Stochastic modelling and risk analysis of groundwater pollution using FORM coupled with automatic differentiation

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Abstract

The first order reliability method (FORM) has been widely used in probabilistic modelling of groundwater problems. The FORM approach requires an iterative optimization procedure to find out the system failure point (the most probable point).

The advantages of this approach are that it does not require many computations in comparison with other methods when applied to simple problems, and it produces reasonably accurate results. However, it has been found that the computations of FORM can equal or exceed that of other methods in case of large number of variables.

In this paper, a new implementation of FORM was proposed with more efficiency and accuracy than the traditional FORM method. In the proposed approach, automatic differentiation is used to obtain the gradient vector of the limit state function, which is required by FORM, instead of using finite difference estimation. This way, the first order derivative was obtained with a very good accuracy, and with less computational effort. Based on the obtained results, it is found that the proposed implementation of FORM is a very good tool for probabilistic risk assessment and uncertainty analysis in groundwater problems.
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1. Introduction

Contaminant transport modelling is an important tool for any management or remediation scheme of groundwater aquifers. Because of increase in groundwater pollution load resulted from industrial, and agricultural stresses on water resources, such a remediation action is essential. Numerical modelling of groundwater contamination is a powerful tool and can be relied on; however, groundwater modelling is not an easy task. To build a predictive model, and to get reliable results, input data should be accurate and representative of the real situation in the field. Because of heterogeneity of the aquifers and uncertainties in model input data, including chemical, physical and hydrogeolog-ical parameters, modelling process turns into a complicated task. In addition, mathematical modelling implies many assumptions and estimations, which increase the uncertainty of the model output. To eliminate this problem, many data are needed with as much accuracy as possible. Since there are different sources of uncertainty related with groundwater modelling, it is so difficult, if not impossible, to collect all the required data with a high degree of accuracy. As a result, the output of numerical modelling of groundwater pollution has always a certain degree of uncertainty.

Several methods of uncertainty analysis in groundwater modelling can be found in the literature. Among these methods, the most familiar one is the Monte Carlo simulation (MCS) [34]. Monte Carlo simulation has been used as a probabilistic uncertainty propagation technique in different environmental problems, and uncertainty analysis (e.g. [20,28]). The advantages of MCS are that it is easy to

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implement, and requires few data. However, MCS requires a huge number of computations to get reliable results. For events with low probability of occurrence, or for contaminant transport problems with a huge number of variables, MCS becomes inefficient. The number of samples required to estimate event probability p is in the order of $100/p$ to get a coefficient of variation of the estimate of 0.10 [6]. For instance, to estimate an event with a probability of 0.001 using MCS, some 100,000 runs are needed. The problem is rather difficult in the case of complex groundwater problems with too many variables. Therefore, it is not efficient to use MCS in real groundwater problems since they have always a large number of variables.

The method of first order second moment (FOSM) is another method used in uncertainty analysis. This method has been used in different groundwater modelling and uncertainty problems (e.g. [8,21]). Although FOSM does not require too many number of runs, but its accuracy is poor especially with low probability events.

The first order reliability method (FORM) was recently used in groundwater modelling to account for uncertainty in input parameters. However, application of FORM in its current form implies optimisation procedure that requires gradient evaluation, and thus, the uncertainties of the obtained results may increase. Some studies have used FORM in reliability and risk analysis of groundwater problems [12–14]. All these studies, however, have applied FORM with theoretical examples and the obtained results were not validated or compared with other methods.

In this study, a new implementation of FORM was proposed to increase its accuracy. Results of the proposed method were checked against results from other methods.

2. Theory of reliability analysis

Deterministic models are usually used to solve groundwater and contaminant transport problems. These models assume that all the input parameters are known in time and space, and consequently, a deterministic value for each parameter can be assigned. However, this assumption is not true because of heterogeneity of hydrogeological parameters. Therefore, deterministic modelling might result in poor output, and thus, the objectives of numerical modelling cannot be achieved. The reliability of the system (P_s) is defined as the probability of non-failure in which the resistance of the system (R) exceeds the load (L). System resistance and load have different meanings according to the problem of concern. In hydrogeology, system failure occurs when the stresses on the aquifer, which can be pollution load or groundwater discharge, exceed the system resistance. Resistance of the system in this context means the aquifer can be exposed to the stresses without damage or deterioration. If R and L were expressed in stochastic format, the probability of non-failure P_s can be obtained as follows:

$$P_s = P(L_s - R_s) \tag{1}$$

where P is the probability, L_s, and R_s are the load and resistance of the system in stochastic form, respectively. Similarly, the probability of failure P_f is the compliment of the reliability, which can be expressed as

$$P_f = P(L_s > R_s) = 1 - P_s \tag{2}$$

Input variables for any hydrogeological system are composed of different parameters. These parameters are classified into two categories: certain and uncertain parameters. For example, groundwater discharge from a certain well can be precisely known and considered as a certain parameter. In contrary to well discharge, the hydraulic conductivity of the aquifer cannot be known because of heterogeneity of the aquifer, and therefore, can be considered as uncertain parameter or random variable. The random variables of the system can be presented in the form of random vector $X = (x_1, x_2, \ldots, x_n)$. The limit state function (sometimes called the performance function) is a scalar function of the input variables, and it defines the failure domain as shown in Fig. 1. In a case of a groundwater flow problem, the limit state function $G(X)$ represents the model output (the value of groundwater head at a certain time and a certain location). The limit state function is formulated such that $\{x : G(X) = 0\}$, represents the limit state surface. The G-function is expressed with the convention that if $G(x_1, x_2, \ldots, x_n) > 0$, the component survives, whereas if $G(x_1, x_2, \ldots, x_n) \leqslant 0$, the component fails. Thus, the space of the physical random variables is divided into two domains: safe, and failure domain. The probability of failure is given by

$$p_f = p[G(X) \leqslant 0] = \int_{G(X) \leqslant 0} f_x(X) \, dx \tag{3}$$

where $f_x(X)$ is the joint probability density function of the random variables $X = (x_1, x_2, \ldots, x_n)$. Because of the difficulties involved in solving the probability function, probabilistic methods were developed to solve (3).
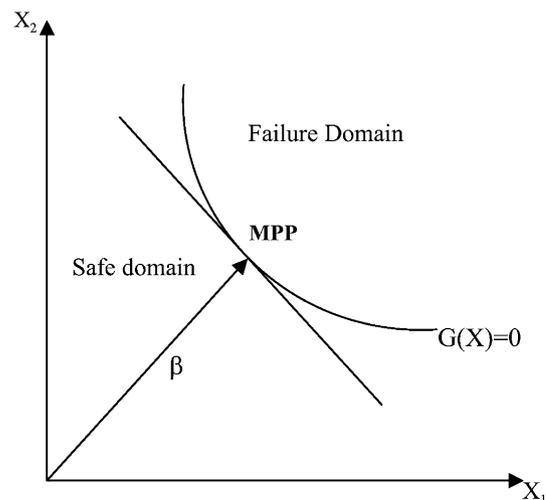

Fig. 1. Limit state function and reliability index.

Almost all methods of reliability analysis have been derived from that one, which is called first order second moment (FOSM). FOSM method uses the first terms of a Taylor series expansion of the performance function to approximate the mean value and the variance of the function [27]. The method is called second moment because it is the highest order term used in FOSM [4]. In all reliability methods, the intended goal is to find out the reliability index (β), as shown in Fig. 1. This index can be used as a measure of comparative reliability, and it is computed as follows:

$$\beta = \left(\frac{\mu_G}{\sigma_G} \right) \tag{4}$$

where μ_G is the mean of the limit state function and σ_G is the standard deviation of the limit state function.

The reliability (or the probability of non-failure) can be computed as follows:

$$P_s = \Phi(\beta) \tag{5}$$

where Φ is the standard normal cumulative distribution function.

3. First order reliability method (FORM)

The idea of the first order reliability method (FORM) was introduced in the early 70s in structural engineering by Hasofer and Lind [15] as alternative to MCS method. The FORM method of Hasofer and Lind was developed later by Rackwitz and Fiessler [30]. It was used to assess the risk of low probability events in structural engineering [9]. The method was recently used in hydrological engineering and risk assessment of groundwater pollution [14,31].

The method of Hasofer–Lind and Rackwitz–Fiessler is referred to as HL–RF approach, and it depends on the linear approximation of the performance function at a point on the limit state, which is called the design point or *the most probable point* MPP. HL–RF approach assumes the existence of the critical level of the system performance, which divides the parameters of the system domain into two parts: the acceptable or *safe domain* and the unacceptable or *failure domain* (Fig. 1).

The optimisation approach of HL–RF depends on the linearization of the limit state function at the closest point to the origin in the standard normal space as illustrated in Fig. 2. Therefore, the first step in FORM is to transform input variables from the physical space (X) to the standard normal space (U) depending on the probability distribution of each random variable. Transformation approach from physical space X to standard normal space U was developed by Liu and Der Kiureghian [22]. Based on their transformation approach, the non-normal random variables $X = (x_1, x_2, \ldots, x_n)$ can be transformed to the corresponding normal standard variables $U = (u_1, u_2, \ldots, u_n)$ as follows:

$$Z_i = \Phi^{-1}[F^i(x_i)] \tag{6}$$

where Z_i is the equivalent standard normal random variable; $F^i(x_i)$ is the cumulative distribution function (CDF) of a random variable x_i and $\Phi^{-1}(\cdot)$ is the inverse of the standard normal distribution function.

