

On the stochastic simulation procedure of estimating critical hydraulic gradient for gas storage in unlined rock caverns

Jitae Kim

Woncheol Cho

Il-Moon Chung*

Jun-Haeng Heo

National Institute for Disaster Prevention, 121-719, Korea

Department of Civil Engineering, Yonsei University, 120-749, Korea

Hydrology Research Division, Korea Institute of Construction Technology, 411-712, Korea

Department of Civil Engineering, Yonsei University, 120-749, Korea

ABSTRACT: We investigated some aspects of spatial variability and their effect on critical hydraulic gradient which is essential for gas containment of underground storage caverns. Monte Carlo technique can be effectively applied to obtain an approximate solution to the two-dimensional steady flow of a stochastically defined non-uniform medium. For the stochastic simulation we generated hydraulic conductivity field on the selected grid resolution using HYDRO_GEN with estimated (based on actual data) ln-K statistics with mean, variance, anisotropic integral scales. In this study, among various covariance functions, a Gaussian covariance function (GCF) was used. To find the critical value of the hydraulic gradient, probability density functions (PDFs) using 1000 outputs at an interested cell were developed. The results obtained in this study were compared with previous results for an exponential covariance function (ECF). It was found that in a stationary ln K field the uncertainty of hydraulic head and gradient depend not only on the variance and integral scale of the ln K field but also on the shape of its covariance function. From these results we can conclude that the critical range of hydraulic gradient is significantly affected by the type of covariance function. Thus, when critical hydraulic gradient is to be determined one should consider shape of covariance function as well as statistical parameters such as mean, variance and correlation scale.

Key words: gas containment; underground storage cavern; spatial variability of hydraulic conductivity, critical hydraulic gradient, covariance function

1. INTRODUCTION

Unlined cavern storage is one of a number of storage techniques for highly pressurized gas. The essence of gas containment for this type of storage consists of maintaining a necessary difference between the water pressure in the rock mass and the gas pressure in the storage. To improve the gas containment capacity of such a storage it is necessary to construct a water curtain; a system of boreholes for water injection into the rock mass at some distance from the cavern (Söder, 1994). In general, the accepted criterion for gas leakage into the rock mass is based on water pressure conditions in the rock mass (Åberg, 1977 and Goodall et al., 1988); if the water pressure is larger than the gas pressure

along all possible leakage paths, then no gas can escape. An important contribution to the understanding of the gas leakage process was presented by Åberg (1977), who also concluded that gas leakage could be divided into two separate problems: gas entry and gas migration. The most important conclusion was that the critical factor in gas migration is the hydraulic gradient and that the criterion for no gas leakage may be expressed as a vertical gradient larger than one. Goodall (1986) continued Åberg's work through laboratory tests in a Hele-Shaw model; he also performed numerical simulations and analyzed numerous geometries, both on the local and the global scale.

The numerical flow analyses commonly used for the evaluation of gas containment around the storage cavern can be classified roughly into three types which are the equivalent continuum methods, discrete fracture methods, and stochastic continuum methods, respectively. The most relevant gas loss mechanism for compressed storage was believed to be for migration along fracture planes (Söder, 1994). Jang et al. (1996) developed the fracture network model to analyze the requirements of hydraulic containment for underground oil storage cavern in Korea. Guerin and Billaux (1993) presented a method of estimating the validity of the continuum assumption for a rock mass. From joint mapping statistics, a three-dimensional joint network was constructed and a hydraulic gradient was imposed on the model in different directions. For each of these directions, the flow through the model and the corresponding directional permeability was calculated. From these directional permeabilities, a variability index for the permeability was calculated, which decreases when the behavior approaches that of a porous medium. Söder (1994) pointed out that the hydraulic behavior of a jointed rock mass is a scale dependent problem. Detailed models on the scale below that which is implied by the size of the REV can be achieved by a discrete joint model. However, a geometrical realization of the actual joint system is a time-consuming process, unless an efficient method is implemented; the method suggested by Dershowitz et al. (1991) seems less complicated in this respect. Furthermore, this type of model requires validation field test data in order

*Corresponding author: imchung@kict.re.kr

to give reliable results.

For large-scale prognosis, the continuum approach is believed advantageous due to its simple nature. So far, most of analyses for designing gas containment criteria have been conducted by deterministic flow analysis using the equivalent continuum concept (GEOSTOCK, 1984; Komada, 1985; Goodall et al., 1988; Liang and Lindblom, 1994). The main problem in these methods is to choose a representative mean value for the hydraulic parameters, normally the hydraulic conductivity, from field tests.

Stochastic continuum methods constitute a type of continuum models where the hydraulic conductivity is represented by a statistical distribution rather than a constant value. From a set of hydraulic conductivities, forming a pre-defined distribution, each value is implemented randomly in a model. From a number of simulations of such realizations, a so called Monte-Carlo simulation, a more correct description of the hydraulic behavior of a rock mass is possible. The comprehensive studies on the stochastic simulation technique have been performed in the hydrological and hydrogeological area (Freeze, 1975; Smith and Freeze, 1979; Smith and Schwartz, 1980; Delhomme, 1979; Matheron, 1973; Mantoglou and Wilson, 1982; Griffiths et al., 1994; Shin et al., 1998).

The object of this study is to widen the use of stochastic hydraulic safety factor for gas containment based on stochastic approach. A part of the present investigation has already been reported in Chung et al. (2003) who aimed at the investigation of a hydraulic safety factor for an underground storage cavern in a fractured rock massive by using stochastic simulation to overcome the limitation of deterministic flow modeling.

