

USER'S GUIDE

PREMChlor: Probabilistic Remediation Evaluation Model for Chlorinated Solvents

ESTCP Project ER-0704

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A new probabilistic remediation model, Probabilistic Remediation Evaluation Model for Chlorinated solvents (PREMChlor), has been developed for simultaneously evaluating the effectiveness of source and plume remediation considering the uncertainties in all major parameters. This development was conducted as an Environmental Security Technology Certification Program (ESTCP) research project (ER-0704), which was a joint effort between Clemson University, GSI Environmental Inc., and Purdue University. The technical foundation of PREMChlor is the U.S. Environmental Protection Agency (USUSEPA) REMChlor (for Remediation Evaluation Model for Chlorinated solvents) model [Falta, 2008]. REMChlor is a significant improvement on existing chlorinated solvent transport models, because it can simultaneously account for both source and plume remediation. REMChlor includes a source model based on a power function relationship linking the source mass to the source discharge and an analytical plume model based on one-dimensional advection, with three-dimensional dispersion. The plume model simulates natural attenuation or plume remediation for parent and daughter compounds in the first-order sequential decay chain. Plume model also calculates the cancer risks posed by carcinogenic compounds assuming that the contaminated water is used in a house for drinking, bathing, and other household uses. PREMChlor is developed by linking the analytical model REMChlor to a Monte Carlo modeling package GoldSim via a FORTRAN Dynamic Link Library (DLL) application. In PREMChlor, all of the uncertain input parameters are treated as stochastic parameters represented by probability density functions (PDFs). The outputs from PREMChlor are probability distributions and summary statistics of the distributions. Cost analysis of common technologies for dense non-aqueous phase liquid (DNAPL) source removal and dissolved plume treatment are included. PREMChlor gives users a single platform where cost, source treatment, plume management, monitored natural attenuation, and risk assessment can all be evaluated together, and where uncertainty can be incorporated into the site decision making process. A license-free file containing the user-friendly graphical user interface (GUI) has been generated to make PREMChlor available for use by others.

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Acronym List

EPA	Environmental Protection Agency
CVOC	Chlorinated volatile organic compound
DCE	dichloroethylene
DLL	Dynamic Link Library
DNAPL	dense non-aqueous phase liquid
GUI	graphical user interface
LB	Lower Bound
NAPLs	Non-aqueous phase liquid
NPV	present net value
NRC	National Research Council
O&M	Operation & Management
PAT	pump-and-treat
PCE	tetrachloroethylene
PDFs	Probability density functions
PRBs	Permeable reactive barriers
REMChlor	Remediation Evaluation Model for Chlorinated solvents
TCE	trichloroethylene
UB	Upper bound
VC	vinyl chloride

Overview

Abstract

A new probabilistic remediation model, Probabilistic Remediation Evaluation Model for Chlorinated solvents (PREMChlor), has been developed for simultaneously evaluating the effectiveness of source and plume remediation considering the uncertainties in all major parameters. This development was conducted as an Environmental Security Technology Certification Program (ESTCP) research project (ER-0704), which was a joint effort between Clemson University, GSI Environmental Inc., and Purdue University.

The technical foundation of PREMChlor is the U.S. Environmental Protection Agency (USUSEPA) REMChlor (for **R**emediation **E**valuation **M**odel for **C**hlorinated solvents) model [Falta, 2008]. REMChlor is a significant improvement on existing chlorinated solvent transport models, because it can simultaneously account for both source and plume remediation. REMChlor includes a source model based on a power function relationship linking the source mass to the source discharge and an analytical plume model based on one-dimensional advection, with three-dimensional dispersion. The plume model simulates natural attenuation or plume remediation for parent and daughter compounds in the first-order sequential decay chain. Plume model also calculates the cancer risks posed by carcinogenic compounds assuming that the contaminated water is used in a house for drinking, bathing, and other household uses.

PREMChlor is developed by linking the analytical model REMChlor to a Monte Carlo modeling package GoldSim via a FORTRAN Dynamic Link Library (DLL) application. In PREMChlor, all of the uncertain input parameters are treated as stochastic parameters represented by probability density functions (PDFs). The outputs from PREMChlor are probability distributions and summary statistics of the distributions. Cost analysis of common technologies for dense non-aqueous phase liquid (DNAPL) source removal and dissolved plume treatment are included. PREMChlor gives users a single platform where cost, source treatment, plume management, monitored natural attenuation, and risk assessment can all be evaluated together, and where uncertainty can be incorporated into the site decision making process. A license-free file containing the user-friendly graphical user interface (GUI) has been generated to make PREMChlor available for use by others.

DISCLAIMER OF LIABILITY

With respect to **PREMChlor** software and documentation, neither the United States Government, Clemson University, GSI Environmental Inc., Purdue University, nor any of their employees, assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed. Furthermore, software and documentation are supplied "as-is" without guarantee or warranty, expressed or implied, including without limitation, any warranty of merchantability or fitness for a specific purpose.

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Software Installation and Computer Requirements

1. PREMChlor is the probabilistic version of USEPA REMChlor deterministic model [Falta, 2008 and U.S. USEPA, 2007]. The user is assumed to be familiar with the REMChlor deterministic model before running the probabilistic model.
2. PREMChlor is run under the GoldSim Player software. To open and run the model file (with an extension name of .gsp), the user needs to download and install the GoldSim Player (www.goldsim.com, version 9.60 SP4, GoldSim 2009). The GoldSim Player may be downloaded from <http://www.goldsim.com/Content.asp?PageID=430> or <http://www.goldsim.com/downloads/software/GSP9604.exe> . Make sure to download the version of 9.60 SP4 (GSP9604.exe). After downloading GSP9604.exe, double click it to install GoldSim Player. Once GoldSim Player is installed, the model file may be opened in two ways. One way is to double click the model file and the other is to open the GoldSim Player, then click the **OPEN MODEL** option and select a model file.
3. A Fortran Dynamic Link Library (DLL) file is also required for the simulation. The DLL file links the REMChlor Fortran source code to the probabilistic model. In order to run the model properly, the probabilistic model file (with the extension name of .gsp) and the DLL file (with the extension name of .dll) need to be in the same directory.
4. This program should run on any recent personal computer using the Microsoft Windows XP, Vista, and Windows 7 operating systems.

PREMChlor Description

Background

Contamination of groundwater by dense, non-aqueous phase liquids (DNAPLs), such as chlorinated solvents, poses a widespread and serious threat to groundwater supplies due to their toxicity. While the solubilities of DNAPLs are very low, they are typically several orders of magnitude higher than drinking water standards [Pankow et al., 1996]. DNAPLs tend to act as continuous long-term sources of groundwater contamination and form large dissolved contaminant plumes.

Technologies have been developed for both DNAPL source control and plume treatment. Source control includes either removal or destruction of the contaminant source, or its physical isolation. For chlorinated solvent source remediation, in-situ technologies include thermal methods (e.g. steam flooding and electrical heating), chemical oxidation, surfactant flooding and cosolvent flooding, soil vapor extraction, and air sparging [Reddi, 1996; Brusseau et al., 1999; Kaluarachchi, 2001; USEPA, 2004b; Mayer and Hassanizadeh, 2005]. To prevent or reduce the source contaminant loading to the plume, source containment methods, such as slurry walls, clay caps and sealable joint sheet pile walls can be used for isolating the contaminant source.

Chlorinated solvents in dissolved plumes can be removed by pump-and-treat (PAT) systems, by natural attenuation processes including biodegradation processes, or they can be controlled by reactive barriers. Currently, enhanced in-situ biodegradation is commonly employed if the natural attenuation as a remedy is not sufficient. These enhanced biodegradation processes can include reductive dechlorination, aerobic oxidation, anaerobic oxidation, and aerobic co-metabolism [Wiedemeier et al. 1999; National Research Council (NRC), 2000; Alvarez and Illman, 2006].

DNAPL source and plume remediation efforts are capital intensive. Partial source removal can cost from several hundred thousand dollars to tens of millions of dollars [McDade et al., 2005]. Due to the lower capital costs, plume remediation costs are normally considered to be smaller than those for source remediation. Plume remediation would be the most cost-effective strategy for sites where the source is almost depleted by natural dissolution or other processes [Falta, 2008]. However, at some sites, source mass is significant. Without source removal, the resulting plume longevity would require a long period of time to treat and manage. The operating and managing cost of plume remediation systems for such sites can be comparable to the source remediation costs. For many sites, a cost-effective remediation design requires some combination of source and plume remediation. It is therefore necessary to simultaneously evaluate the transient effects of source and plume remediation.

Analytical site modeling tools have played important role in the remediation selection process. The widely used screening-level models, BIOSCREEN [Newell et al. 1996] and BIOCHLOR [Aziz et al. 2000] simulate remediation by natural attenuation of dissolved hydrocarbons at petroleum fuel release sites and dissolved solvents at chlorinated solvent release sites, respectively. Several three-dimensional

multiphase numerical models focus on the source zone behavior, such as T2VOC [Falta et al., 1992] and UTCHEM [Pope and Nelson, 1978; Delshad et al., 1996]. Recently, a new analytical screening level model, REMChlor, has been developed [Falta et al., 2005ab and Falta, 2008]. REMChlor is a significant improvement on existing analytical chlorinated solvent transport models, because it can simultaneously account for both source and plume remediation. REMChlor includes a source model based on a power function relationship linking the source mass to the source discharge and an analytical plume model based on one-dimensional advection, with three-dimensional dispersion.

Process and parameter uncertainty that occurs in source and plume remediation is a key factor that has made decision-making about DNAPL site remediation alternatives difficult. Uncertainties arise from hydrogeological and biogeochemical properties (e.g. hydraulic conductivity), from the site condition and history (e.g. size and timing of contaminant releases and discharge to groundwater), from the effectiveness of remediation (e.g. fraction of source removed), and from the cost of remediation. The conventional deterministic modeling approach used in models and tools summarized above does not reflect these uncertainties. It is therefore useful to develop a model that can fully assess the uncertainties in process and system parameters in order to select a robust remediation alternative.

In this section, a new probabilistic remediation model, PREMChlor, is presented. The new PREMChlor model takes into account the uncertainties in all major parameters and allows for quick simulations of different combinations of source and plume remediation scenarios to evaluate remediation alternatives. PREMChlor is developed by linking the analytical model REMChlor to a Monte Carlo modeling package GoldSim [<http://www.goldsim.com/>] via a FORTRAN DLL application.

In PREMChlor, all of the uncertain input parameters are treated as stochastic parameters represented by probability density functions (PDFs). The outputs from PREMChlor are probability distributions and summary statistics of the distributions. Cost analysis of common technologies for DNAPL source removal and dissolved plume treatment are included. PREMChlor gives users a single platform where cost, source treatment, plume management, monitored natural attenuation, and risk assessment can all be evaluated together, and where uncertainty can be incorporated into the site decision making process. A license-free file containing the user-friendly GUI has been generated to make PREMChlor available for use by others.

REMChlor Analytical Model

This section includes a brief description of the REMChlor analytical model based on the work by Falta et al [2005a, b]; Falta [2007] and Falta [2008]. For more detailed description of REMChlor, please refer to the REMChlor user's manual [Falta, 2007].

REMChlor model is the technical foundation of the new probabilistic model. This transport model fully couples the source remediation to the plume remediation. It is not specific to any remediation technology. The contaminant source remediation is simulated as a fractional removal of source mass at a future time after the initial release; plume remediation is modeled by considering time and distance dependent decay rates of parent and daughter compounds in the first-order sequential decay chain [Falta, 2008].

