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Uncertainty in applying the temperature time-series method to the field under heterogeneous flow conditions

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SUMMARY

Due to the irregular distributions of aquifer hydraulic properties, the detail on the characterization of flow field cannot be anticipated. There can be a great degree of uncertainty in the prediction of heat transport processes anticipated in applying the traditional deterministic transport equation to field situations. This article is therefore devoted to quantification of uncertainty involving predictions over larger scales in terms of the temperature variance. A stochastic frame of reference is adopted to account for the spatial variability in hydraulic conductivity and specific discharge. Within this framework, the use of the first-order perturbation approximation and spectral representation leads to stochastic differential equations governing the mean behavior and perturbation of the temperature field in heterogeneous aquifers. It turns out that the mean equation developed in this sense is equivalent to the traditional deterministic transport equation and the temperature variance gives a measure of the prediction uncertainty from the traditional transport equation. The closed-form expression for the temperature variance developed here indicates that the controlling parameters such as the correlation scale of specific discharge, which measures the spatial persistence of the flow field, and the periodicity of the source term tend to increase the variability in temperature field in heterogeneous aquifers. The uncertainty of the traditional heat transport model increases as the penetration depth of thermal front through the aquifer increases. This suggests that prediction of temperature distribution using the traditional heat transport model in heterogeneous aquifers is expected to be subject to large uncertainty at a large depth (in the downstream region). For the management purpose, the variance of temperature could serve as a calibration target when applying the traditional model to field situations. It may be more reasonable to make conclusions from, say, the mean temperature with one or two standard deviations rather than only the mean temperature drawn from the traditional heat transport equation.

1. Introduction

It is well known that the transport of heat in aquifers is partly driven by the flowing groundwater. Especially vertical water fluxes are prone to propagate temperature differences. The fluctuations in aquifer properties are often viewed as random processes as a result of the details of which cannot be described precisely. The spatial variations in hydraulic conductivity cause a non-uniform velocity field. Many practical problems of heat transport involve predictions over much larger scales than these at which direct measurements are possible. It can thus be expected that there can be large uncertainty in predictions of heat transport in the field based on the traditional deterministic heat transport equation for a homogenous porous medium. Therefore, it is useful to provide a quantitative measure of uncertainty, such as the variance of the predicted temperature, as a calibration target when applying the deterministic model to field situations. This could be performed using a stochastic approach.

Stochastic modeling of subsurface flow and transport recognizes hydrological properties of the porous medium to be affected by uncertainty and regards these as random. This randomness leads to predictions of the flow or transport process in terms of a relatively small number of statistical properties, such as the first and second moments of hydraulic head or concentration (namely, the mean and variance, respectively). With the introduction of statistical inference, a field-scale equation containing effective coefficients such as effective hydraulic conductivities or macrodispersivities is developed to model the ensemble mean behavior of the dependent variable. In the case of natural formations, the mean stochastic

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Nomenclature

A	amplitude of temperature variations
C	specific heat capacity of the fluid–rock matrix
C_w	specific heat capacity of the fluid
G	Eq. (11)
K	hydraulic conductivity
K_e	effective thermal conductivity
L	length of the domain
P	period of temperature variations
R	wave number
S_{qq}	specific discharge spectrum
T	temperature
$\overline{T}$	mean temperature
T'	fluctuation in temperature
T'^*	complex conjugate of T'
U	$=\gamma q$
Z	vertical space coordinate
dZ_{q_z}	complex random amplitude of specific discharge process
q_i	ith component of the specific discharge vector
$\bar{q}_i$	ith component of the mean specific discharge vector
q_i'	fluctuation in ith component of the specific discharge vector
q	$=\bar{q}_Z$
t	time
Γ_1	Eq. (22)
Γ_2	Eq. (23)
Θ_{Tq}	transfer function
λ_1	Eq. (14)
λ_2	Eq. (15)
Ξ	$=(\sigma^2 T/A^2)^{0.5}$
Φ_1	Eq. (24)
Φ_2	Eq. (25)
Φ_3	Eq. (26)
Ψ	$=\overline{T}/A$
α_e	$=K_e/(\rho C)$
β	$=\pi\alpha_e/(UL)$
γ	$=\rho_w C_w/(\rho C)$
ε	Eq. (16)
η	$=PU/L$
λ	correlation scale of $\ln K$
μ_1	$=4\pi^2\upsilon^2+1$
μ_2	$=\pi^2\upsilon^2+1$
ζ	$=Z/L$
ρ	density of the fluid–rock matrix
ρ_w	density of the fluid
σ_f^2	variance of $\ln K$
σ_q^2	variance of the specific discharge
σ_T^2	variance of temperature
τ	$=\pi^2\alpha_e t/L^2$
ν	$=\lambda/L$
ϖ	$=\exp(-1/\upsilon)$

solution is useful to make decisions (e.g., Andricevic and Cvetkovic, 1996; Maxwell et al., 1999) in real life transport events, but there will be variations around the mean. Therefore, for a successful prediction a quantification of the degree of variability around the predicted mean behavior (the variance) should be established.