Several covariance functions for log hydraulic conductivity fields, $Y = \log K$, have been proposed in the literature (e.g., de Marsily, 1986) for characterizing spatial covariance structure. The most popular is the exponential covariance function (ECF), shown as the solid curve in Figure 1.

$$C_Y(x, z) = \sigma_Y^2 \exp \left\{ - \left[\left(\frac{x}{\lambda_x} \right) + \left(\frac{y}{\lambda_y} \right)^2 \right]^{1/2} \right\} \quad (1)$$

λ_x, λ_y : the directional $\ln K(\mathbf{x})$ correlation length scales
 σ_Y^2 : the variance of $\ln K(\mathbf{x})$.

Also, the Gaussian covariance function is expressed as

$$C_Y(x, z) = \sigma_Y^2 \exp \left\{ - \left[\left(\frac{x}{\lambda_x} \right) + \left(\frac{y}{\lambda_y} \right)^2 \right] \right\} \quad (2)$$

and is shown as the dashed curve in Figure 1.

Zhang and Di Federico (1998) have conducted solute transport analysis in three-dimensional heterogeneous media with a Gaussian covariance of log hydraulic conductivity

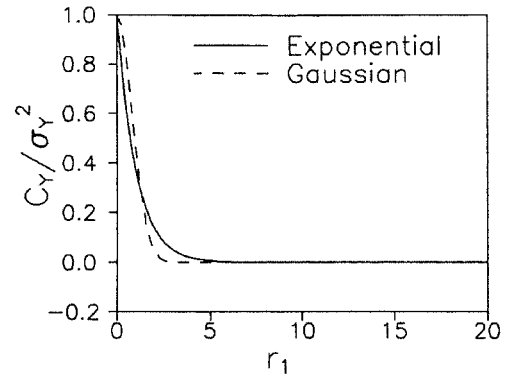


Fig. 1. The exponential covariance (the solid curve) and the Gaussian covariance (the dashed curve) of $\log K$, which are normalized by the variance of $\log K$, σ_Y^2 , as functions of the dimensionless separation distance along the mean flow direction r_1 (from Zhang and Di Federico, 1998).

and found that in a stationary $\ln K$ field the spreading of a solute plume depends not only on the variance and integral scale of the $\ln K$ field but also on the shape of its covariance function. We also present herein an extended application using the Gaussian covariance function (GCF) of logarithmic hydraulic conductivity, to see the effect of the shape of covariance function. The results obtained in this study were compared with previous results for an exponential covariance function (ECF) and discussed.

2. PREVIOUS STUDIES ON GAS CONTAINMENT CRITERIA

A number of works on the gas containment criteria have been conducted during the past decades and summarized by Söder (1994). The first theoretical explanation of the physical process involved was reported by Åberg (1977); it is summarized below. Åberg started with pointing out that a fracture above the cavern with stagnant or slowly moving water towards the storage was not sufficient to prevent leakage of gas. Since the downward rate of water flow in fractures above the storage must reach a certain value, the process of gas leakage in the opposite direction must be in the form of bubbles. He proposed that a vertical hydraulic gradient greater than 1.0 around a cavern should be maintained through the rock fractures surrounding a storage cavern during gas containment operations. Goodall (1988) concluded that bubble migration away from the gas source was prohibited if the gradient was directed towards the gas source. He used physical model (Hele-Shaw model) as well as numerical model. Nakagawa et al. (1987) also used Hele-Shaw model in a study for compressed air storage. The results were compared with a numerical model which included relative permeability for gas and water saturation ratio and porosity. GEOSTOCK (1984) proposed hydraulic margin expressed in Eq. (3)

$$H > P_{\max} + P + S \quad (3)$$

where

H: height from the ceiling of a cavern to groundwater level (m)

$P_{\max}$: maximum tolerable gas pressure expressed as a head in the cavern (m)

P: Shape factor (m)

S: Safety factor (m)

Liang and Lindblom (1994) suggested the 'critical gas pressure' defined as the maximum tolerable gas pressure for a given storage system at no gas leakage conditions. In order to achieve the required degree of confinement, the water curtain system is installed to increase the hydraulic pressure in relation to the cavern operating pressures. The water curtain will be an active back pressure system designed to create a control envelope to the pressurized gas. The curtain will be established principally over the crown zone of the cavern anticipating a vertically upwards gas migration path. However, these criteria are designed by using the deterministic flow analysis which does not consider the spatial variability of hydraulic conductivity, Chung et al. (2003) proposed a novel criteria called 'stochastic hydraulic safety factor' expressed in Eq. (4) by using the stochastic simulation.

$$H > P_{\max} + P + S + S_s \quad (4)$$

Where S_s is a stochastic safety factor (m) under a given probability.

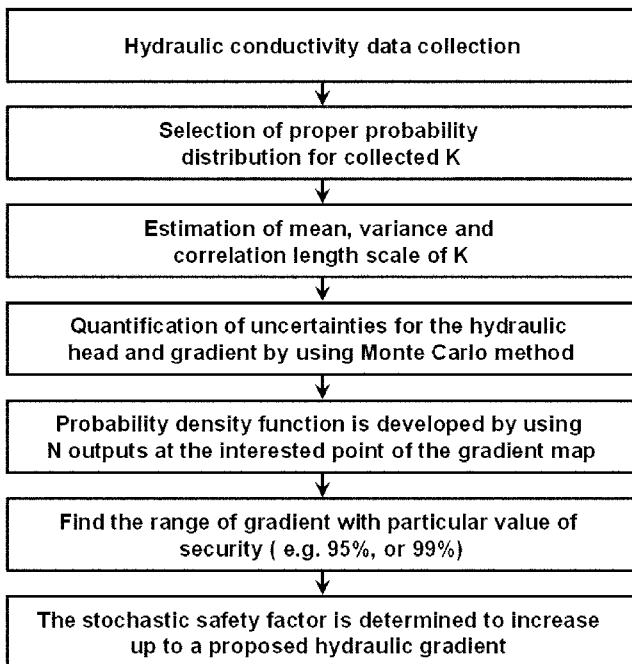


Fig. 2. The procedure to determine stochastic hydraulic safety factor.

The whole procedure to determine this factor is well described in Figure 2.