At the failure point (or MPP), two constraints should be satisfied:

1. Minimisation of the distance from the origin to the tangent of the limit state surface: $\min |U|$.
2. The MPP should be located at the limit state surface; that is: $G(U) = 0$.

The optimisation procedure is used to find the shortest distance from the origin to the limit state surface (Fig. 2). This distance represents the reliability index β. As β decreases, the probability of non-failure $\Phi(p)$ decreases and the complement probability $(1 - \Phi(p))$ increases. Therefore, the closest point on the limit state surface to the origin is that one with the highest probability of failure. The HL–RF approach can now be summarised as follows:

(1) Starting with an initial arbitrary value of random variables vector $X = (x_1, x_2, \ldots, x_n)$ to start FORM iterations. (Usually the initial value is the vector of the mean values of random variables.)
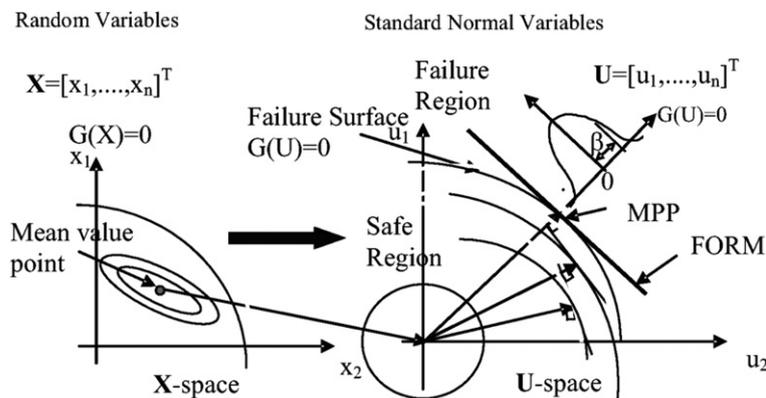

Fig. 2. HL–RF approach.

(2) Transformation of statistical descriptors (mean and standard deviation) of all input random variables $X = (x_1, x_2, \ldots, x_n)$ to their equivalent standard normal descriptors as follows:

$$\mu_{x_i}^{N} = x_i - \sigma_{x_i} \Phi^{-1}[F(x_i)] \tag{7}$$

$$\sigma_{x_i}^{N} = \frac{\phi(\Phi^{-1}[F(x_i)])}{f(x_i)} \tag{8}$$

where $\mu_{x_i}^{N}$ and $\sigma_{x_i}^{N}$ are the mean and standard deviation of a random parameter x_i in the standard normal space respectively. $f(x_i)$ is the probability density function of the parameter x_i, and σ_{x_i} is the standard deviation of the parameter in the physical space.

(3) Evaluation of the partial derivative of the system output with respect to input random variables at the current iteration as follows:

$$\nabla[G(X)] = \left(\frac{\partial[G(X)]}{\partial x_1}, \frac{\partial[G(X)]}{\partial x_2}, \ldots, \frac{\partial[G(X)]}{\partial x_n} \right) \tag{9}$$

where n is the number of random variables.

(4) Evaluation of the performance function and the associated gradient at the current point.

(5) Moving to the new point according to the following equation:

$$\begin{aligned} X_{n+1} = {}& \mu_n^{N} + C(X)_n^{N} \nabla[G(X)]_n \\ & \times \frac{[X_n - \mu_n^{N}]^{t} * \nabla[G(X)]_n - G(X)_n}{\nabla[G(X)]_n^{t} * C(X)_n^{N} * \nabla[G(X)]_n} \end{aligned} \tag{10}$$

where X_{n+1} is the vector of random variable at iteration $n + 1$ in the normal space; X_n is the vector of random variable at iteration n in the normal space; $\mu_{X_i}^{N}$ is the vector of mean values of the random variables in the normal space at iteration n; $C(X)$ is the correlation matrix of random variables in the normal space; $\nabla[G(X)]_n$ is the gradient vector of the limit state function at iteration n with respect to each random variable; $\nabla[G(X)]_n^{t}$ is the transpose of $\nabla[G(X)]_n$.

(6) Check the required accuracy as follows:

$$\|X_{n+1} - X_n\| < \varepsilon \tag{11}$$

where ε is the tolerance value (maximum permissible error); X_n is the vector of random variables at iteration n; X_{n+1} is the vector of random variables at iteration $n + 1$.

If the condition in (11) is satisfied, proceed to the next step, otherwise repeat steps from 2 to 6.

(7) The solution should be revised based on the new value of X.

(8) Calculation of the safety index β can be done as follows:

$$\beta = \left[-\frac{\nabla[G(X)]}{|\nabla[G(X)]|} \right]^{t} X^{*} \tag{12}$$

where X^{*} is the vector of random variables at the design point (most probable point), and t indicates the transpose of the matrix.

One advantage of FORM is that the sensitivity information of the random variables can be obtained without any extra computations. Unlike the mean value method, FORM expands the solution around the most probable point, which is not necessarily the mean value point [24]. However, it was found that FORM procedure in its current form requires many computations especially with complicated contaminant transport problems that contain thousands of nodes. Although the FORM approach is efficient and advantageous when used with simple problems, compared with MCS, it is found that FORM requires more computational effort than MCS [32,33]. As a result, FORM method with its current implementation is not efficient to be used in complicated groundwater and contaminant transport problems.

4. Alternative implementation of FORM

The HL–RF optimisation procedure requires calculating of the gradient vector at each iteration. There are different methods to obtain gradient of the functions. These methods can be summarised as follows:

- *Manual*: This can be done by hand using fundamental calculus rules. Manual differentiation, however, requires a huge effort and the output accuracy is questionable.
- *Finite difference*: The method of finite difference is very common and has been widely used. It depends on estimation of the first derivative by finite difference. The accuracy of the method is highly dependent on the complexity of the function of concern and the increment of the difference.
- *Automatic differentiation*: Automatic differentiation relies on the fact that any mathematical function, regardless to its complexity, is executed on the computer as a series of elementary operation. By applying chain rule on the function repeatedly to the composition of those elementary operations, the derivative of the function can be then computed in a mathematical way.

Automatic differentiation is a good alternative for evaluating the gradient vector instead of using the crude finite difference method or manual method. The advantages of automatic differentiation are that it is easy to implement and does not require any knowledge of the original code contents. The accuracy of automatic differentiation is up to machine precision since it does not imply any cancellation, truncation or estimation. In terms of time requirements, it is also superior when compared to other differentiation methods.

4.1. Automatic differentiation of FORTRAN (ADIFOR)

Derivatives of functions are used very often for different purposes such as sensitivity analysis, optimisation problems, inverse modelling, etc. If the function is simple, the derivative of the function can be obtained analytically

using calculus rules. However, in case of large applications and complex functions like large computer codes, it is very complicated to obtain the derivative analytically. Therefore, other methods have been used to obtain the derivative of the complex functions. The most familiar method used for derivative estimation is the finite difference method. This method suffers from poor accuracy and its result is highly dependent on the increment value of the finite difference. In addition, the method is slow and requires solving the function many times to obtain the derivative.

ADIFOR [5] is a FORTRAN pre-processor to generate a code that computes the partial derivatives of all dependent variables with respect to all independent variables. The processor of ADIFOR needs two input files: the first one lists all the dependents and independents variables, and the second file identifies all the subroutines of the program for which the derivative code should be obtained. Using automatic differentiation, all the errors associated with finite difference method (such as round of error, increment size, etc.) can be eliminated. Any computer code, regardless to its length, is composed of set of mathematical operations such as summation, multiplication, etc. ADIFOR applies chain rule of calculus on all mathematical operation in the code to obtain the derivative of a dependent variable with respect to independent one. The theory of ADIFOR can be illustrated as follows: assuming that the independent variables for a certain function are:

$$X_i = f_i(x_1, x_2, \ldots, x_{i-1}), \quad i = n+1, n+2, \ldots, m \qquad (13)$$

and the dependent variables are:

$$x_{n+1}, x_{n+2}, \ldots, x_m \qquad (14)$$

There are two basic approaches to get the derivative code using automatic differentiation: the forward mode and backward mode.

In the *forward mode*, the computer holds a value and a storage location for all derivatives up to the desired degree. Automatic differentiation breaks the code down into elementary unary and binary operations. Then, for each mathematical operation in the code, the derivatives are calculated by chain rule as follows:

$$\frac{\partial x_i}{\partial x_j} = \sum_{k=1}^{i-1} \frac{\partial f_i}{\partial x_k} \frac{\partial x_k}{\partial x_j}, \quad j = 1, 2, \ldots, n \qquad (15)$$

Since f_i is unary or binary, the sum in (15) consists of a single term or a sum of two terms [29].