The source model is based on a mass balance of the source zone where mass is removed by dissolution and advection with some type of additional decay [Falta et al., 2005a and Falta, 2008]:

$$\frac{dM(t)}{dt} = -Q(t)C_s(t) - \lambda_s M(t) \quad (1)$$

where $Q(t)$ is the water flow rate through the source zone due to infiltration or groundwater flow, $C_s(t)$ is the average contaminant concentration leaving the source zone, $M(t)$ is the contaminant mass in the

source zone, and λ_s is the additional decay term to account for chemical or biological destruction of mass in the source zone.

The source mass is linked to the source discharge through a power function [Rao et al. 2001; Rao and Jawitz, 2003; Parker and Park, 2004; Zhu and Sykes, 2004; Falta et al., 2005a ; Falta, 2008]:

$$\frac{C_s(t)}{C_0} = \left(\frac{M(t)}{M_0} \right)^\Gamma \quad (2)$$

where C_0 is the flow-averaged source concentration corresponding to the initial source mass, M_0 . The exponent, Γ , determines the shape of the source discharge response to changing source mass (Figure 1). When $\Gamma=1$, the source mass and source discharge decline exponentially with time [Newell and Adamson, 2005 and Newell et al., 2006]. When $\Gamma>1$, the source is never fully depleted, and the source discharge is always greater than zero. When $\Gamma<1$, the source is eventually depleted, and the source discharge equals zero in the end. When $\Gamma=0.5$, the source discharge declines linearly with time. When $\Gamma=0$, the source discharge remains constant until the source is completely depleted [Falta et al., 2005a; Falta, 2007 and 2008].

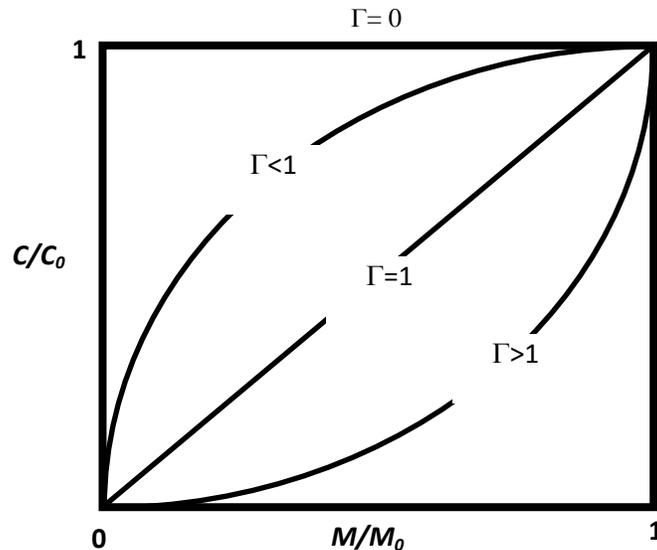


Figure 1. Power function illustration of source mass and source discharge relationship.

Field, laboratory, and theoretical evaluations of the source mass/source discharge response suggest that Γ may vary between about 0.5 and 2 at real sites [Rao and Jawitz, 2003; Falta et al., 2005a; Newell and Adamson, 2005; Fure et al., 2005; Jawitz et al., 2005; McGuire et al., 2006; Newell et al., 2006]. Simulation studies suggest that sites with DNAPL located predominantly in low permeability zones exhibit $\Gamma>1$ and sites with DNAPL in high permeability zones exhibit $\Gamma<1$ [Falta et al., 2005 a, b]. Park and Parker [2005] suggest Γ values greater than 1 for finger-dominated residual DNAPL and less than 1 for DNAPL pools. Essentially, Γ should be considered as an uncertain parameter, whose mean value can be roughly estimated, but whose actual value may never be precisely known at a site.

The solution of Equation 1 with the power function (Equation 2) can be used to predict the time-dependent depletion of the source zone mass by dissolution. The time-dependent mass is then used in Equation 2 to calculate the time-dependent source discharge. If Q is constant, the solutions are given by Falta et al. [2005b]:

$$M(t) = \left\{ \frac{-QC_0}{\lambda_s M_0^\Gamma} + \left(M_0^{1-\Gamma} + \frac{QC_0}{\lambda_s M_0^\Gamma} \right) e^{(\Gamma-1)\lambda_s t} \right\}^{\frac{1}{1-\Gamma}} \quad (3)$$

$$C_s(t) = \frac{C_0}{M_0^\Gamma} \left\{ \frac{-QC_0}{\lambda_s M_0^\Gamma} + \left(M_0^{1-\Gamma} + \frac{QC_0}{\lambda_s M_0^\Gamma} \right) e^{(\Gamma-1)\lambda_s t} \right\}^{\frac{1}{1-\Gamma}} \quad (4)$$

This source model can account for aggressive source remediation efforts (such as excavation, thermal treatment, alcohol or surfactant flooding, or chemical oxidation) that remove a certain fraction of the source mass over a short period of time [Falta et al., 2005a]. By rescaling the equations following the removal of source mass, the source mass and source discharge due to source remediation are presented by Falta et al. [2005b] as:

$$M(t) = \left\{ \frac{-QC_2}{\lambda_s M_2^\Gamma} + \left(M_2^{1-\Gamma} + \frac{QC_2}{\lambda_s M_2^\Gamma} \right) e^{(\Gamma-1)\lambda_s (t-t_2)} \right\}^{\frac{1}{1-\Gamma}} \quad (5)$$

$$C_s(t) = C_2 \left(\frac{M(t)}{M_2} \right)^\Gamma \quad (6)$$

$$M_2 = (1-X)M_1 \quad (7)$$

$$C_2 = C_0 \left(\frac{(1-X)M_1}{M_0} \right)^\Gamma \quad (8)$$

where t_2 is the time when the remediation ends; M_1 is the source mass before remediation, and M_2 is the source mass at t_2 ; X is the fraction of source mass removed during the remediation. This approach is not technology specific, and it allows for a realistic and mass conservative assessment of the effects of source remediation on source longevity and discharge. The source model serves also as a time-dependent mass flux boundary condition to the analytical plume model.

The plume model considers one-dimensional advection, retardation, and three-dimensional dispersion with first order decay of parent compound into daughter products. The governing equation for the dissolved concentration of each contaminant compound in the plume is as follows [Falta et al., 2005b and Falta, 2008]:

$$R \frac{\partial C}{\partial t} = -v \frac{\partial C}{\partial x} + \alpha_x v \frac{\partial^2 C}{\partial x^2} + \alpha_y v \frac{\partial^2 C}{\partial y^2} + \alpha_z v \frac{\partial^2 C}{\partial z^2} + rxn(x, t) \quad (9)$$

where C is the dissolved concentration, and R is the retardation factor, α_x , α_y and α_z are the longitudinal, transverse, and vertical dispersivities, respectively, v is the pore velocity, and $rxn(x,t)$ is the rate of generation (+) or destruction (-) of the dissolved compound due to biological or chemical reactions that may vary temporally and spatially.

A streamtube approach is used to decouple the solute advection and reactions from the longitudinal dispersion. The one-dimensional advective streamtube model is characterized by a constant pore velocity and solute retardation factor. Plume reactions are included in this advective streamtube model. The entire plume is divided into different zones where the reaction rates are time and distance dependent. As illustrated in Figure 2, nine reaction zones are used to represent different conditions downgradient from a contaminant source over the life of a plume. The first time zone after the release, $0 < t < t_1$, could represent a period of natural attenuation following the contaminant spill. The second time zone after the release, $t_1 < t < t_2$ could represent a temporary period of active plume remediation (i.e. enhanced reductive dechlorination). The final time zone, $t > t_2$, could represent long term conditions in the plume after the plume remediation ended (another period of natural attenuation). Similarly, the distance from the source is divided into three zones. For $x < x_1$, one set of natural or engineered biogeochemical conditions are present, while downstream, at $x_1 < x < x_2$, another set of conditions could predominate. For $x > x_2$, conditions could again revert back to natural background conditions. This “reaction-zone” approach provides REMChlor with flexibility to simulate the effect of plume natural attenuation or plume remediation on different contaminant compounds spatially and temporally [Falta, 2007 and 2008].

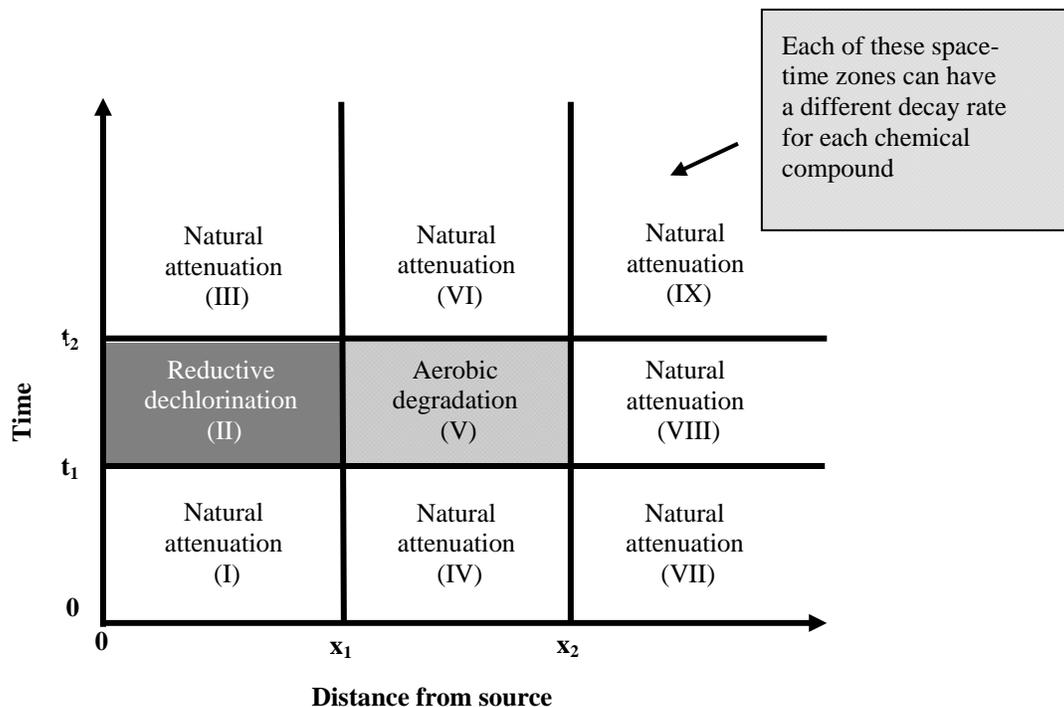


Figure 2. Illustration of plume space-time zones.

The analytical solution for these multiple reaction zones is derived using the residence time in each zone to develop the batch reaction solution for that zone. For more details about the solutions, see Falta [2007

and 2008]. This plume model considers first order parent-daughter decay/production reactions for a four-component system. The batch reaction equations and solutions for four compounds are given by Falta [2007 and 2008].

Longitudinal dispersion is accounted for by considering a collection of streamtubes with a normally distributed pore velocity [Falta, 2008]. With a mean pore velocity, \bar{v} , a standard deviation of pore velocity, σ_v , and a mean front location \bar{x} , longitudinal dispersivity, α_x , at (x,t) is calculated by Equation (10) [Falta, 2008]:

$$\alpha_x = \frac{1}{2} \frac{\sigma_v^2}{\bar{v}} t = \frac{1}{2} \frac{\sigma_v^2}{\bar{v}^2} \bar{x} = a\bar{x} \quad (10)$$

Transverse and vertical dispersions are modeled using Domenico's [1987] approximation. The longitudinal, transverse and vertical dispersivities are made scale dependent by being different linear functions of the mean front location. The plume model assumes dispersion occurring in the positive and negative y directions, but only in the positive z direction [Falta, 2008]. The solution with 3-D dispersion is given by Falta [2007 and 2008].

