

Conditional expectation for evaluation of risk groundwater flow and solute transport: one-dimensional analysis

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Received 24 July 1995; revised 3 December 1996; accepted 30 January 1997

Abstract

A one-dimensional groundwater transport equation with two uncertain parameters, groundwater velocity and longitudinal dispersivity, is investigated in this paper. The analytical uncertainty of the predicted contaminant concentration is derived by the first-order mean-centered uncertainty analysis. The risk of the contaminant transport is defined as the probability that the concentration exceeds a maximum acceptable upper limit. Five probability density functions including the normal, log-normal, gamma, Gumbel, and Weibull distributions are chosen as the models for predicting the concentration distribution. The risk for each distribution is derived analytically based on the conditional probability. The mean risk and confidence interval are then computed by Monte Carlo simulation where the groundwater velocity and longitudinal dispersivity are assumed to be lognormally and normally distributed, respectively. Results from the conditional expectation of an assumed damage function show that the unconditional expectation generally underestimates the damage for low risk events. It is found from the sensitivity analysis that the mean longitudinal dispersivity is the most sensitive parameter and the variance of longitudinal dispersivity is the least sensitive one among those distribution models except the gamma and Weibull distributions. © 1997 Elsevier Science B.V.

Keywords: Ground water; Monte Carlo analysis; Risk assessment; Sensitivity analysis; Solute transport

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Notation

b	a constant in the damage function ϕ
c	concentration of sample contaminant, (ML ³)
c_0	source constant concentration at $x = 0$, (ML ³)
C	random variable of the contaminant concentration
c^*	maximum acceptable upper limit of contaminant concentration, (ML ³)
c_l	lower bound of concentration for each distribution of the predicted concentration, (ML ³)
D	dispersion coefficient, (L ² /T)
d_i	sensitivity of functional output, Y , to the i th random variable, X_i
d_v	sensitivity of C with respect to V
d_{α_L}	sensitivity of C with respect to α_L
$f_c(c)$	probability density function (pdf) of C
$F_c(c)$	cumulative distribution function (CDF) of C
$f_G(g)$	pdf of the damage G
$F_G(g)$	CDF of the damage G
$f_L(l)$	pdf of the loading L
$F_L(l)$	CDF of the loading L
$f_S(s)$	pdf of strength S
$F_S(s)$	CDF of strength S
G	random variable of the damage
G_c	conditional expectation of damage
\bar{G}	unconditional expectation of the damage
L	loading
M	number of Monte Carlo runs
N	number of generated data or sampling points
p_i	probability of a partitioning points on the probability axis of G
\bar{R}	sample mean risk
R	risk
Re	reliability
R_θ	sensitivity of the risk with respect to the parameter θ
S	strength
s^*	deterministic upper limit of strength
S_θ	sensitivity coefficient of the risk with respect to the parameter θ
s_R	sample standard deviation of risk
t	time, (T)
$t_{\beta\alpha/2, n-1}$	variate of the students' t -distribution with the degree of freedom $n - 1$
V	uniform groundwater velocity, (L/T)
v_i	sample variate of the velocity used in the Monte Carlo simulation, (L/T)
x	distance from the source of contaminant, (L)
Z_θ	log-transformed sensitivity coefficient
α_L	longitudinal dispersivity, (L)
α_{L_i}	sample variate of α_L used in the Monte Carlo simulation, (L)
β_c	significance level
γ_i	the risk that $C > c^*$, and corresponds to the point g_i on the probability axis of G
κ	dimensionless concentration of sample contaminant, (ML ³)
μ_{α_L}	mean value of α_L , (L)
μ_C	mean value of contaminant concentration C
μ_κ	mean value of dimensionless concentration κ in terms of τ and ρ
μ_V	mean value of V , (L/T)
ρ	dimensionless distance
σ_C	standard error of the predicted concentration C
σ_V	standard deviation of V
σ_{α_L}	standard deviation of α_L

σ_{κ}	standard error of κ in terms of τ and ρ
τ	dimensionless time
ϕ	damage function
φ	general function of the risk R

1. Introduction

Uncertainties are involved in any engineering planning and design as well as groundwater contamination problems. Generally, uncertainties involved in a water-resources project include hydrologic, hydraulic, structural and economic uncertainties (Tung and Mays, 1980). Yet only hydrological and hydraulic uncertainties are considered in this paper for the problem of groundwater contamination. Hydrologic uncertainties originate from the inherent randomness of natural hydrologic processes, the selection of the probability model, and the evaluation of the corresponding parameters used in the probability model; however, hydraulic uncertainties are attributed to the simplification of mathematical models in describing natural physical phenomena, imprecise dimensions of hydraulic structures, non-uniformity of construction materials, and various operational conditions (Lee and Mays, 1983). Uncertainty, commonly analyzed by the concept of random variable, is represented by the variance or standard error of the variable.

Full distribution analyses and first and second moment analyses are the two primary groups for uncertainty analysis (Dettinger and Wilson, 1981). Monte Carlo simulation and the method of derived distribution are the two most important procedures for full distribution analyses. Freeze (1975) and Smith and Freeze (1979) used Monte Carlo simulation to investigate the uncertainty of one-dimensional groundwater flow field in non-uniform homogeneous media. Perturbation and Taylor series expansion methods are the fundamental approaches for the first and second moment analyses. Bakr et al. (1978) and Gutjahr et al. (1978) used the perturbation approach to analyze the groundwater flow field by taking the spatial variability of the hydraulic conductivity into consideration. Method of Taylor series expansion is more straightforward than the perturbation method. Dettinger and Wilson (1981) used the first-order uncertainty analysis to evaluate the uncertainty in numerical models of groundwater flow. Applications of this method on the flood levee design and groundwater management problems can be found respectively in Tung and Mays (1981) and Tung (1986, 1987).

Probability concepts were introduced into engineering projects because of the existence of uncertainties in the natural environment or simply because of lack of data. Reliability analysis or, in its reverse sense, risk analysis has, therefore, made prominent progress in recent years among various fields. Definition of risk or reliability in terms of probability associated with the concept of loading and strength can be found in many books (e.g. Ang and Tang, 1984; Chow et al., 1988; Kapur and Lamberson, 1977). First-order reliability analysis was applied by Shinozuka (1983) and Der Kiureghian and Lin (1986) in structural reliability analysis. Expanding the Taylor series at a specific linearization point instead of the mean value is the primary feature of this approach. The general procedures in risk and reliability analyses using an example of culvert design have previously been described by Yen (1987). Furthermore, risk analysis was applied by Tung and Mays (1981) and Lee and

Mays (1983) towards the design of levees. Sitar et al. (1987) applied the first-order reliability approach to the analysis of groundwater flow and contaminant transport. However, the example provided in their work only considered the advection dominant effect in the transport equation.

Evaluating the relationship between unconditional and conditional expectations for risk-based decision-making problems is of recent interest (Asbeck and Haimes, 1984; Petrakian et al., 1987; Karlsson and Haimes, 1988a, b). In general, mathematical unconditional expectation was applied in the conventional decision-making processes. However, this approach may possibly conceal some information regarding extreme events as verified by Karlsson and Haimes (1988a). Therefore, conditional expectation was introduced to account for this deficiency. Conditional expectation could be calculated through partitioning the probability axis of the dependent random variable (Asbeck and Haimes, 1984). One of the capabilities of this approach is being able to consider events with different levels of significance. This approach could also be introduced into groundwater contamination problems if one is interested in estimating the damage caused by an extreme event.

An analytical solution of a one-dimensional transport equation is used here to investigate the risk owing to groundwater contamination. The uncertainty of the predicted contaminant concentration is calculated by the first-order mean-centered uncertainty analysis. Risk is derived from the concept of the conditional probability of failure for five probability distribution models of the predicted concentration. A conceptually hypothesized relationship between risk and damage is then assumed. Finally, sensitivities of the risk with respect to various model parameters are evaluated.