In the *backward mode*, a computational graph for all the mathematical operations have to be constructed to represent the computations at each variable x_i, $i = 1, 2, \ldots, m$ and links to nodes for the operands of operation. A storage location for the derivative of each node has to be allocated. All the variables are considered as independent at the beginning. Therefore, the derivatives are all zero except at nodes for f where the derivative value is 1. Then going backward one by one, the variables change to dependent and the derivative updated using chain rule as follows:

$$\frac{\partial f^{\text{new}}}{\partial x_k} = \frac{\partial f^{\text{old}}}{\partial x_k} + \frac{\partial f}{\partial x_i} \frac{\partial f_i}{\partial x_i}, \quad k = 1, 2, \ldots, i - 1 \qquad (16)$$

At a binary node, $\frac{\partial f_i}{\partial f_k}$ is zero for all but one value of k. Unlike forward approach, the computations required by backward approach are independent on the number of non-zero derivatives.

ADIFOR deploys a hybrid forward/backward scheme, and thus, reduces the required time. That is, ADIFOR is generally based on forward mode, but it uses the backward mode to compute the gradient of the assignment statements containing complex expressions.

In this study, ADIFOR was used to generate the derivative code of the two-dimensional finite element groundwater flow and contaminant transport model (MCB2D) [36]. The resulted code is a FORTRAN subroutine including the derivative code for the pre-defined input parameters, in addition to the original model code. All the work, which has to be done, is to identify the dependent parameters (in this case the concentration of pollutant) and the independent parameters (hydraulic conductivity, and groundwater recharge). As a result, the derivative code of the original model was obtained and the required gradient vector was evaluated with a very good accuracy and fewer computations in comparison to finite difference method.

4.1.1. ADIFOR and other automatic differentiation methods

There are different tools and software for derivative calculation using automatic differentiation. A good survey of these tools can be found in [17,35]. In this research, we are interested in a method that can be applied directly to the model code, and produce the derivative code for a pre-defined dependent and independent variables. The groundwater model, which was used in this study, is written in Fortran language. Therefore, it was preferable to use a tool works with FORTRAN.

Tools of automatic differentiation are classified into two groups according to the computer language: (1) GRESS, PADRE-2, ADIFOR, and Odyssee are automatic differentiation for FORTRAN codes, and (2) ADOL-C and ADIC work with C codes. GRESS, PADRE-2, and ADOL-C generate a trace of computation by writing down the particulars of each operation performed. Thus, the code gets very huge and the time required is large [35].

ADIFOR, Odyssee, and ADIC transform the source into the derivative code by applying the rules of automatic differentiation. Odyssee uses the backward mode, and it imposes certain restrictions on the FORTRAN input and runtime environment. ADIFOR deploys a hybrid forward/backward scheme, and thus, reduces the required time. Generally, the advantages of ADIFOR over other automatic differentiation tools are:

1. *Ease of usage*: It can be used without any run-time support and it can be easily used with different computing environments.

2. *Portability*: It supports all Fortran 77 codes including arbitrary calling sequences. Since the majority of groundwater models are written in Fortran, this makes ADIFOR good suited for these models.
3. *Accuracy*: The produced derivative code is accurate up to machine precision.
4. *Efficiency*: The time requirement of ADIFOR is less than that of finite difference. It does not require any change of the original code but identification of dependent and independent variables.

5. Case study: probabilistic contaminant transport modelling

Fig. 3 shows the area of study with the land use and sources of pollution. The area is located in Bait Lahia, which is in the northern part of the Gaza Strip, Palestine. The study area is about 23 km^2 and the water-bearing layer is composed of gravel and sandstone covered with sand dunes from the Quaternary era. Therefore, the area is highly vulnerable to groundwater pollution.

A waste water treatment plant is the main source of groundwater pollution in the area. Bait Lahia treatment plant has been in operation since 1973, and it is one of the plants, which have been inherited from the Israeli government by the Palestinian Authority after the Oslo agreement. Because of increasing population and increasing inflow, the sewage influent has been constantly overflowing the designed capacity. The amount of sewage influent is about 8000–10,000 m^3/day, and less than 30% of the influent is currently being treated. As the area is well recharged from rainfall and the infiltration rate is high because of the existence of sandy dunes, the Bait Lahia treatment plant is near groundwater bodies of high-quality. High-level of nitrate concentrations were detected from the aquifer nearby, and it is most likely that the excess wastewater influent is responsible for the deterioration of the water quality of the aquifer.

5.1. Model description

MCB2D is a two-dimensional finite element groundwater flow and transport model written in FORTRAN computer language. The model couples groundwater flow with contaminant transport using a Multiple Cell Balance Method [36] to solve the two-dimensional advection dispersion equation.

The model in this study consists of 532 nodes and 977 elements. Of course this model is not so large when compared to other models, but it is large enough to show the efficiency of the proposed FORM. The intensity of elements was increased at the location of the pollution sources (e.g. wastewater treatment plant) as shown in Fig. 4. The aquifer in the area is phreatic with groundwater depth varies between 20 and 35 m. Calcareous sandstone, and gravel
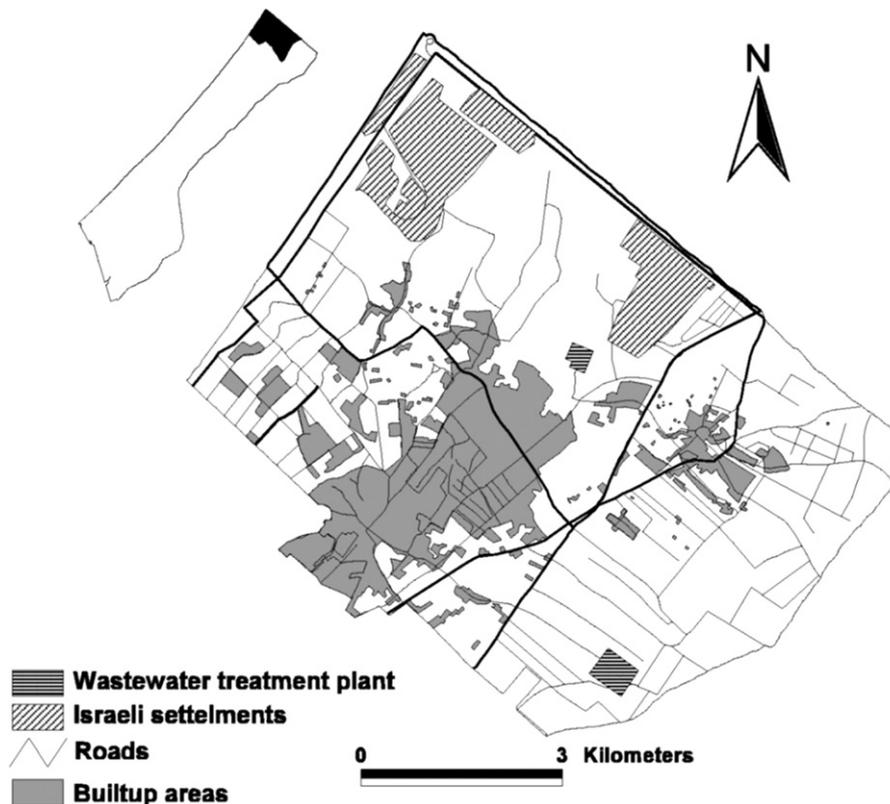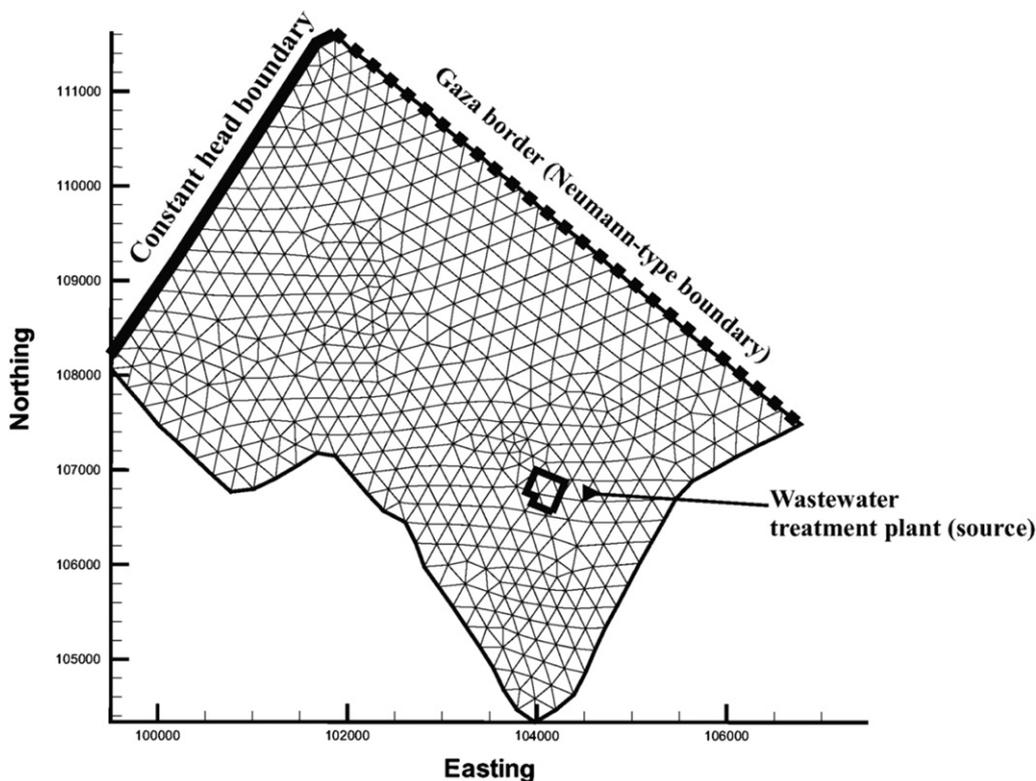

Fig. 3. The study area.

