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2	Bayesian Estimation of the Transmissivity Spatial Structure from Pumping
3	Test Data
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5	Mehmet Taner Demir <sup>1</sup> , Nadim K Copty <sup>1</sup> , Paolo Trinchero <sup>2</sup> , Xavier Sanchez-Vila <sup>3</sup>
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7	<sup>1</sup> Institute of Environmental Sciences, Bogazici University, Istanbul, 34342 Turkey
8	<sup>2</sup> AMPHOS 21 Consulting S.L., Passeig de García i Faria, 49-51, 1 – 1 E08019 – Barcelona,
9	Spain
10	<sup>3</sup> Department of Civil and Environmental Engineering, Universitat Politecnica de Catalunya
11	- UPC, Jordi Girona 31, 08034 Barcelona, Spain
12	

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#### ABSTRACT

Estimating the statistical parameters (mean, variance, and integral scale) that define the 14 15 spatial structure of the transmissivity or hydraulic conductivity fields is a fundamental step 16 for the accurate prediction of subsurface flow and contaminant transport. In practice, the 17 determination of the spatial structure is a challenge because of spatial heterogeneity and data 18 scarcity. In this paper, we describe a novel approach that uses time drawdown data from 19 multiple pumping tests to determine the transmissivity statistical spatial structure. The 20 method builds on the pumping test interpretation procedure of Copty et al. (2011) 21 (Continuous Derivation method, CD), which uses the time-drawdown data and its time 22 derivative to estimate apparent transmissivity values as a function of radial distance from the 23 pumping well. A Bayesian approach is then used to infer the statistical parameters of the 24 transmissivity field by combining prior information about the parameters and the likelihood 25 function expressed in terms of radially-dependent apparent transmissivities determined from 26 pumping tests. A major advantage of the proposed Bayesian approach is that the likelihood 27 function is readily determined from randomly generated multiple realizations of the 28 transmissivity field, without the need to solve the groundwater flow equation. Applying the 29 method to synthetically-generated pumping test data, we demonstrate that, through a 30 relatively simple procedure, information on the spatial structure of the transmissivity may 31 be inferred from pumping tests data. It is also shown that the prior parameter distribution has 32 a significant influence on the estimation procedure, given the non-uniqueness of the 33 estimation procedure. Results also indicate that the reliability of the estimated transmissivity 34 statistical parameters increases with the number of available pumping tests.

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#### 36 1. INTRODUCTION

37 The modeling of groundwater flow and contaminant transport has evolved in recent decades 38 into a valuable tool for the analysis of subsurface systems. Such modeling efforts require 39 mapping the flow parameters - most notably transmissivity (T) or hydraulic conductivity (K)40 - over the domain of interest. Numerous field investigations have however demonstrated that 41 hydrogeological parameters are highly heterogeneous, displaying complex patterns of spatial 42 variability (e.g., Gelhar 1993; Rubin, 2003, Sudicky et al. 2010). Because flow and transport 43 are strongly influenced by the heterogeneity of the subsurface system, incorporating the 44 spatial variability of the underlying parameters is essential for the accurate evaluation of 45 groundwater resources, and in particular for the prediction of contaminant transport as a 46 necessary step for the design and implementation of groundwater remediation activities (e.g., 47 Sanchez-Vila and Fernandez-Garcia, 2016).

48 Complexity in hydrogeological patterns and the lack of detailed data have led researchers to 49 formulate the flow and transport problem within a stochastic framework. With such an 50 approach, flow parameters are defined by spatial random functions whose spatial structure 51 can adequately be expressed in terms of few low-order statistical parameters, namely the 52 spatial mean, variance, and integral scale, which jointly define the covariance function or 53 semi-variogram (Kitanidis, 1997; Renard, 2007). These statistical parameters are typically 54 determined from measurements of the attribute of interest, provided that a sufficiently large 55 number of data with adequate spatial coverage is available.

56 Groundwater flow and solute transport are strongly affected by the spatial distribution of T. 57 At most sites, the number of T estimates determined from the interpretation of pumping tests is quite limited, hindering the accurate determination of the T covariance function. 58 59 Moreover, traditional pumping test interpretation methods, such as those based on log-log 60 plots (Theis, 1935) or semilog plots (Cooper and Jacob, 1946), generally yield single 61 estimates of the flow parameters, which hardly provide information about the underlying 62 heterogeneity. In fact, this averaging process results in T estimates with a smaller variance 63 and a larger integral scale as compared to the actual point distributions, and hence, cannot 64 be used to simulate the impact of small to medium scale variability, which is of interest in 65 many field applications.

These limitations motivated many researchers in the last three decades to examine the impact of spatial heterogeneity on the analysis of pumping tests and investigate whether information about the spatial variability of the flow parameters can be inferred from pumping tests (a 69 review of methods and solutions was provided by Sanchez-Vila et al., 2006). A very early 70 study is Barker and Herbert (1982), who considered the effect of a high hydraulic 71 conductivity anomaly embedded in an otherwise uniform aquifer. Butler (1988) used the 72 *Cooper and Jacob* (1946) method to investigate the effect of a *T* anomaly on the interpreted 73 transmissivity; it was shown that, for observation wells located at large distances from the 74 pumping well, the perturbed non-uniform aquifer behaves as a homogeneous aquifer. On the 75 other hand, Butler (1990) showed that the T values estimated with the Theis (1935) method 76 place more weight on the local T, defined as the T in the vicinity of the pumping well. Feitosa 77 et al. (1994) developed an inverse procedure for the estimation of the transmissivity as a 78 function of distance from the pumping well for the case when the transmissivity field 79 consists of a series of concentric homogeneous rings.