3. TRADITIONAL APPROACH TO EVALUATE GAS CONTAINMENT

The study site is a propane storage cavern in Korea. The representative vertical cross section for flow analysis is shown in Figure 3 and the outline of propane storage cavern in study sites is shown in Table 1. Total hydraulic pressure above the ceiling of cavern maintained by water curtain system was 120 m in head. Since the gas pressure is equivalent to 86 m in head, thus the head difference between cavern and water curtain is 34 m, which is the hydraulic safety factor ($P+S$) in Eq. (3).

Although the influence of individual fissures on groundwater flow in fractured rock masses might not be negligible, the analysis results presented in this study are based on following assumptions: The groundwater flow obeys Darcy's law and the medium is continuous, heterogeneous, and anisotropic. The groundwater flow is steady; that is, groundwater conditions are constant and groundwater is incompressible. Rocks around storage caverns are saturated with rock water. The governing differential equation is the Laplace equation in two dimensions. The finite element program presented in this paper was developed by Chung et al. (1997) which was made for the simulation of groundwater flow caused by water curtain around underground storage cavern. This program is able to deal with stochastic random input of hydraulic conductivity for a large number of simulations. The modeling area is 100 m wide and 100 m deep. The number of finite elements is 400. Linear rectangular elements are used in conjunction with a linear basis function. The mean value of hydraulic conductivity is $1.6 \times 10^{-7} \text{ m s}^{-1}$.

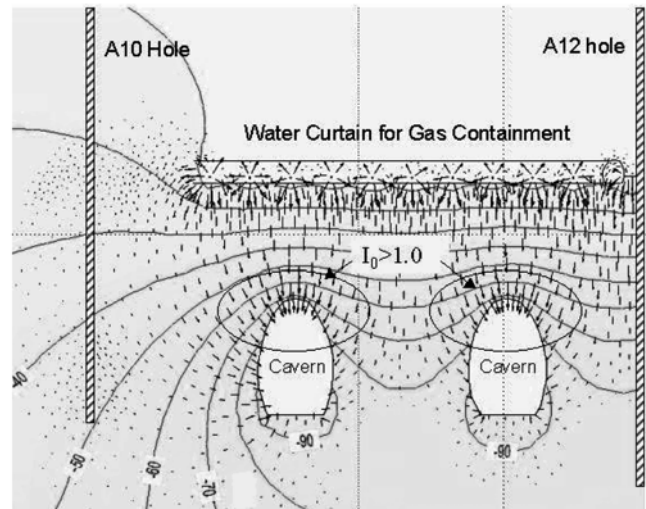
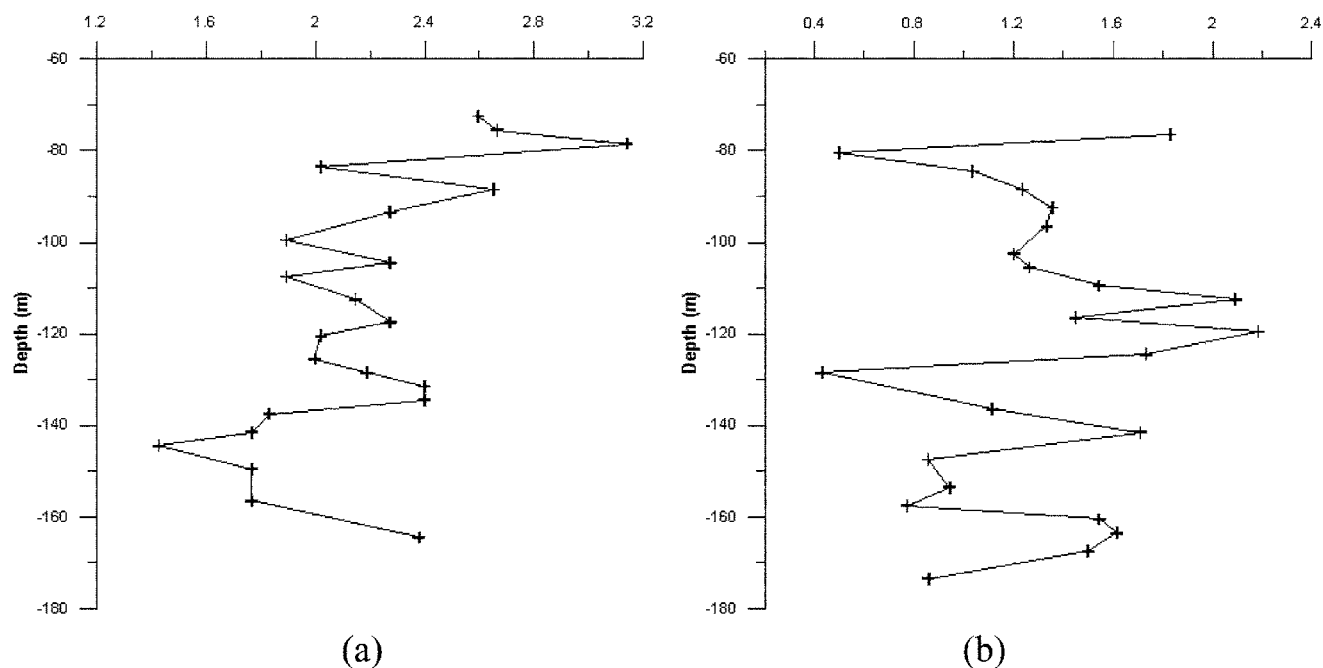
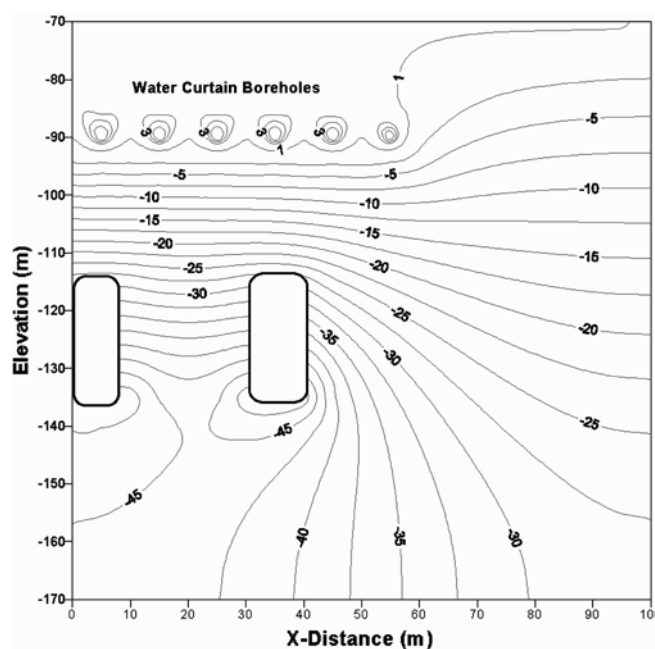