Determination of ground water flux using the analytical solution to the one-dimensional heat transport model has been demonstrated and applied to situations of stream–aquifer interactions (e.g., Stallman, 1965; Silliman et al., 1995; Hopmans et al., 2002; Hatch et al., 2006; Keery et al., 2007; Rau et al., 2010; Jensen and Engesgaard, 2011) and groundwater recharge (e.g., Suzuki, 1960; Taniguchi, 1993; Taniguchi and Sharma, 1993; Tabbagh et al., 1999; Bendjoudi et al., 2005; Cheviron et al., 2005). Interpretation of field observations using one-dimensional analytical results appropriate for a homogenous system may lead to significant errors in the predicted vertical flux in situations where the flow field is non-uniform (e.g., Shanafield et al., 2010; Schornberg et al., 2010; Jensen and Engesgaard, 2011; Ferguson and Bense, 2011; Rau et al., 2012b; Roshan et al., 2012; Cuthbert and Mackay, 2013). In other words, the prediction can be subject to high levels of uncertainty.

As will be seen in the next section given below, the mean heat transport equation is identical to the traditional equation except that the mean specific discharge is replaced by the local specific discharge. The traditional analytical result describing the temperature distribution may be interpreted as the mean of temperature distribution, while the temperature variance may then be viewed as the uncertainty anticipated in applying the deterministic analytical result. For the prediction of an actual temperature distribution in the field, it may be more reasonable to draw conclusions from the mean value (the analytical result) and the variance rather than only the mean temperature. This research is primarily concerned with the development of a quantification of deviation around the mean temperature field in a non-uniform flow field and the analysis of the influence of controlling parameters on that. The analysis we perform is relevant mainly to shallow subsurface situations that receive and transfer cyclic temperature fluctuations (i.e., daily or seasonal) over depth. The temperature fluctuations are damped with depth depending on their periodicity, so the solution generally applies to the surficial zone (Anderson, 2005). We hope that the findings provided here will be useful for interpretation of field data.

2. Mathematical statement of the problem

The heat transport equation for three-dimensional saturated flow in a porous medium at the local level can be written as (e.g., de Marsily, 1986; Demenico and Schwartz, 1998)

$$\frac{K_e}{\rho C}\frac{\partial^2 T}{\partial X_i^2} - \frac{\rho_W C_W}{\rho C}\frac{\partial}{\partial X_i}(q_i T) = \frac{\partial T}{\partial t} \quad i = 1, 2, 3 \tag{1}$$

where T is the temperature, K_e is the effective thermal conductivity, C and ρ are specific heat capacity and density of the fluid–rock matrix, respectively, C_w and ρ_w are specific heat capacity and density of the fluid, respectively, and q_i is the ith component of the specific discharge vector $\boldsymbol{q} = (q_1, q_2, q_3)$. The effective thermal conductivity takes into account the effects of thermal dispersion and conduction through the rock–fluid matrix. It is worth mentioning that the effect of thermal dispersion is very small and negligible (Bear, 1972; Hopmans et al., 2002; Rau et al., 2012a). The parameters in Eq. (1), such as K_e, C_w, C, ρ_w and ρ, are considered fixed parameters for their variations in space and time may be assumed to be negligible (e.g., Demenico and Schwartz, 1998; Anderson, 2005).

To account for the natural heterogeneity of geological formations, the log hydraulic conductivity $\ln K$ is regarded as the spatially correlated random function. Spatially correlated random heterogeneity in $\ln K$ field results in spatial perturbations in specific discharge in Eq. (1) and in turn in the modeled temperature field.

Spatial flux variability has been discussed recently based on small-scale experimental observations by Rau et al. (2012b). On a larger scale, the propagation of the temperature signal over depth in a heterogeneous streambed environment and its implications on flux estimates have been investigated numerically (e.g., Ferguson, 2007; Schornberg et al., 2010; Ferguson and Bense, 2011).

In this study, the flow field we are concerned with is under the steady-state condition, i.e., $\partial q_i/\partial X_i = 0$. This simplifies (1) to

$$\frac{K_e}{\rho C}\frac{\partial^2 T}{\partial X_i^2} - \frac{\rho_W C_W}{\rho C} q_i \frac{\partial T}{\partial X_i} = \frac{\partial T}{\partial t} \tag{2}$$

Consider a decomposition of variables q_i and T in space into a mean and a fluctuation about the mean represented, respectively, by

$$T = \overline{T} + T' \tag{3a}$$

and

$$q_i = \overline{q_i} + q_i' \tag{3b}$$

In Eq. (3) the bar represents the mean value while the prime denotes the small perturbation about the mean. The perturbation is considered to be a zero-mean, spatial stochastic process. In general, it is preferable to work with perturbations which are small such that the products of perturbations are small and negligible.