Cancer risks posed by carcinogenic compounds in the plume are calculated assuming that the contaminated water is used in a house for drinking, bathing, and other household uses [Falta 2007]. The plume model currently considers the inhalation and ingestion cancer risk from water that is piped into the house from a well, but it does not consider vapor transport through the vadose zone. The calculation approach follows USEPA's method [USEPA, 1989 and Falta, 2007].

Probabilistic Modeling Approach

A deterministic modeling approach takes a single value for each parameter and gives a single prediction of the system response (Figure 3a). Typically, these single values selected for different parameters are "best case estimates" or sometimes "worst case estimates", resulting in overestimates or underestimates of results. In reality, however, the hydrogeologic, geochemical, and process parameters used in a model are either variable, uncertain, or both variable and uncertain. The deterministic model does not consider the nature of overall uncertainty in a simulation. A widely used approach for incorporating this uncertainty is probabilistic modeling (e.g., using the Monte Carlo technique), where uncertain parameters are represented by PDFs, and the result itself is also represented by a probability distribution (Figure 3b). The probabilistic modeling approach has been widely used to perform risk assessment in contaminated sites (USEPA, 1997; Hope and Stock, 1998; Slob and Pieters, 1998; Chang, 1999; USEPA, 2001; Liu et al., 2004; Li et al., 2007). However only a few models allow running Monte Carlo simulations and stochastic analysis regarding contaminant fate and transport, such as MODFLOW2000 within GMS v5.0 (<http://www.scisoft-gms.com/>) and Groundwater Vistas v4.0 (<http://www.groundwater models.com/>). PREMChlor has been developed by the linkage between the deterministic REMChlor model and the probabilistic simulation package GoldSim (<http://www.goldsim.com>). GoldSim is a probabilistic simulation software package for visualizing and conducting dynamic, probabilistic simulation to support management and decision-making in business, engineering and science [GoldSim User's Guide, 2007]. It has a great flexibility to link to other external programs and process models. GoldSim has been used in the nuclear industry for conducting performance/safety assessment calculations [Robinson et al., 2003]. GoldSim conducts the probabilistic simulation using a Monte Carlo approach. The Monte Carlo approach is the common technique for propagating the uncertainty in the input parameters of a system to the predicted results and performance. In Monte Carlo simulation, the entire system is simulated a large

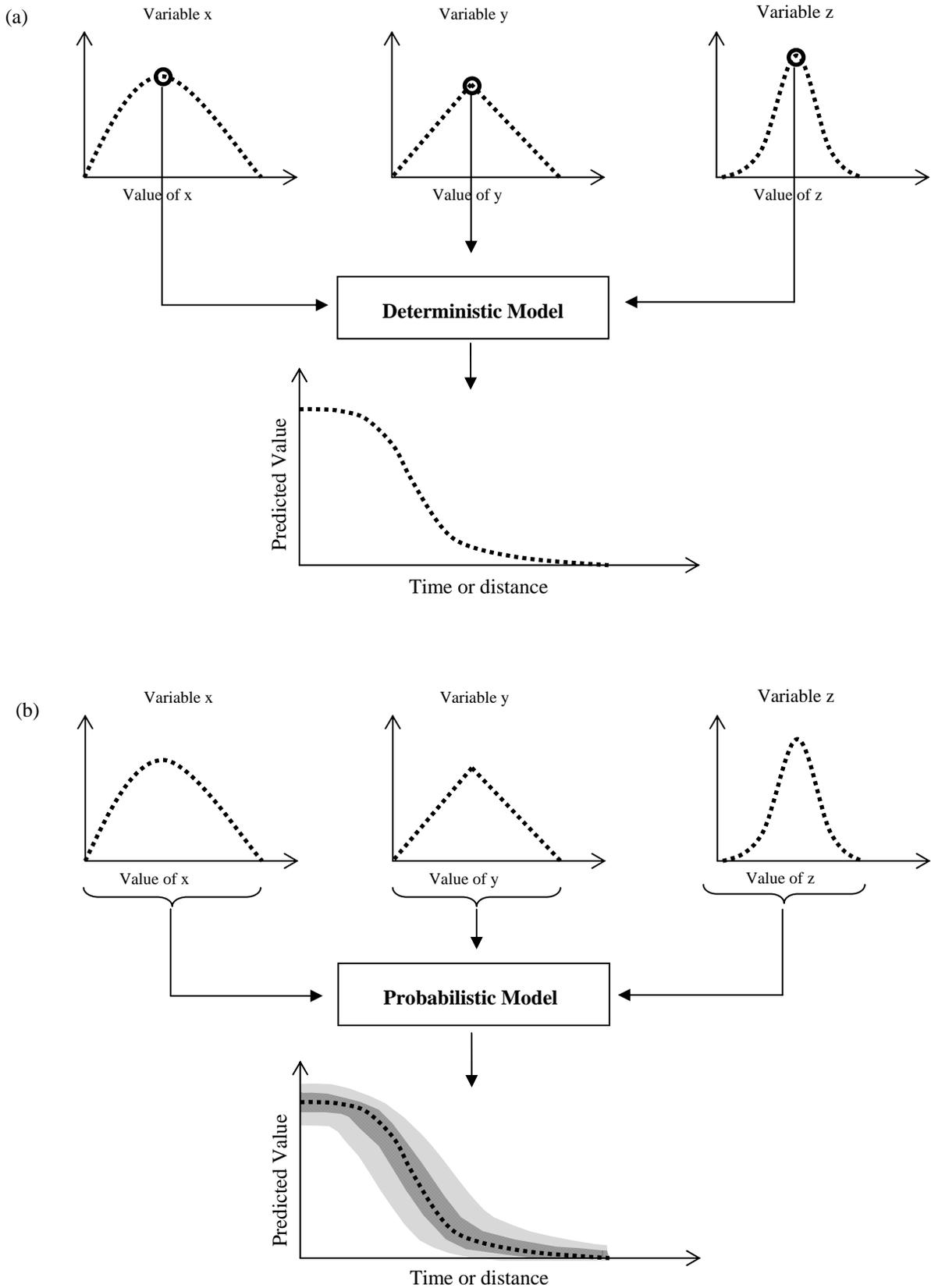


Figure 3. Illustration of deterministic (a) and probabilistic (b) modeling approaches.

number of times. Each simulation is independent and equally likely, referred to as a realization of the system. For each realization, all of the uncertain parameters are sampled from the specified distributions. The performance of the system from one realization is then computed or evaluated and the result is saved. After repeating many realizations, the results of the independent simulations are assembled into probability statistics and distributions.

A probabilistic simulation consists of hundreds or thousands of deterministic Monte Carlo realizations. As illustrated in Figure 4, during the probabilistic simulation, GoldSim is used to specify the probability distributions for all stochastic parameters and specify the Monte Carlo parameters, such as the total simulation duration, time step, and the total realization number for the probabilistic simulation. Inside the Monte Carlo loop, for each realization, GoldSim is used to sample the value for each uncertain parameter through its PDF and specify the value to each deterministic parameter and assigns the values to REMChlor. The REMChlor FORTRAN source code is called via a FORTRAN DLL application to perform the analytical calculation and calculation results are passed back to GoldSim. After all of the realizations are completed, all of the results of REMChlor calculations are stored in GoldSim and assembled into probability distributions and probability statistics.

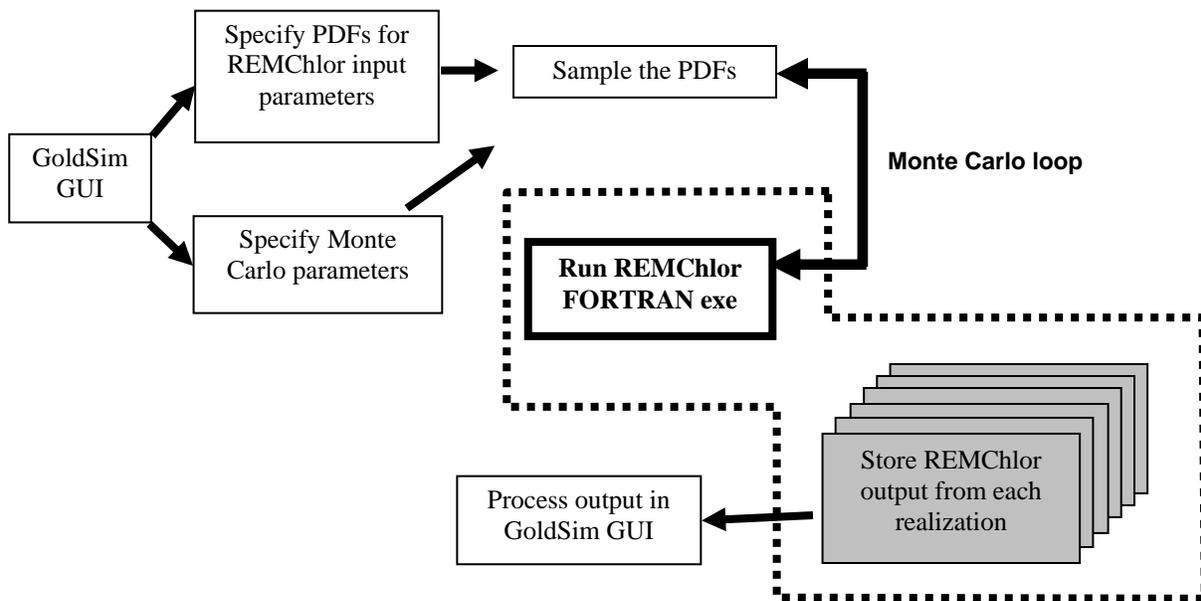


Figure 4. Flow chart of the DLL linkage during the probabilistic simulation.

PREMChlor can be run in two different modes: the probabilistic simulation mode and the deterministic simulation mode. Under the probabilistic simulation mode, model runs multiple realizations. Each realization is deterministic and uses a different probabilistic value for a stochastic parameter. Under the deterministic simulation mode, only one realization is run in which a deterministic value is used for every parameter.

PREMChlor allows two different types of input information, either deterministic or probabilistic values. Deterministic values are provided as the inputs to the model when the user knows the specific values the

model requires. When the required information is uncertain, the user provides probability distribution parameters, such as mean, standard deviation etc., as the inputs to define the distribution for a stochastic parameter.

PREMChlor Inputs and Outputs

There are 86 input parameters in PREMChlor. Among those, 18 are treated as deterministic and 68 are treated as stochastic. Deterministic parameters usually have less or no variability and can be defined in a certain way. For example, two parameters, the times when remediation starts and ends, are treated as deterministic because they are known parameters for a remediation design. Stochastic parameters are normally associated with much uncertainty. For example, groundwater Darcy velocity is treated as stochastic parameter. Stochastic input parameters are defined by distributions. During the probabilistic simulation, PREMChlor samples the different values from the distribution for each realization. In PREMChlor, distributions include the triangular distribution, normal distribution, log-normal distribution, beta distribution (Figure 5). A triangular distribution is defined by a minimum value, a most likely value and a maximum value. A normal distribution is defined by a mean and a standard deviation. A log-normal distribution is defined by a geometric mean and a geometric standard deviation. A beta distribution is defined by a minimum value, a mean, a standard deviation and a maximum value. More information about these distributions can be found in GoldSim User's Guide [2007].