Fig. 4. Finite element mesh and boundary conditions.

with high hydraulic conductivity are the main components of the aquifer media. The aquifer parameters were input into the model based on the statistical analysis of these parameters. Values of hydraulic conductivities were obtained from the literature [10,25,37], and from pumping tests data. Groundwater recharge data were obtained from the literature based on different methods of recharge analysis [2,10,16,25]. Historical data of pumping rates were obtained from the Palestinian Water Authority (PWA), and input into the model. The derivative code of the model, which was obtained using ADIFOR, was coupled with the proposed FORM approach code. Input parameters, which were considered as uncertain, are the groundwater recharge and hydraulic conductivity. The first and second moments of these variables were obtained from statistical analysis.

5.2. Boundary and initial conditions

The boundary conditions for both flow and transport problems are shown in Fig. 4. A Dirichlet-type of boundary condition was assigned to the western part of the model (sea line) at which the head is constant. The head at this boundary was assumed to be zero. Neumann-type boundaries of specified flow were assumed at the residual parts of the model boundaries. Based on groundwater monitoring in the area, it was found that the groundwater flow direction is generally from east to west (i.e., the contour lines are almost parallel to the sea). The flow amounts at these

boundaries were obtained from groundwater contour maps, and from the literature [3,26]. For the transport problem, nitrate was considered as the main pollutant in the aquifer. Therefore, a constant source of nitrate was assumed beneath the wastewater treatment plant.

The computed nitrate concentrations in the model domain were expressed in dimensionless form as a percentage of those infiltrate beneath the treatment plant. Steady state conditions were assumed at the beginning of the simulation (year 1995), then the results of the steady state simulation were used for the transient state (from 1995 to 2005).

The accuracy of the numerical solution is influenced by the resolution of spatial discretisation (i.e., grid size), and the time discretisation (i.e., time-stepping). Selection of the time step is not easy because it affects the accuracy, and the convergence of solution. In one hand, small time steps increase the accuracy of output to some extent. On the other hand, small time steps lead to numerical diffusion and oscillations, require much computations, much computer storage, and more input data. Time discretisation for the simulation of solute transport can be expressed by a stability criterion, the Courant number [1], which is defined as the ratio of groundwater velocity multiplied by the minimum time step divided by the characteristic distance between grid nodes. Therefore, the time step should satisfy the Courant number equation:
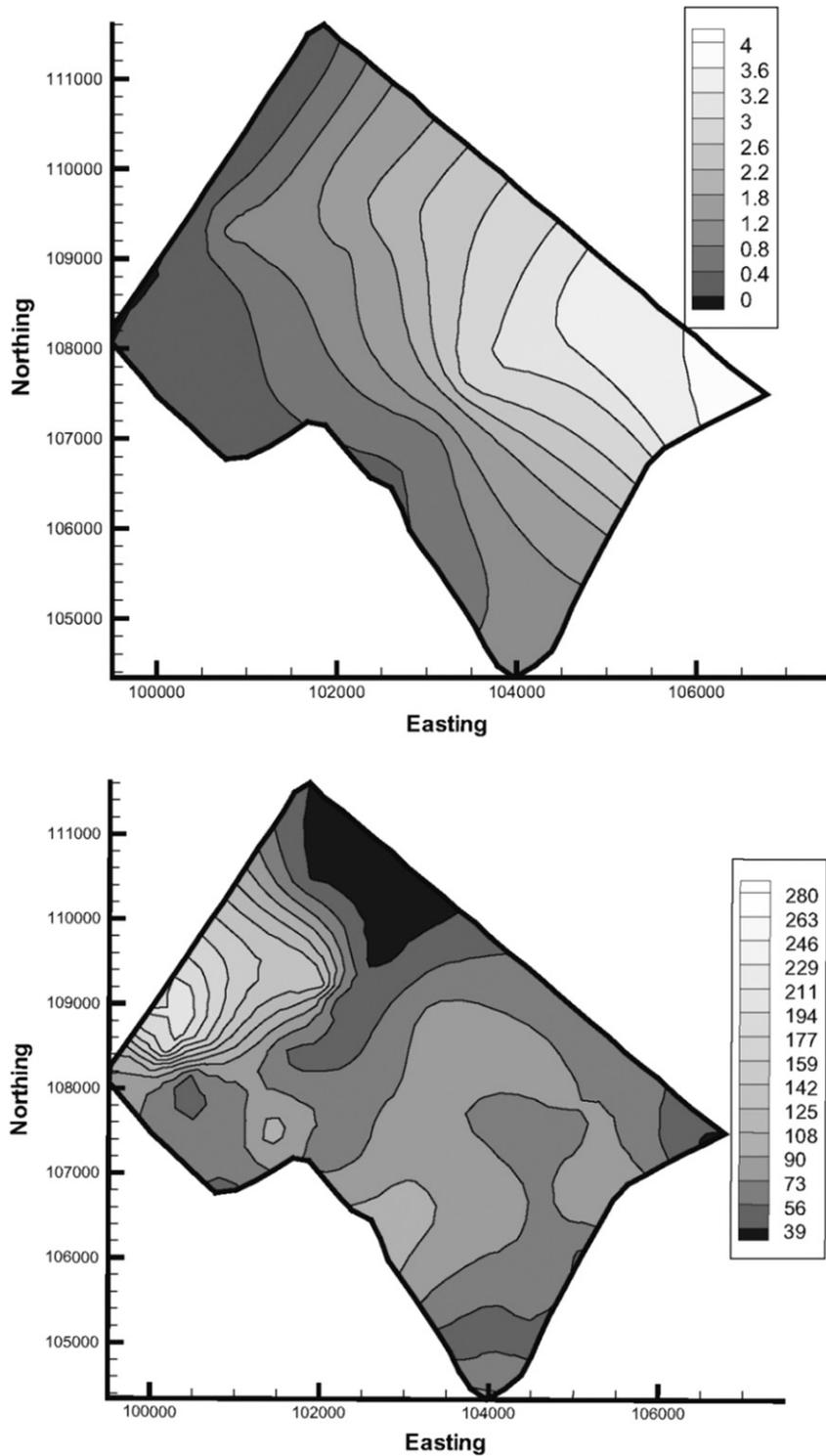
$$\Delta_t \leqslant \frac{\Delta_x}{V} \tag{17}$$

Fig. 5. Initial conditions for groundwater head (upper map [meters above m.s.l.]), and nitrate concentrations (lower map [mg/l]).

where Δ_t is the time step, Δ_x is the distance between nodes and V is the groundwater velocity.

Since the nitrate concentration records in groundwater are available on annual basis, a 1-year time step was assigned. It is found that a 1-year time step satisfies the condition of Eq. (17). Fig. 5 shows the initial groundwater head and nitrate concentrations in the year 1995.

5.3. Coupling FORM with derivative code and MCB model

MCB2D model is written in FORTRAN77 language and has 1770 lines of code. It needed 10 s to run the transient flow and transport code for this study area using a AMD-1000MHz processor. The results of the flow model
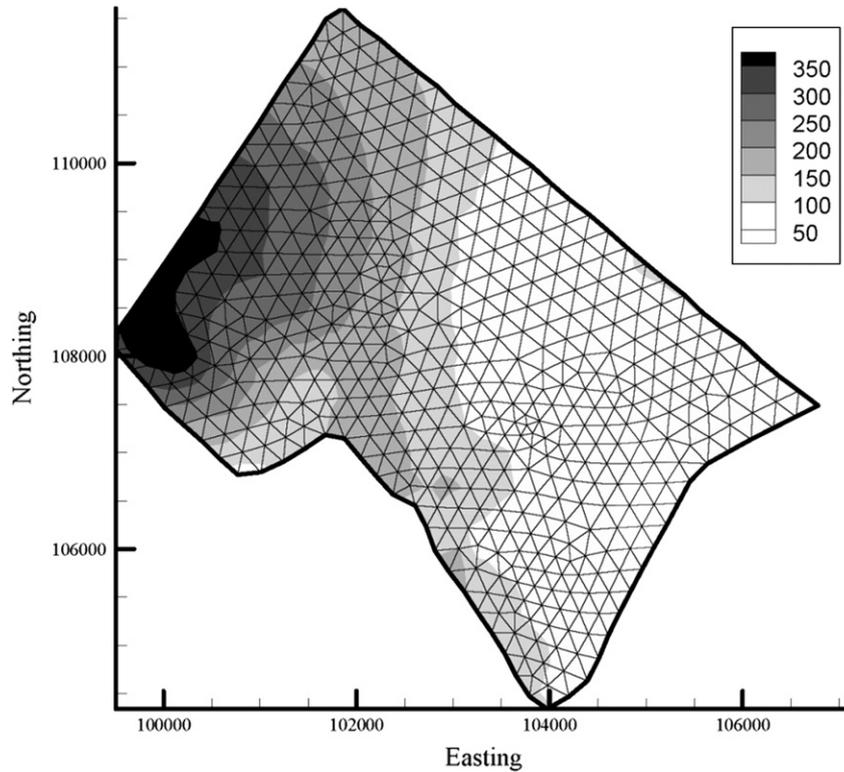
Fig. 6. Nitrate concentration at the end of 10 years contaminant transport simulation [mg/l].

were checked against groundwater monitoring data, and modelling results of the Gaza Strip from the literature [26]. Fig. 6 shows the nitrate concentrations at the end of the 10 years transient simulation period.