Following the approach of Gelhar and Axness (1983), we substitute (3) into (2) and subsequently take the expectation of the resulting equation to yield the equation governing the mean temperature:

$$\frac{K_e}{\rho C}\frac{\partial^2 \overline{T}}{\partial X_i^2} - \frac{\rho_W C_W}{\rho C} \overline{q_i} \frac{\partial \overline{T}}{\partial X_i} = \frac{\partial \overline{T}}{\partial t} \tag{4}$$

In the development of Eq. (4), terms involving products of the perturbations are disregarded. The differential equation governing the perturbations of temperature, T', is then obtained by subtracting the mean Eq. (4) from (2), after using (3) into (2):

$$\frac{K_e}{\rho C}\frac{\partial^2 T'}{\partial X_i^2} - \frac{\rho_W C_W}{\rho C} \overline{q_i} \frac{\partial T'}{\partial X_i} - \frac{\rho_W C_W}{\rho C} q_i' \frac{\partial \overline{T}}{\partial X_i} = \frac{\partial T'}{\partial t} \tag{5}$$

In the present study we are interested in the case where only the mean vertical heat transport is preponderant (e.g., Reiter, 2001). i.e., $\partial\ \overline{T}/\partial X_3 \gg \partial \overline{T}/\partial X_1$ and $\partial \overline{T}/\partial X_2$, and $\partial^2 \overline{T}/\partial X_3^2 \gg \partial^2 \overline{T}/\partial X_1^2$ and $\partial^2 \overline{T}/\partial X_2^2$. We also consider here the steady-state flow assumption, where the uniform mean flow is in the vertical direction (Z-direction or X_3-axis), $\bar{q}_1 = \bar{q}_2 = 0$ and $\bar{q}_3 = q$, but perturbations to the flow are in three dimensions. As such, (4) and (5) reduce, respectively, to

$$\alpha_e \frac{\partial^2 \overline{T}}{\partial Z^2} - \gamma q \frac{\partial \overline{T}}{\partial Z} = \frac{\partial \overline{T}}{\partial t} \tag{6}$$

$$\alpha_e \frac{\partial^2 T'}{\partial Z^2} - \gamma q \frac{\partial T'}{\partial Z} - \gamma q_Z' \frac{\partial \overline{T}}{\partial Z} = \frac{\partial T'}{\partial t} \tag{7}$$

where $\alpha_e = K_e/(\rho C)$, $\gamma = \rho_W C_W/(\rho C)$, and q_Z' is the perturbation to the flow in the Z-direction. Note that in the development of Eq. (7), the contribution of conduction and thermal dispersion in the transverse heat transport process is disregarded.

The mean transport Eq. (6) is identical in form to the traditional one-dimensional heat transport equation for a deterministic system if the mean specific discharge parameter in Eq. (6) is replaced with the local specific discharge parameter. The third term on the left-hand side of Eq. (7) is the sink term and reflects the dissipation produced by the mean temperature gradient interacting with the fluctuations in specific discharge. Therefore, the solution to Eq. (7), providing the relationship between the temperature and specific discharge perturbations, forms the basis for characterizing the variability (or uncertainty) of the mean (or traditional) heat transport model. Determination of the variation of temperature field from the use of the representation theorem is the line of the research pursued here.

Note that the representation theorem applied by this work is referred to the expectation of the product of the Fourier-Stieltjes integral representation for T' and its complex conjugate together with the orthogonality property of random Fourier increments of q_Z'. The representation theorem has been widely applied to compute the variances of hydraulic head and concentration fields in the stochastic subsurface hydrology literature (e.g., Gelhar, 1993; Zhang, 2002; Rubin, 2003).

To provide a complete description of the heat transport processes given by Eqs. (6) and (7), it is necessary to specify the initial and boundary conditions. The conditions we are concerned with are deterministic and similar to those imposed by Hatch et al. (2006):

$$\overline{T}(Z,0) = 0 \tag{8a}$$

$$\overline{T}(0,t) = A\cos\left(\frac{2\pi}{P}t\right) \tag{8b}$$

$$\overline{T}(L,t) = 0 \tag{8c}$$

and

$$T'(Z,0) = 0 \tag{9a}$$

$$T'(0,t) = 0 \tag{9b}$$

$$T'(L,t) = 0 \tag{9c}$$

where A and P are the amplitude and the period of temperature variations at the upper boundary, respectively (Stallman, 1965), and L denotes the maximal depth so that $Z \in [0,\ L]$. Note that Hatch et al. (2006) reformulated Stallman's solution (1965) to reveal the amplitude and phase features.

In the next section, we proceed to develop the analytical solution of Eq. (7), which requires (6) to be solved first in order to know the mean temperature gradient.

3. Solution to the stochastic perturbation equation

The analytical solution to Eq. (6) with boundary conditions (8) can be found by using the method of eigenfunction expansions (e.g., Farlow, 1993; Haberman, 1998) as:

$$\begin{aligned}\overline{T}(Z,t) =& 2AL^2\sum_{n=1}^{\infty}\frac{1}{n\pi}\sin\left(\frac{n\pi}{L}Z\right)\exp\left(\frac{UZ}{2\alpha_e}\right)\frac{1}{G}\left\{\exp\left[-\left(\frac{n^2\pi^2\alpha_e}{L^2}+\frac{U^2}{4\alpha_e}\right)t\right]\right.\\ &\times(64\alpha_e^2L^2\pi^2+4\alpha_e^2n^2P^2U^2\pi^2+L^2P^2U^4)\\ &\left.-[L^2P^2U^4+4\alpha_e^2\pi^2(16L^2+n^2P^2U^2)]\cos\left(\frac{2\pi}{P}t\right)+32\alpha_e^3n^2P\pi^3\sin\left(\frac{2\pi}{P}t\right)\right\}\\ &-2A\sum_{n=1}^{\infty}\frac{1}{n\pi}\sin\left(\frac{n\pi}{L}Z\right)\exp\left(\frac{UZ}{2\alpha_e}\right)\exp\left[-\left(\frac{n^2\pi^2\alpha_e}{L^2}+\frac{U^2}{4\alpha_e}\right)t\right]\\ &+A\frac{L-Z}{L}\exp\left(\frac{UZ}{2\alpha_e}\right)\cos\left(\frac{2\pi}{P}t\right)\end{aligned} \tag{10}$$

where $U = \gamma q$ and

$$G = 16\alpha_e^4n^4P^2\pi^4 + L^4P^2U^4 + 64\alpha_e^2L^4\pi^2 + 8\alpha_e^2L^2n^2P^2U^2\pi^2 \tag{11}$$

In the large-time limit $\alpha_e t/L^2 \gg 1/\pi^2$, we arrive at a simplified form of Eq. (10) as:

$$\overline{T}(Z,t) = \frac{2}{\pi}A\exp\left(\frac{\pi}{2}\frac{\xi}{\beta}\right)\sin(\pi\xi)\left\{\exp\left[-\left(1+\frac{1}{4}\frac{1}{\beta^2}\right)\tau\right](\Lambda_1-1) + \Lambda_2\sin\left(2\frac{\tau}{\beta\eta}\right) - \Lambda_1\cos\left(2\frac{\tau}{\beta\eta}\right)\right\} + A(1-\xi)\exp\left(\frac{\pi}{2}\frac{\xi}{\beta}\right)\cos\left(2\frac{\tau}{\beta\eta}\right) \tag{12}$$

and its spatial gradient takes the form

$$\frac{\partial\overline{T}}{\partial Z} = \frac{A}{L}\exp\left(\frac{\pi}{2}\frac{\xi}{\beta}\right)\left\{\left[\exp\left[-\left(1+\frac{1}{4}\frac{1}{\beta^2}\right)\tau\right](\Lambda_1-1) + \Lambda_2\sin\left(2\frac{\tau}{\beta\eta}\right) - \Lambda_1\cos\left(2\frac{\tau}{\beta\eta}\right)\right]\left[\frac{1}{\beta}\sin(\pi\xi) + 2\cos(\pi\xi)\right] + \left[\frac{\pi}{2}\frac{1}{\beta}(1-\xi) - 1\right]\cos\left(2\frac{\tau}{\beta\eta}\right)\right\} \tag{13}$$

where $\zeta = Z/L$, $\beta = \pi\alpha_e/(UL)$, $\tau = \pi^2\alpha_e t/L^2$, $\eta = PU/L$, and

$$\Lambda_1 = \frac{64(\beta^2/\eta^2) + 4\beta^2 + 1}{\varepsilon} \tag{14}$$

$$\Lambda_2 = 32\frac{\beta^3}{\eta\varepsilon} \tag{15}$$

$$\varepsilon = 16\beta^4 + 8\beta^2 + 64(\beta^2/\eta^2) + 1 \tag{16}$$

Eq. (13) puts us in a position to develop the analytical solution to Eqs. (7) and (9).

To determine the variance of temperature using the representation theorem, we need to construct a wave domain solution to Eqs. (7) and (9). When the specific discharge, the input parameter in Eq. (1), is defined as a second-order stationary process, its perturbed quantities can then be represented by a Fourier-Stieltjes integral representation

$$q'_Z = \int_{-\infty}^{\infty}\exp[iRZ]dZ_{q_Z}(R) \tag{17}$$

where $dZ_{q_1}(R)$ is a complex random amplitude of the process and R is the wave number. It is important to know that although the heat transport process analysis is carried out herein within a one-dimensional framework, the perturbation flow field is not a strictly one-dimensional flow. However, to simplify the analysis, Gelhar (1993) pointed out that the variability in longitudinal specific discharge can be determined within the context of such a quasi-one-dimensional treatment by using that obtained from a three-dimensional analysis. Duffy (1982) and Gelhar and Gutjahr (1982) used that conceptual framework in analysis of the one-dimensional transport problem. That is why the one-dimensional representation for the longitudinal specific discharge perturbation in Eq. (17) is used.