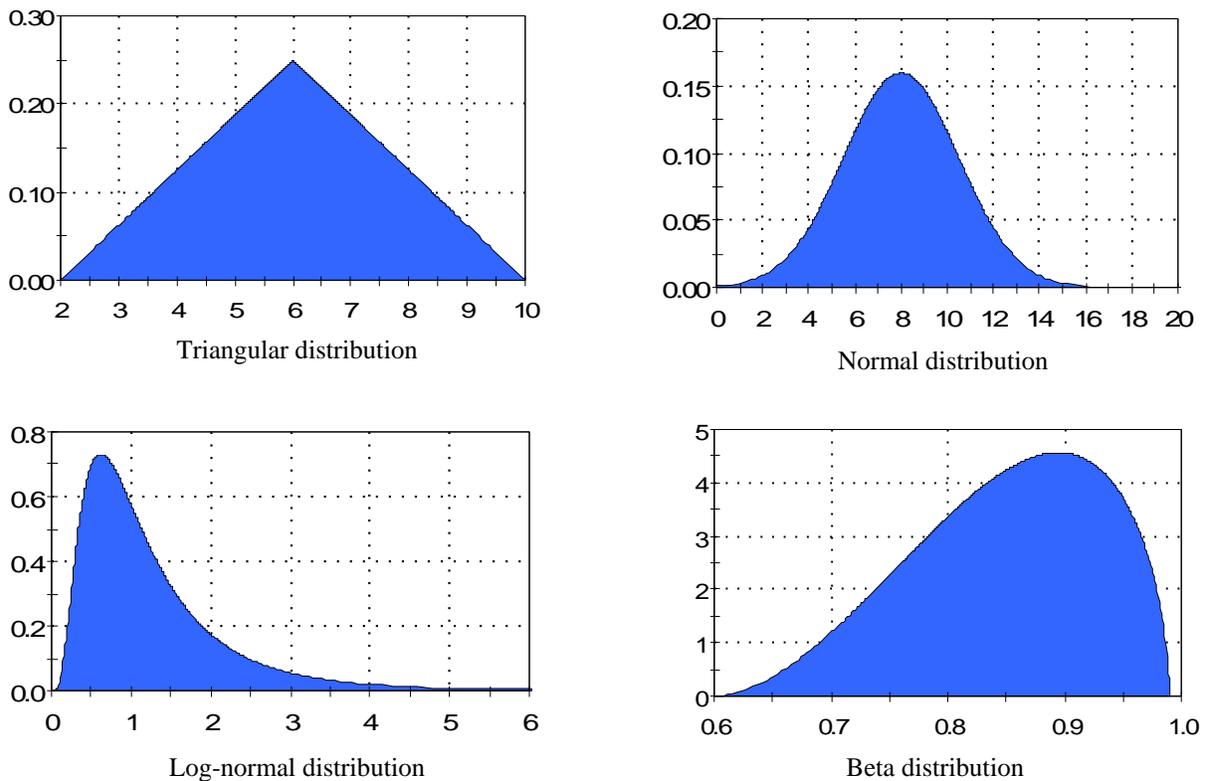


Figure 5. Distributions used for input parameters in PREMChlor.

PREMChlor provides many intermediate and final outputs. Eighteen useful final outputs can be accessed after simulation. PREMChlor considers up to four parent-daughter compounds. These results include the concentration of each component and the total concentration, the mass discharge of each component and the total mass discharge, and the cancer risk posed by each component and the total cancer risk. Contaminant concentration, mass discharge, and cancer risk are the commonly used metrics to assess the performance of the remediation. In PREMChlor, the changes of concentrations, mass discharges and cancer risks over time (time-histories) are calculated for a specified location (x,y,z). PREMChlor allows users to specify such a location by entering any x, y and z value. The final results also include the source remediation cost, the plume remediation cost, and the total remediation cost. Each output has multiple values computed from different realizations. All these values and observations are assembled into the probability statistics and the probability distribution. Probability statistics include the lower and upper bounds, and different percentiles. Lower bound (LB) and upper bound (UB) are the lowest and highest values for an output among all of the realizations, respectively. A percentile is the value of an output below which a certain percent of observations fall. The 50th percentile, also known as the median, is the value below which 50 percent of the observations may be found. Such probability statistics are useful to evaluate the remediation alternatives.

The probability statistics of an output are displayed by the time histories in the form of the probability histories. An example of the probability histories display of concentration vs. time at a location (x, y, z) during natural attenuation is shown in Figure 6. The x axis is the simulation duration time and the y axis is the concentration. The concentration shown here is the plume centerline mass concentration and the location is defined by x=100 m, y=0 m, z=0 m. The solid line is the median of the concentration over the time among all of the realizations. From the median line upward, the outline of the light dot filled area is the 75th percentile, the outline of light diagonal filled area is the 95th percentile, and the outline of dark dot filled area is the upper bound. From the median line downward, the outline of the light dot filled area is the 25th percentile, the outline of light diagonal filled area is the 5th percentile, and the outline of dark dot filled area is the lower bound. The probabilistic statistics also are displayed in tabular form (Figure 7). In this natural attenuation example, the concentration at the 30th yr has the lower bound of 49 ug/L, 5th percentile of 128 ug/L, 25th of 419 ug/L, median of 647 ug/L, 75th of 929 ug/L, 95th of 1185 ug/L, and the upper bound of 1337 ug/L.

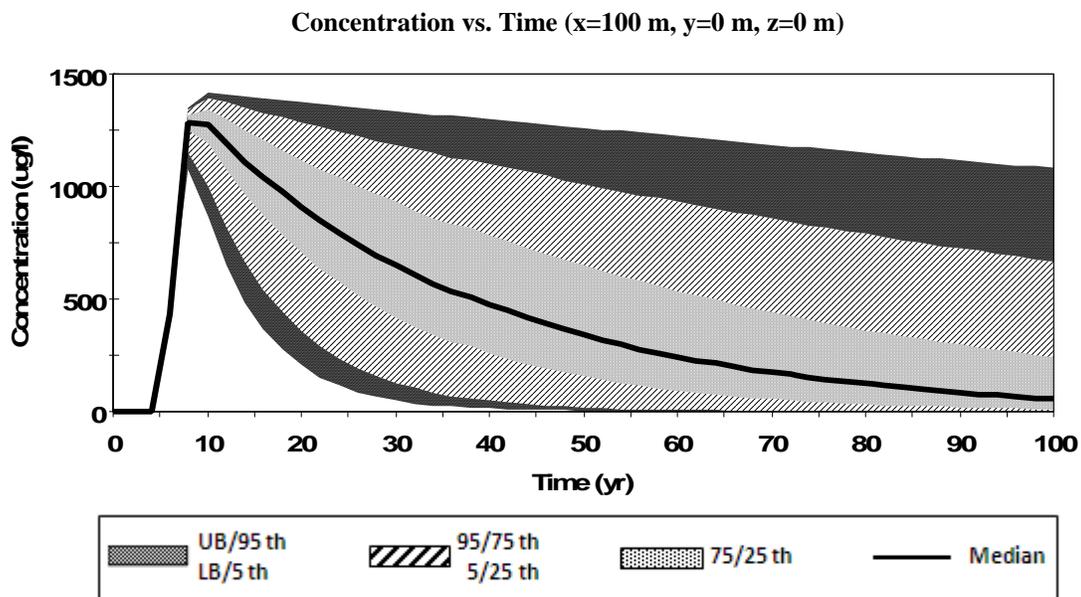


Figure 6. Probability histories of an output: Graphic view.

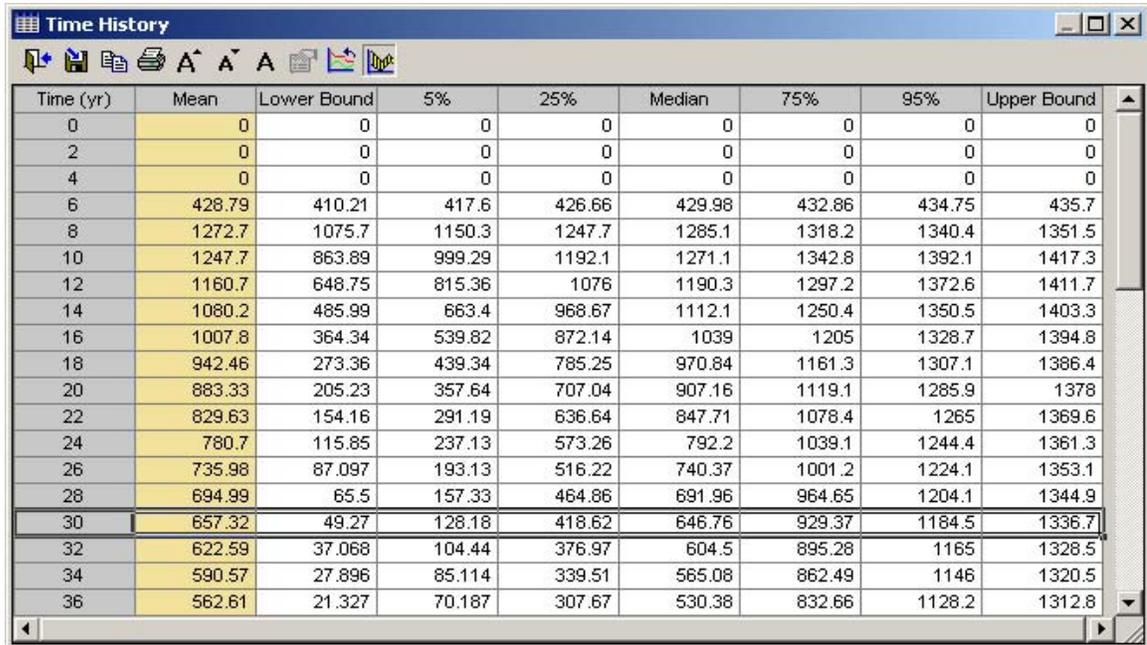


Figure 7. Probability histories of an output: Table view.

The probability distribution summary includes the distribution statistics, such as the mean, standard deviation, skewness and kurtosis, and the PDF for an output. The histogram of the PDF is generated by placing the final values of an output from all of the realizations into a discrete number of “bins”. The PDF of an output reflects the overall uncertainty posed by the uncertainties in the input parameters. An example of the probability distribution summary for an output is shown in Figure 8. The left table shows the distribution’s percentiles below which the distribution statistics are shown. The histogram on the right side is the PDF.

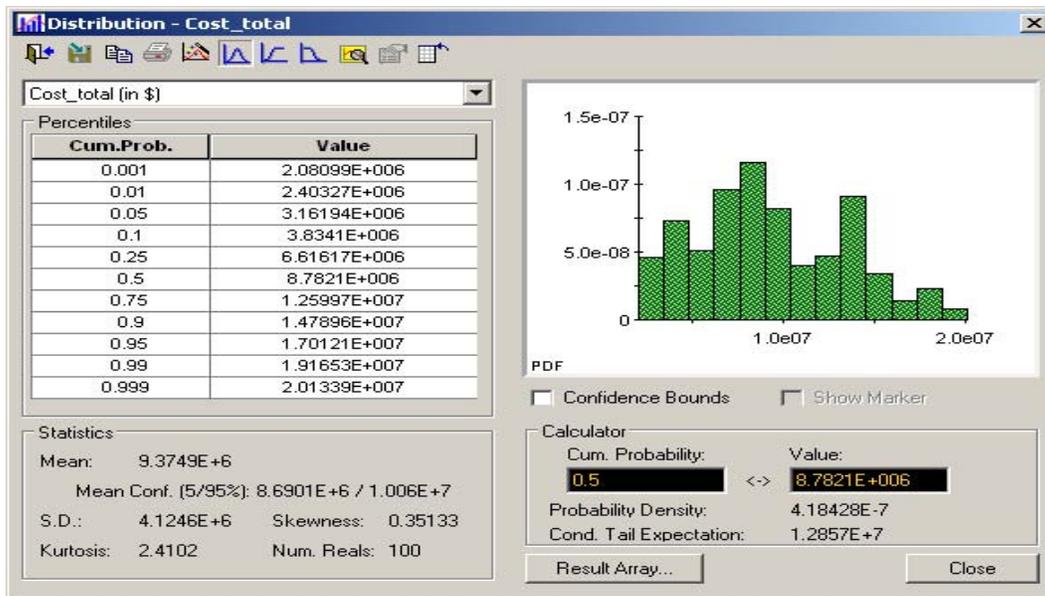


Figure 8. Probability distribution summary of an output.