2. Mathematical background

A saturated groundwater system with a uniform flow field is considered. The one-dimensional transport equation if the chemical reaction and adsorption are absent is

$$\frac{\partial C}{\partial t} = -V \frac{\partial C}{\partial x} + D \frac{\partial^2 C}{\partial x^2} \quad (1)$$

where C is the concentration of a contaminant; V is the uniform groundwater velocity; and D is the dispersion coefficient and is assumed to be a constant. The dispersion coefficient may be expressed as the product of the longitudinal dispersivity (α_L) and the uniform groundwater velocity, that is $D = \alpha_L V$, when neglecting the molecular diffusion. The first term on the right-hand side of Eq. (1) represents the advection component and the second term represents the dispersion component. The initial and boundary conditions related to Eq. (1) are

$$C(x, 0) = 0 \quad (2)$$

$$C(0, t) = c_0$$

$$C(\infty, t) = 0$$

where c_0 , a fixed value, represents the source concentration at $x = 0$. The solution of Eq. (1)

subjected to the initial and boundary conditions of Eq. (2) is (Freeze and Cherry, 1979)

$$C = \frac{c_0}{2} \left\{ \operatorname{erfc} \left[\frac{x - Vt}{\sqrt{4\alpha_L Vt}} \right] + \exp \left(\frac{x}{\alpha_L} \right) \operatorname{erfc} \left[\frac{x + Vt}{\sqrt{4\alpha_L Vt}} \right] \right\} \quad (3)$$

where $\operatorname{erfc}()$ is the complementary error function.

3. Uncertainty analysis

Consider a general function, Y , which is assumed to be composed of n random variables X_1, X_2, \dots, X_n . Expanding Y at the mean of each random variables $\mu_1, \mu_2, \dots, \mu_n$ and neglecting the second-order and higher-order terms, the first-order mean-centered Taylor series approximation of Y is

$$Y = Y(\mu_1, \mu_2, \dots, \mu_n) + \sum_{i=1}^n \frac{\partial Y}{\partial X_i} (X_i - \mu_i) \quad (4)$$

The first-order mean of Y derived from Eq. (4) is (Ang and Tang, 1984)

$$E(Y) = \mu_Y \cong Y(\mu_1, \mu_2, \dots, \mu_n) \quad (5)$$

and, the first-order variance of Y is

$$\operatorname{Var}(Y) = \sum_{i=1}^n d_i^2 E[(X_i - \mu_i)^2] + \sum_{i=1}^n \sum_{j=1}^n d_i d_j \operatorname{Cov}(X_i, X_j) \quad (6)$$

where d_i and d_j respectively represent the partial derivatives $\partial Y/\partial X_i$ and $\partial Y/\partial X_j$ evaluated at $\mu_1, \mu_2, \dots, \mu_n$. These partial derivatives are specifically defined as the sensitivities of Y with respect to X_i . Assuming that the random variables X_1, X_2, \dots, X_n are statistically independent of each other, then Eq. (6) can then be reduced to

$$\operatorname{Var}(Y) \approx \sum_{i=1}^n d_i^2 \operatorname{Var}(X_i) = \sigma_Y^2 \quad (7)$$

Eqs. (5) and (7) are the first-order mean and variance, respectively of the random variable Y . The square root of $\operatorname{Var}(Y)$ is, thus, the first-order mean-centered uncertainty Y . Following the rule of notation adopted in this section, a capital letter refers to a random variable and a lower-case letter refers to the realization of that random variable. For example, C refers to the random variable of the contaminant concentration and c refers to the realization of C .

3.1. Application to transport equation

Two random variables, velocity and longitudinal dispersivity, are involved in Eq. (3). The velocity is linearly related to the hydraulic conductivity on the basis of Darcy's law. Freeze (1975) pointed out that the hydraulic conductivity is a lognormally distributed random variable. Therefore, the velocity is also considered as a random variable. Dispersivity was traditionally treated as a constant. Yet, uncertainties of up to 20% are very likely in measuring field dispersivity (Bedient et al., 1994, p. 147). Therefore, the

longitudinal dispersivity is considered as another uncertain parameter in Eq. (3). The first-order mean (μ_C) and standard deviation (σ_C) of contaminant concentrations can be derived from Eqs. (5), (6) and (7) as

$$\mu_C = \frac{c_0}{2} \left\{ \operatorname{erfc} \left[\frac{x - \mu_V t}{\sqrt{4\mu_{\alpha_L} \mu_V t}} \right] + \exp \left(\frac{x}{\mu_{\alpha_L}} \right) \operatorname{erfc} \left[\frac{x + \mu_V t}{\sqrt{4\mu_{\alpha_L} \mu_V t}} \right] \right\} \tag{8}$$

$$\sigma_C = \sqrt{d_V^2 \sigma_V^2 + d_{\alpha_L}^2 \sigma_{\alpha_L}^2} \tag{9}$$

where

$$d_V = \frac{\partial C}{\partial V} \Big|_{(\mu_V, \mu_{\alpha_L})} = \frac{c_0 x}{2\sqrt{\pi\mu_{\alpha_L} \mu_V t}} \exp \left[-\frac{(x - \mu_V t)^2}{4\mu_{\alpha_L} \mu_V t} \right]$$

$$d_{\alpha_L} = \frac{\partial C}{\partial \alpha_L} \Big|_{(\mu_V, \mu_{\alpha_L})} = \frac{c_0 x}{2} \left\{ \frac{\exp \left[-\frac{(x - \mu_V t)^2}{4\mu_{\alpha_L} \mu_V t} \right]}{\sqrt{\pi\mu_{\alpha_L} \mu_V t}} - \frac{\exp \left(\frac{x}{\mu_{\alpha_L}} \right) \operatorname{erfc} \left[\frac{(x + \mu_V t)}{\sqrt{4\mu_{\alpha_L} \mu_V t}} \right]}{\mu_{\alpha_L}} \right\}$$

Define the dimensionless variables of time, distance, and concentration respectively as $\tau = \mu_V t / \mu_{\alpha_L}$, $\rho = x / \mu_{\alpha_L}$, and $\kappa = C / c_0$. Then, Eqs. (8) and (9) can be rewritten in dimensionless forms as

$$\mu_\kappa = \frac{1}{2} \left\{ \operatorname{erfc} \left[\frac{\rho - \tau}{\sqrt{4\tau}} \right] + \exp(\rho) \operatorname{erfc} \left[\frac{\rho + \tau}{\sqrt{4\tau}} \right] \right\} \tag{10}$$

$$\sigma_\kappa = \sqrt{\delta_V^2 \sigma_V^2 + \delta_{\alpha_L}^2 \sigma_{\alpha_L}^2} \tag{11}$$

where

$$\delta_V = \frac{d_V \mu_V}{c_0} = \frac{\rho}{2\mu_V \sqrt{\pi\tau}} \exp \left[-\frac{(\rho - \tau)^2}{4\tau} \right]$$

$$\delta_{\alpha_L} = \frac{d_{\alpha_L} \mu_{\alpha_L}}{c_0} = \frac{\rho}{2\mu_{\alpha_L}} \left\{ \frac{1}{\sqrt{\pi\tau}} \exp \left[-\frac{(\rho - \tau)^2}{4\tau} \right] - \exp(\rho) \operatorname{erfc} \left[\frac{\rho + \tau}{\sqrt{4\tau}} \right] \right\}$$

4. Evaluation of risk and damage

Reliability (or risk) problems are usually formulated as the relationship between two random variables: loading (or stress) and strength (or capacity). The reliability is defined as the probability that the loading is less than the strength. The risk, however, is the complement of reliability and is defined as the probability that the strength is less than

