AN INVERSE ANALYSIS OF HYDRAULIC CONDUCTIVITY DISTRIBUTION IN A HETEROGENEOUS AQUIFER

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ABSTRACT
Stochastic inverse methods are occasionally employed to deal with the uncertainties in groundwater flow problems. In this paper, the adjoint state method combined with cokriging is used to solve an inverse problem of groundwater flow, in which the distribution of hydraulic conductivity in an aquifer is estimated. The variability in the hydraulic heads and hydraulic conductivities are considered in the analysis. The adjoint equation is used to calculate the hydraulic heads and the distribution of adjoint states at all locations at different times. The results are used to obtain the Jacobian, which is needed as input for the maximum likelihood analysis to obtain the statistical parameters of the model. Using the resulting statistical parameters as input in the cokriging analysis, the distribution of the log hydraulic conductivity of the aquifer is obtained. A hypothetical model is presented as an example of the usefulness of the method.

RÉSUMÉ
Les méthodes stochastiques inverses sont occasionnellement utilisées pour composer avec les incertitudes inhérentes aux problèmes de flux d'eau souterraine. Dans cet article, la méthode de l'état adjoint est combinée au cokrigeage pour résoudre un problème inverse de flux d'eau souterraine. Dans ledit problème, la distribution de la conductivité hydraulique dans un aquifère est estimée. La variabilité des charges hydrauliques et des conductivités hydrauliques sont considérées dans l'analyse. L'équation adjointe est utilisée pour calculer à différents temps les charges hydrauliques et la distribution des états adjoints en tout endroit dans l'aquifère. Les résultats obtenus permettent la détermination du Jacobien qui est utilisé dans l'analyse du maximum de vraisemblance afin d'obtenir les paramètres statistiques du modèle. Les paramètres statistiques obtenus sont utilisés comme entrées dans l'analyse cokrigeant pour déterminer la distribution du logarithme de la conductivité hydraulique de l'aquifère. Un modèle hypothétique est présenté pour illustrer l'utilité de la méthode présentée dans cet article.

1. INTRODUCTION

The groundwater flow in heterogeneous aquifers is a random process. The randomness can be due to the natural variability in the aquifer characteristics such as the hydraulic properties of subsurface soil, the recharge or discharge of groundwater from and to a stream, and the amount of recharge from precipitation. It is difficult to represent these kinds of variability in a deterministic analysis because there is no exact value to be used as input for the parameters. In this case, stochastic approaches are usually employed.

Stochastic methods in groundwater flow studies have been used increasingly in the last two decades. Kaluarachchi et al. (1990) and Myers (2002) stated that stochastic methods give better and more meaningful results compared to the deterministic methods in many surface and groundwater flow studies. This approach provides probabilistic predictions regarding the behaviour of aquifers by considering that the parameters are random variables (de Marsily, 1986; Gelhar, 1986; Dagan, 2002). The probability density functions (pdf) of parameters in an area are provided as input for the analysis. The resulting equations are in the form of differential equations of dependent variables. Therefore, the dependent variables obtained from these equations can also be represented as probability density functions (Dagan, 2002).

In this paper, the stochastic finite element method of inverse solution based on the work of Neuman (1980), Sun and Yeh (1992), and Sun (1999) is utilized for the solution of a transient groundwater flow problem. A hypothetical model is presented to show the usefulness of the method. Subsequently, different values of statistical parameters are used in the analysis to find their effects on the distribution of the estimated hydraulic conductivity values in the aquifer.