Fig. 3. The representative cross section for flow analysis (after Chung et al., 2003).

Table 1. Outline of propane storage cavern in study sites

Gas pressure in hydraulic head (m)	Elevation of ceilings of caverns (El.m)	Head of water curtains (El.m)	Total hydraulic pressure above the cavern (m)	Safety factor (P+S) (m)
86	-115	5	120	34 (=120-86)

**Fig. 4.** Vertical distribution of hydraulic conductivity data (Korea Petroleum Development Cooperation, 1985) (a) A10 hole, (b) A12 hole.**Fig. 5.** The Computed Hydraulic Head by Deterministic Modeling (from Chung et al., 2003).

which is computed by using the 45 data from A10 and A12 boreholes adapted from Korea Petroleum Development Cooperation (1985) shown in Figure 4.

The shape of the cavern is simplified as rectangular whose height is 20 m and the width is 10 m. Two types of boundary condition (constant head boundary at the water curtains and the caverns and no flow boundary for both sides) were used. Figure 5 shows the deterministic contours of computed hydraulic head. As shown in Figure 6, in most cells surrounding upper part of the caverns (marked by dashed line), the Åberg's gas tightness condition was satisfied because the hydraulic gradients are greater than 1. However, in a cell within the crown surrounding upper part of the cavern B ($x = 27.5$, $z = -122.5$), mean hydraulic gradients are less than 1, it shows that the Åberg's condition was not satisfied.

4. STOCHASTIC APPROACH TO EVALUATE GAS CONTAINMENT

The concept of stochastic hydrology can be simply summarized as shown in Figure. 7. The process of aquifer characterization can be seen as that of providing the "correct input" to a transfer function which represents some hydro-

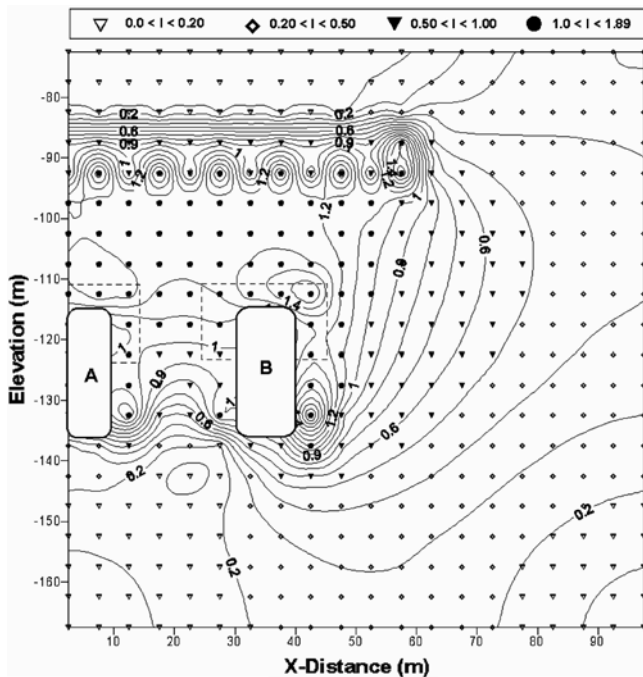


Fig. 6. The Computed Hydraulic Gradient by Deterministic Modeling (from Chung et al., 2003).

geological process. For example, the transfer function may be a numerical simulator of transport, requiring the spatial distributions of the hydraulic conductivity and porosity, and perhaps some chemical reaction parameters, and the output may be the probability distribution function (PDF) of the travel times between a potential contamination source and some regulatory plane of compliance (Delleur, 1998).

Namely, stochastic analysis of groundwater systems is a method of incorporating the flow model into a statistical description of aquifer variability, and this leads to a statistical description of the associated head field (Mizell et al.,

1982). The Monte Carlo type approach generally makes use of generators of random space-time functions (Matheron, 1973; Mejia and Rodriguez-Iturbe, 1974; Gutjahr, 1989; Bellin and Rubin, 1996) to generate fields with specified spatial-temporal covariance structures (Rodriguez-Iturbe et al., 1998).

In this study, Monte Carlo simulation has been used to quantify the impact of the hydraulic conductivity on the hydraulic gradient variation in order to evaluate the potential risk of gas leakage. The proposed methodology consists in three steps: (1) a stochastic approach to generate synthetic realizations of random spatially correlated parameters K , (2) a modeling study, based on a two dimensional finite element groundwater model, to simulate for each realization of heads and hydraulic gradients around underground storage caverns, and (3) a statistical analysis of the simulated fields. With this strategy, we attempt to cover the uncertainty of the model parameter K in the prediction of hydraulic head and gradient for the study site.

