# Groundwater

Technical Commentary/

# Uncertainty Estimation in One-Dimensional Heat Transport Model for Heterogeneous Porous Medium

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# **Abstract**

In many practical applications, the rates for ground water recharge and discharge are determined based on the analytical solution developed by Bredehoeft and Papadopulos (1965) to the one-dimensional steady-state heat transport equation. Groundwater flow processes are affected by the heterogeneity of subsurface systems; yet, the details of which cannot be anticipated precisely. There exists a great deal of uncertainty (variability) associated with the application of Bredehoeft and Papadopulos' solution (1965) to the field-scale heat transport problems. However, the quantification of uncertainty involved in such application has so far not been addressed, which is the objective of this wok. In addition, the influence of the statistical properties of log hydraulic conductivity field on the variability in temperature field in a heterogeneous aquifer is also investigated. The results of the analysis demonstrate that the variability (or uncertainty) in the temperature field increases with the correlation scale of the log hydraulic conductivity covariance function and the variability of temperature field also depends positively on the position.

# Introduction

Heat as a natural groundwater tracer has been used frequently to assess the interchange of groundwater and surface water in groundwater basins by various approaches (e.g., Anderson 2005; Ferguson and Woodbury 2005; Brookfield et al. 2009; Saar 2010; Lewandowski et al. 2011). The analytical approaches afford fast and straightforward means for determining surface water infiltration rates from temperature measurements. Bredehoeft and Papadopulos (1965) developed an analytical solution for temperature profiles to describe the vertical steady flow of groundwater and heat through an isotropic, homogeneous, and fully saturated semiconfining

layer. A graphical type curve solution method based on temperature-depth profiles for estimating groundwater velocities also presented by them. Building on their work, the rates for ground water recharge and discharge in basins were predicted in many studies (e.g., Cartwright 1970; Taniguchi 1993, 1994; Ferguson et al. 2003; Schmidt et al. 2006; Anibas et al. 2009; Schornberg et al. 2010).

It has been generally recognized that dispersion of soluble plumes in groundwater is caused by large-scale spatial heterogeneities of geologic formations. The natural heterogeneity of the subsurface environment (including spatial variations of soil properties such as hydraulic conductivity) results in a nonuniform velocity field. The spatial fluctuations of velocity enhance the spreading of solutes and contribute to the highly irregular character of the concentration distribution in field-scale plumes. Because of the analogy between the contaminant transport and heat transport, it is expected that the heterogeneity of natural formations also plays an important role in influencing the heat advection at field scale. Therefore, the prediction of field-scale heat transport from the classical heat transport equation in the uniform velocity field,

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developed at the local scale, is subject to a great deal of uncertainty.

The hydraulic properties of the aquifer materials are known to be highly variable in space. In most practical situations, there are never enough data in describing the spatial distributions of these properties in detail. Those problems may result in large uncertainty in predicting field-scale heat transport. From the practical application point of view, the classical deterministic heat transport equation may be viewed as an averaging one in a stochastic sense, and the uncertainty (variability) needs to be recognized when applying the mean transport model. As such, the primary purpose of this study is to provide a quantitative measure of uncertainty in assessing the heat transport model of Bredehoeft and Papadopulos (1965) applied to field situations.

# **Temperature Perturbation**

As the starting point, we assume that the temperature distribution in a locally saturated porous medium under the steady-state condition can be characterized by the Darcy-scale transport equation expressed as (e.g., de Marsily 1986)

$$\alpha_{\rm e} \frac{\partial^2 T}{\partial X_i \partial X_j} - \frac{\partial}{\partial X_i} (q_i T) = 0, \ i, j = 1, 2, 3$$
 (1)

where T is the temperature,  $\alpha_e = K_e/\rho_w C_w$ ,  $K_e$  is the effective thermal conductivity,  $C_w$  and  $\rho_w$  are specific heat and density of the fluid, respectively, and  $q_i$  is the ith component of the specific discharge vector  $\mathbf{q} = (q_1, q_2, q_3)$ . In Equation (1),  $K_e$ ,  $\rho_w$ , and  $C_w$  are considered as constants. The effect of varying the effective thermal conductivity is small when compared with the effect of varying the hydraulic conductivity (e.g., Bear 1972; Hopmans et al. 2002; Anderson 2005) so that the effective thermal conductivity in Equation (1) is treated as a constant.