80 For spatially variable T fields (i.e., T fields that are not defined in terms of a deterministic 81 perturbation but that are individual realizations of a random field), Meier et al. (1998) and 82 Sanchez-Vila et al. (1999) showed that the transmissivity obtained with the Cooper and 83 Jacob (1946) is close to the spatial geometric mean of the T field, regardless of the location 84 of the observation point. On the other hand, the estimated storativity (S) varies spatially, 85 demonstrating how the interpretation method significantly translates the heterogeneity in 86 transmissivity into spatially variable S estimates. This finding was further confirmed by Trinchero et al. (2008b), who provided an analytical relationship between the estimated 87 88 storativity and the porosity inferred from tracer test data (the latter parameter was considered 89 as an indicator of transport connectivity).

90 Copty and Findikakis (2004a) examined the sensitivity of transient drawdown in pumping 91 tests to the statistical parameters describing the spatial structure of T, and noted that the time 92 derivative of the drawdown is particularly sensitive to the heterogeneity in T. Oliver (1993) 93 and Knight and Kluitenberg (2005) used the Frechet kernel to evaluate the sensitivity of the 94 drawdown to the spatial variability of T and S. Leven and Dietrich (2006) used sensitivity 95 coefficients to assess the influence of the spatial variability of T and S on the interpretation 96 of pumping tests, leading to time-dependent interpreted parameters. Avci et al. (2011, 2013) 97 developed a numerical method for the estimation of the variability of the T and S as a 98 function of pumping time; the method could be used as a diagnostic tool to identify some 99 aquifer system characteristics. Avci et al. (2014) evaluated the performance of a number of 100 analytical methods for the estimation of the variation of the transmissivity with radial 101 distance. Recently, *Pechstein et al.* (2016) discussed the relationship of the interpreted T 102 values derived from pumping tests to the underlying spatial variability of the T field. The 103 authors showed numerically that the interpreted T value that best reproduces the pumping 104 test data in confined heterogeneous aquifers is a weighted average of the point T values 105 which uses the temporal derivative of the Frechet kernel as a spatial weight.

106 Copty et al. (2008) and Trinchero et al. (2008a) considered the influence of spatial variability 107 of the transmissivity on pumping tests conducted in leaky aquifers. A significant difference 108 between flow towards a well in a confined non-leaky versus a leaky aquifer is that in the 109 former case the cone of depression continues to expand with time, while in the latter a steady 110 state condition is reached. As a result, the response of a pumping test in a leaky aquifer is 111 more sensitive to variations in the local transmissivity in the vicinity of the well, as compared 112 to the case of a confined aquifer.

113 A number of studies have attempted to estimate directly, from pumping test data, the 114 statistical spatial structure of the transmissivity field, commonly expressed in terms of two 115 statistical parameters: variance and integral scale. Copty and Findikakis (2004b) examined 116 the relation of the time-derivative of the drawdown to the integral scale and the variance of 117 the log-transmissivity field. Neuman et al. (2004, 2007) developed a graphical approach that 118 uses steady-state drawdown data for the estimation of the T variance and integral scale. Riva 119 et al. (2009) applied this type-curve method to field data from the site of Poitiers, France. 120 Firmani et al. (2006) used an expression of the equivalent hydraulic conductivity for steady-121 state radially convergent flow towards a well in a heterogeneous aquifer to estimate the 122 variance and integral scale of K. Zech et al. (2012) developed an analytical expression for 123 the steady state drawdown due to pumping in a heterogeneous aquifer using the Coarse 124 Graining upscaling method (Attinger, 2003), a method subsequently applied to real pumping 125 test data from the Horkheimer Insel test site in Germany (Zech et al., 2015). This latter paper 126 also discusses the quantity and spatial coverage of the data needed to obtain reliable 127 estimates of the statistical parameters of the transmissivity field. Zech et al. (2016) extended 128 the analysis to transient flow and showed that the number of measurements needed to obtain 129 reliable estimates of the transmissivity spatial structure is reduced compared to steady state 130 pumping tests.

In parallel efforts, and to overcome the scarcity of hydrological data commonly encountered in field applications, a number of researchers have proposed incorporating additional secondary data in the identification of subsurface parameters such as geophysical data (see recent reviews such as *Binley et al.*, 2015; *Slater*, 2007; *Rubin and Hubbard*, 2005). Novel 135 field data acquisition techniques, such as hydraulic tomography (e.g., Butler et al., 1999; 136 Yeh, and Liu, 2000; Zhu and Yeh, 2005; Yin and Illman, 2009; Illman et al., 2015) and direct 137 push technologies (Butler et al., 2007; Dietrich et al., 2008; Bohling et al., 2012) have also 138 been proposed. These approaches have been shown to have several benefits; most notably 139 they allow for the collection of dense hydraulic head data in response to groundwater 140 pumping that allows for the estimation of the three-dimensional hydraulic conductivity 141 distribution in the vicinity of the tests. Despite these advantages, their application to routine 142 field problems remains limited due to the relatively large costs associated and the difficulty 143 of solving the groundwater inverse problem.