2. AN INVERSE ANALYSIS USING THE ADJOINT FINITE ELEMENT METHOD

This method of calculation has been used previously by Neuman (1980), Sun and Yeh (1992), Sun (1999), and Neupauer and Wilson (2001) in groundwater flow studies. In this method, it is assumed that the coefficient of storage is constant in the entire aquifer. The random field Y is characterized by a constant mean and an isotropic, exponential covariance as follows. In the present study, Y represents the logarithm of hydraulic conductivity.

$$E[Y] = \mu_Y \quad [1]$$

$$Cov_{YY}(x_i, x_j) = \sigma_Y^2 \exp\left(\frac{-d_{ij}}{l_Y}\right) \quad [2]$$

where σ_Y^2 is the variance of log hydraulic conductivity, l_Y is the log hydraulic conductivity correlation length, d_{ij} is the distance between points x_i and x_j, μ_Y is the mean of log hydraulic conductivity.

In the small perturbation method, the hydraulic conductivity and hydraulic head are presented as their means plus a small variation about their means as written below.

$$Y = F + f \quad \text{and} \quad \phi = H + h \qquad [3]$$

where ϕ is the hydraulic head, F is the expected value of Y, i.e. F=E[Y], H is the expected value of ϕ, i.e. H=E[ϕ], f is the variation of Y about the mean value, and h is the variation of ϕ about the mean value.

In the adjoint state method, Eq. 3 is substituted into the classical groundwater flow equation. In this study, a transient groundwater flow in a confined aquifer is analyzed. After introducing an objective function and the adjoint state or importance function, ψ, into the resulting equation from the previous step and using the Green's first identity, the following equations are obtained (see Sun and Yeh, 1992).

$$\frac{\partial G}{\partial h} = S\frac{\partial \psi}{\partial t} + e^F\left[\frac{\partial}{\partial x}\left(b\frac{\partial \psi}{\partial x}\right) + \frac{\partial}{\partial y}\left(b\frac{\partial \psi}{\partial y}\right)\right] \qquad [4]$$

$$\frac{\partial J}{\partial f} = \int_0^T \int_B \left\{\frac{\partial G}{\partial f} + e^F b\left[\frac{\partial \psi}{\partial x}\frac{\partial H}{\partial x} + \frac{\partial \psi}{\partial y}\frac{\partial H}{\partial y}\right]\right\} dB dt \qquad [5]$$

Equation 4 represents the adjoint problem of the groundwater flow equation and Eq. 5 is the functional derivatives of the objective function of Eq. 4 (Neuman, 1980; Sun and Yeh, 1992). In Eqs. 4 and 5, J is the objective function, G is a user-chosen function, B is the flow region, T or t is time, and x and y are the Cartesian coordinates. By solving Eq. 4, the adjoint state, ψ, is obtained. Equation 5 is used to calculate the functional derivatives needed in the calculation of Jacobian.

In the finite element method, the following equations are utilized (Neuman, 1980, and Sun and Yeh, 1992).

$$[A]\{H\}^{t+\Delta t} = \{M\} + [D]\{H\}^t \qquad [6]$$

$$[A]\{\psi\}^{t+\Delta t} = \{E\} + [D]\{\psi\}^t \qquad [7]$$

$$\frac{\partial h(x_l, t_k)}{\partial f_i} = \sum_{n=1}^{NNODE} \sum_{m=1}^{NNODE} B_{inm} \sum_k \int_k^{t_{k+1}} \psi_n H_m dt \qquad [8]$$

where [A] is a characteristic matrix, [D] is a matrix that accommodates the storage coefficient in the calculation, {M} is a column matrix that contains source or sink terms, and {E} is a column matrix that contains the G function, and

$$B_{inm} = \int_R \nabla N_n . \nabla N_m . N_i(x, y) dR \qquad [9]$$

Equations 6, 7, and 8 are used to calculate the expected hydraulic heads, the adjoint states, and the functional derivatives, respectively. These values are needed in the calculation of covariance matrices used in the maximum likelihood (MLE) analysis to obtain the statistical parameters and in the calculation of the distribution of estimated hydraulic conductivities using the cokriging method.