In addition, the non-stationary Fourier-Stieltjes integral representation (e.g., Li and McLaughlin, 1991) for the perturbed quantities allows us to relate the output (T') to input (q'_Z) perturbations in the following way

$$T' = \int_{-\infty}^{\infty}\Theta_{Tq}dZ_{q_z}(R) \tag{18}$$

where Θ_{Tq} represents the transfer function which describes the relationship between spectral fluctuations in specific discharge and spatial fluctuations in temperature. Introducing (17) and (18) into (7) yields

$$\alpha_e\frac{\partial^2\Theta_{Tq}}{\partial Z^2} - U\frac{\partial\Theta_{Tq}}{\partial Z} - \gamma\exp(iRZ)\frac{\partial\overline{T}}{\partial Z} = \frac{\partial\Theta_{Tq}}{\partial t} \tag{19}$$

where $\partial\overline{T}/\partial Z$ is defined in Eq. (13). Transformation of the initial and boundary conditions leads (9) to

$$\Theta_{Tq}(Z,0) = 0 \tag{20a}$$

$$\Theta_{Tq}(0,t) = 0 \tag{20b}$$

$$\Theta_{Tq}(L,t) = 0 \tag{20c}$$

For the case of $\alpha_e t/L^2 \gg 1/\pi^2$, the transfer function can be expressed as:

$$\Theta_{Tq}(Z,t;R) = 4\pi\frac{\gamma A}{LU^2\varepsilon}\exp\left(\frac{\pi}{2}\frac{\xi}{\beta}\right)\sin(\pi\xi) \times\left\{4\alpha_e\Gamma_1(\tau)[1-\exp(iRL)]\frac{R+i(U/\alpha_e)}{R(L^2R^2-4\pi^2)} + \Gamma_2(\tau)\left[\frac{LU-2\alpha_e(1+\exp[iRL])}{L^2R^2-\pi^2} - i2L^2U(1+\exp[iRL]) \times\frac{K}{(L^2R^2-\pi^2)^2}\right]\right\} \tag{21}$$

where

$$\Gamma_1(\tau) = \Phi_1\exp\left[-\left(1+\frac{1}{4}\frac{1}{\beta^2}\right)\tau\right] + \Phi_2\sin\left(2\frac{\tau}{\eta\beta}\right) - \Phi_3\cos\left(2\frac{\tau}{\eta\beta}\right) \tag{22}$$

$$\Gamma_2(\tau) = (4\beta^2+1)\left\{\cos\left(2\frac{\tau}{\eta\beta}\right) - \exp\left[\left(1+\frac{1}{4}\frac{1}{\beta^2}\right)\tau\right]\right\} + 8\frac{\beta}{\eta}\sin\left(2\frac{\tau}{\eta\beta}\right) \tag{23}$$

$$\Phi_1 = (4\beta^2+1)\Lambda_1 + 8\frac{\beta}{\eta}\Lambda_2 + \varepsilon(\Lambda_1-1)\frac{\tau}{4\beta^2} \tag{24}$$

$$\Phi_2 = (4\beta^2+1)\Lambda_2 - 8\frac{\beta}{\eta}\Lambda_1 \tag{25}$$

$$\Phi_3 = (4\beta^2+1)\Lambda_1 + 8\frac{\beta}{\eta}\Lambda_2 \tag{26}$$

Combining (21) with (18) gives

$$T' = 4\pi\frac{\gamma A}{LU^2\varepsilon}\exp\left(\frac{\pi}{2}\frac{\xi}{\beta}\right)\sin(\pi\xi) \times\int_{-\infty}^{\infty}\left\{4\alpha_e\Gamma_1(\tau)[1-\exp(iRL)]\frac{R+i(U/\alpha_e)}{R(L^2R^2-4\pi^2)} + \Gamma_2(\tau)\left[\frac{LU-2\alpha_e(1+\exp[iRL])}{L^2R^2-\pi^2} - i2L^2U(1+\exp[iRL])\frac{K}{(L^2R^2-\pi^2)^2}\right]\right\}dZ_{q_z}(R) \tag{27}$$

4. Variance of temperature

It follows from the use of the representation theorem for T' that

$$\sigma_T^2 = \langle T'T'^*\rangle = 16\pi^2\frac{\gamma^2A^2}{L^2U^4\varepsilon^2}\exp\left(\pi\frac{\xi}{\beta}\right)\sin^2(\pi\xi) \times\int_{-\infty}^{\infty}\left\{32\alpha_e^2\Gamma_1^2\frac{[R^2+(U/\alpha_e)^2][1-\cos(RL)]}{R^2(L^2R^2-4\pi^2)^2} + 8\alpha_e\Gamma_1\Gamma_2\left[\frac{LU[1-\cos(RL)]}{(L^2R^2-4\pi^2)(L^2R^2-\pi^2)} + \frac{(LU^2/\alpha_e-4U)\sin(RL)}{R(L^2R^2-4\pi^2)(L^2R^2-\pi^2)} - 4\frac{L^2UR\sin(RL)}{(L^2R^2-4\pi^2)(L^2R^2-\pi^2)^2}\right] + \Gamma_2^2\left[\frac{L^2U^2+8\alpha_e^2-4LU\alpha_e}{(L^2R^2-\pi^2)^2} + 4\frac{(2\alpha_e^2-\alpha_eLU)\cos(RL)}{(L^2R^2-\pi^2)^2} + 4\frac{L^3U^2R\sin(RL)}{(L^2R^2-\pi^2)^3} + 8\frac{U^2L^4R^2[1+\cos(RL)]}{(L^2R^2-\pi^2)^4}\right]\right\}S_{qq}(R)dR \tag{28}$$

where $\sigma^2 T$ is the variance of temperature, the angle bracket denotes the expected value operator, T'^* is the complex conjugate of T', and $S_{qq}(R)$ is the specific discharge spectrum in wave number domain. Eq. (28) provides a means of quantifying the temperature variability for the mean heat transport process or the uncertainty in applying the traditional (deterministic) heat transport model.