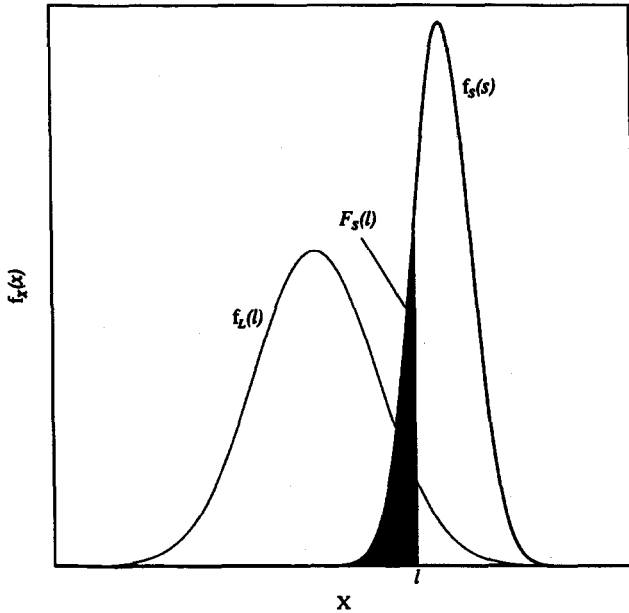


Fig. 1. Probability density function of the loading $f_L(l)$ and strength $f_S(s)$ (source: Ang and Tang, 1984).

the loading. Let the random variables S and L refer respectively to the strength and the loading, the reliability (Re) and the risk (R) can be defined as $Re = Pr(L < S)$ and $R = Pr(S < L)$. Alternatively, the risk can be expressed by the conditional probability as

$$R = Pr(S < L) = \sum_{\text{all } l} Pr(S < l)Pr(L = l) \tag{12}$$

$$R = Pr(L > S) = \sum_{\text{all } s} Pr(L > s)Pr(S = s)$$

if the loading and strength are statistically independent. Furthermore, the risk can be written as the following formulas if the probability density functions (pdfs) of S and L are known (Ang and Tang, 1984; Kapur and Lamberson, 1977):

$$R = \int_{-\infty}^{\infty} F_S(l)f_L(l)dl \text{ or } R = \int_{-\infty}^{\infty} [1 - F_L(s)]f_S(s)ds \tag{13}$$

where $f_S(s)$ and $F_S(s)$ are respectively the pdf and cumulative distribution function (CDF) of S , as are $f_L(l)$ and $F_L(l)$ for L . The shaded area under the pdf of S shown in Fig. 1 is the probability or risk, for $S < l$, that is, $F_S(l)$. If the strength is a deterministic value, Eq. (13) reduces to

$$R = Pr(L > s^*) = \int_{s^*}^{\infty} f_L(l)dl$$

where s^* is the deterministic strength as indicated in Fig. 2.

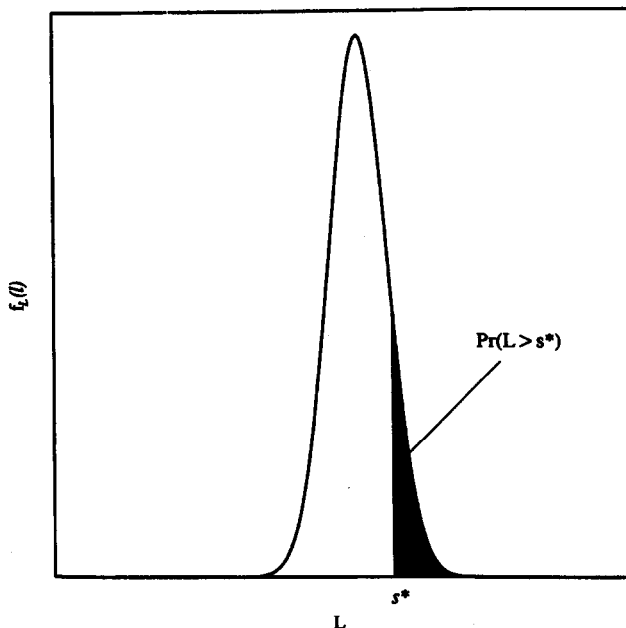


Fig. 2. Alternative definition of risk for deterministic strength s^* .

4.1. Risk of groundwater contamination

Since Eq. (3) involves two random variables α_L and V , the predicted concentration, C , is also a random variable and has the mean and standard deviation respectively expressed in Eqs. (8) and (9). Consider the loading as the predicted concentration C , and the strength as the maximum acceptable upper limit of contaminant concentration, c^* , the risk then becomes

$$R = Pr(C > c^*) \quad (14)$$

If the probability distribution of C is known, the risk can be directly calculated by Eq. (14). Yet, specifying a precise distribution of C is generally impossible owing to finite sampling data available for most contamination cases. Thus, the distribution for sample concentration data may be represented by a chosen probability distribution based on the results of goodness of fit tests and/or the graphical plot of data.

4.2. Choice of probability model for predicted concentration

The probability distribution for the contaminant concentration has to be known prior to computing the risk. However, the sampling data and probability information concerning the contamination are usually limited. Therefore, the adopted probability model is generally not able to completely describe the natural randomness. The method of χ^2 statistics and sample likelihood were previously used by Castano et al. (1978) for choosing suitable

probability models. They suggested that a composite model could be used such that different weights can be given to models with different ranks. A composite model was also employed by Tung and Mays (1981) towards the evaluation of flood levee design. All the techniques, however, require sample data. Yet, collecting a representative set of sample data may require a great effort in engineering practice.

Contamination caused by multiple sources with variable release concentration and pattern which frequently happens in the real world, makes the distribution of the contaminant concentration hard to predict. Therefore, five probability distribution models are considered here to represent the possible distributions of the contaminant concentrations. These models include the normal, lognormal, gamma, Gumbel, and Weibull. The normal distribution (N) is the most widely used and most important probability distribution function (Hann, 1977, p. 84). It is symmetrically distributed and the magnitude of the variate can range from negative infinity to positive infinity. However, hydrologic quantities and environmental data are usually positive. Also, as the adverse effects of environmental pollution usually are associated with very high concentration, interest customarily focuses on the tails of the probability distributions (Ott, 1995). The lognormal distribution (LN) which considers only the positive random variables is, therefore, more realistic. The concentration of contaminants in environmental media is usually lognormally distributed (Ott, 1990). It has been used to model many kinds of environment contaminant data, for example, air quality data (Mage, 1974), radionuclide data sets (Horton et al., 1980), and dissolved solids in groundwater (David, 1966). The gamma distribution (GA) has been used to fit total suspended particulate data (Lynn, 1974). Sherwani and Moreau (1975) analyzed water quality data from monitoring stations to determine the best fits of three probability models: the normal, lognormal, and gamma, to the observed frequency distributions. Both the Gumbel and Weibull distributions are extreme value distributions. The Gumbel distribution is the largest extreme value type I and the Weibull distribution is the smallest extreme type III distribution (Ang and Tang, 1984). The Gumbel distribution (GB) was first used to analyze the frequencies by Gumbel (1954). It is often used for maximum type events and results from any initially unlimited distribution of exponential type which converges to an exponential function (Kite, 1977). Roberts (1979) reviewed extreme value theory for its applicability to air pollution problems, and Kinnison (1985) applied it to a variety of problems such as environmental pollution and forecasting floods. The Weibull distribution (WB) was found to be well suited for describing spatial and temporal distributions of atmospheric radioactivity (Apt, 1976). Furthermore, Georgopoulos and Seinfeld (1982) discussed the applications of the gamma and Weibull distributions to air pollution concentrations. Derived formulas to compute the risk based on these five probability distribution models are given in Appendix A. The method of moments is used in this paper to estimate the parameters of those distribution models.

4.3. Conditional probability

Physically interesting values of the contaminant concentration are in the range between zero and c_0 . Yet, the predicted concentration by a chosen probability distribution model may attain values beyond that range. It is, therefore, necessary to truncate the infeasible values from the original distribution. Mood et al. (1988) introduced a method for deriving

a truncated distribution. The truncation of the pdf of the predicted contaminant concentration should add more weight to the remaining distribution if the random variable is out of the range of (c_l, c_0) where c_l represents the lower bound of each distribution. Thus, the truncated pdf can be expressed as

$$f_C(C) = \frac{f_C(C)I_{(c_l, c_0)}}{F_C(c_0) - F_C(c_l)}, \text{ where } I_{(c_l, c_0)} = \begin{cases} 1 & \text{if } c_l \leq C \leq c_0 \\ 0 & \text{otherwise} \end{cases} \quad (15)$$

Furthermore, Eq. (14) can be rewritten through usage of the conditional probability. Define two events A and B such that $A = \{C|C > c^*\}$ and $B = \{C|c_l \leq C \leq c_0\}$, where event A accounts for the original risk region and event B stands for the physically possible region of the predicted concentration. The risk can then be expressed as the conditional probability of event A given event B , that is

$$R = Pr(A|B) = \frac{Pr(A \cap B)}{Pr(B)} = \frac{F_C(C) - F_C(c^*)}{F_C(c_0) - F_C(c_l)} \quad (16)$$

where $F_C()$ is the CDF of C .