3. CALCULATION OF STATISTICAL PARAMETERS AND THE DISTRIBUTION OF HYDRAULIC CONDUCTIVITIES

Following Kitanidis and Vomvoris (1983), and Sun and Yeh (1992), the MLE is used to estimate the statistical parameters, which appear in Eqs. 1 and 2. The negative log-likelihood equation is

$$L(z|\theta) = \frac{LT}{2}\ln(2\pi) + \frac{1}{2}\ln|Q_D| + \frac{1}{2}(z-\mu)^T Q_D (z-\mu) \qquad [10]$$

where θ is the statistical parameter vector. The elements of θ are μ_Y, σ_Y^2, and l_Y, the values of which are not known. In Eq. 10, l_y is the correlation length, z is the measurement vector, LT is the total number of measurements, Q_D is the measurement covariance matrix, and μ is the mean vector of measurements. Both Q_D and μ are functions of unknown statistical parameters. The structure of Q_D can be found in a paper of Sun and Yeh (1992). The details of the calculation using the MLE are given in Kitanidis and Lane (1984).

Once the statistical parameters are obtained, the distribution of the hydraulic conductivities in the aquifer can be estimated by using cokriging. The general equation of cokriging is as follows (Isaaks and Srivastava, 1989).

$$\hat{Y}_0 = \sum_{k=1}^{K}\sum_{l=1}^{L}\mu_{l,k}(\phi_{l,k} - H_{l,k}) + \sum_{m=1}^{M}\lambda_m Y_m \qquad [11]$$

where $\hat{Y}$ is the estimate of logarithm of K, μ and λ are the cokriging coefficients, and the subscripts k, l, and m indicate the number of observation times, hydraulic heads, and hydraulic conductivities, respectively.

The variance of cokriging can be estimated by the following equation (Isaaks and Srivastava, 1989).

$$Var[\hat{Y}_0 - Y_0^*] = \sigma_Y^2 - \sum_{m=1}^{M}\lambda_m Cov[Y(x_m), Y(x_0)] - \sum_{k=1}^{K}\sum_{l=1}^{L}\mu_{l,k} Cov[\phi(x_l, t_k), Y(x_0)] - \upsilon \qquad [12]$$

where

$Cov[\phi(x_l, t_k), Y(x_0)]$ = the covariance between the hydraulic head observation at point x_l and time t_k and logarithm of K measurement at point x_0.

$Cov[Y(x_m), Y((x_0)]$ = the covariance between the logarithm of K measurement at point x_m and point x_0.

ν = the Lagrange multiplier.

The details of cokriging method can be found in Isaaks and Srivastava (1989) and Kitanidis (1997).

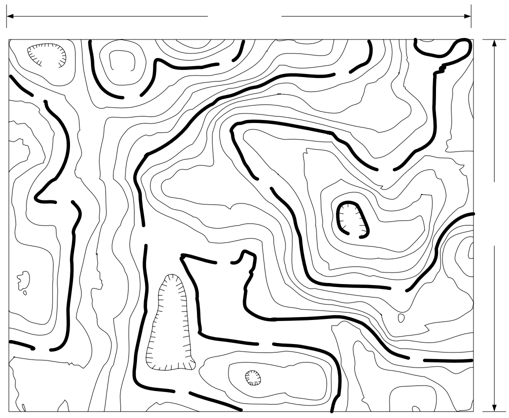
To compare the resulting distribution of estimated hydraulic conductivities with the distribution of the "true" hydraulic conductivity values, the L2-norms for the logarithm of K and for prediction errors, as written below, are used (Sun and Yeh, 1992).

$$CY = \left\| Y^* - \hat{Y} \right\|_{L2} = \left[\frac{1}{M} \sum_{m=1}^{M} \left(Y_i^* - \hat{Y}_i \right)^2 \right]^{1/2} \qquad [13]$$

$$CP = \left\| P\left(Y^*\right) - P\left(\hat{Y}\right) \right\|_{L2} \qquad [14]$$

