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