In the absence of sources or sinks, the conservation of total mass for a steady state fluid flow:

$$\frac{\partial q_i}{\partial X_i} = 0 \tag{2}$$

is imposed. This simplifies Equation (1) to

$$\alpha_{\rm e} \frac{\partial^2 T}{\partial X_i \partial X_i} - q_i \frac{\partial T}{\partial X_i} = 0 \tag{3}$$

In the following analysis, we concern the case where both temperature and specific discharge are realizations of space random fields. In addition, they can be decomposed and expressed in terms of their mean and perturbation around the mean as

$$T = \overline{T} + T^{'} \tag{4}$$

$$q_{i} = \overline{q_{i}} + q'_{i} \tag{5}$$

where the bar represents the mean value and the prime denotes the perturbation of the quantity. Substituting the perturbed forms (4) and (5) into Equation (3) and retaining only first-order terms (i.e., removing terms involving products of the perturbations) gives

$$\alpha_{e} \frac{\partial^{2}}{\partial X_{i} \partial X_{j}} \left( \overline{T} + T' \right) - \overline{q_{i}} \frac{\partial \overline{T}}{\partial X_{i}} - \overline{q_{i}} \frac{\partial T'}{\partial X_{i}} - q'_{i} \frac{\partial \overline{T}}{\partial X_{i}} = 0$$
(6)

The expectation of Equation (6) results in

$$\alpha_{\rm e} \frac{\partial^2 \overline{T}}{\partial X_i \partial X_j} - \overline{q_i} \frac{\partial \overline{T}}{\partial X_i} = 0 \tag{7}$$

which governs the mean temperature field. Subtracting the mean Equation (7) from Equation (6) leads to the first-order perturbation equation for T', that is,

$$\alpha_{\rm e} \frac{\partial^2 T'}{\partial X_i \partial X_j} - \overline{q_i} \frac{\partial T'}{\partial X_i} - q_i' \frac{\partial \overline{T}}{\partial X_i} = 0 \tag{8}$$

For the case of the mean groundwater flow aligned with the  $X_1$  direction so that  $\overline{q}_1 = q$  and  $\overline{q}_2 = \overline{q}_3 = 0$ , the mean and perturbation equations, Equations (7) and (8), take the forms, respectively, as

$$\alpha_{\rm e} \frac{\partial^2 \overline{T}}{\partial X_1^2} - q \frac{\partial \overline{T}}{\partial X_1} = 0 \tag{9}$$

$$\alpha_{\rm e} \frac{\partial^2 T'}{\partial X_i^2} - q \frac{\partial T'}{\partial X_1} - q_1' \frac{\partial \overline{T}}{\partial X_1} = 0 \tag{10}$$

For the case of vertical one-dimensional heat transport through an isotropic, homogeneous, and fully saturated porous medium, Equation (3) can be simplified to

$$\alpha_{\rm e} \frac{\partial^2 T}{\partial X_1^2} - q_1 \frac{\partial T}{\partial X_1} = 0 \tag{11}$$

An analytical solution to this equation constrained with prescribed temperatures  $T_0$  and  $T_L$  specified at  $X_1 = 0$  and  $X_1 = L$ , respectively, is in the form (Bredehoeft and Papadopulos 1965)

$$T = T_0 + (T_L - T_0) \frac{\exp[X_1/\mu] - 1}{\exp[L/\mu] - 1}$$
 (12)

where  $\mu = \alpha_e/q_1$ . A temperature profile consisting of a few measurement points with depth and the temperatures at the upper and lower boundaries are sufficient to obtain a fit with Equation (12) and then to obtain reasonable flux estimates (Schmidt et al. 2007; Anibas et al. 2009). Jensen and Engesgaard (2011) mentioned that the steady-state solution is most suitable in the period where

there is a marked difference in temperature between the groundwater and the boundary.

Lu and Ge (1996) presented an extension of the Bredehoeft and Papadopulos model by introducing an additional source (or sink) term in accounting for constant horizontal flows of water and heat. Their analytical results demonstrated that the horizontal flows of heat and fluid have a negligible effect on the vertical temperature distribution if the rates are less than 10% of the vertical. But the effect becomes significant when it is comparable to the vertical. In addition, from the numerical simulations of stochastic models of heat and fluid flow in a twodimensional porous medium, Ferguson and Bense (2011) concluded that one-dimensional analytical solution can provide good estimates of specific discharge into streams for the specific discharge ranging between  $1 \times 10^{-7}$ and  $1 \times 10^{-5}$  m/s for the case with variance of log hydraulic conductivity less than 1.0 m<sup>2</sup>/s<sup>2</sup>. However, conduction into areas with the specific discharge less than  $10^{-7}$  m/s from adjacent areas can lead to significant errors.