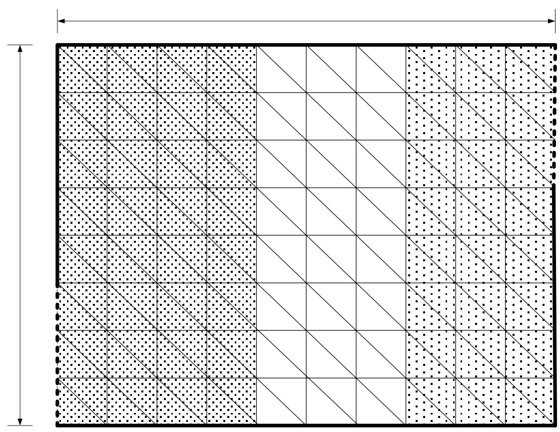
4. HYPOTHETICAL MODEL

The case study used in this paper makes use of the two-dimensional stationary random field provided in a publication by Mantoglou and Wilson (1982). In their paper, the stationary random field was generated using the turning bands method that was first introduced by Matheron (1973). In generating this random field, they used a mean value of five for the region, an exponential covariance with correlation length b^{-1}, number of points in the P field, NP = 8000, number of lines, L = 16, the discretization length (band width), $\Delta\zeta = 0.012\ b^{-1}$, the number of harmonics along the lines, M = 100, $\sigma^2 = 1$, and the maximum frequency at which the spectrum is truncated, $\Omega = 40$ b. The reproduction of the random field is presented in Fig. 1. The distribution of hydraulic conductivities presented in this figure is considered as the "true" values of hydraulic conductivities in the aquifer. In the real life problems these values are not known everywhere.



Note: in this paper, it is assumed that b^{-1} = 833.33 m

Figure 1. The reproduction of random field provided in a paper by Mantoglou and Wilson (1982), which is used in the hypothetical model



Legend: X = the pumping well
O = observation wells

Figure 2. Plan view of the hypothetical aquifer

In this paper, the hypothetical confined aquifer is 1000 metres long and 800 metres wide as shown in Fig. 2. The aquifer region is discretisized into 160 triangular elements with 99 nodes. The aquifer has a constant depth of 100 metres with the value of storage coefficient 0.0009 everywhere. The hydraulic heads between A and B and between D and E along the boundaries are assumed to be constant at values of 200 m and 190 m, respectively. At the other sides of the region, there is no flow across the boundaries. The aquifer is divided into three parameter zones 1, 2, and 3 that are indicated by different types of shading. There is a pumping well located at node 49 with the discharge of 5000 cubic metres per day. The initial values of hydraulic heads in the aquifer before pumping are shown in Fig. 3. The pumping well is also used as an observation well. There are two more observation wells located at nodal points numbered as 25 and 78. The hydraulic heads that are observed at 3 observation wells are presented in Table 1. The observed hydraulic conductivities in these wells are also shown in Table 1.

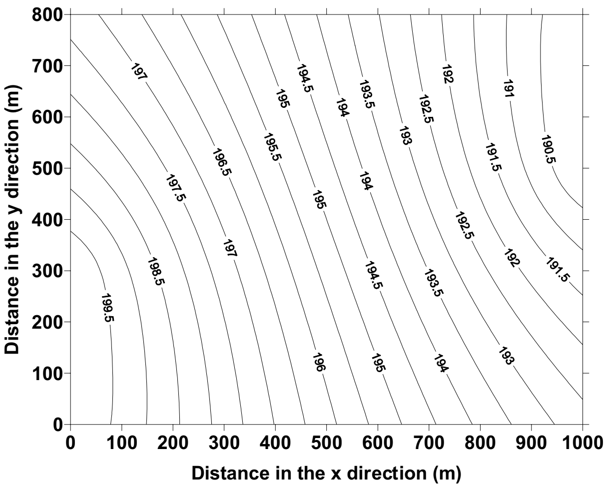


Figure 3. The initial hydraulic heads before pumping

Table 1: The observed hydraulic heads and hydraulic conductivities

Time (days)	Observed hydraulic heads (m)		
	Node #25	Node #49	Node #78
0.1	196.32	190.58	192.03
0.5	194.77	188.91	191.18
1	194.14	188.27	190.73
5	193.81	187.94	190.50
10	193.78	187.91	190.48
20	193.76	187.89	190.46
Observed Hydraulic conductivities (m/d)	5.64	5.05	3.90

