < 0$), alpha= α , and beta=1, which returns the value of ψ_q . In the limit $C_{sK} \rightarrow 0$, the factor within brackets in Eq. (33) tends to the standard normal quantile z_p . Specifically

$$\lim_{C_{sK} \rightarrow 0} \left(\frac{\Psi_q C_{sK}}{2} - \frac{2}{C_{sK}} \right) \rightarrow z_p \quad (36)$$

so that the quantile K_p in Eq. (33) becomes $K_p = \bar{K} + z_p \sigma_K$. In other words, the gamma PDF approaches the normal PDF when the coefficient of skew tends to zero.

Extensions of Gamma PDF: Log-Gamma Distributed Hydraulic Conductivity

A variant of the gamma PDF is the log-gamma PDF (also called log-Pearson Type III), which is used by federal agencies in the United States to fit annual streamflow peaks at gaged sites (see, e.g., USGS 1982; Koutrouvelis and Canavos 1999). When using the log-gamma PDF it is assumed that the logarithm of the hydraulic conductivity K [i.e., $Y = \ln(K)$] follows the gamma PDF in Eq. (20) with the shape and scale parameters replaced by α_Y and β_Y , respectively. In this instance, $\theta = \theta_Y$ in Eq. (20) denotes the lower bound of Y when $\beta_Y > 0$, or its upper bound when $\beta_Y < 0$. The log conductivity Y has the following PDF:

$$g_Y(s) = \frac{\left(\frac{s - \theta_Y}{\beta_Y} \right)^{\alpha_Y} |s - \theta_Y|^{-1} \exp \left[- \left(\frac{s - \theta_Y}{\beta_Y} \right) \right]}{\Gamma(\alpha_Y)},$$

$$s \geq \theta_Y \text{ if } \beta_Y > 0, \quad s \leq \theta_Y \text{ if } \beta_Y < 0 \quad (37)$$

Evidently, $K = e^Y$, which is positive with lower or upper bound e^{θ_Y} depending on whether $\beta_Y > 0$ or $\beta_Y < 0$, respectively. The PDF of log-gamma distributed K is

$$h_K(s) = \frac{\left[\frac{\ln(s) - \theta_Y}{\beta_Y} \right]^{\alpha_Y} |\ln(s) - \theta_Y|^{-1} \exp \left\{ - \left[\frac{\ln(s) - \theta_Y}{\beta_Y} \right] \right\}}{s \Gamma(\alpha_Y)} \quad (38)$$

in which $s \geq e^{\theta_Y}$ if $\beta_Y > 0$, or $0 < s \leq e^{\theta_Y}$ if $\beta_Y < 0$. Key properties of the log-gamma-distributed hydraulic conductivity K are derivable from its PDF Eq. (38). These are presented next.

Statistics of Log-Gamma PDF

The following are statistics of the log-gamma PDF:

Expected value

$$\bar{K} = \frac{e^{\theta_Y}}{(1 - \beta_Y)^{\alpha_Y}} \quad (39)$$

Geometric mean

$$K_G \equiv e^{E(Y)} = e^{\alpha_Y \beta_Y + \theta_Y} \quad (40)$$

The estimator of K_G is $\exp[(1/n)(\hat{Y}_1 + \hat{Y}_2 + \dots + \hat{Y}_n)]$, whose expected value can be shown to be $\exp(\theta_Y) / [1 - (\beta_Y/n)]^{n\alpha_Y}$ when the log-conductivity observations are mutually independent. This result proves that the sample estimator of K_G is biased in this instance, that is, its expected value differs from $\exp[\alpha_Y \beta_Y + \theta_Y]$. On the other hand, the sample estimator is consistent, that is, its expected value tends to $\exp[\alpha_Y \beta_Y + \theta_Y]$ when $n \rightarrow \infty$. The magnitude of the bias of the estimator of K_G is unknown when the log-conductivity observations are correlated.

Median

$$K_{0.50} = e^{\psi_{0.50} \beta_Y + \theta_Y} \quad (41)$$

in which $\psi_{0.50}$ is obtained from the solution of the integral Eq. (25).

Mode, when $\alpha > 1$

$$\bar{K}_M = \exp \left[(\alpha_Y - 1) \frac{\beta_Y}{\beta_Y + 1} + \theta_Y \right] \quad (42)$$

the mode equals e^{θ_Y} if $0 < \alpha_Y \leq 1$.