Note that under the assumption of uniform mean flow (or a uniform mean head gradient) in the  $X_1$  direction, the mean heat transport equation (9) in this study will be equivalent to the classical one-dimensional transport equation proposed by Bredehoeft and Papadopulos (1965) if the specific discharge in their transport equation is replaced with the mean specific discharge. Equation (12) may then be read as the expression for the mean temperature distribution with the gradient of

$$\Lambda = \frac{\partial \overline{T}}{\partial X_1} = \eta \exp\left[X_1/\mu\right] \tag{13}$$

where

$$\eta = \frac{T_L - T_0}{\mu} \frac{1}{\exp\left[L/\mu\right] - 1} \tag{14}$$

The variable  $\mu$  in Equation (13) is now defined as  $\mu = \alpha_{\rm e}/q$ . Through Equation (13), Equation (10) may be rewritten as

$$\alpha_{\rm e} \frac{\partial^2 T^{\prime}}{\partial X_{\rm i}^2} - q \frac{\partial T^{\prime}}{\partial X_{\rm 1}} - q^{\prime}_{1} \Lambda = 0 \tag{15}$$

# **Temperature Variance**

In this section we attempt to quantify the uncertainty (temperature variance) to be anticipated in applying Equation (12). This can be done through the application of the spectral representation theorem (e.g., Gelhar 1986) for the temperature perturbations.

The space-dependent  $\Lambda$  in Equation (15) causes the nonstationarity in the temperature fields, a transfer-function approach (or nonstationary spectral representation) (Li and McLaughlin 1991) is therefore used to solve Equation (15). On the other hand, because of the uniform mean flow assumption, the only source of variability

in specific discharge is the hydraulic conductivity perturbation field. In this work, the logarithm of hydraulic conductivity  $(\ln K)$  is modeled as a realization of a stationary random field and, in turn, stationarity of the specific discharge field is presumed.

If the specific discharge perturbation field is expressed in a Fourier spectral framework as

$$q_{1}^{'} = \int_{-\infty}^{\infty} \exp\left[i\mathbf{R} \cdot \mathbf{X}\right] dZ_{q_{1}}(\mathbf{R})$$
 (16)

then the temperature perturbation field will admit the following form in terms of a transfer function  $\Phi_{Ta}$  as

$$T' = \int_{-\infty}^{\infty} \Phi_{Tq} dZ_{q_1}(\mathbf{R})$$
 (17)

In Equations (16) and (17),  $dZ_{ql}(\mathbf{R})$  is a complex random amplitude, which is a function of a vector of wave numbers  $\mathbf{R} = (R_1, R_2, R_3)$ . Introducing Equations (16) and (17) into Equation (15) leads to

$$\int_{-\infty}^{\infty} \{ \alpha_{e} \frac{\partial^{2} \Phi_{Tq}}{\partial X_{i}^{2}} - q \frac{\partial \Phi_{Tq}}{\partial X_{1}} - \Lambda \exp\left[i\mathbf{R} \cdot \mathbf{X}\right] \} dZ_{q_{1}}(\mathbf{R}) = 0$$
(18)

Making use of the uniqueness of the spectral representation in Equation (18) with  $\Lambda = \eta \exp[X_1/\mu]$  in Equation (13) results in

$$\alpha_{\rm e} \frac{\partial^2 \Phi_{Tq}}{\partial X_i^2} - q \frac{\partial \Phi_{Tq}}{\partial X_1} - \eta \exp\left[i\mathbf{R} \cdot \mathbf{X} + X_1/\mu\right] = 0 \quad (19)$$

Equation (19) admits the following solution:

$$\Phi_{Tq} = -\eta \frac{\exp\left[i\mathbf{R}\cdot\mathbf{X} + X_1/\mu\right]}{q\left(\mu R^2 - iR_1\right)}$$
(20)

where  $R^2 = R_1^2 + R_2^2 + R_3^2$ . It follows from Equations (17) and (20) that

$$T^{'} = -\eta \exp\left[X_{1}/\mu\right] \int_{-\infty}^{\infty} \frac{\exp\left[i\boldsymbol{R} \cdot \boldsymbol{X}\right]}{q\left(\mu R^{2} - iR_{1}\right)} dZ_{q_{1}}(\boldsymbol{R})$$
(21)