Unit Cost and Remediation Efficiency

PREMChlor considers common technologies for DNAPL source removal and dissolved plume treatment. Source remediation methods are thermal treatments, surfactant/cosolvent flooding, chemical oxidation/reduction, and enhanced bioremediation. The efficiency of source remediation is represented by the fraction of mass removed. In addition, efficiency of enhanced source bioremediation has another option as it can alternately be represented by the enhanced decay rate. In PREMChlor, each remediation technology corresponds to a specific unit cost (cost per volume treated) and specific remediation efficiency. These parameters are treated as uncertain variables represented by the PDFs. The distributions and the parameters of unit costs and remediation efficiencies were interpolated based on literature resources.

McDade et al. [2005] presented a comprehensive cost analysis of DNAPL source depletion technologies. This study reviewed more than 60 sites and performed the cost analysis for 36 field sites across the United States that had sufficient size, cost, and performance data to evaluate. The unit costs were reported for enhanced bioremediation (11 sites), chemical oxidation (13 sites), surfactant/cosolvent flooding (6 sites), and thermal treatment (6 sites). The reported statistics were used to determine the distribution function of the unit cost. Different types of distribution functions available in GoldSim were tested to fit the reported values. It was found that the beta distribution fit the reported value best. In PREMChlor, the mean, minimum (min) and maximum (max) values of the interpolated beta distribution are the reported median, minimum and maximum values [McDade et al., 2005], respectively. The standard deviation of the beta distribution was adjusted by matching the interpolated PDF with the histogram generated based on the reported unit costs.

McGuire et al. [2006] presented a performance evaluation of DNAPL source remediation technologies at 59 chlorinated solvent contaminated sites. Data were collected and compiled from similar sources as in McDade et al. [2005]. The concentration reduction percentages of parent chlorinated volatile organic compound (CVOC) compound were reported for enhanced bioremediation (26 sites), chemical oxidation (23 sites), thermal treatment (6 sites) and surfactant/cosolvent flooding (4 sites). Since the mass reduction/removal data were not reported, we assumed the value of the exponent of Equation (2), Γ , in order to estimate the mass reduction/removal from concentration reduction percentage. By assuming Γ is equal to one, the ratio of mass reduction to concentration reduction is 1:1. In PREMChlor, only the parent CVOC compound was considered in the source zone. Therefore the reported concentration reduction percentages for parent CVOC compound [McGuire et al., 2006] were used as the source mass removal percentages in PREMChlor.

The reported statistics of the concentration reduction percentages for parent CVOC compound were used to determine the distribution function for the source removal efficiency. Different types of distribution functions available in GoldSim were tested to fit the reported values. It was found that the beta distribution fit the reported value best. In PREMChlor, the mean, minimum (min) and maximum (max) values of the interpolated beta distribution are the reported median, minimum and maximum values [McGuire et al., 2006], respectively. The standard deviation of the beta distribution was adjusted by matching the interpolated PDF with the histogram generated based on the reported values. Due to lack of information, the enhanced decay rate, which is another option to represent the remediation efficiency of enhanced bioremediation, is assumed to have a triangular distribution.

The plume treatment methods mainly are enhanced biodegradation. PREMChlor can also simulate permeable reactive barriers (PRBs). Plume PRB treatment can be modeled by assigning a very high first-order degradation rate for contaminant in a narrow reaction zone. The application of PREMChlor to a plume PRB treatment can be found in Liang [2009]. Due to the lack of information, the unit cost and degradation rate for plume treatment are assumed to have triangular distributions.

More information about unit cost and remediation efficiency can be found in Liang [2009].

Calculation of Remediation Cost

Remediation costs of source removal and plume treatment are included in the probabilistic simulation model. Remediation cost analysis is conducted outside the FORTRAN DLL link. The total remediation cost consists of the source remediation cost and the plume remediation cost. For source remediation, the probabilistic model considers a one-time capital cost, which is the product of the unit cost of the source remediation and the volume of the treated source zone. For plume remediation, cost includes a one-time capital cost and a total operation & management (O&M) cost in present net value (NPV) for a certain remediation period. The probabilistic model allows two plume remediation zones. For each remediation zone, the one-time capital cost is the product of the unit cost of the plume remediation and the volume of the remediation zone. The calculation of the total O&M cost in NPV is based on the formula in ITRC [2006]:

$$\begin{aligned} TotalNPV &= \sum_1^n \frac{AnnualCostinYeartwithInflation}{(1 + InterestRate)^{t-1}} = \sum_1^n \frac{AnnualCost(1 + i)^{t-1}}{(1 + r)^{t-1}} \\ &= AnnualCost \sum_1^n \frac{(1 + i)^{t-1}}{(1 + r)^{t-1}} = AnnualCost \frac{1 - \left(\frac{1 + i}{1 + r}\right)^n}{1 - \frac{1 + i}{1 + r}} \end{aligned} \quad (11)$$

where AnnualCost is the current annual cost and it is assumed to be constant, i is the average annual inflation rate, r is the average annual interest rate, t is the year, and n is the total period of time for plume operation and management. In Equation (11), the numerator accounts for the total O&M cost in current dollar considering inflation, and the denominator accounts for the interest rate. This formula accounts for the inflation and interest factors at the beginning of the second year.

Graphical User Interface

Main Interface

Once the model is opened, the main interface with the **Run Controller** will appear. This main interface shows the overall layout of the model. The left-hand side of the main interface has six tabs to direct the user to other interfaces. On the right side, the user can specify the observation location and view the simulation results. The various model interfaces are described in the following.

The **Run Controller** allows the user to run, monitor, pause and step through the simulation. The **Reset** tab on the GoldSim **Run Controller** clears all of the results and allows the user to edit model settings and start a new simulation. The **Run Controller** also allows the user to jump to any interface. To do this, click **Go** tab and select the desired interface. For more information about the **Run Controller**, see the GoldSim Player Help file. To access the GoldSim Player Help file, click the **Explore Model** tab on the main interface, and then click the **Help** menu on the top tool bar.

Simulation Settings

The **Simulation Settings** tab directs the user to the interface where the user can specify the simulation duration time and the Monte Carlo settings. Under the **Time** tab, the **Basic Time Settings** allows the user to choose either an elapsed time simulation or a date-time simulation. In both cases, the number of time steps needs to be specified (**#Steps** in the **Time Phase Settings** portion of the dialog). For more information about the Simulation Settings, see the Player Help file. To access the GoldSim Player Help file, click the **Explore Model** tab on the main interface, and then click the **Help** menu on the top tool bar.

Explore Model

The **Explore Model** tab directs the user to the model structure. The user can explore how the model is set up and view the details of the model. For more information about the model structure, see the work by Liang [2009].

Source Zone Parameters

The **Source Zone Parameters** tab directs the user to the interface that allows the user to specify source zone parameters, such as the initial concentration, initial mass, power function exponent Gamma, and source dimensions.

Transport Parameters

The **Transport Parameters** tab directs the user to the interface that allows the user to specify transport parameters, such as darcy velocity, porosity, retardation factor and scale-dependent dispersivity parameters.

Source Remediation

The **Source Remediation** tab directs the user to the interface that allows the user to specify source zone remediation parameters for different source depletion technologies.

Plume Decay Rates

The **Plume Decay Rates** tab directs the user to the interfaces that allow the user to set up all of the chlorinated solvent plume parameters, such as the plume decay rates, yield coefficients and cancer risk slope factors for all components. The user also can specify the plume treatment parameters, such as treatment rates, treatment zone dimensions and costs. More details about plume parameter settings are described in the **Basic Operation** section.

Viewing Model Output

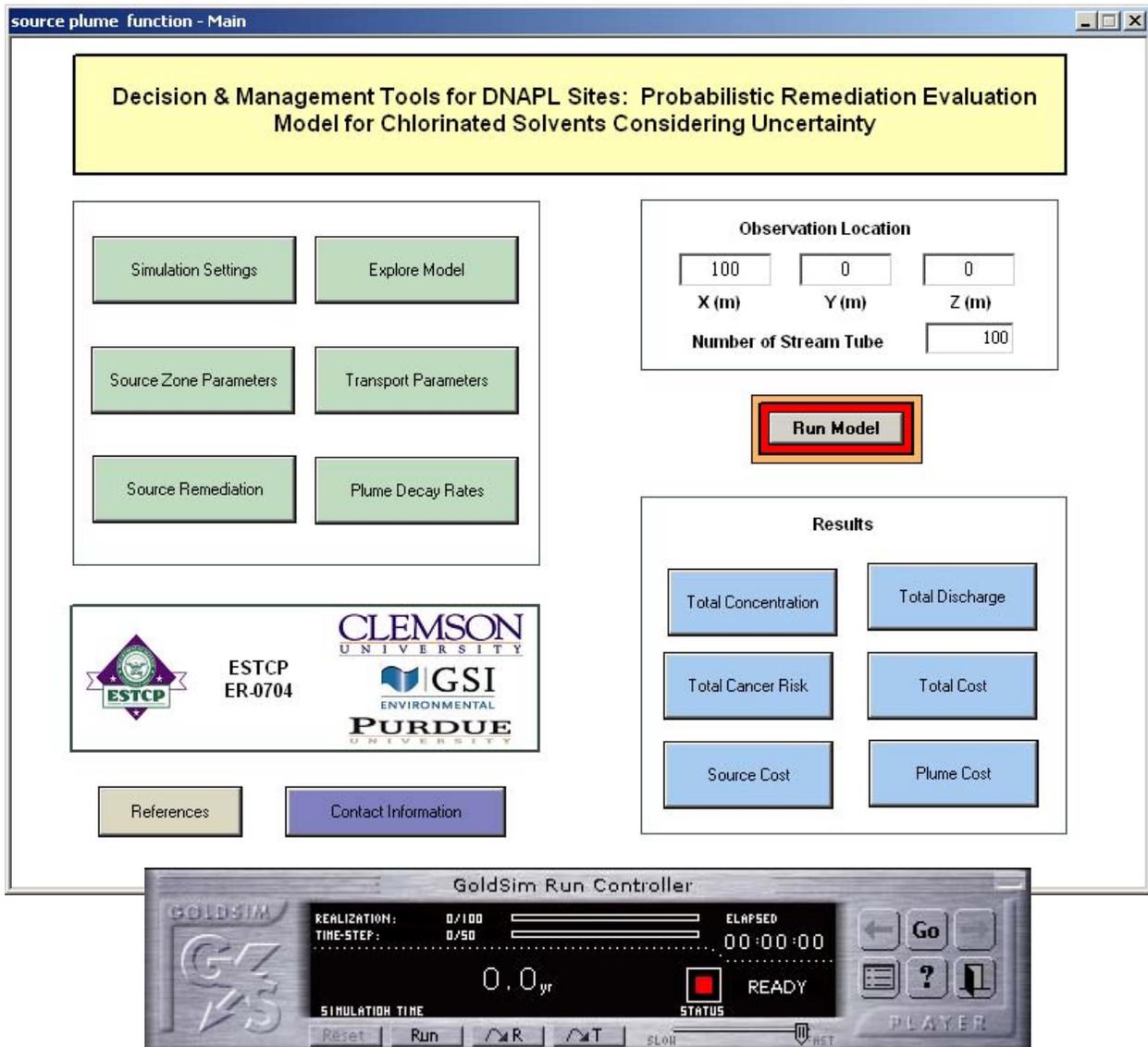
View Graphical or tabular Output

Major model output can be viewed by clicking the result tabs on the main interface. The default output for **Total Concentration**, **Total Mass Discharge** or **Total Risk Factor** versus time for any location is the chart view. The default output for **Total Cost**, **Source Cost**, or **Plume Cost** is also the chart view. The user, however, can switch the output format between the chart view and table view under the output view window for both cases.