Variance

$$\sigma_K^2 = \bar{K}^2 \left\{ \left[\frac{(1 - \beta_Y)^2}{(1 - 2\beta_Y)} \right]^{\alpha_Y} - 1 \right\} \quad (43)$$

in which \bar{K} (the expected value of K) is given by Eq. (39).

Coefficient of variation

$$C_{vK} = \left\{ \left[\frac{(1 - \beta_Y)^2}{(1 - 2\beta_Y)} \right]^{\alpha_Y} - 1 \right\}^{1/2} \quad (44)$$

Coefficient of skew

$$C_{sK} = \frac{\left[\frac{(1 - \beta_Y)^3}{(1 - 3\beta_Y)} \right]^{\alpha_Y} - 3 \left[\frac{(1 - \beta_Y)^2}{(1 - 2\beta_Y)} \right]^{\alpha_Y} + 2}{C_{vK}^3} \quad (45)$$

in which C_{vK} is given by Eq. (44).

Moment estimators of the log-conductivity parameters α_Y , β_Y , and θ_Y are obtained by resorting to the fact that $Y = \ln(K)$ is gamma distributed. Letting \bar{Y} , σ_Y , and C_{sY} be the mean, standard deviation, and coefficient of skew of Y , respectively, one obtains

$$\alpha_Y = \frac{4}{C_{sY}^2} \quad (46)$$

$$\beta_Y = \frac{\sigma_Y C_{sY}}{2} \quad (47)$$

$$\theta_Y = \bar{Y} - \frac{2\sigma_Y}{C_{sY}} \quad (48)$$

in which \bar{Y} , σ_Y , and C_{sY} are replaced in Eqs. (46)–(48) by the standard sample estimators of the mean, variance, and coefficient of skew of the log conductivity Y , respectively.

Quantiles of the hydraulic conductivity: for $0 < p < 1$, $P(K \leq K_p) = p$ defines the p th quantile (K_p). In particular, $K_{0.50}$ = the median. In general, K_p is given by the following equation:

$$K_p = \exp \left[\bar{Y} + \left(\frac{\Psi_q C_{sY}}{2} - \frac{2}{C_{sY}} \right) \sigma_Y \right] \quad (49)$$

in which Ψ_q must be obtained from the following integral equations ($0 < p < 1$):

$$\frac{1}{\Gamma(\alpha_Y)} \int_0^{\Psi_q} e^{-v} v^{\alpha_Y - 1} dv = p \quad \text{if } C_{sY} > 0 \text{ (i.e., } \beta_Y > 0) \quad (50)$$

in which $\alpha_Y = 4/C_{sY}^2$, or

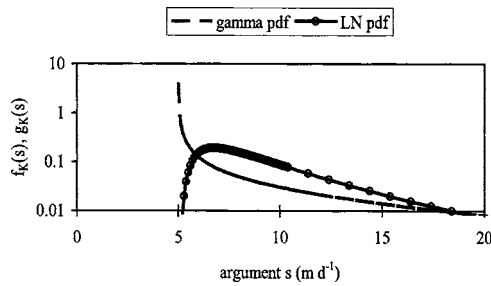


Fig. 1. Graphs of gamma and lognormal (LN) PDFs of hydraulic conductivity (K). Lower bound (θ), mean (\bar{K}), standard deviation (σ_K), and coefficient of skewness (C_{sK}) are 5, 10, 10, and 4, respectively. The first three parameters are in meters day⁻¹. Argument s represents realization of hydraulic conductivity in Eqs. (1) and (20).

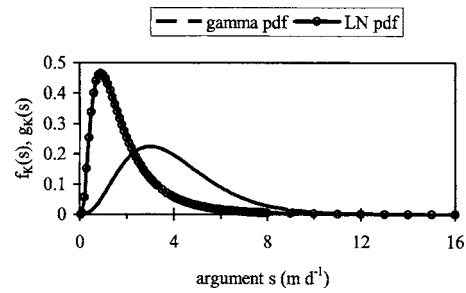


Fig. 3. Graphs of gamma and lognormal (LN) PDFs of hydraulic conductivity (K). Lower bound (θ), mean (\bar{K}), standard deviation (σ_K), and coefficient of skewness (C_{sK}) are 0, 4, 2, and 1, respectively. First three parameters are in meter day⁻¹. Argument s represents realization of hydraulic conductivity in Eqs. (1) and (20).