144 Despite these recent developments, the determination of the underlying statistical spatial 145 structure of the transmissivity field from pumping test data remains a challenge. In a recent study, *Copty et al.* (2011) developed an interpretation method for pumping tests, denoted as 146 147 the Continuous Derivation (CD) method. The CD method uses the transient drawdown data 148 and its time derivative to estimate interpreted transmissivities as a function of the radial 149 distance,  $T_i(r)$ . It was shown by Copty et al. (2011) that  $T_i(r)$  is close to the geometric mean of the T values over a radially increasing volume,  $T_g(r)$ . The function  $T_g(r)$  varies from the 150 151 transmissivity at the well for small values of r, to the geometric mean of the entire field, for 152 large r values. In the current study, we extend the work of *Copty et al.* (2011) by examining 153 whether  $T_i(r)$  can be used to infer the spatial structure of the transmissivity field. The goal is 154 thus to develop a relatively simple pumping test interpretation method that can help in the 155 definition of relevant characteristics of the local scale transmissivity spatial structure without 156 the need for complex inverse modeling. We primarily focus on time-drawdown data derived 157 from pumping tests, which remains a widely used technique for subsurface parameter 158 estimation.

For the sake of completion, we present in Section 2 the main features of the CD method, followed by the presentation of the Bayesian approach used to infer the spatial structure of the transmissivity field, namely the variance and the integral scale. Section 3 describes a numerical application of the proposed Bayesian method and discusses its potential applications and limitations.

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#### 165 **2. Pumping Test Interpretation Method**

166 **2.1. The Continuous Derivation Method (CD)** 

For pumping tests conducted in heterogeneous aquifers, the cone of depression due to pumping expands in time. At early times the apparent transmissivity is close to the T value in the immediate vicinity of the well (order of few meters), while at later times it is some weighted average of the transmissivity of a much larger region around the well. The term "apparent" is used here in accordance with the terminology of Sanchez-Vila et al., 2006 which refers to an estimate of the parameter that is function of space and that satisfies some

relationship such as the Theis solution (*Theis*, 1935). The CD method (*Copty et al.*, 2011) 174 captures the full temporal transition between the local T value and the estimate obtained 175 using late time data. The estimation method relies on the time-derivative of the drawdown 176 because this is more sensitive than the drawdown itself to spatial variation of transmissivity 177 (e.g., Bourdet, 2002).

For two-dimensional flow towards a well in a confined aquifer, the time-dependent 178 drawdown is given by the classical Theis' solution:  $s(t,r) = \frac{Q}{4\pi T}W(u)$ , where  $u = \frac{r^2 S}{4\tau T}$ , 179 180 W(u) is the well (i.e., the exponential integral) function, Q is the pumping rate, r is the 181 separation distance between the pumping and observation wells, t is time, and S is storativity. 182 The ratio of the drawdown to the drawdown time derivative, s'(t,r), can be written as (*Copty*) 183 *et al.*, 2011):

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$$\gamma_c = \frac{2.3s}{s'} = W(u) \exp(u) \tag{1}$$

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A plot of the function  $\gamma_c$  is shown in Figure 1. It is observed that  $\gamma_c$  increases monotonically 186 187 with dimensionless 1/u (equivalent to a dimensionless time). For a given pumping test, the 188 ratio of the observed drawdown at any time t to its time derivative provides an estimate of u 189 from (1). From the estimated u value, the interpreted transmissivity and storativity ( $T_i$  and 190  $S_i$ , respectively) corresponding to that particular moment in time are then estimated as:

191 
$$T_{i}(t) = \frac{Q}{4ps(t)}W(u); \qquad S_{i}(t) = \frac{4tT_{i}u}{r^{2}}$$
(2)

192 Applying the above procedure repetitively to the full duration of the test yields time-193 dependent estimates of the flow parameters. Thus, the CD method provides estimates of the 194 flow parameters that change with time, in contrast to conventional methods (e.g., the Theis 195 method) that lump all observed drawdown together to estimate single representative values 196 of T and S.



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Figure 1. Plot of  $\gamma_c$  as a function of 1/u (modified from *Copty et al.*, 2011)

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Through sensitivity analysis of the drawdown and its derivative to variations in the transmissivity, the interpreted transmissivity  $T_{i}$ -t relationship is mapped into a  $T_{i}$ -r\* relationship, where  $r^*$  is an radial distance computed as (*Copty et al.*, 2011):

204 
$$r^* = \sqrt{\frac{4tT}{1.65S}}$$
 (3)

205 Equation (3) indicates that there is a direct mapping between the values of  $r^*$  and t. Copty et 206 al. (2011) applied the CD method to synthetically generated 2D aquifers and found that the 207 curves  $T_i(r^*)$  match well to the function  $T_g(r)$ , defined as the geometric mean of the 208 transmissivity, computed over a circular area of the aquifer centered around the pumping 209 well and with radius r. As r increases,  $T_g(r)$  approaches the geometric mean of the entire 210 transmissivity field. Therefore, observation points located at a small distance from the 211 pumping well (compared to the integral scale of *T*) would yield the most information about 212 the spatial variability of *T*.