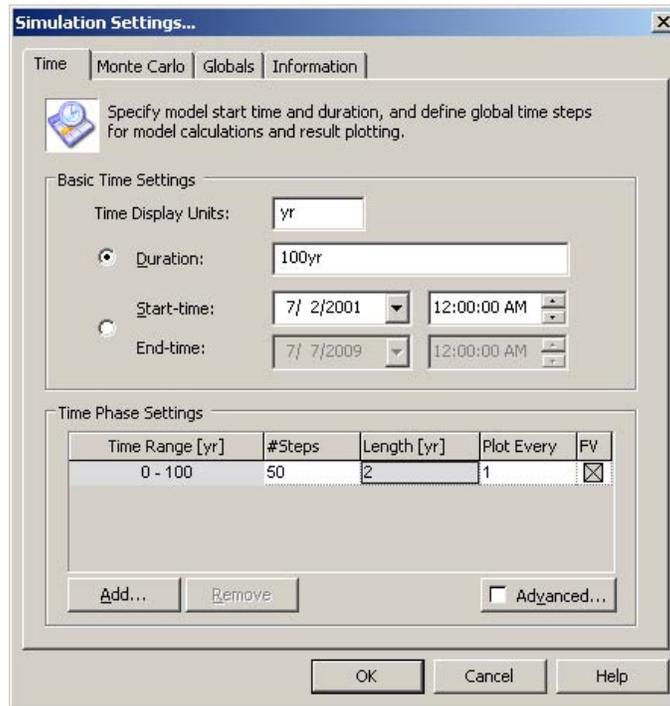
Basic Operation

The following simple operation illustrates the most basic functions and capabilities of the graphical user interface for PREMChlor.

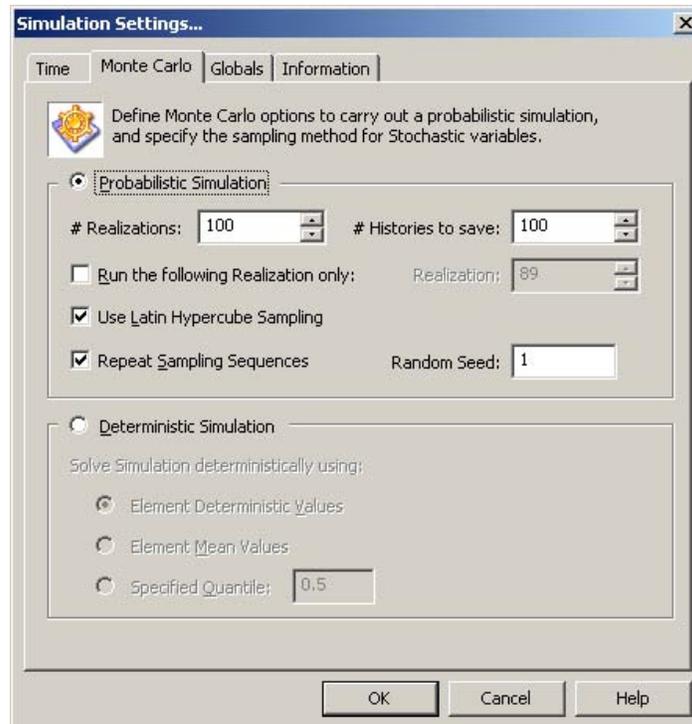
1. Double-click the model sample file (Sample.gsp) to start the application. The following screen will appear:



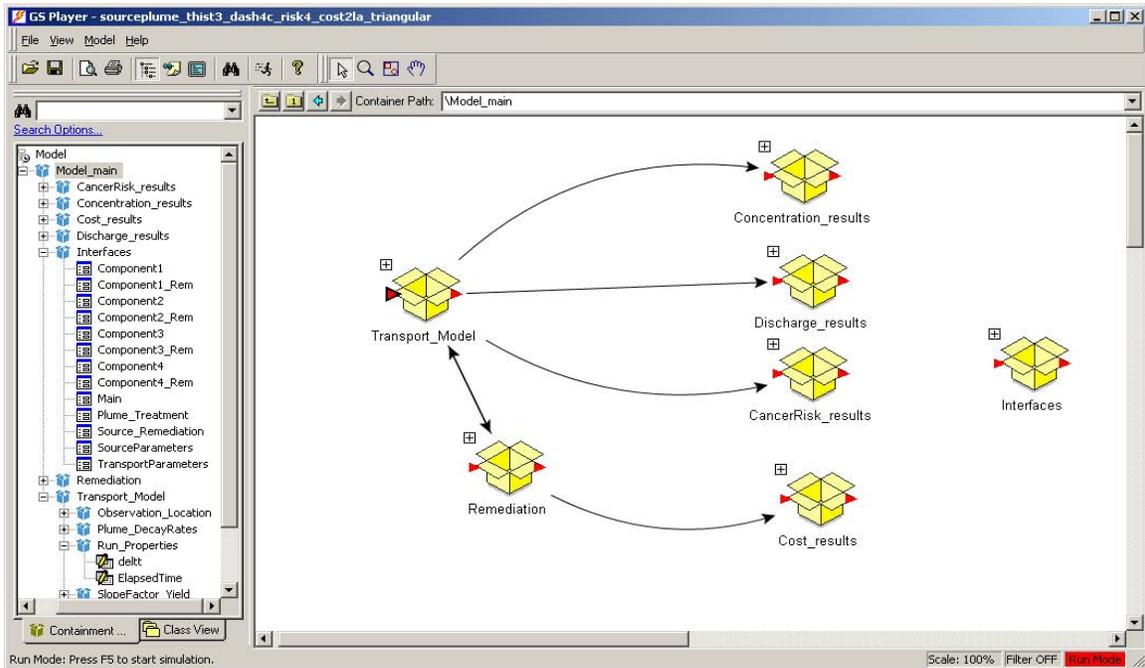
- Click on the **Simulation Settings** tab and the following screen will appear. This **Time** setting screen shows the **Basic Time Settings**, including simulation duration and the **Time Phase Settings**, including time steps:



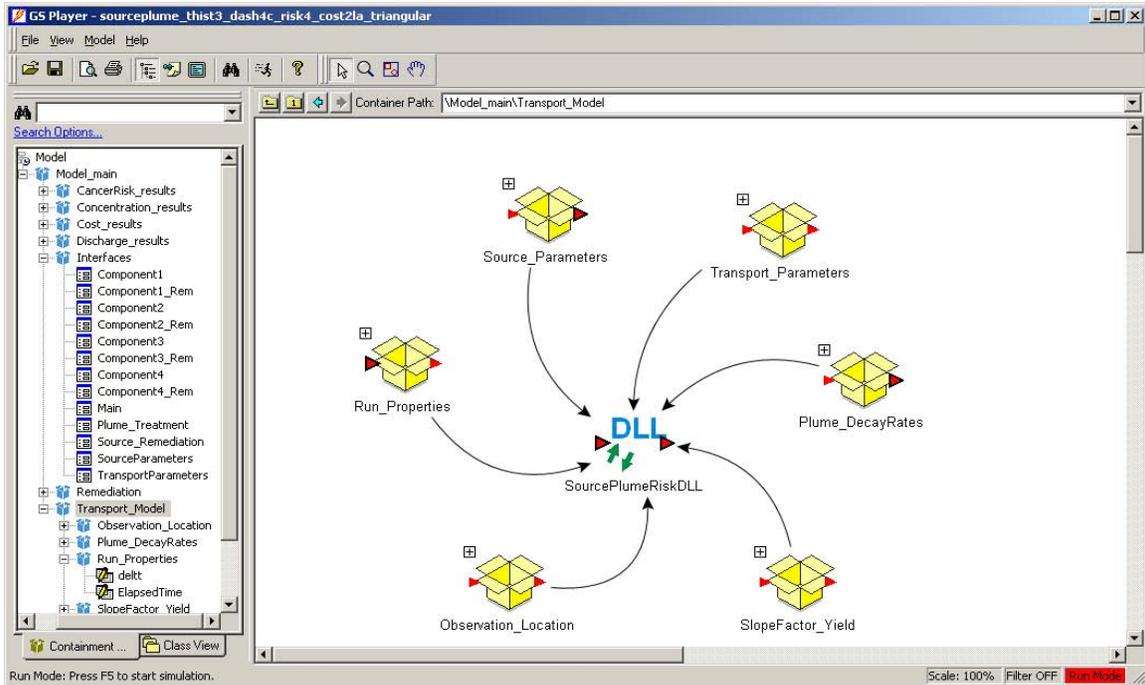
Click the **Monte Carlo** tab to view the Monte Carlo options. Click **OK** to go back to the main interface.



- Click on the **Explore Model** tab and the following screen showing top level of the model structure will appear:



This model is organized in a top-down manner. The level of detail increases as the user “push down” into the container hierarchy. For example, click the plus sign on the top left side of the **Transport_Model** container, the structure of the transport model will appear as shown below. The user may explore the every detail of the model as navigating through the model hierarchy. For more details about model structure, see Liang [2009]. To go back to the main interface anytime, click the **Go** tab on the Run Controller and select **Main**.



- Click on the **Source Zone Parameters** tab and the following source zone parameters screen will appear:

Source Parameters

Initial Concentration (g/L)

0.005 0.01 0.02

Min Likely Max

If checked, use Deterministic Value 0.01

Initial Mass (kg)

500 1620 3000

Min Likely Max

If checked, use Deterministic Value 1620

Power Function Exponent

1 1.41

Mean Stdv

If checked, use Deterministic Value 1

Source Dimensions

Source Width (m)

3 10 30

Min Likely Max

If checked, use Deterministic Value 10

Source Depth (m)

0.5 3 10

Min Likely Max

If checked, use Deterministic Value 3

Source Length (m)

3 10 30

Min Likely Max

If checked, use Deterministic Value 10

Main Interface

To go back to the main interface, click the **Main Interface** tab. To jump to another interface, click the **Go** tab on the Run Controller and select an interface.

- Click on the **Transport Parameters** tab and the transport parameters screen will appear:

Transport Parameters

Darcy Velocity (m/yr)		Porosity			Retardation Factor		
Mean	Stdv	Min	Likely	Max	Min	Likely	Max
20	2	0.2	0.3333	0.4	0.01	2	20
<input checked="" type="checkbox"/> If checked, use Deterministic Value	20	<input checked="" type="checkbox"/> If checked, use Deterministic Value	0.3333		<input checked="" type="checkbox"/> If checked, use Deterministic Value	2	

Scale-dependent Dispersivity Parameters

	Min	Likely	Max	If checked, use Deterministic Value
Longitudinal	0.001	0.01	0.1	<input checked="" type="checkbox"/> 0.01
Transverse	0.0001	0.001	0.01	<input checked="" type="checkbox"/> 0.001
Vertical	1e-5	0.0001	0.001	<input checked="" type="checkbox"/> 0.0001

Main Interface

To go back to the main interface, click the **Main Interface** tab. To jump to another interface, click the **Go** tab on the Run Controller and select an interface.