$$\frac{1}{\Gamma(\alpha_Y)} \int_0^{\psi_q} e^{-\nu} \nu^{\alpha_Y-1} d\nu = 1 - p \quad \text{if } C_{sY} < 0 \quad (\text{i.e., } \beta_Y < 0) \quad (51)$$

in which $\alpha_Y = 4/C_{sY}^2$. The left-hand side of Eqs. (50) and (51) can be evaluated using the GAMMAINV (probability, alpha, beta) function in the software EXCEL, with probability $q=p$ (if $C_{sY} > 0$) or $1-p$ (if $C_{sY} < 0$), $\alpha = \alpha_Y$, and $\beta = 1$, which returns the value of ψ_q . In the limit $C_{sY} \rightarrow 0$, the factor within parentheses in Eqs. (50) and (51) tends to the standard normal quantile z_p .

Eqs. (46)–(51) are sufficient to characterize the log-gamma distributed hydraulic conductivity. In the limit $C_{sY} \rightarrow 0$, the factor within brackets in Eq. (49) tends to the standard normal quantile z_p . Specifically

$$\lim_{C_{sY} \rightarrow 0} \left(\frac{\psi_q C_{sY}}{2} - \frac{2}{C_{sY}} \right) \rightarrow z_p \quad (52)$$

so that the quantile K_p in Eq. (49) becomes

$$K_p = \exp(\bar{Y} + z_p \sigma_Y) \quad (53)$$

In other words, the log-gamma PDF approaches the log-normal PDF when the coefficient of skew tends to zero [compare Eq. (53) with Eq. (11), after setting $\theta=0$ in the latter].

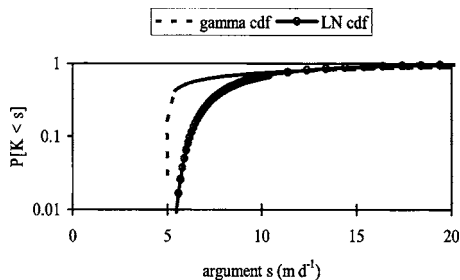


Fig. 2. Graphs of gamma and lognormal (LN) CDFs of hydraulic conductivity (K). Lower bound (θ), mean (\bar{K}), standard deviation (σ_K), and coefficient of skewness (C_{sK}) are 5, 10, 10, and 4, respectively. First three parameters are in meter day⁻¹. Argument s represents realization of hydraulic conductivity in Eqs. (1) and (20).

Examples of Positively and Negatively Skewed Hydraulic Conductivity

Fig. 1 shows two graphed PDFs. One is a gamma PDF [Eq. (20)] with properties $\theta=5$, $\bar{K}=10$, $\sigma_K=10$ (these three in meter day⁻¹), $C_{sK}=4$ (and, therefore, $\alpha=1/4$ and $\beta=20$). The other is a lognormal PDF [Eq. (1)] with properties identical to those of the gamma PDF, i.e., $\theta=5$, $\bar{K}=10$, $\sigma_K=10$, $C_{sK}=4$ (and, therefore, $\bar{Y}=1.2629$, $\sigma_Y=\sqrt{\ln 2}=0.8326$). A $C_{sK}=4$ implies a high degree of asymmetry for hydraulic conductivity. Therefore, the graphs in Fig. 1 portray a graphical representation of PDFs with unusually pronounced skew. The two PDFs in Fig. 1 have remarkably different shapes in spite of sharing the same lower bound, mean, variance, and coefficient of skew. Fig. 2 shows the cumulative distribution functions (CDFs) corresponding to the PDFs of Fig. 1. The graphs in Fig. 2 reveal that the gamma CDF is larger than the lognormal CDF for most values of hydraulic conductivity in this example.