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### 215 **2.2. Bayesian Approach for the Estimation of the Variance and Integral Scale**

Since the estimation of the transmissivity variance and integral scale is generally difficult and therefore associated with a high level of uncertainty, we define these two parameters as random functions. Denoting V and I as the variance and integral scale random functions, respectively, the primary goal of this paper is to estimate their conditional joint probability

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density function (pdf),  $f_{V,I}^{c}(v,i|Y_1\cdots Y_N)$ , where  $Y_1\cdots Y_N$  denotes the drawdown data from *N* available pumping tests. The superscript *c* denotes conditional.

222 Using the CD method, the drawdown data from each pumping test is converted to the geometric mean of the transmissivity as a function of radial distance from the well,  $T_g(r)$ . 223 224 Interpretation of each pumping test is done separately. If data from more than one 225 observation well are present for the same pumping test, they would yield similar T estimates 226 as they would be sampling the same aquifer volume. Under such conditions, it is sufficient 227 to use data from only one observation well. This redundancy in information has also been 228 noted by other researchers, such as Leven and Dietrich (2006) and Bohling and Butler 229 (2010), who demonstrated the issue of reciprocity of sequential pumping tests when pumping 230 and monitoring wells are reversed. Limitations of reciprocity have been also explored 231 elsewhere (e.g., Delay et al., 2012; Sanchez-Vila et al., 2016). Substituting each pumping 232 test by the transmissivity functions derived from the available pumping tests, the conditional joint pdf is rewritten as  $f_{V,I}^c(v,i|T_{g,1}(r)\cdots T_{g,N}(r))$ , where  $T_{g,1}(r)\cdots T_{g,N}(r)$  denotes the 233 234 transmissivity estimates derived from pumping tests 1,...N. In other words, the goal here can 235 be restated as the estimation of the joint pdf of V and I conditioned on the estimates of the 236 geometric mean of the T field as a function of radial distance derived from all available pumping tests. To simplify the notation, the variable r is dropped from the ensuing 237 derivations. It is however important to note that  $T_{e,k}$  is not a single value but rather a full 238 239 function of *r*.

240 Using Bayes' Theorem on conditional probability (e.g. *Tarantola*, 1987), the joint pdfs are:

241 
$$f_{V,I}^{c}(v,i|Y_{1}\cdots Y_{N}) = f_{V,I}^{c}(v,i|T_{g,1}\cdots T_{g,N}) = \frac{f_{T}(T_{g,1}\cdots T_{g,N}|v,i) \times f_{V,I}(v,i)}{f_{T}(T_{g,1}\cdots T_{g,N})}$$
(4)

242 where

243  $f_T(T_{g,1}\cdots T_{g,N}|v,i)$  is the likelihood of observing  $T_{g,k}$  given that variance and integral scale 244 values are *v* and *i*, respectively. This pdf can be seen as the reverse of the 245 desired pdf,  $f_{V,I}^c(v,i|T_{g,1}\cdots T_{g,N})$ 

246  $f_T(T_{g,1}\cdots T_{g,N})$  is the unconditional pdf of observing  $T_{g,1}\cdots T_{g,N}$ 

- 247  $f_{V,I}(v,i)$  is the prior joint pdf of observing the variance and integral scale values 248 v and i, respectively.
- The pdf in the denominator of (4) is denoted as ω, and can be expressed from the definitions
  of the marginal and conditional probabilities (*Tarantola*, 1987) as:
- 251  $\omega = f_T \left( T_{g,1} \cdots T_{g,N} \right) = \int_{V,I} f_T \left( T_{g,1} \cdots T_{g,N} \middle| v, i \right) \times f_{V,I} \left( v, i \right) dv di$ (5)

In words, the pdf of  $T_{g,1} \cdots T_{g,N}$  is equal to the probability of observing  $T_{g,1} \cdots T_{g,N}$  given that V = v and I = i, integrated over all possible values of V and I;  $\omega$  is a normalizing parameter that guarantees that (4) is a proper pdf; that is:  $\int_{V,I} f_{V,I}^c (v,i|T_{g,1} \cdots T_{g,N}) dv di = 1$ 

If the separation distances between the different pumping tests is large such that the cones of depression do not significantly overlap (consequently, there is little redundancy in the data), then the pumping tests can be treated as independent (i.e., they sample different volumes of the aquifer). The likelihood function  $f_T(T_{g,1} \cdots T_{g,N} | v, i)$  can be re-written as a product of the individual pdfs:

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$$f_{V,I}^{c}(v,i|Y_{1}\cdots Y_{N}) = \frac{1}{\omega}f_{T}(T_{g,1}|v,i)..f_{T}(T_{g,N}|v,i)f_{V,I}(v,i)$$
(6)

261 where

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$$\omega = \int_{V,I} f_T \left( T_{g,1} | v, i \right) \dots f_T \left( T_{g,N} | v, i \right) f_{V,I} \left( v, i \right) dv \, di \tag{7}$$

Equation (6) states that the pdf of *V* and *I* conditional on the available pumping test data can be expressed in terms of products of N+I pdfs. The first one,  $f_{V,I}(v,i)$ , is the prior joint pdf of *V* and *I*, which reflects the level of knowledge of the site *prior* to conducting the pumping tests. Such information can be derived from previously conducted geologic or geophysical studies, or adopted from other sites with similar characteristics. In the absence of information,  $f_{V,I}(v,i)$ , can be taken as some uniform (uninformative) distribution that includes all possible values, reflecting the lack of knowledge of the site.