4.4. Confidence interval of the mean risk

Random variables are generally represented by point estimators or interval estimation. The most commonly seen point estimators are mean and variance. Since the true mean and true variance of the risk are actually unknown, the interval estimation, or the confidence interval, is, therefore, used for representing the true mean risk. By assigning the significance level β_c , the confidence interval of the mean risk is (Devore, 1987)

$$\left(\bar{R} - t_{\frac{\beta_c}{2}, n-1} \cdot \frac{s_R}{\sqrt{n}}, \bar{R} + t_{\frac{\beta_c}{2}, n-1} \cdot \frac{s_R}{\sqrt{n}} \right) \quad (17)$$

where n is the sample size, \bar{R} is the sample mean of risk, s_R is the sample standard error of risk, and $t_{\beta_c/2, n-1}$ is the variate of the students' t -distribution given that the significance level is P , and the degree of freedom is $n - 1$.

4.5. Conditional expectation of the damage

The conventional approach in risk analysis uses mathematical expectation as an index for evaluating the damage. Many practical problems, however, are essentially multi-objective. In addition, some probabilistic information such as extreme events which are of great concern may have been lost by using only one expected value. In other words, the mathematical expectation may either underestimate the low probability events or overestimate the high probability events. A new approach with the capability of considering extreme events is, therefore, necessary.

The definition of damage can be different in many aspects. Five categories of damage are commonly reported in flood damage estimation: direct damages, indirect damages, secondary damages, intangible damages, and uncertainty damages (Mays and Tung,

1992). They indicated that the empirical depth-damage curve is the most common method in estimating flood damage. However, it requires a property survey which is usually insufficient or difficult in most cases. Empirical or hypothesized damage function are, therefore, necessary. In analysing a flood levee reliability problem, Wood (1977) used a hypothesized damage function which indicated that the damage increased quadratically with exceedance discharge. Asbeck and Haines (1984) assumed a power series damage function for considering the resource damage and the emission level of sulfur dioxide. Based on a data set of damage and the predicted concentration, Petrakian et al. (1987) showed that the discrete probability density function of damage can be derived from the CDF of the predicted concentration. Therefore, the damage function, or the pdf of damage, may be derived from past experience, curve fitting, or a given relationship between the predicted concentration and damage.

Because of the scarcity of data relating the predicted concentration to the damage, a hypothesized damage function is assumed herein. The function is subject to the following three constraints: (1) the damage increases with higher values of the predicted concentration; (2) the rate of increase of damage is at least linear; (3) a lower limit of damage exists when the predicted concentration is zero. One can, then, propose the following hypothetical damage function, ϕ , as

$$G = \phi(C) = b \left(e^{\frac{C}{C_0}} - 1 \right) \quad (18)$$

where G is the damage and b is a constant that converts the value of concentration into a measurement of damage in monetary units. The value of b here is assumed to be 100. The lower bound of Eq. (18) is zero if C is equal to zero. The damage G in Eq. (18) is a random variable because of the randomness of the predicted concentration C . In addition, the pdf of G can be related to the pdf of C by a derived distribution. If two random variables, Q and W , have a functional relationship, $W = h(Q)$ and the pdf of Q is known as $f_Q(q)$, the pdf of W may be expressed as (Ang and Tang, 1975)

$$f_W(W) = f_Q(q) \left| \frac{dh^{-1}}{dw} \right| \quad (19)$$

where h^{-1} is the inverse function of the function $h(Q)$. The notation of the absolute value in Eq. (19) can be dropped if the function h is monotonically increasing. Substituting Eq. (18) into Eq. (19) gives $f_G(g) = f_C(\phi^{-1}(g)) |d\phi^{-1}(g)/dg| = f_C(\phi^{-1}(g))/b$. Having derived the pdf of damage, the conditional expectation can be defined as (Karlsson and Haines, 1988b)

$$G_c = \frac{1}{p_{i+1} - p_i} \int_{F_G^{-1}(p_i)}^{F_G^{-1}(p_{i+1})} g f_G(g) dg \quad (20)$$

where f_G is the pdf of G , p_i and p_{i+1} are the probabilities of the two partitioning points on the probability axis of G . Choosing these two partitioning points such that p_i corresponds to the case where the risk, γ_i , equals to the mean risk \bar{R} , and p_{i+1} corresponds to the case where the risk, $\gamma_{i+1} = 1$. That is,

$$p_i = F_G(g_i) = F_G[\phi(c_i)] = F_G\{\phi[F_C^{-1}(\gamma_i)]\} \quad (21)$$

$$p_{i+1} = F_G\{\phi[F_C^{-1}(\gamma_{i+1})]\}$$

and $\gamma_i = \bar{R}$ and $\gamma_{i+1} = 1$. The CDF of damage, F_G , can be related to the CDF of the random variable C by $F_C(c) = Pr(C \leq c) = Pr(G \leq g) = Pr[G \leq \phi(c)] = F_G[\phi(c)]$. The point with the cumulative probability of p_i on the axis of the random variable G , which corresponds to the risk γ_i on the axis of C , is $g_i = \phi[F_C^{-1}(1 - \gamma_i)]$. Substituting Eq. (21) into Eq. (20) yields

$$G_c = \frac{\int_{\phi[F_C^{-1}(\bar{R})]}^{\phi[F_C^{-1}(1)]} g f_G(g) dg}{F_G\{\phi[F_C^{-1}(1)]\} - F_G\{\phi[F_C^{-1}(\bar{R})]\}} \tag{22}$$

The unconditional expectation of the damage can be derived in a way similar to that used for deriving the mean of concentration. The damage function can be expanded to the second-order as

$$G = \phi(\bar{C}) + \frac{\partial \phi}{\partial C}(C - \bar{C}) + \frac{1}{2} \frac{\partial^2 \phi}{\partial C^2}(C - \bar{C})^2 \tag{23}$$

Taking the expectation of Eq. (23) then yields the mean of damage as $\bar{G} = be^{\mu_c}(1 + \sigma_c^2/2) - b$.

5. Sensitivity analysis

Sensitivity is a measurement of the influence of a system input onto the system output. Kabala and Milly (1990) declared that three commonly used approaches for sensitivity analysis are perturbation, direct and adjoint methods. The perturbation method is simple but may be limited by the choice of perturbation and the computational effort. The direct approach examines sensitivity by partially differentiating system equations with respect to parameters. The adjoint approach can be employed for solving the system output and sensitivities simultaneously by describing the system and its sensitivities by means of the governing equation and its adjoint. Sykes et al. (1985) used the adjoint operators to analyze the sensitivities of piezometric head and velocity in groundwater flow. McElwee and Yukler (1978) calculated the sensitivity of drawdown with respect to transmissivity and storage coefficient with the direct method. The sensitivity coefficients in this paper are obtained through combining the concepts of the perturbation method and differentiation.

5.1. Sensitivity coefficient

The risk can be expressed in a general function, φ , for each predicted distribution of the contaminant concentration as $R = \varphi(x, t, \mu_v, \mu_{\alpha_1}, \sigma_v, \sigma_{\alpha_1}, c^*)$ where the four statistics and c^* compose the input parameters of the system. The sensitivity coefficient of the system output to a parameter θ , in a dimensionless form, can be defined as

$$S_\theta = \frac{dR/R}{d\theta/\theta} = \frac{\partial R}{\partial \theta} \frac{\theta}{R} \tag{24}$$

which is a measure of the change of system output owing to the change of system input. Besides, the partial derivative in Eq. (24) is defined as the sensitivity, R_θ where $R_\theta = \partial R / \partial \theta$.