5. RESULTS AND DISCUSION

The results of the inverse analysis are discussed. The hydraulic conductivities in each zone resulting from the inverse analysis are 5.7 m/d, 4.66 m/d, and 4.22 m/d for zones 1, 2, and 3, respectively.

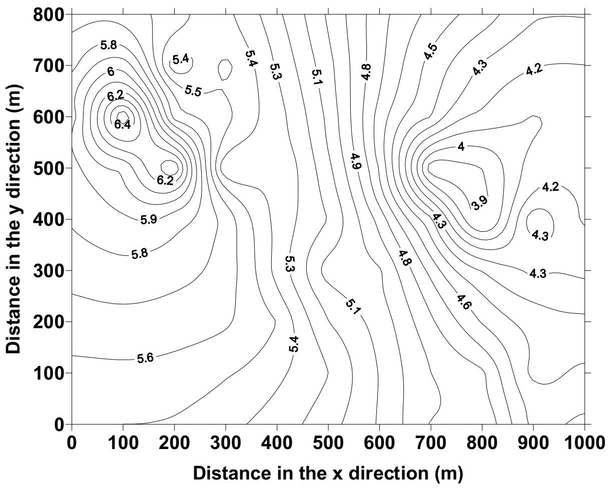


Figure 4. The distribution of estimated hydraulic conductivities in the aquifer (m/d) -- μ_Y = 1.61, σ_Y^2 = 0.05, and l_Y = 900 m

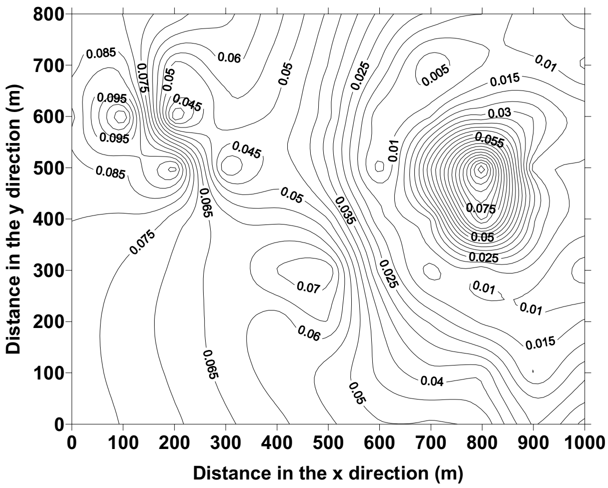


Figure 5. The distribution of variance of the estimated hydraulic conductivities in the aquifer -- μ_Y = 1.61, σ_Y^2 = 0.05, and l_Y = 900 m

The resulting statistical parameters of the model are μ_Y = 1.61, σ_Y^2 = 0.05, and l_Y = 900 m. The distribution of the estimated hydraulic conductivities in the aquifer is shown in Fig. 4 and the distribution of variance of the estimated hydraulic conductivities is presented in Fig. 5.

The distribution of the estimated hydraulic conductivities shown in Fig. 4 indicates an agreement, in most locations, with the distribution of the "true" values of hydraulic conductivities shown in Fig. 1. The degree of agreement between the two distributions of hydraulic conductivities can also be shown by calculating the value of L2-norm of the hydraulic conductivity values. The value of L2-norm in this case is 0.12, which is an indication of a good agreement. Moreover, the amount of agreement also can be determined by using the value of L2-norm calculated for the prediction errors. The L2-norm of the prediction errors is found to be 0.33 in this comparison.