Before evaluation of Eq. (28) can be completed, it is necessary to select the spectrum of the specific discharge process. We consider a particular form for S_{qq}(R) (Bakr et al., 1978; Duffy, 1982)

$$S_{qq}(R) = \frac{2}{\pi}\frac{\Lambda^3 R^2}{(1+\Lambda^2 R^2)^2}\sigma_q^2 \tag{29}$$

which is widely applicable to modeling of natural phenomena. In Eq. (29), where λ and σ_q^2 represent the correlation scale and the variance of the specific discharge process.

$$\begin{aligned}\sigma_T^2 = {}& 64A^2\frac{\beta^2}{\varepsilon^2}\frac{\sigma_q^2}{q^2}\exp\left(\pi\frac{\xi}{\beta}\right)\sin^2(\pi\xi)\Bigg\{32\Gamma_1^2\upsilon^3\left[\frac{1}{4}\frac{\upsilon}{\mu_1^2}-\frac{\upsilon}{\mu_1^3}+\frac{\pi^2}{\beta^2}\left(\frac{1}{16\pi^2}\frac{1}{\mu_1^2}+\frac{1}{4}\frac{1}{\mu_1^2}[1+(1-\upsilon)\varpi-\upsilon^2(1+\upsilon)\varpi+\upsilon^3]+\frac{\upsilon(1-\varpi)(\upsilon^2-1)}{\mu_1^3}\right)\right]\\ &+8\Gamma_1\Gamma_2\upsilon\Bigg[\frac{1}{3\pi\beta}\Bigg(\frac{1}{4}\frac{1}{\mu_1}\left[\frac{4}{3\pi^2}(1/\upsilon-2)\varpi+4\upsilon^2\varpi-\upsilon-(1-\upsilon)\varpi\right]+\frac{1}{2}\frac{1}{\mu_1^2}\left[\frac{4}{3\pi^2}\varpi+\frac{16}{3}\upsilon^2-\upsilon(1-\varpi)(4\upsilon-1)\right]\\ &+\frac{1}{4}\frac{1}{\mu_2}\left[\upsilon+(1-\upsilon)\varpi-4\upsilon\varpi+\frac{4}{3\pi^2}(2-1/\upsilon)\varpi\right]+\frac{1}{2}\frac{1}{\mu_2^2}\left[(\varpi-1)\upsilon-2\upsilon^2(2-1/\upsilon)\varpi-4\upsilon^2\varpi+\frac{4}{3}\upsilon^2-\frac{4}{3\pi^2}\varpi\right]+\frac{4\upsilon^2}{\mu_2^3}[\pi^2\upsilon^2-\varpi]\Bigg)\\ &+\frac{1}{6\beta^2}\left(-\frac{1}{2}\frac{\upsilon\varpi}{\mu_1}+\frac{\upsilon^2(1-\varpi)}{\mu_1^2}+\frac{1}{2}\frac{\upsilon\varpi}{\mu_2}+\frac{\upsilon^2(1+\varpi)}{\mu_2^2}\right)\Bigg]+\Gamma_2^2\upsilon^3\Bigg[2\frac{1+\upsilon-(1-\upsilon)\varpi}{\mu_2^2}-8\frac{\upsilon(1+\varpi)}{\mu_2^3}+\frac{\pi}{\beta}\left(\frac{(1-\upsilon)\varpi-\upsilon-1}{\mu_2^2}+4\frac{\upsilon(1+\varpi)}{\mu_2^3}\right)\\ &+\frac{\pi^2}{\beta^2}\left(\frac{1}{12\pi^2}\frac{-3\pi^2\upsilon+2\pi^2+3}{\mu_2^2}-\frac{\upsilon}{\mu_2^3}[\upsilon+(2\upsilon-1)\varpi-1]-2\frac{\upsilon^2}{\mu_2^4}[3\upsilon+(3\upsilon-4)\varpi]+16\upsilon^3\frac{1+\varpi}{\mu_2^5}\right)\Bigg]\Bigg\}\end{aligned} \tag{30}$$

Substituting (29) into (28) and performing integration yields- where $\upsilon = \lambda/L$, $\varpi = \exp(-1/\upsilon)$, $\mu_1 = 4\pi^2\upsilon^2 + 1$ and $\mu_2 = \pi^2\upsilon^2 + 1$. From a three-dimensional analysis of first-order fluctuations in flow field, the variance of the specific discharge can be expressed in the form (Gelhar and Axness, 1983; Dagan, 1987; Chang and Yeh, 2007)

$$\frac{\sigma_q^2}{q^2} = \frac{8}{15}\sigma_f^2 \tag{31}$$

where σ_f^2 is the variance of ln$K$. With (31), the final result is now given by