Note that to take the advantage of an analytical solution, the perturbation-boundary effect on  $T^\prime$  is assumed very small and negligible in obtaining Equation (20). It is expected that the perturbation-boundary effect is largely limited to a small region close to the medium boundary when dealing with field-scale flow phenomena (e.g., Rubin and Dagan 1988, 1989). A similar assumption has been made by, for example, Li and McLaughlin (1995), Lu and Zhang (2002), and Chang and Yeh (2010) to analyze the behavior of field-scale flow in heterogeneous aquifers.

By taking the expected value of the product of the Fourier-Stieltjes integral representation for T' in

Equation (21) and its complex conjugate together with the orthogonality property of random Fourier increments of  $q'_1$  (virtue of representation theorem), we obtain the variance of temperature as follows:

$$\sigma_{T}^{2} = \left\langle T'T'^{*}\right\rangle = \eta^{2} \exp\left[2X_{1}/\mu\right]$$

$$\times \int_{-\infty}^{\infty} \frac{1}{q^{2} \left(\mu^{2} R^{4} + R_{1}^{2}\right)} \left\langle dZ_{q_{1}}(\mathbf{R}) dZ_{q_{1}}^{*}(\mathbf{R})\right\rangle$$

$$= \eta^{2} \exp\left[2X_{1}/\mu\right] \int_{-\infty}^{\infty} \frac{1}{\mu^{2} R^{4} + R_{1}^{2}} \frac{S_{q_{1}q_{1}}(\mathbf{R})}{q^{2}} d\mathbf{R} \quad (22)$$

where the asterisk superscript identifies the complex conjugation, <> stands for the ensemble average, and  $Sq_1q_1$  is the specific discharge wave number spectrum in the  $X_1$  direction. The reader may be referred to the books, e.g., by Gelhar (1993), Zhang (2002), and Rubin (2003) for a detailed application of representation theorem to the analysis of the field-scale groundwater and solute transport processes in heterogeneous aquifers.

The specific discharge wave number spectrum in the  $X_1$  direction can be computed according to Gelhar and Axness (1983)

$$S_{q_1q_1}(\mathbf{R}) = q^2 \left(1 - \frac{R_1^2}{R^2}\right)^2 S_{ff}(\mathbf{R})$$
 (23)

where  $S_{ff}(\mathbf{R})$  is the spectral density function of the random log hydraulic conductivity field (lnK). Combining Equation (23) with Equation (22) gives the form

$$\begin{split} \sigma_T^2 &= \eta^2 \exp\left[2X_1/\mu\right] \\ &\times \int_{-\infty}^{\infty} \frac{1}{\mu^2 R^4 + R_1^2} \left(1 - \frac{R_1^2}{R^2}\right)^2 S_{ff}\left(\pmb{R}\right) d\pmb{R} \end{split} \tag{24}$$

We proceed to compute Equation (24) explicitly. A hole-type exponential function (Vomvoris and Gelhar 1990) is considered representing the spatial pattern of correlation of random log hydraulic conductivity field  $(\ln K)$ , which has the following wave number spectrum:

$$S_{ff}(R) = \frac{4 \sigma_f^2}{3 \pi^2} \frac{\lambda^5 R^2}{(1 + \lambda^2 R^2)^3}$$
 (25)

(26)

where  $\lambda$  represents the correlation scale of  $\ln K$  and  $\sigma_f^2$  is the variance of  $\ln K$ . With  $S_{ff}(R)$  given in Equation (25), integrating Equation (24) over the wave number domain yields the temperature variance

$$\frac{\sigma_T^2}{(T_L - T_0)^2} = \frac{2}{9} \sigma_f^2 \frac{\exp\left(2\frac{X_1}{L}\frac{L}{\mu}\right)}{\left[\exp\left(\frac{L}{\mu}\right) - 1\right]^2} \times \frac{1}{P} \left[3P^4 - 4P^3 + 6P^2 - 12P + 12\ln(P+1)\right]$$

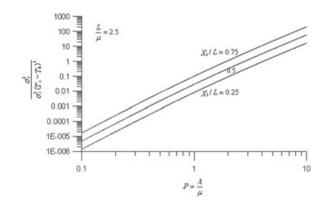


Figure 1. Dimensionless temperature variance as a function of dimensionless correlation length of lnK.

where  $P = \lambda/\mu$ . Due to the assumption of negligible boundary effects on the perturbation solution made above, Equation (26) is not applicable to the small region next to the boundary.