The magnitude of the sensitivity coefficients varies depending on the considered

distribution of the contaminant concentration and the model parameters. Sensitivity coefficients can otherwise be expressed in terms of log-transformed values, that is:

$$Z_\theta = \text{sgn}(\chi_\theta) \log_{10}(|\chi_\theta|) \begin{cases} \chi_\theta = 1 & \text{if } 0 < S_\theta \leq 1 \\ \chi_\theta = -1 & \text{if } -1 \leq S_\theta < 0 \\ \chi_\theta = S & \text{if } |S_\theta| > 1 \end{cases} \quad (25)$$

where S_θ and Z_θ are respectively the original and transformed sensitivity coefficient and $\text{sgn}(\chi_\theta) = 1$ if $S_\theta > 0$; otherwise, $\text{sgn}(\chi_\theta) = -1$. In other words, Eq. (25) implies that Z_θ will be zero if the value of S_θ is between -1 and 1 , and Z_θ will be the log-transformed counterpart of S_θ if it is located beyond the range $(-1, 1)$.

Sensitivity coefficients and sensitivities have the same sign because the parameter, θ , and the risk, R , are always positive. If R_θ is positive, the risk will increase while θ increases or vice versa. If R_θ is negative, the risk will increase if θ decreases.

5.2. Second-order analysis

Results of the first-order uncertainty analysis of C , S_{μ_V} , and $S_{\mu_{\alpha_L}}$ contain respectively the terms $\partial\sigma_C/\partial\mu_V$ and $\partial\sigma_C/\partial\mu_{\alpha_L}$ which involve the second-order derivatives with respect to V and α_L . However, only first-order derivatives with respect to V and α_L are contained in the sensitivity coefficients of the risk to uncertainties of velocity and dispersivity, i.e. $\partial R/\partial\sigma_V$ and $\partial R/\partial\sigma_{\alpha_L}$. Since the sensitivity coefficients of the risk with respect to mean values of V and α_L are generally larger than that with respect to the uncertainties of V and α_L , the influence of the second-order derivatives on the values of sensitivity coefficients may be significant. If one expands the mean concentration to the second order, that is,

$$\mu_C = f(\mu_V \mu_{\alpha_L}) + \frac{\partial^2 f(\mu_V \mu_{\alpha_L})}{2\partial V^2} \sigma_V^2 + \frac{\partial^2 f(\mu_V \mu_{\alpha_L})}{\partial V \partial \alpha_L} \sigma_V \sigma_{\alpha_L} + \frac{\partial^2 f(\mu_V \mu_{\alpha_L})}{2\partial \alpha_L^2} \sigma_{\alpha_L}^2 \quad (26)$$

where $f(\mu_V \mu_{\alpha_L})$ refers to the right-hand side of Eq. (8). The derivative of μ_C with respect to σ_V and σ_{α_L} is then no longer zero and the second-order derivatives also appear in the sensitivity coefficients with respect to σ_V and σ_{α_L} . In short, large deviations among these sensitivity coefficients may result from truncating the second-order and higher order derivatives in uncertainty analysis.

6. An example and discussion

A random and contaminated subsurface field is given herein as an example to demonstrate the calculation of the mean risk, confidence interval, and conditional expectation of damage and sensitivity coefficients. Assume that the groundwater velocity V is log-normally distributed with the mean μ_U and standard deviation σ_U while $U = \ln V$ and the longitudinal dispersivity α_L is normally distributed with μ_{α_L} . Data of $\mu_U = 0.7 \text{ m s}^{-1}$, $\sigma_U = 0.14 \text{ m s}^{-1}$, $\mu_{\alpha_L} = 10.0 \text{ m}$, and $\sigma_{\alpha_L} = 1.2 \text{ m}$ are assumed to be obtained from N sampling points by a hydrogeologic site investigation. The value of the maximum acceptable upper limit of dimensionless concentration is taken as 0.77.

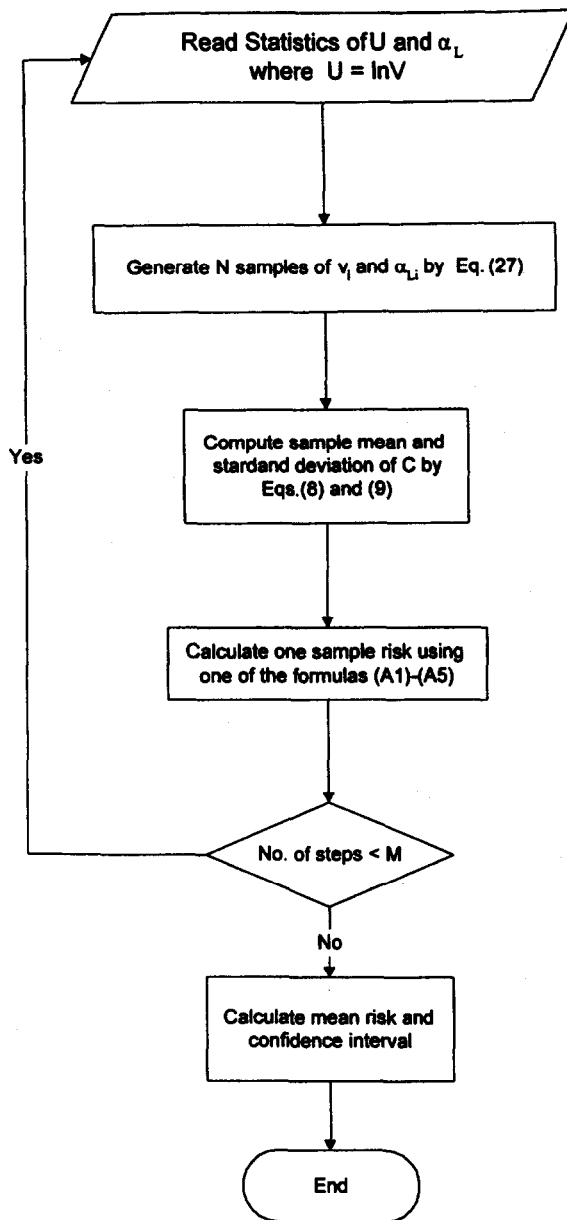


Fig. 3. Algorithm for computing the mean risk and confidence interval for a specific distribution model where M is the number of Monte Carlo runs and N is the number of generated data.

6.1. Monte Carlo simulation

Monte Carlo simulation is employed here to calculate the sample risk. Firstly, a set of v_i and α_{L_i} , with $i = 1, 2, \dots, N$ for the random field is generated by:

$$v_i = \exp(z_i \sigma_U + \mu_U) \tag{27}$$

and

$$\alpha_{L_i} = z_i \sigma_{\alpha_L} + \mu_{\alpha_L}$$

where z_i is the standard normal variate. Sample mean and standard error of V and α_L are calculated using those N -generated data. Then, estimated mean and standard deviation of the predicted concentration can be obtained by plugging the sample statistics of V and α_L into Eqs. (8) and (9). Parameters of each concentration distribution model can be computed according to the estimated statistics of the predicted concentration. Hence, different sample risks can be calculated based on Eqs. (A1) to (A5) in Appendix A for different concentration model. The same procedures described above are carried out M times. The mean risk can then be estimated by M sample risks and the confidence interval of the mean