$$\begin{aligned}\sigma_T^2 = {}& \frac{512}{15}A^2\sigma_f^2\frac{\beta^2}{\varepsilon^2}\exp\left(\pi\frac{\xi}{\beta}\right)\sin^2(\pi\xi)\Bigg\{32\Gamma_1^2\upsilon^3\left[\frac{1}{4}\frac{\upsilon}{\mu_1^2}-\frac{\upsilon}{\mu_1^3}+\frac{\pi^2}{\beta^2}\left(\frac{1}{16\pi^2}\frac{1}{\mu_1^2}+\frac{1}{4}\frac{1}{\mu_1^2}[1+(1-\upsilon)\varpi-\upsilon^2(1+\upsilon)\varpi+\upsilon^3]+\frac{\upsilon(1-\varpi)(\upsilon^2-1)}{\mu_1^3}\right)\right]\\ &+8\Gamma_1\Gamma_2\upsilon\Bigg[\frac{1}{3\pi\beta}\Bigg(\frac{1}{4}\frac{1}{\mu_1}\left[\frac{4}{3\pi^2}(1/\upsilon-2)\varpi+4\upsilon^2\varpi-\upsilon-(1-\upsilon)\varpi\right]+\frac{1}{2}\frac{1}{\mu_1^2}\left[\frac{4}{3\pi^2}\varpi+\frac{16}{3}\upsilon^2-\upsilon(1-\varpi)(4\upsilon-1)\right]\\ &+\frac{1}{4}\frac{1}{\mu_2}\left[\upsilon+(1-\upsilon)\varpi-4\upsilon\varpi+\frac{4}{3\pi^2}(2-1/\upsilon)\varpi\right]+\frac{1}{2}\frac{1}{\mu_2^2}\left[(\varpi-1)\upsilon-2\upsilon^2(2-1/\upsilon)\varpi-4\upsilon^2\varpi+\frac{4}{3}\upsilon^2-\frac{4}{3\pi^2}\varpi\right]+\frac{4\upsilon^2}{\mu_2^3}[\pi^2\upsilon^2-\varpi]\Bigg)\\ &+\frac{1}{6\beta^2}\left(-\frac{1}{2}\frac{\upsilon\varpi}{\mu_1}+\frac{\upsilon^2(1-\varpi)}{\mu_1^2}+\frac{1}{2}\frac{\upsilon\varpi}{\mu_2}+\frac{\upsilon^2(1+\varpi)}{\mu_2^2}\right)\Bigg]+\Gamma_2^2\upsilon^3\Bigg[2\frac{1+\upsilon-(1-\upsilon)\varpi}{\mu_2^2}-8\frac{\upsilon(1+\varpi)}{\mu_2^3}+\frac{\pi}{\beta}\left(\frac{(1-\upsilon)\varpi-\upsilon-1}{\mu_2^2}+4\frac{\upsilon(1+\varpi)}{\mu_2^3}\right)\\ &+\frac{\pi^2}{\beta^2}\left(\frac{1}{12\pi^2}\frac{-3\pi^2\upsilon+2\pi^2+3}{\mu_2^2}-\frac{\upsilon}{\mu_2^3}[\upsilon+(2\upsilon-1)\varpi-1]-2\frac{\upsilon^2}{\mu_2^4}[3\upsilon+(3\upsilon-4)\varpi]+16\upsilon^3\frac{1+\varpi}{\mu_2^5}\right)\Bigg]\Bigg\}\end{aligned} \tag{32}$$

5. Discussion

The analytical results above are developed based on the key assumptions of smallness of the perturbations of specific discharge and temperature (the first-order perturbation approximation), second-order stationarity of the specific discharge perturbations, and nonstationary representation for the temperature perturbation. At this point it is appropriate to review those assumptions. In terms of the variability of ln$K$, the first-order perturbation approximation leading to the analytical results is valid only if the variance of ln$K \ll 1$ (Gutjahr and Gelhar, 1981). That is, the variance of temperature developed here based on the first-order approximation is restricted to the case of mildly heterogeneous media. However, the study of Monte Carlo simulations of flow through heterogeneous formations shows agreement with the small perturbation approximation for the moments of hydraulic head with variance up to 4 (Zhang and Winter, 1999; Guadagnini and Neuman, 1999).

The assumption of stationarity of the specific discharge field is valid when the mean hydraulic head field is uniform (or relatively smooth). In other words, the only source of variability in specific discharge is the hydraulic conductivity perturbation field. The logarithm of hydraulic conductivity in this work is modeled as a realization of a stationary random field and, in turn, stationarity of the specific discharge field is presumed. On the other hand, the space-dependent mean temperature gradient (see Eq. (13)) produces nonstationarity of temperature perturbation process, which excludes the direct applicability of the stationary spectral representation. The nonstationary Fourier-Stieltjes integral representation (Li and McLaughlin, 1991) is then used to represent the temperature perturbation process instead.

The result in Eq. (32) shows that the amplitude of the temperature variance is linearly proportional to the variance of $\ln K$. The textural variations exhibited in natural porous media give rise to spatial variability of their constitutive properties. This implies that the temperature variability increases linearly with the heterogeneity of the aquifer for mildly heterogeneous formations.