It is apparent from Equation (26) that there is a linear relationship between the variability in temperature fields and the heterogeneity of the medium  $(\sigma_f^2)$ . The temperature variation will be large in areas where there exists a large difference in temperature between the groundwater and the boundary. Figure 1 demonstrates how the temperature variance in Equation (26) is influenced by the lnK correlation scale. As indicated in the figure, the variability in temperature field increases with the lnK correlation scale,  $\lambda$ . A larger  $\lambda$  produces a higher persistence of fluctuations in lnK field around the mean. This implies that positive increments in lnK tend to be followed by other positive increments, while negative increments tend to be followed by other negative increments. In other words, the lnK fluctuations are either consistently above or below the mean for a large  $\lambda$ . Those contribute to a greater variance of the specific discharge since the fluctuations in  $\ln K$ field acts as the source of the fluctuations in groundwater specific discharge field. In addition, the convection of heat is carried by the groundwater flow in aquifers. The fluctuations in the temperature field are therefore a direct result of those in the specific discharge in heterogeneous aguifers. Therefore, an increased variability in the specific discharge caused by a larger  $\lambda$  will introduce greater variability of the temperature field around the mean. This is why the variability in temperature field is enhanced by a larger  $\lambda$ . Figure 1 also indicates that the temperature variance is positively related to the position.

# An Example of the Uncertainty of Temperature Profiles

The square root of Equation (26), one standard deviation of the mean values, offers a useful basis to quantify the uncertainty associated with the prediction of temperature profiles in field situations using Equation (12). About 68.2% of the time, the value of temperature falls within the range of mean temperature  $\pm$  one standard deviation.

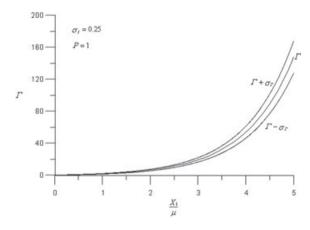


Figure 2. Normalized temperature profiles along with one standard deviation intervals as a function of dimensionless position.

When the temperature profiles and the temperature variance are normalized by the quantity  $\Xi = (T_L - T_0)/[\exp(L/\mu) - 1]$ , respectively, then Equations (12) and (26) can be expressed as

$$\Gamma = \frac{\overline{T} - T_0}{\Xi} = \exp\left[X_1/\mu\right] - 1 \tag{27}$$

$$\sigma_{\Gamma}^{2} = \frac{\sigma_{T}^{2}}{\Xi^{2}} = \frac{2}{9}\sigma_{f}^{2} \left[ \exp\left(\frac{X_{1}}{\mu}\right) \right]^{2} \times \frac{1}{P} \left[ 3P^{4} - 4P^{3} + 6P^{2} - 12P + 12\ln(P+1) \right]$$
 (28)

Figure 2 shows the normalized mean temperature profiles in Equation (27) along with one standard deviation  $(\sigma_{\Gamma})$  intervals plotted as the dimensionless  $X_1$ -coordinate. It reveals that the prediction of temperature distribution at large position in heterogeneous aquifers is subject to large uncertainty. This implies that there can be of large uncertainty anticipated in heat transport prediction in the far-source region (downstream region) based on the analytical solution of Bredehoeft and Papadopulos (1965), corresponding to the mean stochastic solution. For the planning and management of heat resources purposes, it may be more reasonable to draw conclusions, say, from the mean temperature with one or two standard deviations in the downstream region rather than only the mean temperature distribution. Many practical applications of subsurface heat transport modeling involve predictions over a relative large space scale, where direct measurements are not possible in most field cases. Under such conditions, the stochastic theory provides a useful way of assessing the uncertainty about the ensemble mean (or classical deterministic model prediction).

## **Conclusions**

Within the stochastic framework, the solution of the heat transport in heterogeneous porous earth materials is developed in terms of the temperature variance. This variance can be used to quantify the uncertainty (or reliability) anticipated with the application of the classical deterministic heat transport model. From the practical application point of view, the classical heat transport model may be treated as the mean model containing effective parameters. Our result indicates that the  $\ln K$  correlation scale takes a role in increasing the variability in the temperature field and the variability of temperature field increases with the position.

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