Fig. 3 shows gamma and lognormal PDFs with $\theta=0$, $\bar{K}=4$, $\sigma_K=2$ (these three in meter day⁻¹), $C_{sK}=1$. The values of the skew coefficient (=1) and the coefficient of variation (=2/4=0.5) are typical for hydraulic conductivity. In the case of the gamma PDF, $\alpha=4$ and $\beta=1$. For the lognormal PDF, $\bar{Y}=0.426$ and $\sigma_Y=0.731$. In spite of the striking differences between the PDFs shown in Fig. 3, they have identical lower bounds, means, variances, and coefficients of skew. Fig. 4 displays graphs of the CDFs of hydraulic conductivity corresponding

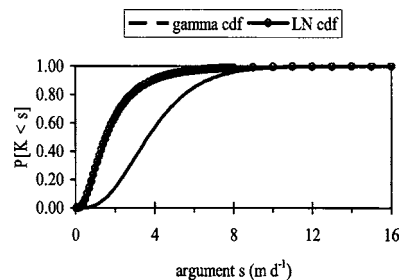


Fig. 4. Graphs of gamma and lognormal (LN) CDFs of hydraulic conductivity (K). Lower bound (θ), mean (\bar{K}), standard deviation (σ_K), and coefficient of skewness (C_{sK}) are 0, 4, 2, and 1, respectively. First three parameters are in meter day⁻¹. Argument s represents realization of hydraulic conductivity in Eqs. (1) and (20).

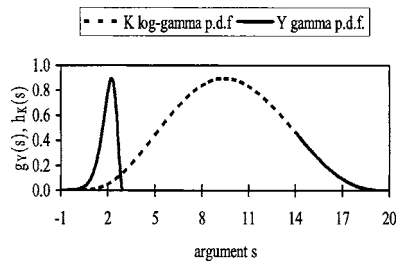


Fig. 5. Gamma PDF of log conductivity Y for which $\bar{Y}=\ln(20)-1=1.996$, $\sigma_Y=1/2$, $C_{sY}=-1$, and upper bound $\theta_Y=\ln(20)=2.996$. Corresponding log-gamma PDF of hydraulic conductivity K is also shown, for which domain is $K \in [0,20]$ in meter day $^{-1}$, with $\bar{K}=8.192$, $\sigma_K=3.450$, and $C_{sK}=+0.260$. Argument s appears in Eqs. (37) and (38).

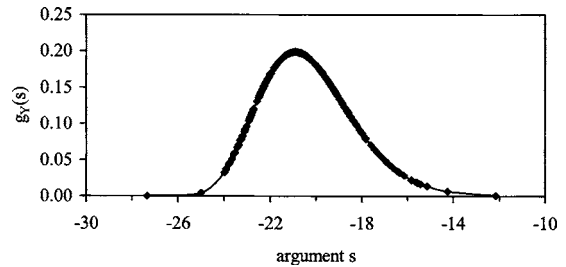


Fig. 7. Gamma PDF of log conductivity $Y=\ln K$ estimated from hydraulic conductivity data shown in Fig. 6. Estimates of minimum, maximum, average, median, and standard deviation of log conductivity were -24.2 , -12.2 , -20.3 , -20.4 , and 2.1 , respectively. Coefficient of skew $C_{sY}=0.59$, and lower bound $\theta_Y=-27.3$. Argument s appears in Eq. (37).

to the PDFs of Fig. 3. In contrast to the CDFs of the previous example (see Fig. 2), the lognormal CDF is larger than the gamma CDF in this instance.

The two previous examples demonstrate that the gamma PDF is a flexible density that can fit positively skewed hydraulic conductivity as well as the lognormal PDF can. It was remarked earlier that the log-gamma PDF can fit positively or negatively skewed log conductivity. The lognormal PDF, on the other hand, can only fit symmetric (that is, nonskewed) log-conductivity. Fig. 5 shows the gamma PDF of log conductivity Y [Eq. (37)] for which $\bar{Y}=\ln(20)-1=1.996$, $\sigma_Y=1/2$, $C_{sY}=-1$, and the upper bound $\theta_Y=\ln(20)=2.996$. The corresponding log-gamma PDF of hydraulic conductivity K [Eq. (38)] is also shown in Fig. 5, for which the domain is $K \in [0,20]$ in meter day $^{-1}$, with $\bar{K}=8.192$, $\sigma_K=3.450$, and $C_{sK}=+0.260$.