Automatic differentiation was used to obtain the following derivatives:

$$\left(\frac{\partial C}{\partial K}\right)_t \tag{18}$$

$$\left(\frac{\partial C}{\partial R}\right)_t \tag{19}$$

where C is the pollutant concentration at any time t; K is the hydraulic conductivity and R is the recharge.

ADIFOR was applied on the original code of MCB2D to generate the derivative code with respect to hydraulic conductivity and groundwater recharge as in (18) and (19). FORM model was considered as the main code, which calls the derivative code and the original function. At each run, FORM reads the input data file, gets the derivative, the function output from the generated code by ADIFOR, and starts the iterations. Iterations stops when the error (i.e., the difference between two successive iterations, as expressed in (11)) does not exceed 1E−05. Thus, iteration procedure continues until the convergence achieved for the pre-defined accuracy. For this case study, the generated derivative code needed 50 s to be executed with the original code coupled with FORM model.

5.4. Limit state function

Different pollutants usually exist in the groundwater as a result of leaching from land use activities. For each type of pollutant, there is a maximum permissible value, which should not be exceeded. Therefore, the main aim of contaminant transport modelling is to investigate if the level of pollutants at a certain location and time exceeds its maximum allowed value. The limit state function in this case can be written as:

$$G(X) = C_t - C(X) \tag{20}$$

where $C(X)$ is the value of concentration obtained by the model, C_t is the maximum permissible value of pollutant concentration. The wastewater treatment plant (refer to Fig. 3) was considered as a continuous source of pollution (nitrate) with a concentration value equals C_0. The formulation of the limit state function was done based on Cawlfield approach [7]. According to this approach, the value of pollutant concentration at a receptor well (C_x) was normalised by the source concentration (C_0). That is, the limit state function was formulated in dimensionless form based on the following equation:

$$G(X) = \left(\frac{C}{C_0}\right)_t - \left(\frac{C_x}{C_0}\right) \tag{21}$$

where C is a pre-defined value of a contaminant concentration at a target location t (maximum permissible value that should not be exceeded); C_0 is the concentration at the

source of pollution and C_x is the value of concentration obtained from the model.

Target concentration was assumed as the maximum permissible value of the pollutant in groundwater in the entire model domain. The results of the proposed FORM model are: the probability of failure contour map for the predefined limit state function, uncertainty analysis, and sensitivity analysis. All computations were carried out based on transient simulations, and the results were obtained at the end of the transient period (10 years).

5.5. Probability of failure

Two input parameters (groundwater recharge and hydraulic conductivity) were considered in this case study as random variables. The hydraulic conductivity and groundwater recharge are assumed constant in the physical space, and variable in the probability space. The required data for the model input were obtained based on field investigations, pumping tests data, and data from literature [11,26]. Tables 1 and 2 list the statistical descriptors of hydraulic conductivity and groundwater recharge in normal and lognormal distributions, respectively.

From the descriptive statistics in Tables 1 and 2, it is obvious that the skewness factor of hydraulic conductivity for lognormal probability is low (0.01) compared to the case of normal distribution (0.675). In addition to skewness factor, the Kolmogorov–Smirnov test, which is used to decide if a sample of data follows a specific probability distribution [19], was carried out. The Kolmogorov–Smirnov parameter (Z) is computed from the largest difference (in absolute value) between the observed and theoretical cumulative distribution functions. It was found from the results of the Kolmogorov–Smirnov test, that the Z parameter for lognormal distribution of hydraulic conductivity equals (0.466), while it is (0.708) in the case of normal distribution. This is also evidence that the hydraulic conductivity is more likely to follow the lognormal distribution rather than the normal distribution. Thus, the hydraulic conductivity was considered to follow the log-normal distribution. Since the hydraulic conductivity values (in general all the hydrogeological parameters) are positive, the log normal distribution is consistent with this fact because the lognormal distribution contains no negative values.

Similarly, the statistical analysis of groundwater recharge reveals that the skewness factor of lognormal distribution equals (0.53), which is less than that of normal distribution (0.87). The results of the Kolmogorov–Smirov test show that the Z value of groundwater recharge for lognormal distribution is smaller than the case of normal distribution (Z equals 0.65, and 0.41 for normal and lognormal distribution, respectively). Therefore, the groundwater recharge is more likely to follow log-normal distribution.

In addition to Kolmogorov–Smirnov test, probability distributions for both parameters were examined using goodness of fit for both normal and lognormal distribution. For the hydraulic conductivity, it was found that the maximum differences between measured and predicted plot is 0.139, and 0.091 for normal and lognormal distributions, respectively. For the rainfall, it was found that the maximum differences are 0.157, and 0.129 for normal and lognormal distributions, respectively. Obviously, the maximum difference between measured and predicted plots is smaller in the case of lognormal distribution than in the case of normal distribution.

The limit state function was formulated as described above in (21), and the transient state simulation was carried out. Nitrate (NO_3) is the simulated pollutant in this case and the maximum permissible value (C_x/C_0) equals 50%. The result of FORM-contaminant transport model at the end of simulation period is presented in Fig. 7. The failure probability map is a function of space for the pre-defined normalised target concentration [$(C_x/C_0) \geqslant 50\%$]. As the groundwater flow direction is generally westward, areas with high probability of failure exist downstream to the west of the sources of pollution (wastewater treatment plant). The eastern and northern areas have low probability of failure. The probability of failure in some areas is almost zero. That means, for the given conditions and for this target concentration, nitrate concentration at these areas will not ever exceed the maximum permissible value.

Table 1
Statistical information of hydraulic conductivity, and groundwater recharge in normal distribution

Statistics	K[a]	Rainfall[b]	R (%)[c]
Normal distribution			
Range	68.00	476.43	21.5
Minimum	15.00	114.57	31.50
Maximum	83.00	591.00	53.00
Mean	41.58	321.00	38.55
Standard deviation	16.69	140.67	5.43
Variance	433.13	19,781.45	29.53
Skewness	0.675	0.381	0.87
Kolmogorov–Smirnov Z	0.708	0.681	0.65

[a] Hydraulic conductivity in m/d.
[b] Rainfall in mm/a.
[c] Net groundwater recharge as a percentage of rainfall.

Table 2
Statistical information of hydraulic conductivity, and groundwater recharge in lognormal distribution

Statistics	K[a]	Rainfall[b]	R (%)[c]
Lognormal distribution			
Range	1.71	1.64	0.52
Minimum	2.71	4.74	3.45
Maximum	4.42	6.38	3.97
Mean	3.60	5.76	3.64
Standard deviation	0.51	0.44	0.14
Variance	0.26	0.19	0.02
Skewness	0.01	−0.45	0.53
Kolmogorov–Smirnov Z	0.466	0.560	0.41

[a] Hydraulic conductivity in m/d.
[b] Rainfall in mm/a.
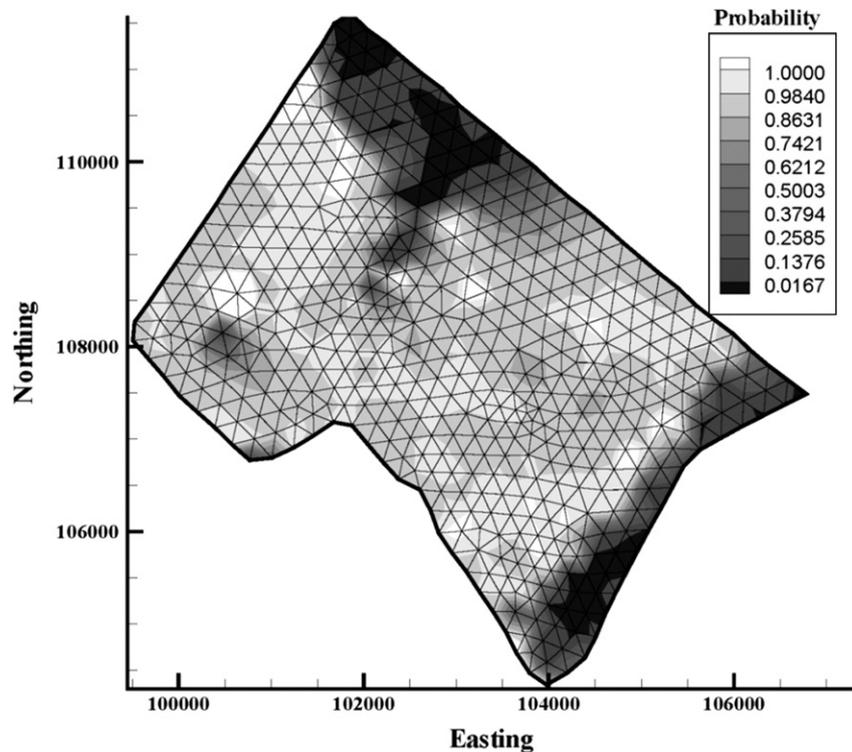[c] Net groundwater recharge as a percentage of rainfall.