At this stage of the investigation, it was decided to find out how the results of the inverse analysis would change if the statistical parameters had different values than those given in the previous paragraph. It was assumed that the statistical parameters of the model had a range of values as indicated next. The mean, μ_Y, ranged between 1.5 and 1.7, the variance, σ_Y^2, ranged between 0.03 and 0.06, and the correlation length, l_Y, varied between 700 and 1000 m in repeated calculations. However, in the calculation of the distribution of hydraulic heads using the cokriging method the value of μ_Y is not needed; therefore, the use of μ_Y is excluded from the comparison. The resulting distribution of hydraulic conductivities calculated by using different values of σ_Y^2 and l_Y are presented in Figs. 6 to 9.

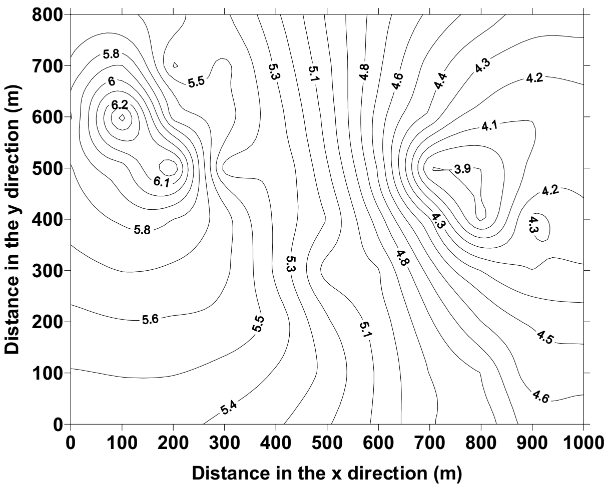


Figure 6. The distribution of estimated hydraulic conductivities in the aquifer (m/d) -- μ_Y = 1.61, σ_Y^2 = 0.05, and l_Y = 700 m

From these figures, it can be seen that the patterns of the distribution of hydraulic conductivities do not change as the value of l_Y increases. However, the contour lines shift slightly toward the edge of the aquifer. The values of L2-norm for the hydraulic conductivity values are 0.11944, 0.11927, 0.11925, 0.11926, and 0.11937 for l_Y values of 700 m, 800 m, 850 m, and 1000 m, respectively. The values of L2-norm for the predicted errors are 0.341531, 0.342174, 0.334046, 0.33713, and 0.337436 for l_Y values of 700 m, 800 m, 850 m, and 1000 m, respectively.

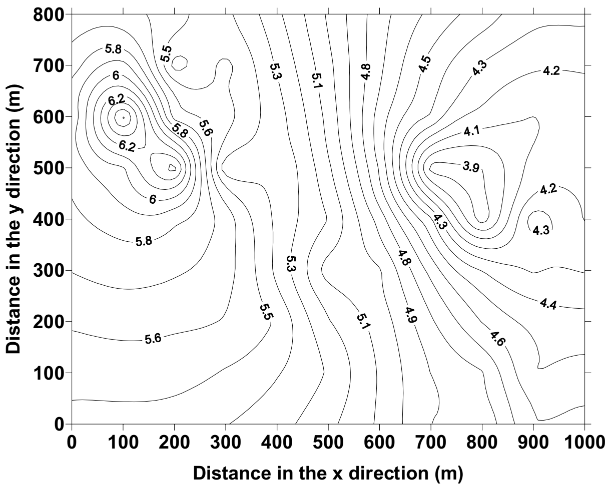


Figure 7. The distribution of estimated hydraulic conductivities in the aquifer (m/d) -- μ_Y = 1.61, σ_Y^2 = 0.05, and l_Y = 800 m

The differences among the values of L2-norm both for the hydraulic conductivities and for the prediction errors are not significant. These values show that the minimum values of L2-norm for the K values and the prediction errors are reached when the value of l_Y is 850 m. However, it was found that the value of σ_Y^2 does not affect the distribution of hydraulic conductivities. This is happening, because, in the calculation of the cokriging coefficients for the estimated hydraulic conductivities using the cokriging method, σ_Y^2 cancels out. The values of σ_Y^2 only affect the distribution of variance of the hydraulic conductivities. A large value of the statistical parameter, σ_Y^2, produces an estimated hydraulic conductivity distribution with a large variance.