In the previous work (Chung et al., 2003), various probability distributions such as the two- and three- parameter gamma (three parameter means scale, shape and location parameter, respectively), General Extreme Value (GEV), Gumbel, two- and three- parameter lognormal, log-Pearson type III are applied and validated to determine probability distribution of hydraulic conductivity data obtained in the study area. Among the 4 models (Gamma-2, GEV, Gumbel, Lognormal-2) which passed statistical validation test, two-parameter lognormal distribution is selected as an appropriate model for the stochastic simulation because this is generally assumed as appropriate for the hydraulic conductivity data, as shown in many studies (McMillan, 1966; Freeze, 1975; Woodbury and Sudicky, 1991; Massmann and Hagley, 1995).

The $\ln K$ field generation has been carried out with the HYDRO_GEN computer code (Bellin and Rubin, 1996) which have been frequently used by researchers and scien-

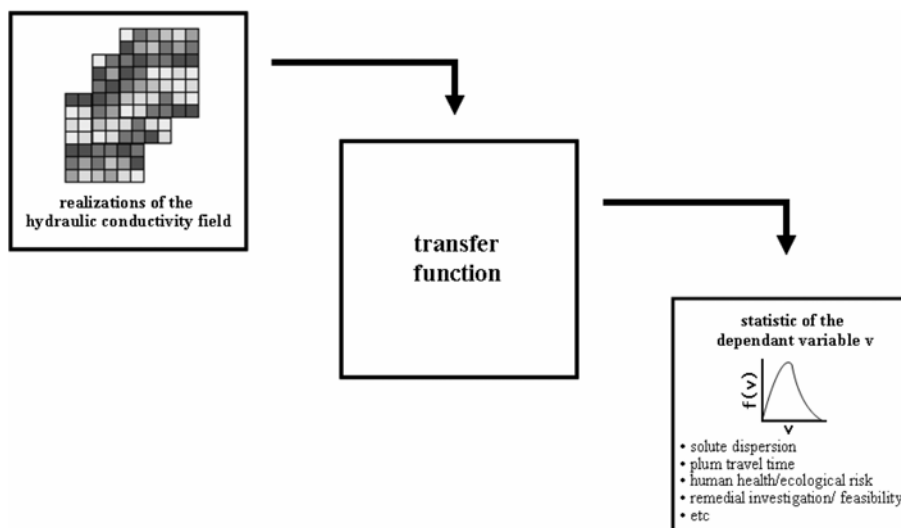


Fig. 7. The Monte Carlo method in aquifer studies (after Delleur, 1998).

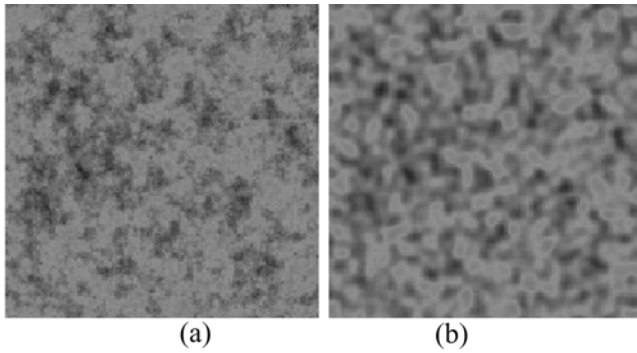


Fig. 8. Hydraulic conductivity field generated using the HYDRO_GEN (Bellin, 2007). (a) an exponential covariance, (b) a Gaussian covariance.

tists to generate spatially correlated random fields, and the validity of this methods has been widely reported in the literature. The two main advantages of this model are its ability to reproduce the prescribed spatial moments as well as the associated computational time. Another feature that directly affects the required computational effort is the accuracy of the resulting output values. The relative ease with which the HYDRO_GEN code was compiled and its free of charge availability were also encouraging factors in selecting this model over other stochastic models. Two simulated examples of hydraulic conductivity fields, having two different types of covariance, are illustrated in Figure 8.

We describe hydraulic conductivity field as a random field and generate 1000 realizations in vertical plane. For each realization, the groundwater head and gradient are solved and results are analyzed statistically. For the stochastic

simulation we generated hydraulic conductivity field on the selected grid resolution using HYDRO_GEN with estimated (based on actual data) $\ln K$ statistics with mean, variance, anisotropic integral scales. In this study, among various covariance functions, a Gaussian covariance function (GCF) was used. The results obtained in this study were compared with previous results (Chung et al., 2003) for an exponential covariance function (ECF).

In our realizations, the mean and standard deviation of the log-transformed hydraulic conductivity data are given as $\mu_Y = -4.79$ ($Y = \ln K$, K in cm/s) and $\sigma_Y = 0.27$. Regarding correlation scales, detailed procedure were already introduced for obtaining proper correlation length scale in which estimated autocorrelation functions for the data from A10 and A12 holes were included (Chung et al., 2003). Gelhar (1993) pointed out that the significant anisotropy of the spatial correlation structure in many sedimentary materials and the vertical scales are an order of magnitude less than the horizontal scale. In that study, referring to the results ($\sigma_Y = 0.4$, $\lambda_{h1} = 8$ m, $\lambda_{v1} = 3$ m) from Goggin et al. (1988) where the vertical scale is 60 m, the value of the horizontal and vertical correlation scales ($\lambda_{h1} = 15$ m, $\lambda_{v1} = 5$ m) were estimated since overall scale of measurement is similar to that work. The smoothed log conductivity fields according to different covariance functions (ECF and GCF) are shown in Figure 9. In particular, it is noteworthy that each field has distinct features, although the ranges of $\ln K$ are similar.