Fig. 6 shows a plot of 201 rising-head slug-test measurements of hydraulic conductivity made in the main clay aquitard that underlies Mexico City (unit one in Vargas and Ortega-Guerrero 2004). Slug-test measurement of the hydraulic conductivity averages K over a domain whose characteristic length is the size of the screened interval in the test well (Vargas and Ortega-Guerrero 2004), consistent with the local scale of groundwater flow. This aquitard is important for the long-term management and protec-

tion of the water resources of Mexico City and its urban environs. The aquitard's effective hydraulic conductivity is central to assessing the degree of connectedness of shallow groundwater and groundwater in the aquifer underlying the aquitard. This degree of hydraulic connection is the key to preventing pollution of the aquifer's groundwater. The spatial characterization of the effective hydraulic conductivity, in particular, is considered potentially valuable in calibrating groundwater-flow models of the Mexico City aquifer system (Vargas and Ortega-Guerrero 2004). The measurement of hydraulic conductivity in the Mexico City aquitard range from 3.1×10^{-11} to 5.2×10^{-6} cm/s, as seen in Fig. 6. Its average, median, and standard deviation are 3.9×10^{-8} , 1.5×10^{-9} , and 3.7×10^{-7} cm/s, respectively. The coefficient of variation $C_{vK} \equiv \sigma_K/\bar{K}=9.4$, indicating inordinate variability of K . Moreover, the K data in Fig. 6 exhibit very large skew $C_{sK}=13.7$, and an estimated lower bound of 1.3×10^{-12} cm/s. The log conductivity $Y=\ln K$ has minimum and maximum measured observations equal to -24.2 and -12.2 , respectively. Its average, median, and standard deviation are -20.3 , -20.4 , and 2.1 , respectively. Notice that this particular sample does not comply with the small-perturbation assumption $\sigma_Y^2 \ll 1$. In addition, the coefficient of skew $C_{sY}=0.59$, and the lower bound is $\theta_Y=-27.3$. Evidently, the logarithmic transformation does not normalize the data in this instance. The log-gamma PDF is the appropriate model to fit the log conductivity in this case. The estimated shape and scale parameters equaled $\alpha_Y=11.4$ and $\beta_Y=0.62$, respectively.

Fig. 7 shows the estimated gamma PDF of the log conductivity of the data in Fig. 6, $g_Y(s)$ [see Eq. (37)]. Fig. 8 contains a graph

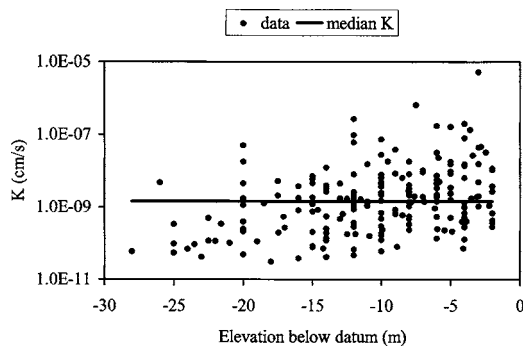


Fig. 6. Hydraulic conductivity measurements made using rising-head slug tests in main clay aquitard underlying Mexico City. Two hundred one measurements were made. Minimum, maximum, average, median, and standard deviation of hydraulic conductivity estimated from measurements were 3.1×10^{-11} , 5.2×10^{-6} , 3.9×10^{-8} , 1.5×10^{-9} , and 3.7×10^{-7} cm/s, respectively. Coefficient of skew $=C_{sK}=13.7$, and lower bound of $K=1.3 \times 10^{-12}$ cm/s.

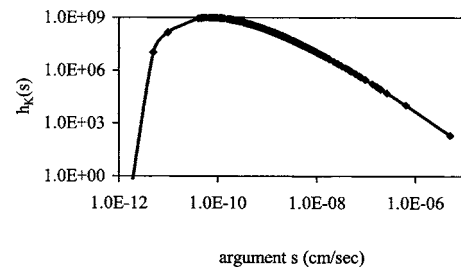


Fig. 8. Log gamma PDF of hydraulic conductivity estimated from data shown in Fig. 6. Main statistics of K are those written in legend of Fig. 6. Notice substantial degree of asymmetry in PDF, whose lower-bound estimate equals 1.3×10^{-12} cm/s. Argument s appears in Eq. (38).

of the log-gamma PDF of the hydraulic conductivity, $h_K(s)$ [see Eq. (38)]. The asymmetry of the latter PDF is evident.