Fig. 7. Probability of exceedance in case $C/C_0 \leqslant 50$.

FORM can also compute the values of individual random parameters in the probability space at the design point (X value in (10)). Since the random variables change in the probability space, these variables can get any value between the maximum and minimum range of each. The values of input random parameters at the design point illustrate the conditions leading to a particular realisation. These values give the highest probability of exceeding the threshold (i.e., $C/C_0 \geqslant 50\%$). The contours of hydraulic conductivity (K) and groundwater recharge (R) at the failure point are shown in Fig. 8. The values of hydraulic conductivity that lead to exceedance are generally higher than the mean value (mean value of hydraulic conductivity is 41.58 m/day). Hydraulic conductivity increases gradually from the source of contamination to the maximum value at other locations (from 40 m/day at the source of pollution to 85 m/day away from it). The contour map of groundwater recharge at the failure point shows also increase of this value along the movement paths of contamination. Similarly, the values of groundwater recharge are generally greater than the mean value as shown in the figure.

5.6. Uncertainty analysis

Coefficient of variation (CV) is a statistical measure of the deviation of a variable from its mean, and it is used to determine the degree of relative dispersion of the population. That is, CV is the standard deviation σ divided by the mean value μ of a population. The probabilistic model

for the previously described limit state function was carried out at different values of CV. First, the CV was changed by changing the mean value only keeping the standard deviation constant. The CV of hydraulic conductivity was given four different values: 0.25, 0.50, 0.75, and 1.00 and the model were run keeping the other parameters constant. Then, the same procedure was followed for groundwater recharge. Finally, both hydraulic conductivity and groundwater recharge were given different values of CV simultaneously, and the results of probability of failure were obtained for each case. This procedure was followed at different nodes in the model domain including the municipal wells locations in the area. A typical result of this analysis at a municipal well location is presented in Fig. 9. This figure shows the probability of failure at different values of CV based on changing mean values, keeping standard deviation constant. The first diagram in the figure (top) is for hydraulic conductivity, the second one (middle) is for groundwater recharge, and the last one (bottom) is for both groundwater recharge and hydraulic conductivity together. Based on the analysis of the results, it is found that the probability of failure decreases always, when the CV increase by decreasing the mean value and keeping standard deviation constant. Also the probability of failure increases when the mean value increases, as a result of increasing output.

Similarly, the CV was changed by increasing the standard deviation only, keeping the mean value constant. Any increase in the CV by increasing the standard deviation leads to dispersion of the probability outcome, and
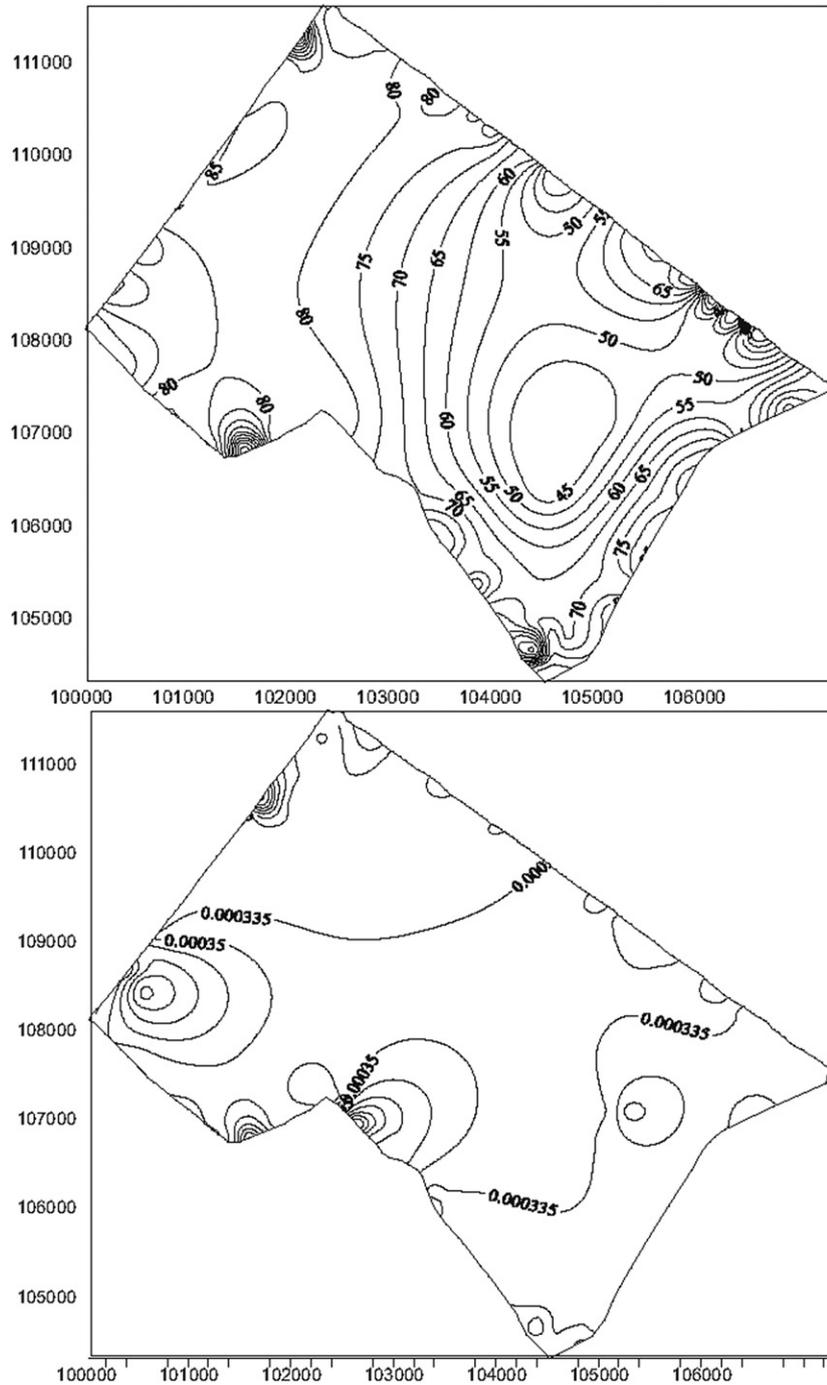
Fig. 8. Contour map of hydraulic conductivity (top [m/d]), and groundwater recharge (bottom [m]) at the failure point.

thus, the probability of failure increases. Fig. 10 illustrates this fact by example of two probability density functions. The population for the two functions is the same as well as the mean, but the standard deviation for population 2 is twice the standard deviation of population 1. Clearly, the distribution of population 2 is dispersed around the mean as a result of increasing the standard deviation. The probability of failure as shown in the figure is the area under the curve to the right of the maximum permissible value. It is obvious that the area under population 2 is lar-

ger than that under population 1. As a result, as the standard deviation increases, the probability of failure increases.

5.7. Sensitivity analysis

In addition to uncertainty analysis, sensitivity of the probability of failure with respect to each random variable was investigated. Sensitivity analysis is important to allocate and design of sampling sites. Since the sampling wells
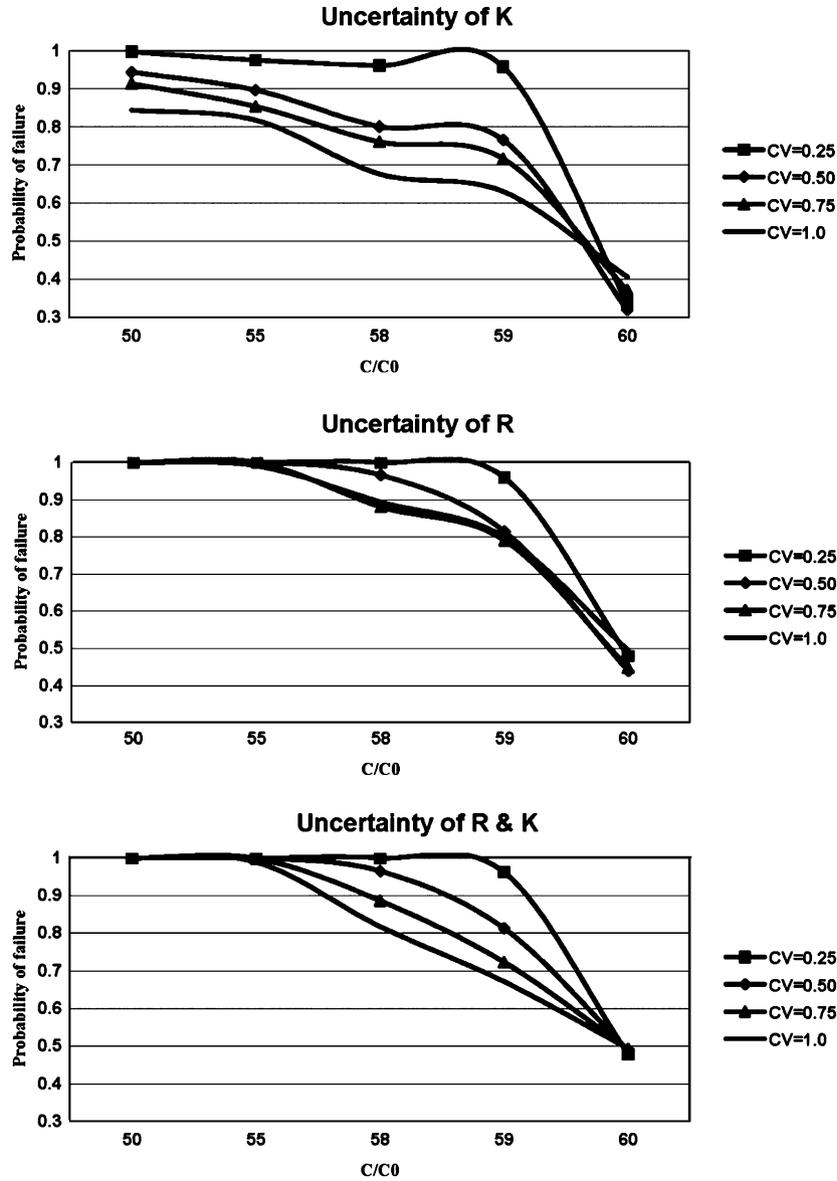
Fig. 9. Effect of CV variation (by varying the mean value of model input) on model output. (Typical figure at municipal well in the area.)