To estimate the effect of spatial variability statistically, the Monte Carlo method is used. The hydraulic conductivity values K_i can be generated by using the following equa-

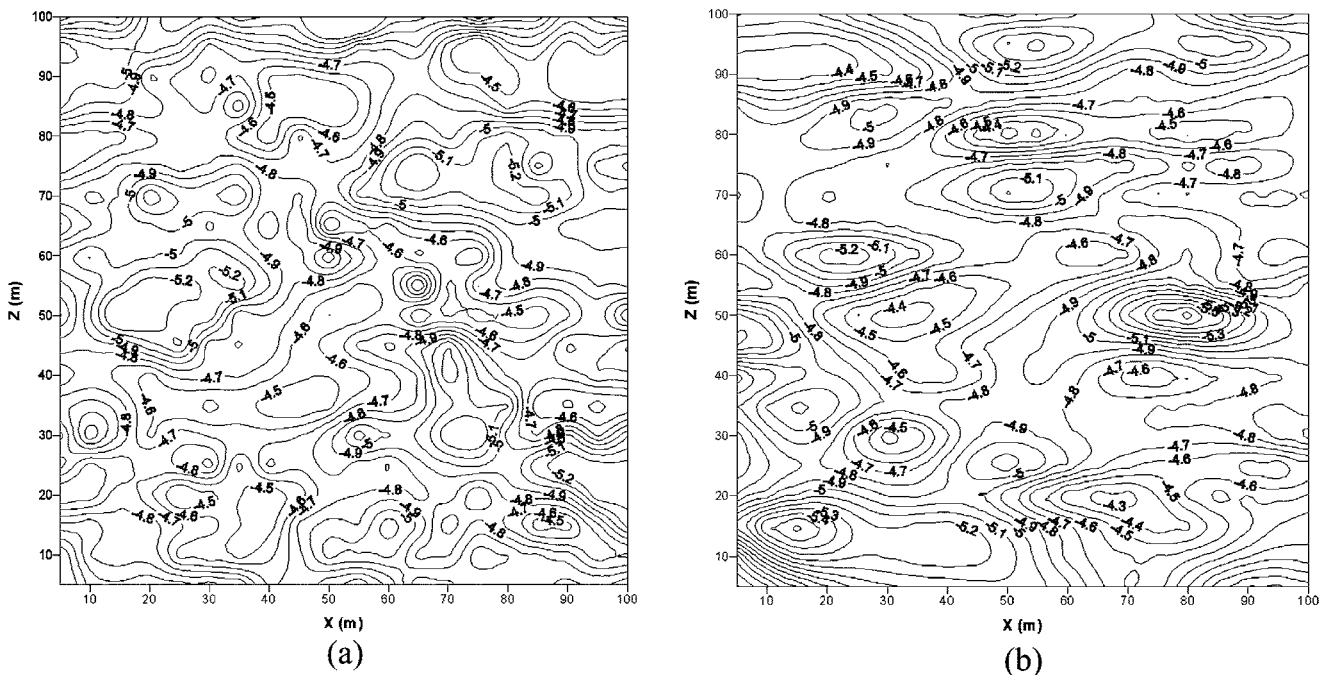


Fig. 9. Smoothed Log Hydraulic Conductivity Contours ($Y = \ln K(x)$, K in cm/s) (a) $\ln K$ field with ECF (b) $\ln K$ field with GCF.

tion.

$$K_i = 10^{y_i}, i = 1, \dots, p \quad (5)$$

where

p = number of finite elements

Then the FEM model is used to solve the head values on a set of nodal points within the flow domain. By repeating the analysis 1000 times, the frequency distributions of hydraulic head and gradient at the nodal points in the finite element grid can be analyzed to estimate the statistical properties representing the uncertainty of the hydraulic head and gradient.

The Figure 10 shows the distribution of standard deviation of hydraulic head (σ_ϕ) for the simulation case 1 (ECF) and case 2 (GCF). Case 1 and Case 2 show very similar uncertainty of hydraulic head ranged from 0 m to 3.1 m (case 1) and 0 m to 3.14 m (Case 2), respectively. But the spatially distributed feature of uncertainty is slightly different. The water curtains have the constant head boundaries in which hydraulic heads are maintained as elevation 5.0 m by artificial management, and the caverns also have the known boundaries in which the gas pressure has been maintained constant for a long time. Especially, σ_ϕ is higher in the upper region of the caverns than in any other region.

The standard deviations of hydraulic gradient (σ_g) are plotted in Figure 11. We can find a different range of uncertainty according to the shape of covariance function as shown in Figure 11a, b. It means that the shape of covari-

ance function has effect on the uncertainty of the hydraulic gradient. When GCF was used, the standard deviations of the hydraulic gradient ranged from 0 to 0.51 (Fig. 11b), compared with the hydraulic gradient ranged from 0 to 0.48 (Fig. 11a) when ECF was used.

As mentioned earlier, the Åberg's gas tightness can be maintained by steady mean hydraulic gradient (I), which is greater than 1 in the periphery of a cavern. However, due to the heterogeneity of $\ln K$, uncertainty in hydraulic gradient could affect the gas tightness of some cells in the upper part of cavern. To find the critical value of the hydraulic gradient, probability density functions (PDFs) using 1000 outputs at two interested cells were developed for both cases (ECF, GCF) as shown in Figure 12. In these PDFs we could set a particular value for the security, i.e. 95% or 99% and find the critical gradient value. According to these PDFs, the possible ranges of hydraulic gradients at a cell in the upper part of cavern B ($x = 27.5$ m, $z = -122.5$ m) is examined with a given probability as shown in Table 2.