6. Click on the **Source Remediation** tab and the source zone remediation parameters screen will appear:

Source Remediation

Remediation Time (yr) Start Time: 30 End Time: 31

Aqueous Phase Source Decay (1/yr) Min: 0 Likely: 0.01 Max: 0.1 If checked, use Deterministic Value: 0.01

	Percent Removed				If checked, use Deterministic Value	Unit Cost (\$/cubic meter)				If checked, use Deterministic Value
	Mean	Stdv	Min	Max		Mean	Stdv	Min	Max	
<input checked="" type="checkbox"/> Thermal Methods	0.97	0.025	0.56	1	<input type="checkbox"/> 0.97	115.1	50	41.85	392.39	<input checked="" type="checkbox"/> 115.1
<input type="checkbox"/> Surfactant Flooding	0.95	0.01	0.91	1	<input type="checkbox"/> 0.95	503.56	375	86.32	7193.7	<input type="checkbox"/> 503.56
<input type="checkbox"/> Chemical Oxidation/Reduction	0.88	0.05	0	1	<input type="checkbox"/> 0.88	163.49	65	26.16	667.52	<input type="checkbox"/> 163.49
<input type="checkbox"/> Bioremediation	0.95	0.02	0.29	1	<input type="checkbox"/> 0.95	37.93	25	2.62	294.29	<input type="checkbox"/> 37.93
<input type="checkbox"/> If checked, use enhanced aqueous phase decay rate for remediation efficiency (1/yr)		0.8	0.6	0.95	<input type="checkbox"/> 0.8					
<input type="checkbox"/> Source Containment										
t_f	0.8	0.02	0.6	0.95	<input type="checkbox"/> 0.8					
n	0.8	0.02	0.6	0.95	<input type="checkbox"/> 0.8					
Q_{in}	0.8	0.02	0.6	0.95	<input type="checkbox"/> 0.8					

Main Interface

To go back to the main interface, click the **Main Interface** tab. To jump to another interface, click the **Go** tab on the Run Controller and select an interface.

7. Click on the **Plume Decay Rates** tab and the following screen will appear. This screen shows the plume decay rates and the cancer risk slope factors of the first component:

Component Name: 1

Time, Years	Period	Zone 1					Zone 2					Zone 3				
		Decay Rate (1,3)			If checked, use Deterministic Value		Decay Rate (2,3)			If checked, use Deterministic Value		Decay Rate (3,3)			If checked, use Deterministic Value	
tplume 2 → 50	Period 3	0.8	1.1	2.4	<input checked="" type="checkbox"/>	1.1	0.8	1.1	2.4	<input checked="" type="checkbox"/>	1.1	0.8	1.1	2.4	<input checked="" type="checkbox"/>	1.1
Time, Years	Period 2	Treatment Zone					Treatment Zone					Decay Rate (3,2)				
	tplume 1 → 30	Treatment Rate					Treatment Rate					0.8	1.1	2.4	<input checked="" type="checkbox"/>	1.1
	Period 1	Decay Rate (1,1)			If checked, use Deterministic Value		Decay Rate (2,1)			If checked, use Deterministic Value		Decay Rate (3,1)			If checked, use Deterministic Value	
		0.8	1.1	2.4	<input checked="" type="checkbox"/>	1.1	0.8	1.1	2.4	<input checked="" type="checkbox"/>	1.1	0.8	1.1	2.4	<input checked="" type="checkbox"/>	1.1
		Min	Likely	Max			Min	Likely	Max			Min	Likely	Max		

× 1 400 × 2 700

Distance From Source, Meters

Component 1
Component 2
Component 3
Component 4

Cancer Risk Slope Factor

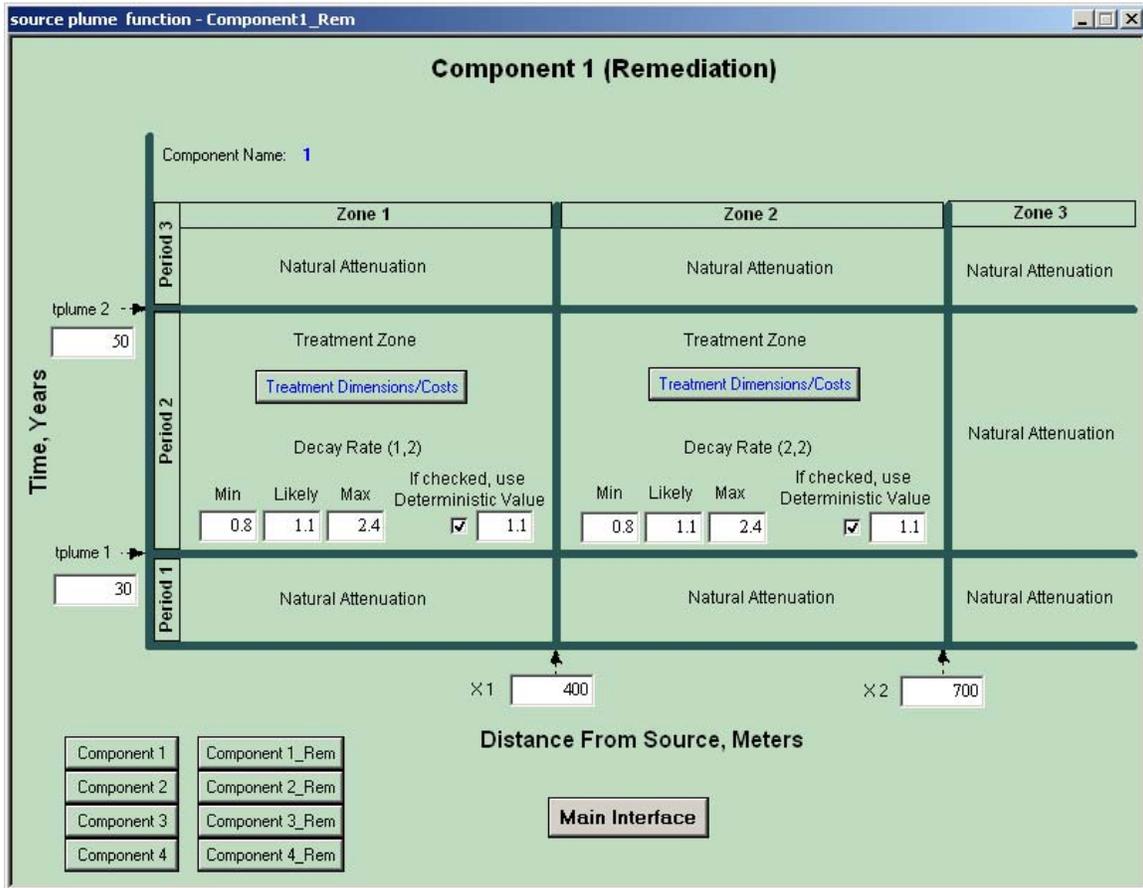
Oral: 0.1 (Min), 0.54 (Most), 0.9 (Max) 0.54 (Deterministic Value)

Inhalation: 0.001 (Min), 0.021 (Most), 0.05 (Max) 0.021 (Deterministic Value)

Main Interface

To access the other component, click the **Component #** tab. To go back to the main interface, click the **Main Interface** tab.

8. Click on the **Treatment Rate** tab on the **Component 1** interface and the following screen will appear. This screen shows the plume decay rates of the first component in two remediation zones:



To go to the other component for the natural decay rates, click the **Component #** tab. To go to the other component for the remediation degradation rates, click the **Component #_Rem** tab. To go back to the main interface, click the **Main Interface** tab.

9. Click on the **Treatment Dimensions/Costs** tab and the following **Plume Treatment** screen will appear:

Plume Treatment

Time, Years	Period	Zone 1	Zone 2	Zone 3
		Period 3	Natural Attenuation	Natural Attenuation
50 (tplume 2)	Period 2	Treatment Zone Treatment Width (m): 5 Treatment Depth (m): 5 Unit Cost (\$/cubic meter): Min: 1, Likely: 10, Max: 100, Deterministic Value: 10 (checkbox) x1: 400	Treatment Zone Treatment Width (m): 50 Treatment Depth (m): 5 Unit Cost (\$/cubic meter): Min: 1, Likely: 10, Max: 100, Deterministic Value: 10 (checkbox) x2: 700	Natural Attenuation
30 (tplume 1)	Period 1	Natural Attenuation	Natural Attenuation	Natural Attenuation

Distance From Source, Meters

Present Annual O&M Cost (\$):
 Min: 1000, Likely: 100000, Max: 1e6, Deterministic Value: 180000 (checkbox)

Treatment Period (tplume2-tplume1, yr): 20
 Inflation Rate (%): 4
 Interest Rate (%): 6

[Treatment Rate](#) [Main Interface](#)

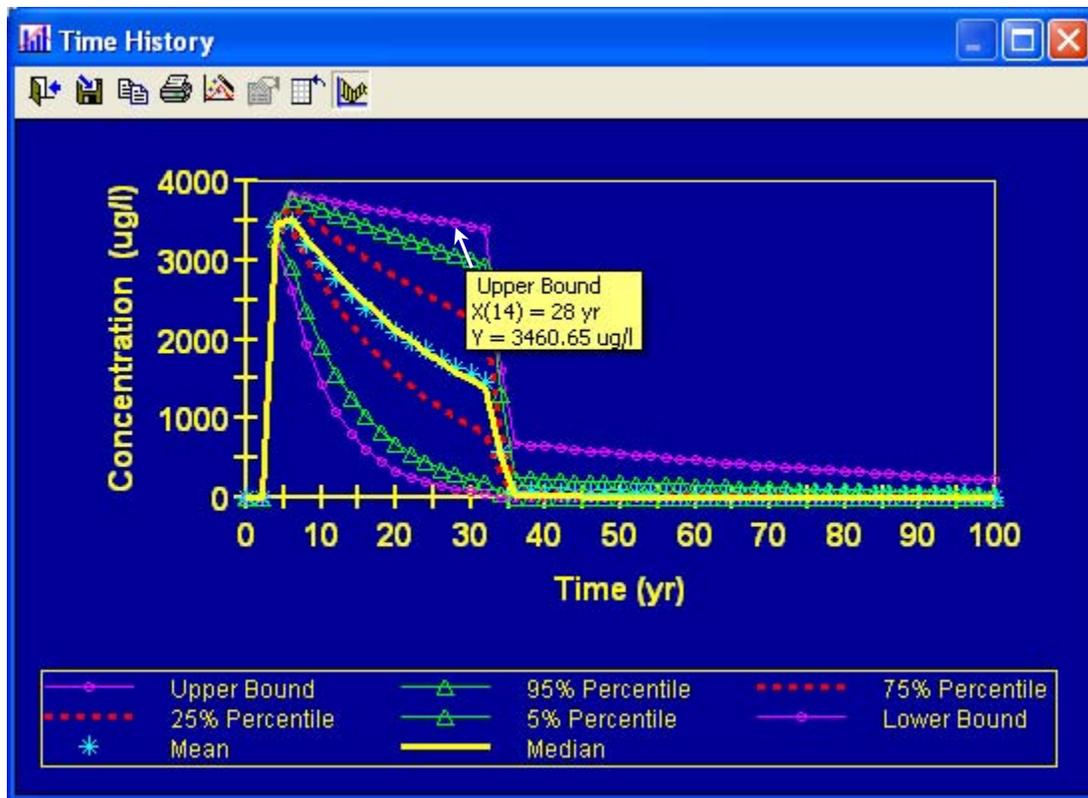
To go back to the previous screen, click the **Treatment Rate** tab. To go back to the main interface, click the **Main Interface** tab.