The remaining *N* pdfs are  $f_T(T_{g,k}|v,i) k = 1, \dots N$ ; i.e., the individual likelihood functions of observing  $T_{g,k}$  given that the aquifer variance and integral scale are *v* and *i*, respectively, in pumping test *k*. As it will be described in the following subsection, the likelihood functions can be readily computed without the need for any inverse modeling by generating multiple realizations of the transmissivity field with different values of *V* and *I*, computing the resultant pdf of the geometric mean of the generated transmissivity fields and then evaluating the likelihood of  $T_{g,k}$ . Hence, it can be seen that the desired pdf,  $f_{V,I}^{c}(v,i|Y_1\cdots Y_N)$  depends on both prior information about the site,  $f_{V,I}(v,i)$ , and the information derived from the pumping test,  $f_T(T_{g,k}|v,i)k = 1, \dots N$ .

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280 Finally, the marginal pdfs of *V* and *I* are computed as:

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$$f_V^c(v|Y_1\cdots Y_N) = \int_I f_{V,I}^c(v,i|Y_1\cdots Y_N) di, \qquad (8)$$

282 
$$f_I^c(i|Y_1\cdots Y_N) = \int_V f_{V,I}^c(v,i|Y_1\cdots Y_N) dv.$$
(9)

283 The expected values of the variance and integral scale can be computed from the integral of 284 the conditional joint pdf of *V* and *I*,  $f_{V,I}^{c}(v,i|Y_1\cdots Y_N)$ :

285 
$$E[I] = \int_{V,I} if_{V,I}^{c} (v, i|Y_1 \cdots Y_N) dv di, \qquad (10)$$

286 
$$E[V] = \int_{V,I} v f_{V,I}^c (v, i | Y_1 \cdots Y_N) dv di.$$
(11)

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# 288 **2.3. Estimation of the likelihood function** $f_T(T_{g,1} \cdots T_{g,N} | v, i)$

This section describes the method used to estimate the likelihood function  $f_T(T_{g,1}\cdots T_{g,N}|v,i)$ It is assumed that  $\ln T$  is a multivariate Gaussian random spatial function with exponential semi-variogram. Other semi-variogram functions could also be considered. Multiple realizations (*n*=1000) of the natural logarithm of the transmissivity were randomly generated for various *V* and *I* values using the Turning band method (*Mantoglou and Wilson*, 1982). The geometric mean of the transmissivity over a circular area with radius *r* located at the center of the generated domain was computed as:

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$$T_g(r) = \exp\left[\int_{r=0}^r \ln(T) dA\right]$$
(12)

Figure 2 displays  $T_g(r)$  for randomly selected transmissivity fields with variance V=1. The radial distance in the figure is normalized by the integral scale, *I*, while the ensemble geometric mean,  $T_{g,o} = T_g(r \rightarrow \infty)$  was used to normalize the vertical axis. It can be seen that the variability of  $T_g(r)$  decreases as *r* increases. For radial distances larger than about 20*I*,  $T_g(r)$  approached the ensemble geometric mean for all of the generated transmissivity fields.

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Figure 2.  $T_g(r)$  as a function of radial distance for randomly selected transmissivity fields with V=1.  $T_g(r)$  is normalized by the ensemble mean of *T* used in data generation. The distance *r* is normalized by the integral scale, *I*.

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309 Figure 3 shows the expected value and upper/lower deciles of  $T_g(r)$  for V=1, 2 and 4. The expected value was computed for each distance r as the arithmetic average of the 1000 310 311 realizations. Similar curves for other values of the variance could be developed readily. 312 Analysis of the generated realizations shows that 1000 simulations were sufficient (with 313 error less than 1%). Figure 3 shows that for r=0 the expected value is simply the arithmetic 314 mean of the transmissivity at the well. For r/I > 20,  $T_g(r)$  of each realization approaches the 315 ensemble geometric mean and hence, the expected value over all realizations would also approach the ensemble geometric mean. The semi-variogram model selected influences the 316 317 rate of change with distance, but not the end points.

Although Figure 3 depicts only the average and upper/lower deciles, it is evident that for a particular value of *V* and *r/I*, there is a range of possible values of  $T_g(r)$ . This range increases with the increase in the variance value, and decreases as *r/I* increases. This figure also shows overlap among the different set of curves; e.g., for a given distance, the possible range of values of  $T_g$  obtained with variance *V*=2 is fully comprised within the range spanned by *V*=4. This overlap has an influence on the Bayesian estimation, as discussed in detail is section3.2.



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Figure 3. Expected value (solid line) and upper/lower deciles (dashed lines) for V=1, 2 and 4. The red, black and blue lines correspond to V=1, 2, and 4, respectively.  $T_g(r)$  is normalized by the geometric mean of the transmissivity,  $T_{go}$  used in data generation.

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Based on the information shown in Figure 3, it is possible to construct a distribution of all possible  $T_g(r)$  values corresponding for each *V* and *r/I* pairs. Figure 4 shows the pdfs of  $T_g(r)$ at 3 different distances: *r/I*=1, 5 and 10, and for *V*=1. As distance increases, the statistical distribution becomes narrower and less skewed. It is important to note that these pdf's are computed only once and can be used in other problems provided the semi-variogram model is kept.