With a given probability of 95%, critical hydraulic gradients can be obtained as 0.662 for case 1 (ECF) and 0.705 for case 2 (GCF) at a cell as shown in Table 2. When the proposed critical hydraulic gradient (e.g., 1.0 for Åberg's criteria) is greater than this critical hydraulic gradient, gas tightness could not be satisfied at that point. Therefore, the hydraulic gradient should be increased as much as the proposed value (e.g., 0.338 for case 1 and 0.295 for case 2 according to Åberg's condition) to prevent gas leakage. With a 99% security, the critical hydraulic gradient was 0.493 for case 1 and 0.560 for case 2. From these results we

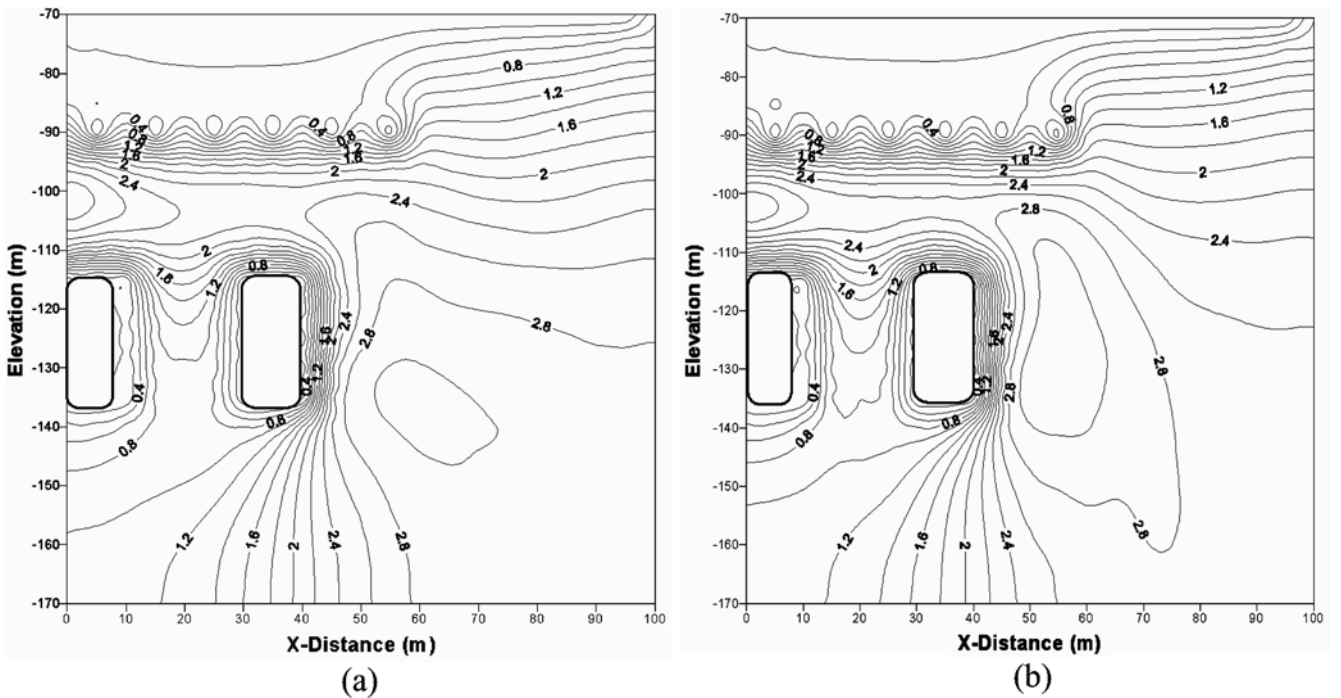


Fig. 10. The Distribution of Standard Deviation of Hydraulic Head (σ_ϕ) (a) Case 1 (ECF) (b) Case 2 (GCF).

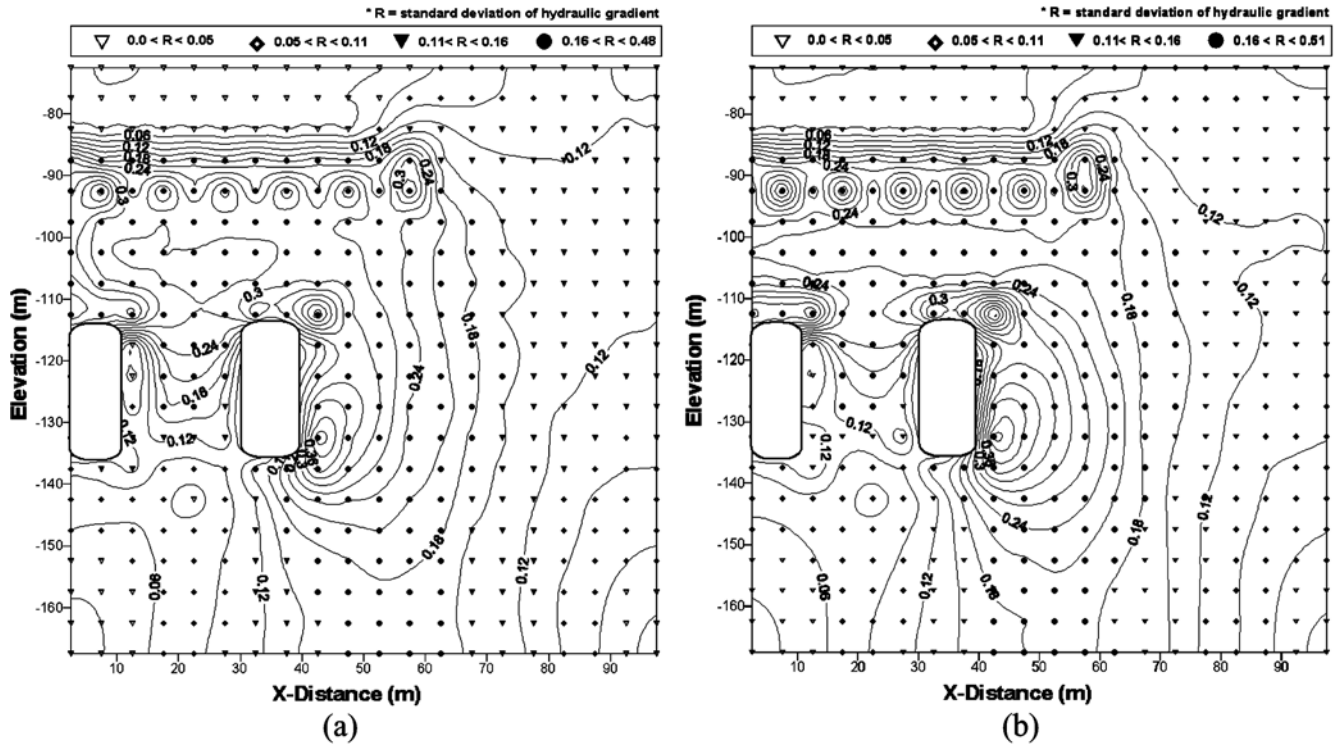


Fig. 11. The Distribution of Standard Deviation of Hydraulic Gradient (σ_g) (a) Case 1 (ECF) (b) Case 2 (GCF).