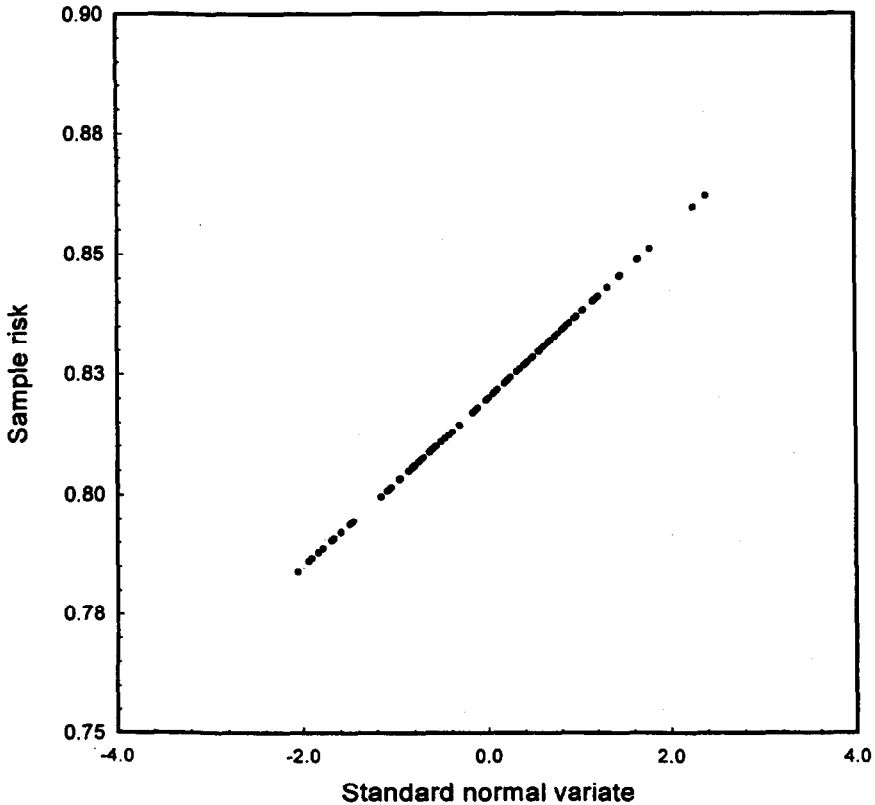


Fig. 4. Probability plot of sample risk from normally distributed concentration for a sample with sample size of 100, where the correlation coefficient is 0.99.

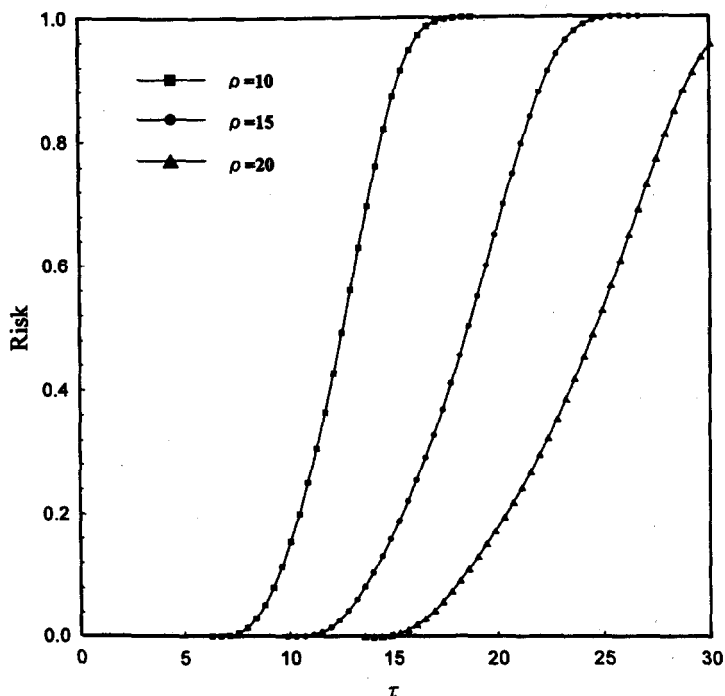


Fig. 5. Risk versus τ at different values of ρ for normally distributed concentration.

risk can be computed by Eq. (17). Fig. 3 presents a flow chart to illustrate the calculation procedures of the mean risk and confidence interval when using the Monte Carlo simulation.

The number of sampling points, N , and the number of Monte Carlo runs M are determined herein by numerical experiments. By trying the values of 100, 500, and 1000 for N , it was found that the computed sample risk approaches to a constant for $N \geq 500$. Eq. (17) requires that the underlying distribution of the sample risk should be approximately normal. Fig. 4 shows that the sample risk data is approximately linearly distributed with respect to the standard normal variate with the correlation coefficient value of 0.99 when M is equal to one hundred. Accordingly, the numbers of N and M are respectively chosen as 500 and 100 for each distribution model.

6.2. Simulation results

Fig. 5 shows the values of the risk versus dimensionless time τ at dimensionless distances of $\rho = 10, 15,$ and 20 , respectively, calculated by Eq. (A1) for the case of normally distributed concentration model. This figure indicates that the risk increases as τ increases from $\tau = 0$ and decreases with increasing ρ . Similar trends predicted by distribution models represented by Eqs. (A2) to (A5) are also exhibited, although not shown in this paper.

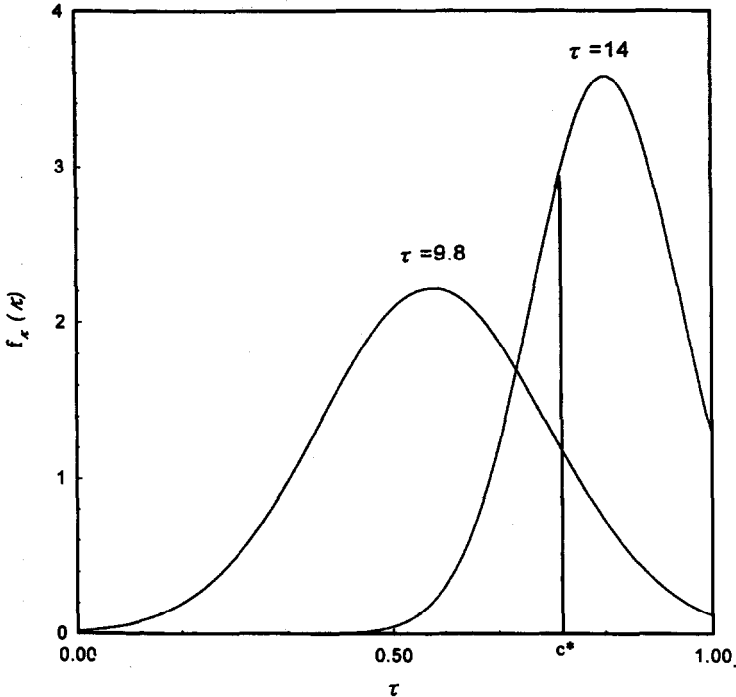


Fig. 6. Illustration for normally distributed pdf of dimensionless concentration κ when $\tau = 9.8$ and 14 at $\rho = 10$.

Fig. 6 illustrates the normally distributed distributions of dimensionless concentration κ for $\tau = 9.8$ and 14 , respectively, at $\rho = 10$. Obviously, the distribution of κ for $\tau = 14$ is more peaked than for $\tau = 9.8$. Therefore, the area under the pdf curve to the right of κ^* while $\kappa^* = c^*/c_0$, for $\tau = 14$ is significantly greater than the area for $\tau = 9.8$. This indicates that the risk increases for increasing τ at a constant ρ . On the other hand, the first-order mean concentration becomes smaller as ρ increases at a constant τ .

Fig. 7 manifests the confidence intervals of the mean risk for the Weibull and Gumbel distribution models at $\rho = 10$. It has been found that the width of the confidence interval is largest in the case of Weibull distribution and smallest in the case of Gumbel distribution among these five distribution models.