Figure 4 also shows a sample calculation of the likelihood function for a  $T_g(r)$  obtained from a given pumping test. Starting from the  $T_g(r)$  values derived from the pumping test, one can calculate the pdf corresponding for each *V* and *I* pairs. Because the pdf's depicted in Figure 4 are for particular values of *V* and *I*, this calculation has to be repeated for all possible *V* and *I* pairs as defined by their prior joint distribution,  $f_{V,I}(v,i)$ . According to the Bayesian formulation (Equation 4), the desired joint conditional pdf of *V* 

341 According to the Dayesian formulation (Equation 4), the desired joint conditional put of v

and *I* is function of the product of the likelihood function and the prior distribution. If for a

given pair (v,i), the product of  $f_{V,I}(v,i)$ , and  $f_T(T_{g,1}\cdots T_{g,N}|v,i)$  is small, the probability of the transmissivity field having these v and i values would also be small. On the other hand, if this product is large, this would mean that this (v, i) pair is more likely.



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Figure 4: pdfs of  $T_g(r)$  at r/I=1, 5 and 10 and for V=1. The red arrow represents the likelihood function for an example *T* value derived from a particular pumping test

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351 The above discussion illustrates the benefits of formulating the parameter estimation within 352 a Bayesian framework. First, it incorporates the information inferred from the pumping test data, as well as any prior information about the site. Second, the Bayesian formulation 353 simplifies the calculation by expressing the desired conditional pdf,  $f_{V,I}^{c}(v,i|T_{g,1}\cdots T_{g,N})$  in 354 terms of its reciprocal,  $f_T(T_{g,1}\cdots T_{g,N}|v,i)$  (Eq. 4). Whereas the former can viewed as a form 355 of the inverse problem and its evaluation is not straight forward,  $f_T(T_{g,1} \cdots T_{g,N} | v, i)$  can be 356 357 readily determined from the randomly generated transmissivity fields corresponding to the 358 v and i values as presented above without the need for any inverse modeling. Third, the 359 Bayesian approach provides an estimate of the entire pdf based on prior information and the 360 pumping test data and, as such, provides a measure of the uncertainty of the estimates.

361 In summary, we list below the main steps for the estimation of the conditional joint pdf of V 362 and I,  $f_{V,I}^{c}(v, i|T_{v,1} \cdots T_{v,N})$ :

363 1. Given *N* pumping tests, the geometric transmissivity as a function of radial distance 364  $T_{g,1}(r)\cdots T_{g,N}(r)$  is estimated using the CD method. Each pumping test is analyzed 365 separately.

366 2. The prior joint pdf of *V* and *I*,  $f_{V,I}(v,i)$ , is defined based on prior information about the 367 site.

3. For the available pumping tests, the likelihood function  $f_T(T_{g,1} \cdots T_{g,N} | v, i)$  is determined 368 369 from Figures 3 and 4. By assuming the pumping tests are sufficiently far and, therefore, 370 can be treated as independent, the likelihood function is expressed as a product of the 371 likelihood functions of the individual pumping tests (Eq. 6). It is important to note that 372 these figures do not require the simulation of the groundwater flow equation; they were 373 developed by generated multiple realizations of the transmissivity field and averaging 374 the T as a function of radial distance. The calculation of the likelihood function is 375 repeated for all possible v and i pairs as defined by their prior distribution (step 2).

376 4. The normalizing parameter, *ω*, is calculated from Eq. (5) or Eq. (7) if the pumping tests
377 treated as independent.

5. The desired conditional pdf is finally computed according to Eq. (4) or Eq. (6). The
marginal distributions of *V* and *I* are determined from Eq (8) and Eq. (9), respectively.

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#### 381 **3. Application**

#### 382 **3.1. Data Generation**

383 To demonstrate the above parameter estimation procedure, the procedure was tested using 384 1000 synthetic pumping tests conducted in confined heterogeneous aquifers. The 385 heterogeneous transmissivity fields were generated using the turning bands method. It was 386 assumed that the natural log transform of the transmissivity is a multivariate Gaussian 387 random spatial function with zero mean  $(T_g=1)$ , an exponential semi-variogram, with variance, V=1, and integral scale, I=8 length units (lu). Storativity was assumed to be 388 389 uniform, as field data usually indicate that the spatial variation in storativity is less than that 390 of the transmissivity. The storativity value used in all simulations was 0.0001; which is a 391 typical value for a confined aquifers (Domenico and Schwartz, 1997).

The flow domain was assumed to be 481 by 481 lu. A fully penetrating pumping well was placed at the center of the domain. The observation point was assumed to be at a distance of *I*/8 from the pumping well. Constant head conditions were prescribed along the outer boundaries of the domain. The duration of the pumping test was  $\tau=1$ , while the pumping rate was fixed at Q=2 (using consistent units for both  $\tau$  and Q). Pumping tests were terminated before the drawdown data were affected by boundary effects.

398 The pumping tests were simulated using MODFLOW (Harbaugh et al., 2000). A uniform 399 grid of 1 by 1 lu was used. The drawdown data were analyzed using the CD method yielding 400 one  $T_g(r)$  for each of the 1000 simulated pumping tests. Using the proposed Bayesian 401 approach, the inferred  $T_g(r)$  was then used to estimate the variance and integral scale. To 402 assess the robustness of the proposed method, a Monte Carlo approach was adopted. First, 403 each of the  $T_{g}(r)$  curves were used independently to estimate the variance and integral scale 404 of the T field. This corresponds to the case when only a single pumping test is present (N=1). 405 The method was then repeated by combining 5 and 10 pumping tests (N = 5 and N = 10, 406 respectively) to test the performance of the method when multiple wells are present.