should be located at points of high sensitivity, this analysis is very helpful in designing site monitoring wells. Therefore, sensitivity is very useful in the design of groundwater monitoring networks. Sensitivity of the probability of failure P_f with respect to each random variable can be computed as follows [23]:

$$\frac{\partial P_f}{\partial x_i} = -\frac{\alpha_{x_i}\phi(\beta)}{\sigma_{x_i}} \tag{22}$$

where σ_{x_i} is the standard deviation of a parameter x_i, ϕ is the standard normal probability density function, and β is the reliability index. The vector α is called alpha sensitivity vector and can be computed for any random parameter x_i as follows:

$$\alpha_{x_i} = -\frac{\nabla x_i G(X)}{|\nabla x_i G(X)|} \tag{23}$$

where $G(X)$ is the limit state function in the standard normal space evaluated at the design point, and ∇x_i is the gradient of the function G with respect to the random variable x_i. The alpha vector in (23) can be obtained within the FORM computations, and thus, no extra computations are needed to calculate the sensitivity.

Figs. 11 and 12 show the sensitivity of the probability of failure with respect to hydraulic conductivity, and groundwater recharge, respectively (α_k, and α_r). From the sensitivity figures, the following conclusions could be drawn:

- In general, the probability of failure is more sensitive to hydraulic conductivity than to groundwater recharge.
- It is also clear the sensitivity of hydraulic conductivity is high at the sources of pollution and in the contamination path.
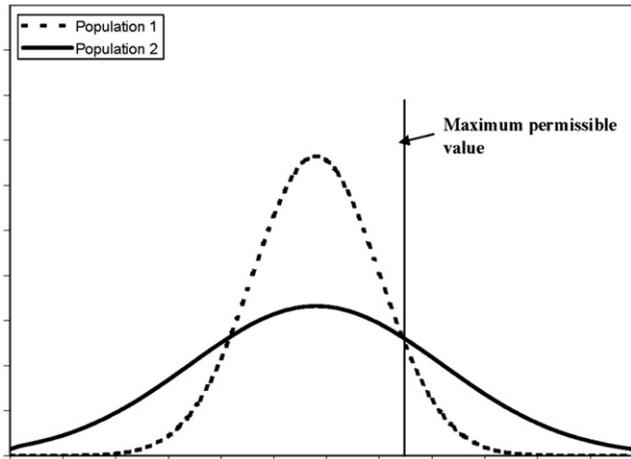
Fig. 10. Example of probability density function with the same mean and different standard deviation.

- The negative values of sensitivity at some locations indicate that any decrease in the value of a parameter at these particular locations leads to increase in the probability of exceedance.

6. Comparison and validation

The obtained results by the developed FORM model were compared with Monte Carlo simulation to check the accuracy and the efficiency of the proposed method. The gradient vector required for FORM simulations was obtained using automatic differentiation. Therefore, the proposed methodology, which couples FORM with auto-matic differentiation (FORM-AD), was compared with FORM model using finite difference method (FORM-FD). The comparison was applied at different locations distributed in the model domain. Fig. 13 shows the probability of failure using the following methods:

- FORM using automatic differentiation to obtain the derivative of the limit state function (FORM-AD model).
- Monte Carlo simulation (MCS).
- First order second moment method (FOSM).
- FORM using finite difference method to obtain the derivative of the limit state function (FORM-FD model).

The same principle of reliability setup, which was discussed above, was used and applied with FOSM method. The intended reliability index β was derived based on (4). FOSM involves the first order expansion around the mean to estimate the first and second moments [18]. So, it depends on Taylor series expansion of the limit state function $G(X)$ around the mean values of random variables [18]. The Taylor series expansion of the limit state function was developed as follows:

$$
\begin{aligned}
G(X) \approx G(\overline{X}) + \sum_{i=1}^{n} \frac{\partial G(\overline{X})}{\partial x_i}(x_i - \mu_i) \\
+ \frac{1}{2!} \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial^2 G(\overline{X})}{\partial x_i \partial x_j}(x_i - \mu_i)(x_j - \mu_j) + \text{H.O.T}
\end{aligned}
\tag{24}
$$

where $G(\overline{X})$ is the limit state function evaluated at the mean values, n is the number of random variables, and
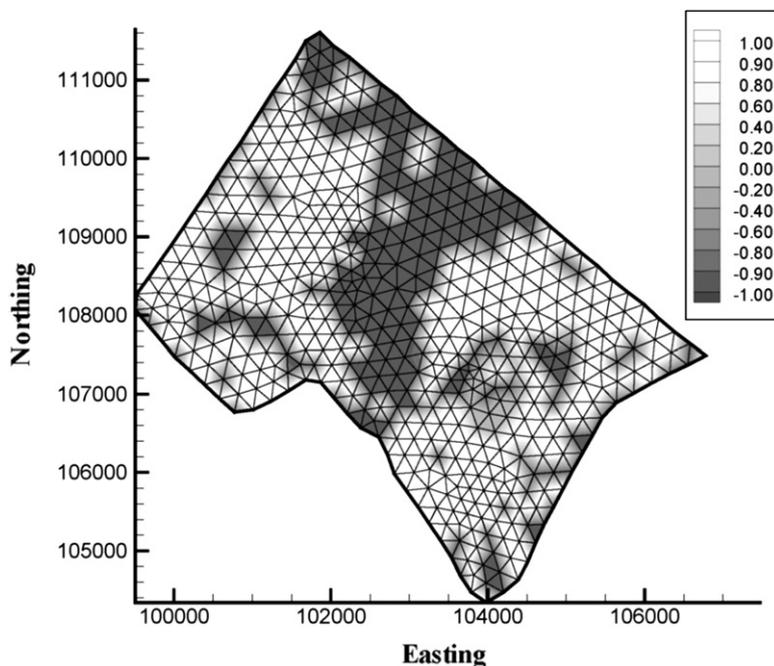

Fig. 11. Sensitivity of contaminant transport model with respect to hydraulic conductivity.
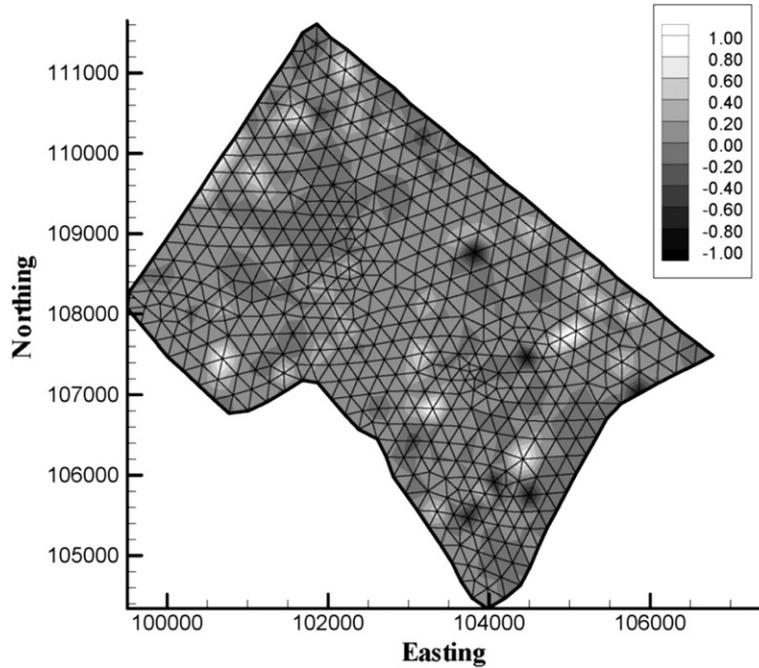
Fig. 12. Sensitivity of contaminant transport model with respect to groundwater recharge.