6.3. Conditional expectation of the damage

The conditional expectation of damage with respect to the risk is shown in Fig. 8 for those five contaminant distribution models. The unconditional expectation of damage, indicated by the solid line, is also shown in the figure. Note that the unconditional expectation of damage, having the upper and lower limits of 0 and 172 respectively if the coefficient b is 100 in Eq. (18), is independent of the concentration distribution. Interestingly, the conditional expectation of damage for each contaminant distribution is significantly greater than the unconditional one if the risk is less than 0.1. This is due to the fact

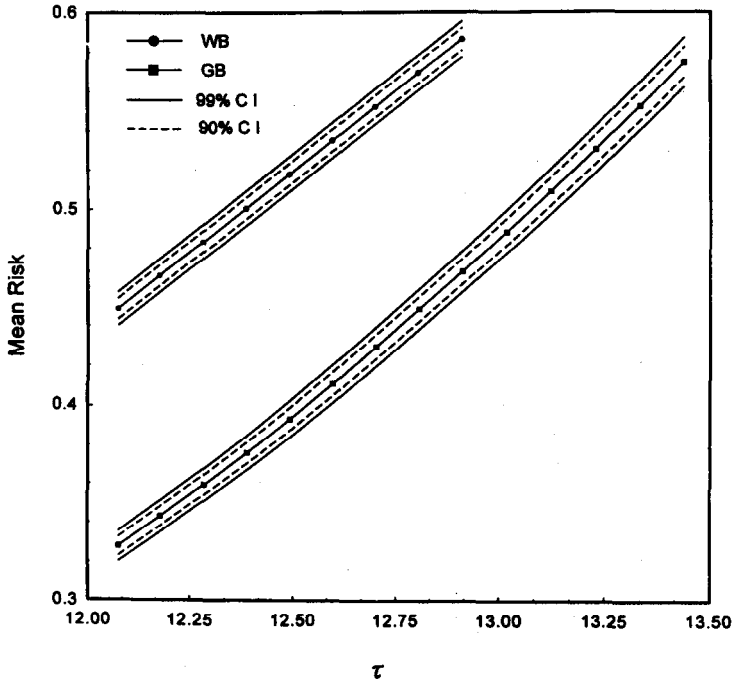


Fig. 7. Confidence interval (CI) of the mean risk for Weibull and Gumbel distribution models at $\rho = 10$.

that these two approaches give different weights to the first moments of the damage. Yet, the limiting case of the conditional expectation of damage, i.e. the risk approaching 1, will approach the unconditional one as indicated in Fig. 8.

The area under a pdf curve between two neighboring values of the random variable is defined as “probability mass”. The expected value of a random variable can then be defined as a weighted sum of the probability mass of that random variable. In the case of unconditional expectation, a constant weight, 1, is applied to each probability mass. However, a weight depending on the level of significance is given to the probability mass in the case of conditional expectation. The probability mass in the case of conditional expectation corresponds to the mass under the pdf curve between two pre-defined points expressed in Eq. (21). Accordingly, the weight for the conditional expectation is the inverse of the cumulative probability between these two points. That is, the smaller the risk, the larger the weight and the larger the conditional expectation of damage. The conditional expectation will obviously approach the conditional expectation if the risk approaches 1.

In short, the critical drawback of the unconditional expectation is that it fails to evaluate the importance of events with low risks. It is also unable to provide different weights to events with different levels of significance. The overall effect of evaluating damage could be underestimated if the unconditional approach is implemented by a decision maker. The conventional unconditional approach which treats the probability mass as a whole may, therefore, be inadequate to describe the low risk events.

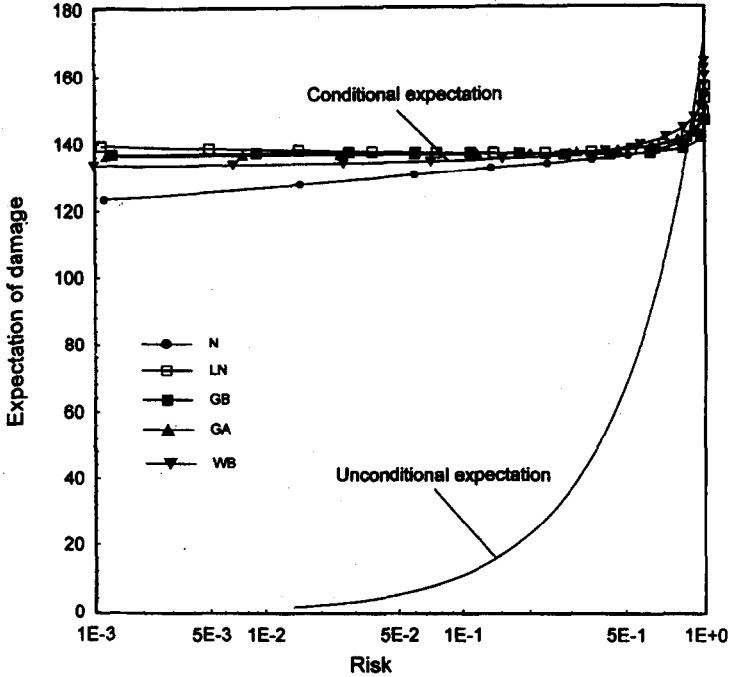


Fig. 8. Conditional and unconditional expectations of damage with respect to the risk for normally distributed concentration at $\rho = 10$.

6.4. Sensitivity coefficients of the risk

Sensitivity coefficients for the case of $\rho = 10$ are considered herein. However, conclusions drawn from this case also apply to other values of ρ . Figs. 9 and 10 show the sensitivity coefficients versus the risk for different concentration distributions models. Fig. 9 demonstrates that the Weibull distribution has the largest absolute sensitivity coefficients with respect to the parameter c^* . For the other four parameters, however, gamma distribution has the largest sensitivity coefficients. The sensitivity coefficient of the risk to μ_v shown in Fig. 10 indicates that the gamma distribution has the largest sensitivity coefficient. It is found that the risk is most sensitive to μ_{α_L} for all distribution models, and least sensitive to σ_{α_L} for each concentration distribution except the gamma distribution, which is least sensitive to c^* . This is illustrated in Fig. 11, where the sensitivity coefficients of the risk to the five parameters for normally distributed concentration at $\rho = 10$ are shown. Therefore, it can be concluded from above observations that the risk is most sensitive to μ_{α_L} , but least sensitive to σ_{α_L} .

7. Conclusion and recommendations

The following conclusions can be drawn from this study:

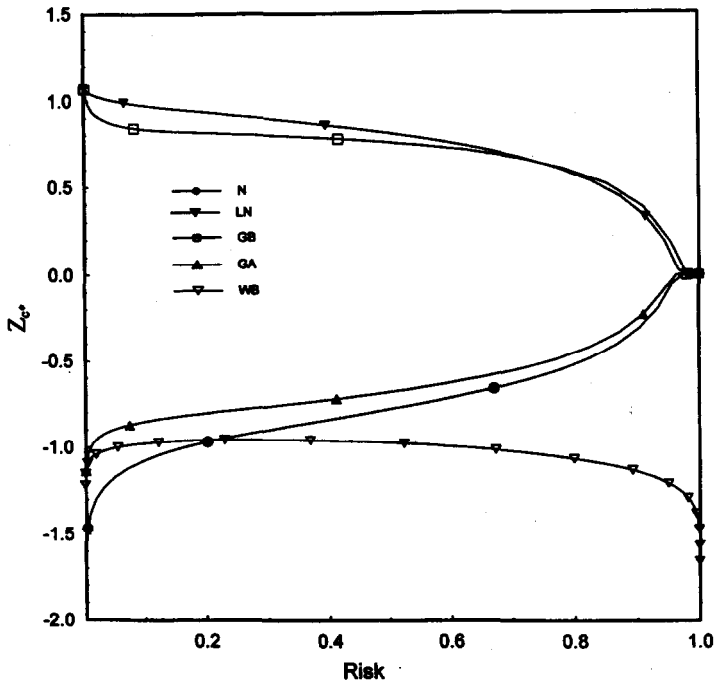


Fig. 9. Log-transformed sensitivity coefficients of the risk to c^* for five concentration distribution models at $\rho = 10$.

1. The risk increases with τ for constant ρ and decreases with ρ for constant τ .
2. Conditional expectation of damage is significantly greater than the unconditional one for events with small risks. The conventional unconditional expectation could possibly underestimate the damage.
3. Mean dispersivity, μ_{α_L} , is the most sensitive parameter among the five distribution models of the predicted concentration. The uncertainty of dispersivity, σ_{α_L} , is the least sensitive parameter among all the distribution models except for the Gamma and Weibull distributions.