407 The Bayesian estimation requires the definition of a prior distribution for the parameters of 408 interest (variance and integral scale). In the present analysis, the prior distribution of the 409 variance was assumed to be uniform between 0 and 5,  $U_V(0,5)$ . This range encompasses 410 typical variance values encountered in the field (Gelhar, 1993). The prior pdf of the integral 411 scale was also assumed to be uniform between 0 and 40 lu,  $U_{I}(0,40)$ . The uniform 412 distributions are the least informative distributions in terms of priors, requiring only the 413 definition of upper limits (5 and 40 lu, respectively). The corresponding joint prior pdf is 414  $f_{V,I}(v,i)=1/5\times1/40=0.005$ . The joint pdf is also uniformly distributed which means that all v 415 and *i* pairs falling between the lower and upper limits of V and I respectively have the same 416 probability of occurring. To assess the sensitivity of the prior distribution on the estimation 417 of the variance and integral scale, the analysis was also repeated assuming the prior 418 distributions of the variance and the integral scale are  $U_V(0,3)$  and  $U_I(0,30)$ , respectively, 419 which are closer to the parameter values used in data generation.

420

#### 421 **3.2. Results**

422 The parameter estimation procedure was repetitively applied to all 1000 pumping tests. 423 Figure 5 shows a randomly selected example of the conditional joint pdf of the variance and 424 integral scale obtained with the Bayesian estimation procedure. The true variance and 425 integral scale used in the data generation are 1 and 8 lu, respectively. The number of available 426 pumping tests was 5. The conditional pdf joint should be contrasted to the prior 427  $f_{V,I}(v,i)=0.005$ . This figure shows that conditioning on the pumping test data shifts the pdf 428 from the diffuse prior towards the true values of the variance and integral scale (v=1, i=8 lu). 429 The range of the more likely values of the variance and integral scale significantly decreased. 430



431

Figure 5. Example of the conditional joint pdf of the variance and integral scale based on data from 5 pumping tests. The prior distributions of the variance and integral scale are  $U_V(0,5)$  and  $U_I(0,40)$  which correspond to a prior pdf  $f_{V,I}(v,i)=0.005$ . The true values are V=1 and I=8 lu.

436

437 The marginal distributions of the integral scale and variance for 3 randomly selected cases 438 are shown in Figure 6. Each of these conditional pdfs were computed assuming 5 pumping 439 tests were available. The mean of the marginal pdfs of the integral scale for the three 440 randomly selected cases were 5.8, 9.2 and 17 lu. The mean of the marginal pdfs of the 441 variance on the other hand were 2.4, 1.8 and 0.86. For comparison, the prior pdfs of V and I 442 are also shown in this figure. The corresponding means of the prior pdfs of the integral scale 443 and variance were 20 lu and 2.5, respectively. These results show that the conditional 444 variance and integral scale marginal pdfs are closer to the true values (V=1, I=8 lu) compared 445 to the initial prior distribution. The conditional marginal pdfs do exhibit a tail that results 446 from the diffuse prior distribution of V and I, and the overlap of the likelihood functions 447 (Figures 3 and 4). 448





Figure 6. Integral scale and variance marginal pdfs for three randomly selected cases. Each of these cases assumes 5 pumping tests are available. The prior distributions of the variance and integral scale are  $U_V(0,5)$  and  $U_I(0,40)$ . The true values are V=1 and I=8 lu.

454 Figure 7 presents the histogram of the conditional expected values of the integral scale (E[I])455 and variance (E[V]), from the 1000 Monte Carlo results. The results are computed using 1, 456 5 or 10 pumping tests. The average of E[V] and E[I] over all realization for N=1, 5, and 10 457 are shown in Table 1, For comparison, the "true" values of V and I used in the generation of 458 the T fields and the expected values of the prior distribution are also included. Figure 7 and 459 Table 1 demonstrate that the Bayesian updating can be viewed as a weighted average of the 460 prior pdf and the results of the pumping test. Conditioning improves the estimation of the 461 considered variables although, because of the overlap of the different likelihood functions 462 (Figures 3), the resulting histograms still show some spread. Provided there is no redundancy 463 in the data, increasing the number of pumping tests causes the estimates of the variance and 464 integral scale to shift towards the true values.