The variance of temperature as a function of correlation scale of specific discharge for various values of η is presented graphically in Fig. 1. Similar to the field-scale solute transport process, the correlation scale λ has a positive influence on the temperature variance. As λ increases, the persistence of correlations increases and the fluctuations spend less time around the mean. This results in a large variability in temperature field. The figure also indicates that increasing period of temperature variations P tends to increase the temperature variance with λ held constant. As pointed out by Goto et al. (2005) and Wörman et al. (2012), the damping of thermal front is related to the periodicity of the source term. The thermal front with small period of temperature variations penetrates more rapidly into the aquifer than the large one does, but is dampened more abruptly with depth, which leads to a less variability in temperature field.

Fig. 2 shows how the variability in temperature field varies with the depth. As the thermal front penetrates large regions of the aquifer, the transported heat responds to larger and larger heterogeneities. There is a change in the size of those heterogeneities with the depth in the associated flow field that affects the movement of heat transport. This is why the temperature variability increases with the depth. The increase of variability in temperature field with the depth reveals that the prediction of temperature distribution is subject to large uncertainty in the far-source region (downstream region) in heterogeneous aquifers.

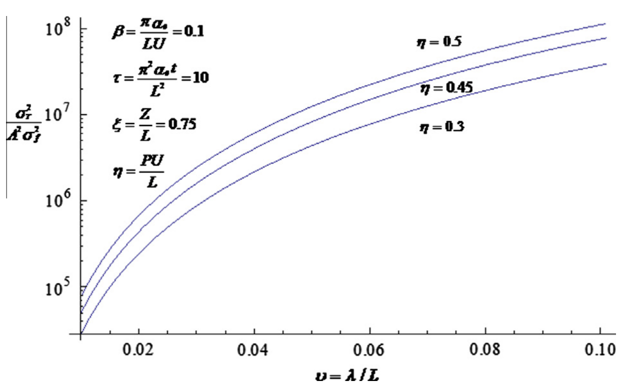

Fig. 1. Dimensionless temperature variance as a function of dimensionless correlation length of specific discharge.

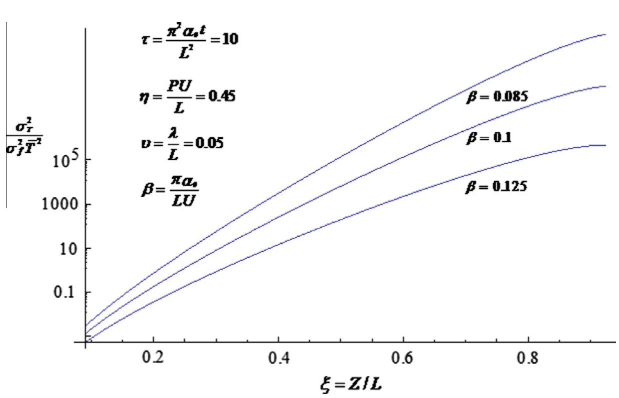

Fig. 2. Dimensionless temperature variance as a function of dimensionless depth.

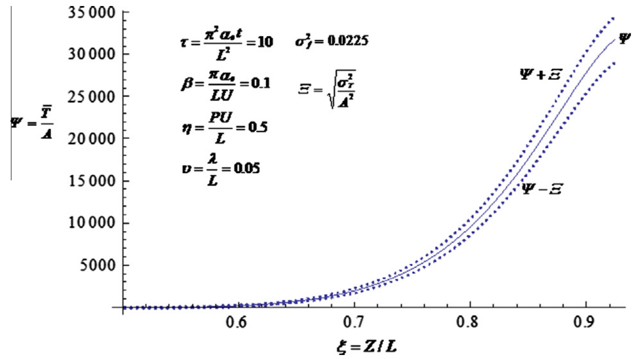

Fig. 3. Dimensionless temperature profile with mean ± one standard deviation envelopes.

The analytical solution (12) to the mean temperature equation described in this work is equivalent to that to the traditional one-dimensional deterministic heat transport equation (e.g., Stallman, 1965). We can anticipate irregular variations in temperature around the mean in natural porous media. Therefore, the variance (32) gives us a quantitative measure of the uncertainty in applying the traditional transport model to field situations. The most challenging types of heat transport problems involve predictions over much larger scales where direct measurements are not possible. Under such conditions, the mean profile along with standard deviations provides a useful way of evaluating the model prediction. For practical applications of heat transport modeling in the field, for example for management purposes, it may be more reasonable to consider, say, the mean temperature with one standard deviation (square root of Eq. (32)) rather than only the mean temperature drawn from the traditional heat transport equation. Fig. 3 indicates that the level of uncertainty grows with the depth and is largest in the downstream. Presented in solid line is the predicted mean temperature field, while the dashed lines present the temperature field corresponding to the ± one standard deviation.

6. Conclusions

The perturbation-based nonstationary spectral techniques have been applied to quantify the variability in temperature field in a heterogeneous aquifer. The closed-form expressions developed here apply to the region of shallow subsurface. We conclude from the analysis of the closed-form expression for the temperature variance that the correlation length scale of the specific discharge and the period of temperature variations have a strong influence on increasing the variability of temperature field. In addition, there can be large uncertainty in the prediction of temperature distribution at a large depth in heterogeneous aquifers. From the practical application viewpoint, a result such as (32) could serve as a calibration target when applying the traditional deterministic transport equation to the field situations.

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