One can make the following recommendations:

1. The conventional unconditional expectation has been shown to be unable to adequately describe the low probability events. The conditional expectation for various levels of significance should be considered in the decision-making process.
2. Each distribution model of the predicted concentration contributes positively in the calculation of risk. Using a composite probability model which combines possible concentration distribution models and gives different weights to each alternative depending on its importance is recommended. This would particularly be suitable for conditional expectation of damage.
3. The mean dispersivity has been shown to be the most sensitive parameter because of the truncation of high-order terms in uncertainty analysis. Second-order uncertainty

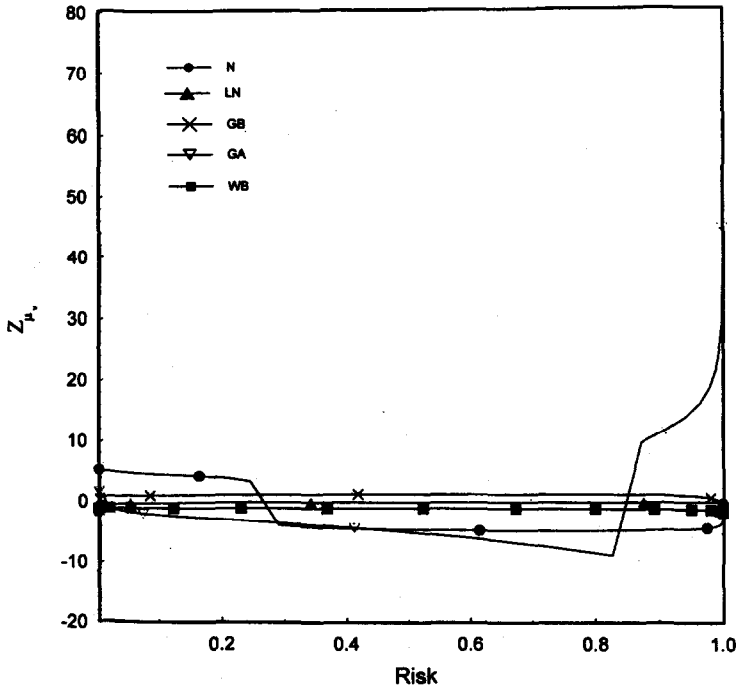


Fig. 10. Log-transformed sensitivity coefficients of the risk to μ_v for five concentration distribution models at $\rho = 10$.

analysis is suggested for application in uncertainty analysis owing to the obtained remarkable differences in sensitive coefficients.

Acknowledgements

This work was partly funded by the National Science Council of the Republic of China under the contract number NSC-82-0410-E-009-080. The authors would like to thank three anonymous reviewers for their valuable and constructive comments that greatly improved the paper.

Appendix A. Formulas of the risk for different distribution models

Appendix A.1. Normal distribution

$$R^N = \frac{\text{erf}\left(\frac{c - \mu_C}{\sqrt{2}\sigma_C}\right) - \text{erf}\left(\frac{c^* - \mu_C}{\sqrt{2}\sigma_C}\right)}{\text{erf}\left(\frac{c_0 - \mu_C}{\sqrt{2}\sigma_C}\right) - \text{erf}\left(\frac{-\mu_C}{\sqrt{2}\sigma_C}\right)} \tag{A1}$$

where μ_C and σ_C are the mean and standard deviation of C.

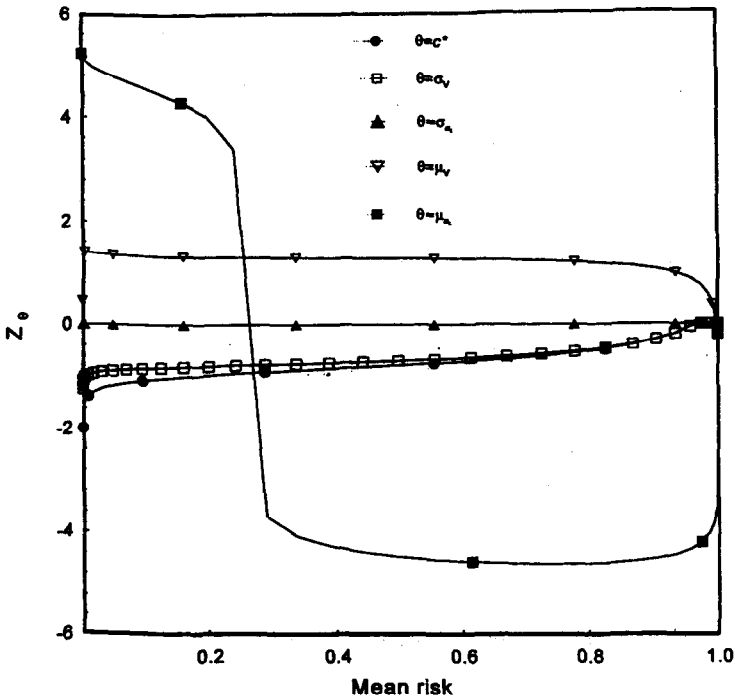


Fig. 11. Log-transformed sensitivity coefficients of the risk to five parameters for normally distributed concentration at $\rho = 10$.

Appendix A.2. Lognormal distribution

$$R^{LN} = \frac{\operatorname{erf}\left(\frac{y - \mu_Y}{\sqrt{2}\sigma_Y}\right) - \operatorname{erf}\left(\frac{\ln c^* - \mu_Y}{\sqrt{2}\sigma_Y}\right)}{\operatorname{erf}\left(\frac{\ln c_0 - \mu_Y}{\sqrt{2}\sigma_Y}\right)} - 1 \tag{A2}$$

where $y = \ln c$, $\sigma_Y^2 = \ln(1 + \sigma_C^2/\mu_C^2)$, and $\mu_Y = \ln \mu_C - \sigma_Y^2/2$.

Appendix A.3. Gamma distribution

$$R^{GA} = \frac{P(\beta_A, \lambda_A c) - P(\beta_A, \lambda_A c^*)}{P(\beta_A, \lambda_A c_0)} \tag{A3}$$

where $\beta_A = \mu_C^2/\sigma_C^2$, $\lambda_A = \mu_C/\sigma_C$, and $P(\cdot)$ is the incomplete gamma function.

Appendix A.4. Gumbel distribution

$$R^{GB} = \frac{\exp\left[-\exp\left(-\frac{c-\mu_G}{\alpha_G}\right)\right] - \exp\left[-\exp\left(-\frac{c^*-\mu_G}{\alpha_G}\right)\right]}{\exp\left[-\exp\left(-\frac{c_0-\mu_G}{\alpha_G}\right)\right] - \exp\left[-\exp\left(\frac{\mu_G}{\alpha_G}\right)\right]} \quad (\text{A4})$$

where $\mu_G = \mu_C - 0.5772\alpha_G$ and $\alpha_G = \sqrt{6}\sigma_C/\pi$.

Appendix A.5. Weibull distribution

$$R^W = \frac{\exp\left[-\left(\frac{c^*}{\alpha_W}\right)^{\beta_W}\right] - \exp\left[-\left(\frac{c}{\alpha_W}\right)^{\beta_W}\right]}{1 - \exp\left[-\left(\frac{c_0}{\alpha_W}\right)^{\beta_W}\right]} \quad (\text{A5})$$

where α_W and β_W are the solutions of the following equations:

$$\frac{\mu_C}{\sigma_C} = \frac{\Gamma\left(1 + \frac{1}{\beta_W}\right)}{\left\{\Gamma\left(1 + \frac{2}{\beta_W}\right) - \left[\Gamma\left(1 + \frac{1}{\beta_W}\right)\right]^2\right\}^{\frac{1}{2}}}$$

and

$$\alpha_W = \frac{\sigma_C}{\left\{\Gamma\left(1 + \frac{2}{\beta_W}\right) - \left[\Gamma\left(1 + \frac{1}{\beta_W}\right)\right]^2\right\}^{1/2}}$$

where $\Gamma()$ is the gamma function.

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