465



467 Figure 7. Histograms of E[V] and E[I] based on the Monte Carlo analysis, assuming 1, 5 or

- 468 10 pumping tests are available. The prior distributions are  $U_V(0,5)$  and  $U_I(0,40)$ , implying
- 469 expected values of 2.5 and 20 lu, respectively. The true values are V=1 and I=8 lu.
- 470

471 Table 1: Average of E[V] and E[I] for all simulations, assuming N=1, 5 or 10 pumping tests

- 472 are available and for different prior distributions of the variance and integral scale. For
- 473 comparison, the true values used in the generation of the transmissivity field are also shown

Prior distributions	Number of	Average of	Average of
	Pumping	E[V]	E[ <i>I</i> ], lu
	Tests		
	0	2.5	20
V: Uniform between 0 and 5	1	1.96	16.7
<i>I</i> : Uniform between 0 and 40 lu	5	1.47	13.9
	10	1.36	12.4
	0	1.5	15
V: Uniform between 0 and 3	1	1.36	13.8
<i>I</i> : Uniform between 0 and 30 lu	5	1.21	12.5
	10	1.17	11.5
"True" Values of <i>I</i> and <i>V</i>		1	8

474 Note: The average values corresponding to *N*=0 are the values of the prior distributions475 before conditioning on the pumping well data

476

477 To assess the impact of the prior V and I distributions, the parameter estimation procedure 478 was repeated with the same pumping tests, but now assuming that the initial distributions of 479 the variance and integral scales are uniformly distributed between 0 and 3 and between 0 480 and 30 lu, respectively. Figure 8 shows the histograms of the E[V] and E[I] for different 481 number of pumping tests. The corresponding average of E[V] and E[I] for all simulations are 482 given in Table 1. With increase in the number of pumping tests, E[V] and E[I] move from 483 the expected values of the prior distributions,  $E^{p}[V] = 1.5$  and  $E^{p}[I] = 15$  lu, towards the true 484 parameter values, V=1 and I=8 lu. Compared to Figure 7, the impact of the number of tests 485 on the estimation is less significant (in particular for E[V]), because the prior estimates were

486 closer to the true values. This demonstrates the benefits of using accurate prior distributions487 in Bayesian estimation procedures provided such information is available.

#### 488



489

490 Figure 8. Histograms of E[V] and E[I], assuming 1, 5 or 10 pumping tests are available.

491 The prior distributions are  $U_V(0,3)$  and  $U_I(0,30)$ , implying expected values of 1.5 and 15 lu, 492 respectively. The true values are V=1 and I=8 lu.

493

## 494 **4. Summary and Conclusions**

495 Modeling of the spatial variability of transmissivity is essential for the accurate simulation 496 of groundwater flow and contaminant transport. The spatial variability of T is commonly 497 defined in terms of a semi-variogram or covariance function that is expressed in terms of 498 two statistical parameters: the variance, V, and integral scale, I. It is therefore important to 499 develop simple techniques for the estimation of these two statistical parameters. Despite the 500 development in recent years of novel data acquisition techniques, the analysis of drawdown 501 data from pumping tests remain the most commonly used technique for the identification of 502 subsurface flow parameters. Traditionally, the interpretation of pumping tests generally yield 503 single representative (apparent) estimates of the flow parameters. Here we explore whether 504 pumping test data can be used to infer the variance and integral scale of the transmissivity, 505 two statistical parameters that describe the spatial variability of the underlying transmissivity 506 field. Estimates of the variance and integral scale can be employed in the analysis of flow 507 and contaminant transport problems and their associated uncertainty, either directly using 508 various analytical expressions found in the literature that relate flow and transport attributes

to the underlying aquifer heterogeneity, or numerically through the generation of multiplerealizations of the transmissivity field.

The starting point of the present study is the Continuous Derivation method (*Copty et al.*, 2011), which uses the drawdown and its time derivative to estimate a function that was shown to be close to the geometric mean of the transmissivity field defined over an increasing radial distance from the pumping well,  $T_g(r)$ . Analysis of  $T_g(r)$  indicated that the early part of the curve is sensitive to the variance of the *T* field while the rate at which it approaches the geometric mean of *T* in the full domain could be related to the integral scale. This provided the basis for attempting to use  $T_g(r)$  for estimating *V* and *I*.

The estimation of V and I was formulated using a Bayesian approach which expresses the conditional pdf of V and I as a weighted function of the prior pdf and the likelihood function that is itself dependent on the pumping test data. An important advantage of this approach is that the likelihood function is readily computed from multiple realizations of the transmissivity without the need to solve potentially complex inverse problems. Another feature of the Bayesian approach is that it provides a measure of the uncertainty of the estimated statistical parameters.

525 The Bayesian estimation procedure was applied to a number of synthetic pumping tests. The 526 analysis assumed that the natural log transform of the transmissivity distribution is a 527 multivariate Gaussian random spatial function with an exponential variogram. The variance 528 and integral scale were assumed to have a uniform joint prior distribution. The diffuse prior 529 distributions considered in this application and the non-uniqueness of the likelihood function 530 means that the results of the estimation procedure can be associated with a significant level 531 of uncertainty, highlighting the challenges of the parameter estimation problem. Single as 532 well as multiple pumping tests (N=5 and N=10) were assumed to be available. In the case 533 when multiple pumping tests were available, it was further assumed that they are located far 534 from each other such they sample different portions of the aquifer.

The significance of the Bayesian estimation procedure becomes apparent when the conditional distribution of V and I is compared to the prior pdf of V and I which represents the level of information available prior to conducting the pumping tests. It is shown that improved estimates of V and I are obtained as the number of available pumping tests increases or when more accurate prior distributions are available. The results of this numerical example show that as little as 5 pumping tests may be sufficient to yield reliable estimates of the statistical parameters of the transmissivity field. 542 Overall, the proposed interpretation procedure can be viewed as an extension of traditional 543 pumping test interpretation procedures, such as the Theis method, that besides best-fit 544 estimates of the storativity and transmissivity, can potentially also provide estimates of the 545 variance and integral scale of the transmissivity field.

546

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