Effective Hydraulic Conductivity for Arbitrary PDF of Hydraulic Conductivity

Dagan (1989) presented a self-consistent approach to obtain the effective hydraulic conductivities in the horizontal plane (K_{eh}) and in the vertical direction (K_{ez}) when the hydraulic conductivity has an axisymmetric covariance. His results are applicable for arbitrary PDF of the hydraulic conductivity and circumvents the assumption of very small log-conductivity variance (i.e., that $\alpha_Y^2 \ll 1$) required in the small-perturbations approach reviewed in a previous section. The results are

$$K_{eh} = \frac{1}{2} \left[\int_{s \in D} \frac{f_K(s) ds}{(s - K_{eh})\eta + 2K_{eh}} \right]^{-1} \quad (54)$$

in which $f_K(s)$ =PDF of the hydraulic conductivity (lognormal, gamma, exponential, log gamma, for example) whose domain, D , may contain only non-negative values. In the case of a log-gamma PDF with upper bound $\exp(\theta_Y)$, for instance, $D=[0, \exp(\theta_Y)]$. Other terms in Eq. (54) are

$$\eta = \frac{\kappa^2}{1 - \kappa^2} \left[\frac{1}{\kappa \sqrt{1 - \kappa^2}} \tan^{-1} \left(\sqrt{\frac{1}{\kappa^2} - 1} \right) - 1 \right] \quad (55)$$

in which the inverse tangent function is expressed in radians, and

$$\kappa = \frac{I_{Kz}}{I_{Kh}} \sqrt{\frac{K_{eh}}{K_{ez}}} \quad (56)$$

$I_{Kh}=I_{Yh}$ and $I_{Kz}=I_{Yz}$ =horizontal and vertical correlation scales of the hydraulic conductivity (and of the log conductivity), respectively.

The vertical effective hydraulic conductivity is

$$K_{ez} = \left[\int_{s \in D} \frac{f_K(s) ds}{s + \eta \cdot (K_{ez} - s)} \right]^{-1} \quad (57)$$

Eqs. (54) and (57) are coupled integral equations. This is so because the factor κ in Eq. (56) contains the ratio K_{eh}/K_{ez} , which appears in both equations via the term η [see Eq. (55)]. Therefore, Eqs. (54) and (57) must be solved jointly to obtain the horizontal and vertical effective hydraulic conductivities. The calculations are tedious but straightforward using mathematical-statistical software such as EXCEL.

If the hydraulic conductivity is isotropic $K_{eh}=K_{ez}=K_e$

$$K_e = \frac{1}{3} \left[\int_{s \in D} \frac{f_K(s) ds}{s + 2K_e} \right]^{-1} \quad (58)$$

Eqs. (54), (57), and (58) can be simplified when the PDF of the hydraulic conductivity is the gamma density [see Eq. (20)]. In this instance, and provided that $\beta > 0$ (that is, the coefficient of skewness C_{sK} is positive), Eq. (54) becomes

$$\frac{2\Gamma(1 - \alpha, \omega) \cdot e^\omega \cdot \omega^{\alpha-1} K_{eh}}{\beta \eta} = 1 \quad (59)$$

in which $\Gamma(1 - \alpha, \omega)$ =(complementary) gamma function (see Gradshteyn and Ryzhik 1994, Eq. 8.350.2)

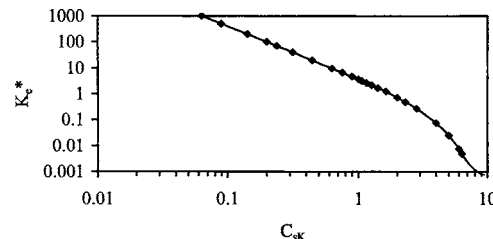


Fig. 9. Dimensionless ratio $K_e^*=K_e/\beta$ as function of coefficient of skewness $|C_{sK}|=2/\sqrt{\alpha}$, based on Eq. (64) for isotropic effective hydraulic conductivity with gamma PDF, in which $\beta > 0$ and lower bound $\theta=0$. To obtain K_e , calculate standard deviation (σ_K) and coefficient of skewness (C_{sK}) from hydraulic conductivity data, enter graph with C_{sK} , and interpolate corresponding K_e/β . Solve for K_e using $K_e=(K_e/\beta) \cdot (\sigma_K C_{sK}/2)$.