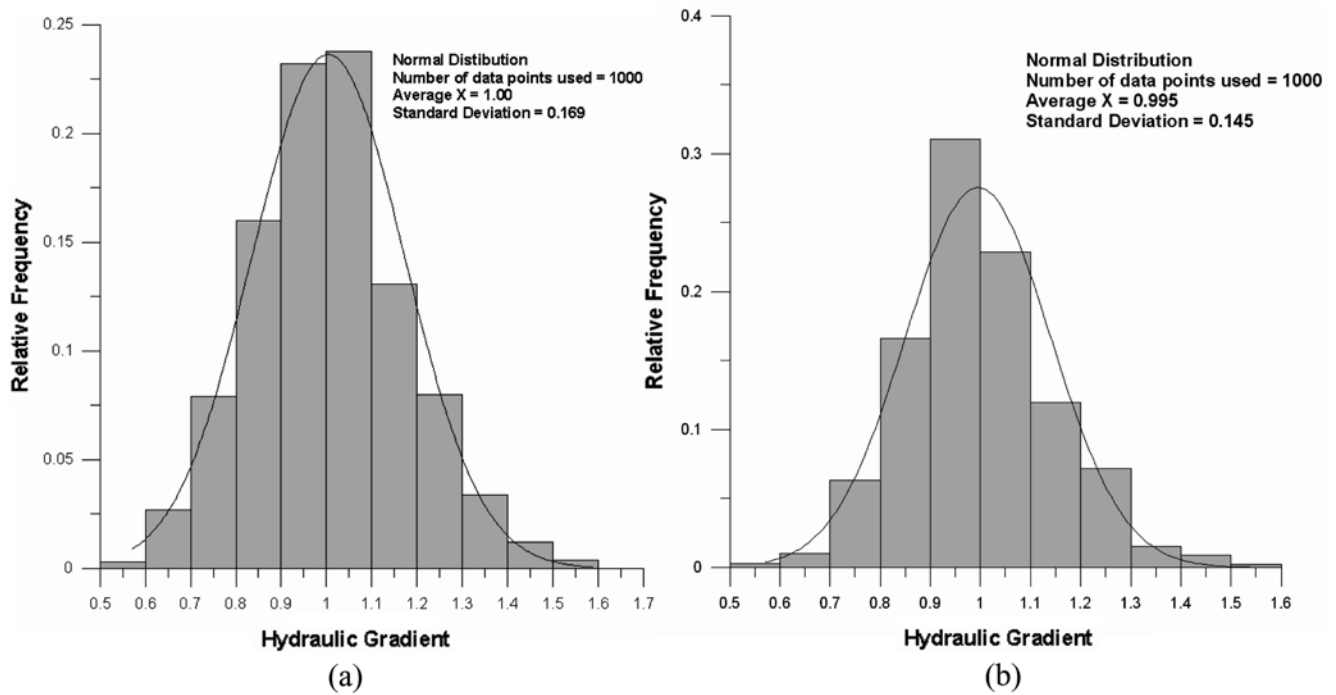


Fig. 12. The Probability Distribution Functions of Hydraulic Gradient at a Cell in the Upper Part of Cavern B ($x = 27.5$ m, $z = -122.5$ m) (a) Case 1 (ECF) (b) Case 2 (GCF).

can conclude that the critical range of hydraulic gradient depends not only on the variance and integral scale of the $\ln K$ field but also on the shape of its covariance function.

6. SUMMARY AND DISCUSSION

In this article, we examined some aspects of spatial vari-

Table 2. Critical Ranges of Hydraulic Gradient with Given Probabilities at a cell in the upper part of cavern B ($x = 27.5$ m, $z = -122.5$ m)

Shape of Covariance Function	Critical range of hydraulic gradient with given probabilities	
	95%	99%
Exponential	$0.662 < I < 1.338$	$0.493 < I < 1.507$
Gaussian	$0.705 < I < 1.285$	$0.560 < I < 1.430$

ability and their effect on hydraulic head and gradient prediction and proposed the method of determining critical hydraulic gradient for gas containment of underground storage cavern by stochastic simulation, considering the heterogeneity of hydraulic conductivity. We described hydraulic conductivity field as a random field and generate 1000 realizations in vertical plane. For each realization, the groundwater head and gradient are solved and results are analyzed statistically. For the stochastic simulation we generated hydraulic conductivity field on the selected grid resolution using HYDRO_GEN code with estimated (based on actual data) $\ln K$ statistics with mean of -4.79 (cm/s), standard deviation of 0.27 and anisotropic integral scales of 15 m and 5 m in horizontal and vertical direction, respectively. In particular, a Gaussian covariance function (GCF) of logarithmic hydraulic conductivity, $\ln K$, was used. The results obtained in this study were compared with previous results for an exponential covariance function (ECF). It was found that in a stationary $\ln K$ field, the hydraulic head and gradient depend not only on the variance and integral scale of the $\ln K$ field but also on the shape of its covariance function. In particular, critical hydraulic gradient with a given probability was significantly affected by the type of covariance function. Thus, when critical hydraulic gradient is to be determined one should consider shape of covariance function as well as statistical parameters such as mean, variance and correlation scale. Since current study is limited to two dimensional analysis, further study should be extended to three dimensional analysis.

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