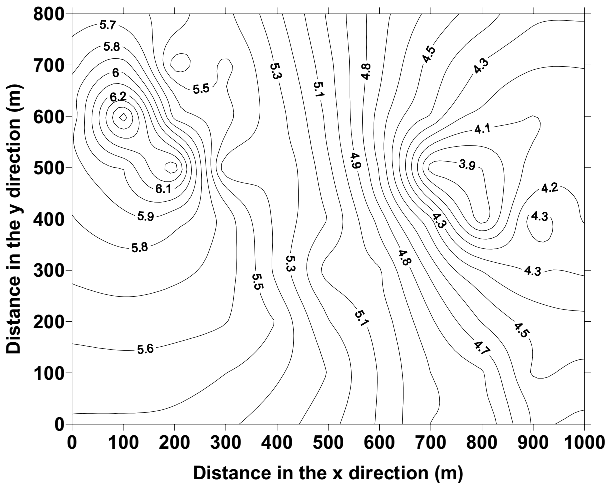


Figure 8. The distribution of estimated hydraulic conductivities in the aquifer (m/d) -- μ_Y = 5, σ_Y^2 = 0.05, and l_Y = 850 m

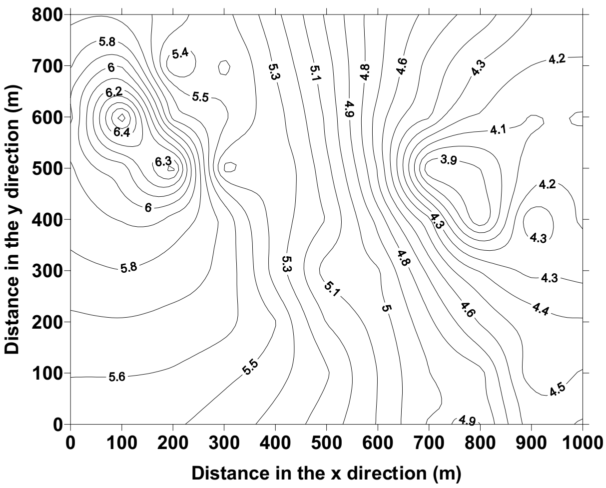


Figure 9. The distribution of estimated hydraulic conductivities in the aquifer (m/d) -- μ_Y = 1.61, σ_Y^2 = 0.05, and l_Y = 1000 m

6. CONCLUSION

The adjoint finite element analysis is a powerful method to estimate the distribution of hydraulic conductivities in an aquifer. In this study, the values of L2-norm between the estimated and true values of hydraulic conductivities are found to be relatively small for different values of l_Y. In addition, L2-norms for the prediction errors in the estimated and true values of hydraulic conductivities are also very small for different values of l_Y. Smallest values of L2-norms, for both the estimated values of hydraulic conductivities and the prediction errors, are obtained when the value of l_y is 850 m. However, L2-norms for different values of l_y are very close to each other for the problem investigated in this study. Further studies are necessary to confirm the generality of this finding. Different values of σ_Y^2 do not affect the resulting distribution of hydraulic conductivities in this particular study. The value of σ_Y^2 only affects the distribution of variance of the hydraulic conductivities. A large value of the statistical parameter, σ_Y^2, produces an estimated hydraulic conductivity distribution with a large variance.

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