$$\Gamma(1 - \alpha, \omega) = \int_{\omega}^{\infty} e^{-v} v^{-\alpha} dt \quad (60)$$

and

$$\omega = \frac{\theta \eta + (2 - \eta) \cdot K_{eh}}{\beta \eta} \quad (61)$$

Using the gamma PDF [Eq. (20)] in Eq. (57) yields (with $\beta > 0$, that is, $C_{sK} > 0$)

$$\frac{\Gamma(1 - \alpha, \vartheta) \cdot e^{\vartheta} \cdot \vartheta^{\alpha-1} K_{ez}}{\beta \cdot (1 - \eta)} = 1 \quad (62)$$

in which

$$\vartheta = \frac{\theta \cdot (1 - \eta) + \eta K_{ez}}{\beta \cdot (1 - \eta)} \quad (63)$$

Eq. (58) for isotropic hydraulic conductivity produces the following integral equation for the effective hydraulic conductivity (K_e) when the gamma PDF Eq. (20) with $\beta > 0$ (and thus with $C_{sK} > 0$) is used

$$\frac{3\Gamma(1 - \alpha, \tau) \cdot e^{\tau} \cdot \tau^{\alpha-1} K_e}{\beta} = 1 \quad (64)$$

in which

$$\tau = \frac{\theta + 2K_e}{\beta} \quad (65)$$

The isotropic solution Eq. (64) takes its simplest form when $\alpha=1$, that is, when the gamma PDF becomes the exponential PDF with parameter $1/\beta > 0$. The isotropic effective hydraulic conductivity is then obtained by solving the following equation:

$$\frac{3\Gamma(0, \tau) \cdot e^{\tau} \cdot K_e}{\beta} = 1 \quad (66)$$

Fig. 9 shows solutions of the isotropic K_e [Eq. (64)] expressed as the dimensionless variable $K_e^*=K_e/\beta$ as a function of the coefficient of skewness $|C_{sK}|=2/\sqrt{\alpha}$, and for a lower bound $\theta=0$. All calculations were performed with the software MATHEMATICA. It is seen in Fig. 9 that the ratio K_e/β decreases with increasing coefficient of skewness. Fig. 9 can be used to estimate the isotropic K_e by first estimating the coefficient of skewness (C_{sK}) and the standard deviation (σ_K) of the hydraulic conductivity data to obtain $\beta=\sigma_K C_{sK}/2$, then reading the K_e/β corresponding to C_{sK}

using the graph in Fig. 9, and, finally, solving for the effective hydraulic conductivity: $K_e = (K_e/\beta) \cdot (\sigma_K C_{sK}/2)$. Notice that the effective conductivity so obtained differs fundamentally from that obtained in the small-perturbations approach [see Eq. (19)] in that the former captures the first-, second-, and third-moment characteristics of the hydraulic conductivity, whereas the latter is based strictly on the first moment of the log conductivity. Although the graph in Fig. 9 corresponds to isotropic effective hydraulic conductivity, the same observation holds regarding the multimoment characteristics of the anisotropic effective hydraulic conductivities presented in this section [see Eqs. (54) and (57)].

Choosing PDF

It can be construed from the previous sections that the log-gamma PDF is a suitable probability model for hydraulic conductivity in the cases of skewed and symmetric data sets. The goodness-of-fit of the log-gamma PDF to a specific sample of hydraulic conductivity values can be investigated formally using the chi-squared test, for example, as illustrated in the context of other hydrologic data in Loáiciga et al. (1992). It has been shown in this paper that if the log conductivity has a negligible coefficient of skew, then the lognormal PDF is an adequate, perhaps the simplest, probability model to fit a sample.

Conclusion

The relative advantages/disadvantages of well-known, asymmetric, PDFs for the statistical characterization of hydraulic conductivity were reviewed in this paper. It was shown that the gamma and log-gamma PDFs possess statistical traits that render them advantageous in comparison with the more commonly used lognormal PDF. In addition, this work reviewed the effect that the choice of hydraulic conductivity PDF has on the estimation of the effective hydraulic conductivity in local-scale groundwater flow. Theoretical results and computational examples using synthetic and field hydraulic conductivity data demonstrated that the log-gamma PDF possesses all the features necessary to model skewed hydraulic conductivity data with lower or upper bounds. The assumption of lognormally distributed hydraulic conductivity with negligible log-conductivity variance was shown to be unnecessary in the statistical characterization of hydraulic conductivity or in the derivation of the effective hydraulic conductivity.

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