H.O.T are the higher order terms. The mean of the function is equal to the expectation value $E[(GX)]$, which is

$$E[G(X)] \approx G(\overline{X}) + \frac{1}{2!} \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial^2 G(\overline{X})}{\partial x_i \partial x_j} E[(x_i - \mu_i)(x_j - \mu_j)]$$
(25)

and the variance can be computed as follows:

$$\sigma^2[G(X)] = E[(G(X) - E[G(X)])^2]$$
$$\approx \sum_{i=1}^{n} \sigma^2(x_i) \left(\frac{\partial G(\overline{X})}{\partial x_i}\right)^2$$
$$+ 2 \sum_{i=1}^{n} \sum_{j=1+1}^{n} C(x_i, x_j) \left(\frac{\partial G(\overline{X})}{\partial x_i}\right) \left(\frac{\partial G(\overline{X})}{\partial x_j}\right)$$
(26)

where $C(x_i, x_j)$ is the covariance between variables x_i and x_j, and $\sigma^2(x_i)$ is the variance of the variable x_i.

Substituting the results of (25) and (26) in (4), the reliability index β, and the probability failure can be computed.

The use of the finite difference method to estimate the derivative of the functions has many drawbacks. Increment size, for example, affects the accuracy of the finite difference estimation, in addition to convergence rate. A small increment is desired to reduce the truncation error of the finite difference estimate but a very small increment size increases subtractive cancellation errors. Based on studies carried out by Hamed et al. [12,13], the increment size in the finite difference should be chosen as a small fraction of the standard deviation of the random variable. Therefore, the increment size was chosen as 0.1 of the standard deviation of each random variable. The FORM-AD model converges

after only 5–10 runs with a very good accuracy as shown in the figure. The reference of accuracy of FORM is the Monte Carlo results. The obtained results of Monte Carlo simulation were based on 1000 model runs. Monte Carlo simulation procedure can be described as follows: the input values of the hydraulic conductivity and groundwater recharge (random variables) were randomly sampled using a random number generator. With this realisation, the transport model was run and the output was obtained. Then, using a new sampling, the transport model was run again, and another set of results were obtained. If the resulted concentration value is less than the pre-defined value, then the hit value equals 0, else, the hit value equals 1. At the end, the probability of failure could be calculated by dividing the number of hits by the total number of runs. The results of Monte Carlo simulations were used as a reference to check the accuracy of other methods and compare them with the proposed method.

The simulations of the above mentioned models were done using a AMD-1000MHz processor. The run time and number of runs for each model are shown in Table 3. Although the finite difference method needs less time to evaluate the model, but it requires more runs to converge. Consequently, the total time required by FORM-FD is more than that required by FORM-AD. In this study, the difference in time between FORM-AD and FORM-FD is not so large. However, we are talking about a model of 532 nodes and 977 elements. It is small in comparison to large models with ten of thousands of nodes. In that case, every extra second in each iteration does affect the total time of run. On the other hand, we are talking about a model of two random variables. If the number of variables increases, the total time required by FORM-FD will increase while

Node 227

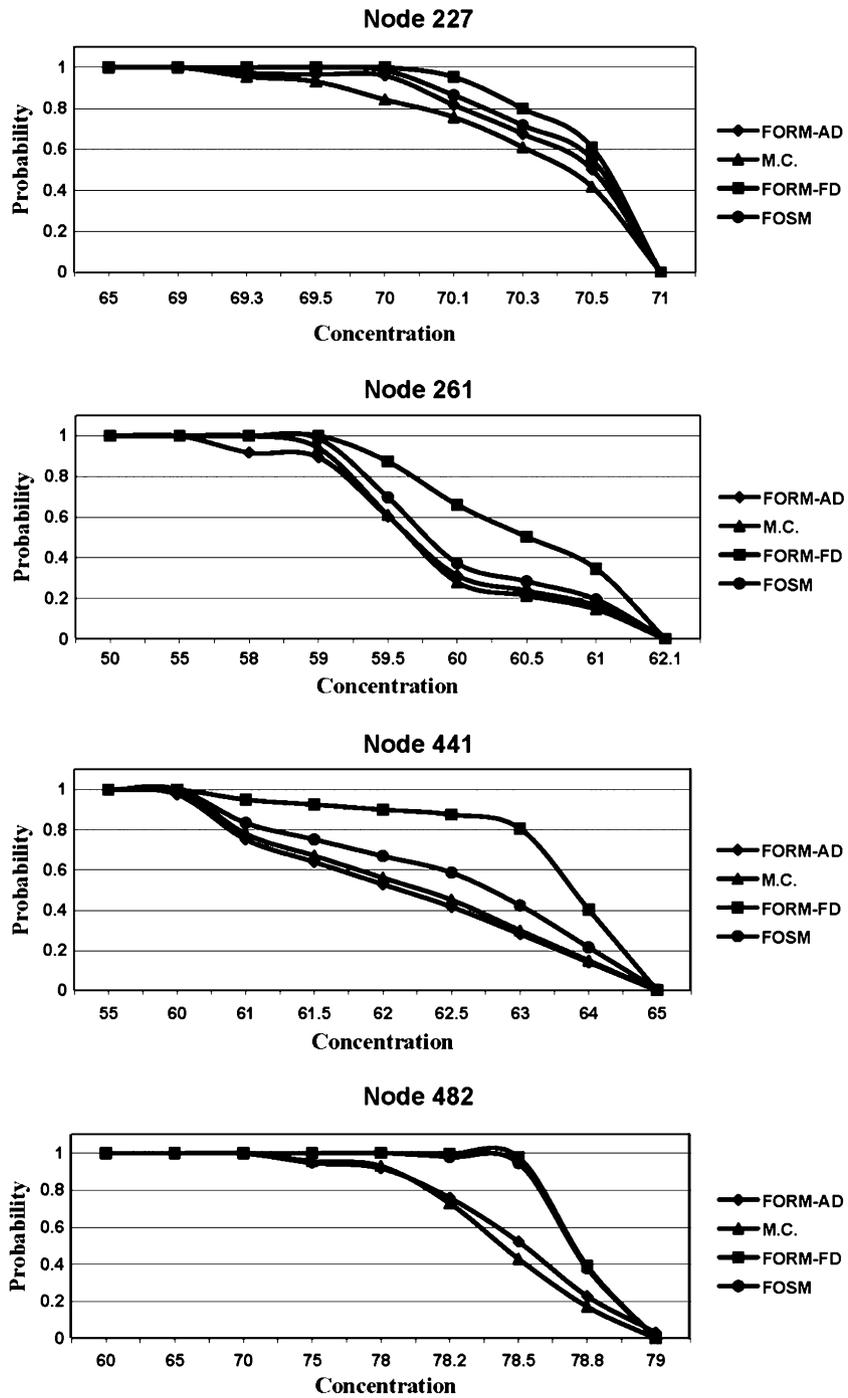**Node 261**

Node 441

Node 482

Fig. 13. Probability of failure using FORM-AD, Monte Carlo, FOSM, and FORM-FD at different model nodes.

Table 3
Efficiency of FORM-AD, MC, and FORM-FD

Method	Model components	Time[a]/run	No. runs	Total time[a]
FORM-AD	Contaminant transport model, derivative code, FORM code	50	7	350
MC	Contaminant transport model, sampling code	10	1000	10,000
FORM-FD	Contaminant transport model, FORM code	10	13 × 3	390

[a] Time in seconds.

that of DORM-FD will not. It is clear from Fig. 13 that the FORM-FD model underestimates the probability of failure. The FOSM approximation is good only when the probability of failure is not extreme. In other words, if the probability of failure is very small or very large, FOSM results are very poor while Monte Carlo requires more runs for such probabilities. Using the finite difference method to estimate the first order derivative is not accurate and leads to cumulative error in FORM-FD.

7. Conclusions

From the analysis of the results obtained in this study, it is found that the modified FORM method provides a very good tool to incorporate the uncertainty in model parameters in groundwater modelling, and to carry out sensitivity analysis. The characteristics of FORM-AD are efficiency and robustness. The proposed FORM-AD method requires only 5–10 runs to converge to the solution with a very good tolerance value (i.e., error is less than 1E−05). When compared to other methods (e.g. Monte Carlo simulation or FORM with finite difference method), the developed FORM-AD method has shown a good efficiency. The use of automatic differentiation in FORM has promoted a solution that is both accurate and efficient. This is obvious since automatic differentiation requires few runs and produces accurate results. From the comparison between different methods of uncertainty analysis, it was found that the proposed FORM with automatic differentiation is more efficient in terms of accuracy and computation effort. Moreover, the FORM-AD method has another advantage when compared to MCS, which is the added inherent sensitivity analysis. FORM-AD produces sensitivity results without any further computations since it is part of FORM optimisation approach.

Results of sensitivity analysis reveal that the hydraulic conductivity has greater effect on the model results than the groundwater recharge. Uncertainty of model input parameters plays a big role in probabilistic model output. Based on the results of uncertainty analysis, it was found that the probability of failure increases as the mean value or the standard deviation of the input parameters increases.

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