Similar operations (steps 7, 8 and 9) for other components.

10. The parameters are set to run the illustration problem. Move the mouse over an input field and a simple explanation of the input will pop up. To run the simulation, click **Run Model** tab or click the **Run** tab on the Run Controller. The Run Controller will show the simulation is running.



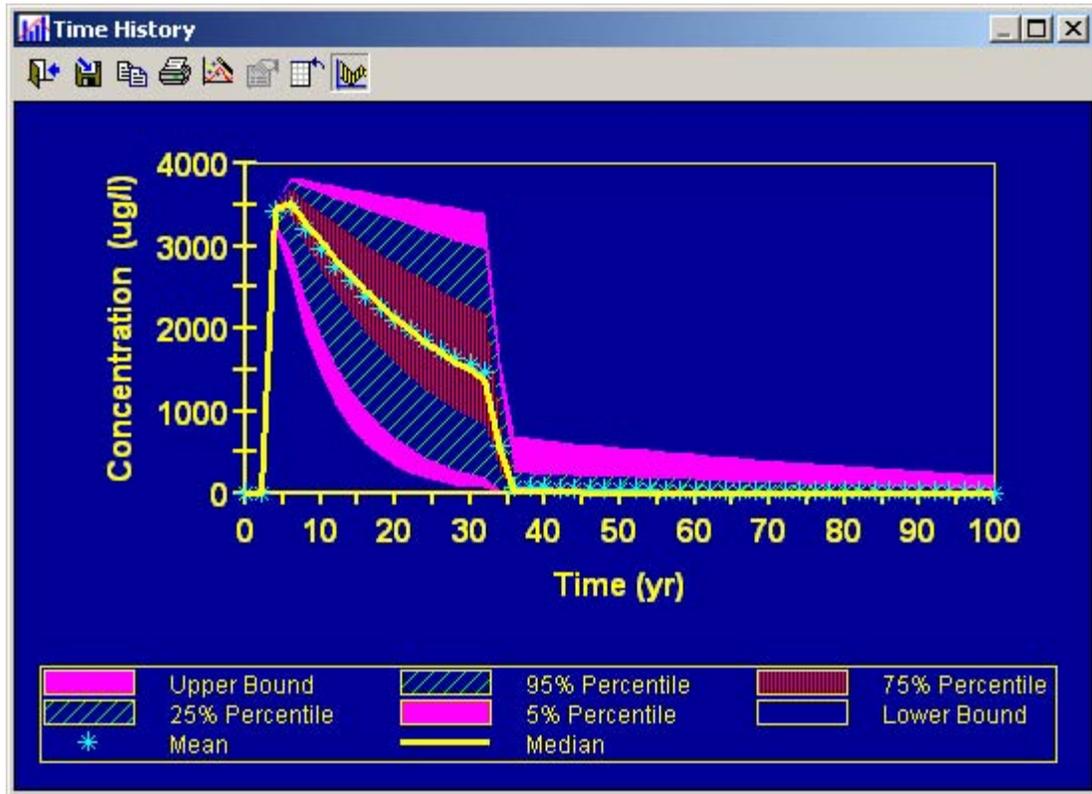
11. After finishing of the run, a small window with the message of “**Simulation Complete!**” will show up. Click **OK** and the simulation results are ready to be viewed now. From the main interface, click **Total Concentration** tab and the following graphical output of the probability history will appear:



This probability history shows the statistics of the results, such as the mean, median, lower/upper bounds, and different percentiles. A percentile is the value of a variable below which a certain percent of observations fall. The 50% percentile (median) is the value below which 50 percent of the observations may be found. From the top to the bottom, the statistics are the upper bound (purple circles), 95% percentile (green triangles), 75% percentile (red dash line), median (yellow solid line), mean (light blue stars), 25% percentile (red dash line), 5% percentile (green triangles), and the lower bound (purple circles), respectively.

Put the cursor at a percentile curve on the graph, a message box will appear and show the exact value for that percentile as the Y value. The message box also shows the X value.

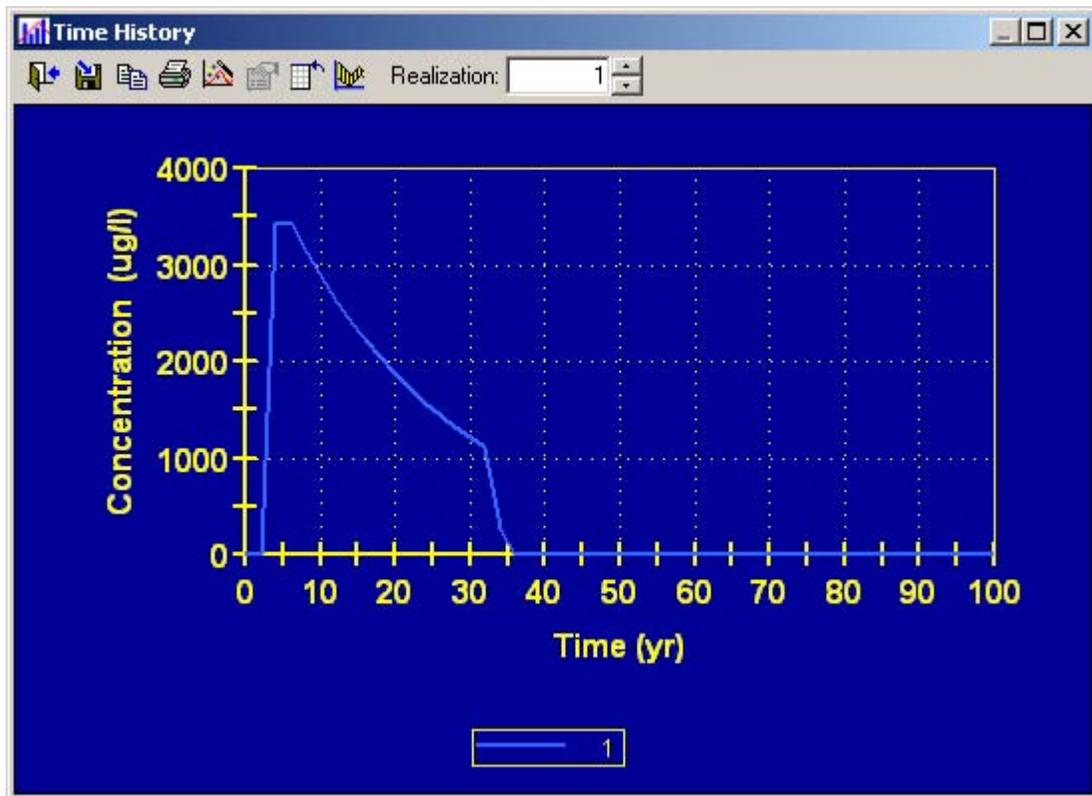
12. The probabilistic statistics can be viewed in another way. Right click the chart window and select **Show as Areas** and the following screen will appear:



From the top to the bottom, the upper outline of the purple area is the upper bound, the upper outline of blue diagonal filled area is the 95% percentile, the upper outline of the red diagonal filled area is the 75% percentile, the yellow solid line is the median, light blue stars are the mean, the bottom outline of the red diagonal filled area is the 25% percentile, the bottom outline of blue diagonal filled area is the 5% percentile, and the bottom outline of the purple area is the lower bound.

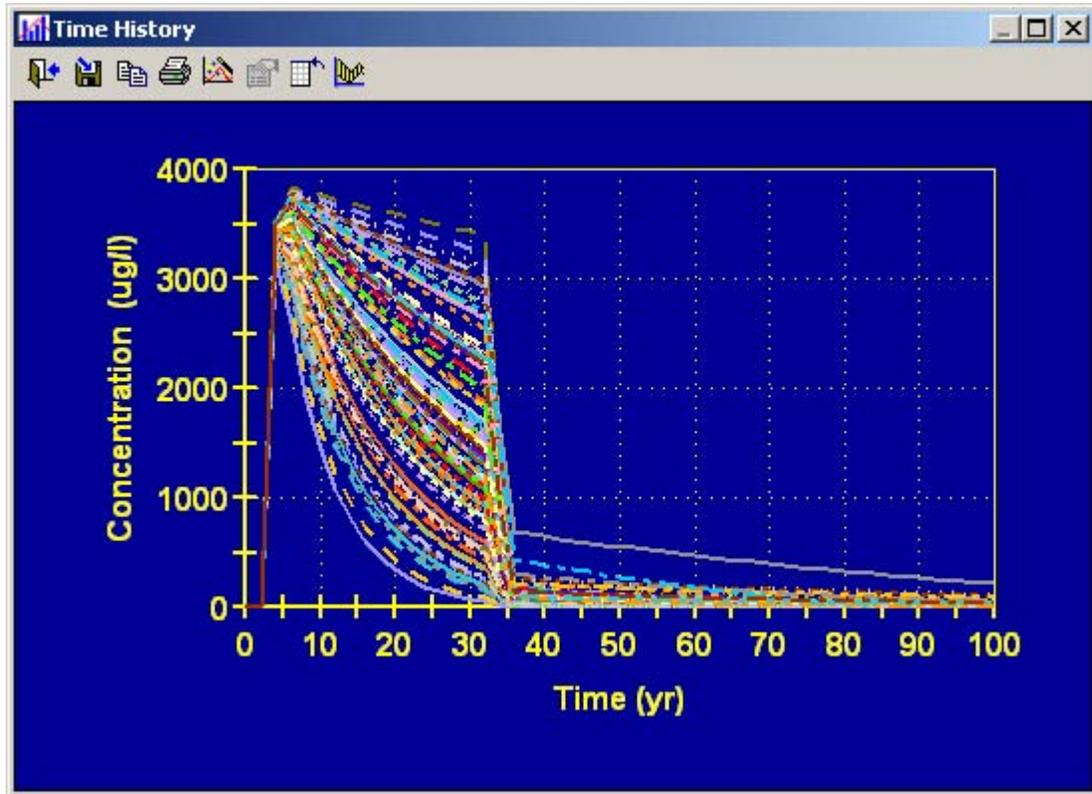
Put the cursor at somewhere on the graph, a message box will appear and show the percentile range in which the Y value at this point falls. The message box also shows the X value and the Y value of the upper limit of that range.

13. Probabilistic output could also be displayed as individual realizations (equivalent to a deterministic simulation result). To do this, right click on the above chart window, unselect **Probability Histories**, and the following single realization screen will appear:



This plot shows the output for a single realization. To view the other single realizations, change the number in the **Realization** field. Put the cursor at somewhere on the curve, a message box will appear and show the realization number, X value and the exact corresponding Y value at that point.

14. Probabilistic output could also be displayed as the results for all realizations. To do this, right click on the single realization chart window, select **Show All Realizations** and a legend window will appear. Then right click on the legend window and select **Hide**, the following screen showing all realizations will appear:



This graph shows the outputs for all realizations. Each curve represents the output of the each single realization. Put the cursor at somewhere on the curves, a message box will appear and show the realization number, X value and the exact corresponding Y value at that point.

15. Click on **Table View** from the top toolbar and the following tabular output screen will appear. The columns correspond to the realizations.

The screenshot shows a window titled "Time History" with a toolbar containing icons for file operations and text formatting. The main area is a table with 8 columns: "Time (yr)", "1", "2", "3", "4", "5", "6", and "7". The rows represent time steps from 0 to 72 in increments of 2. The data values decrease over time, with some values in later rows appearing in scientific notation.

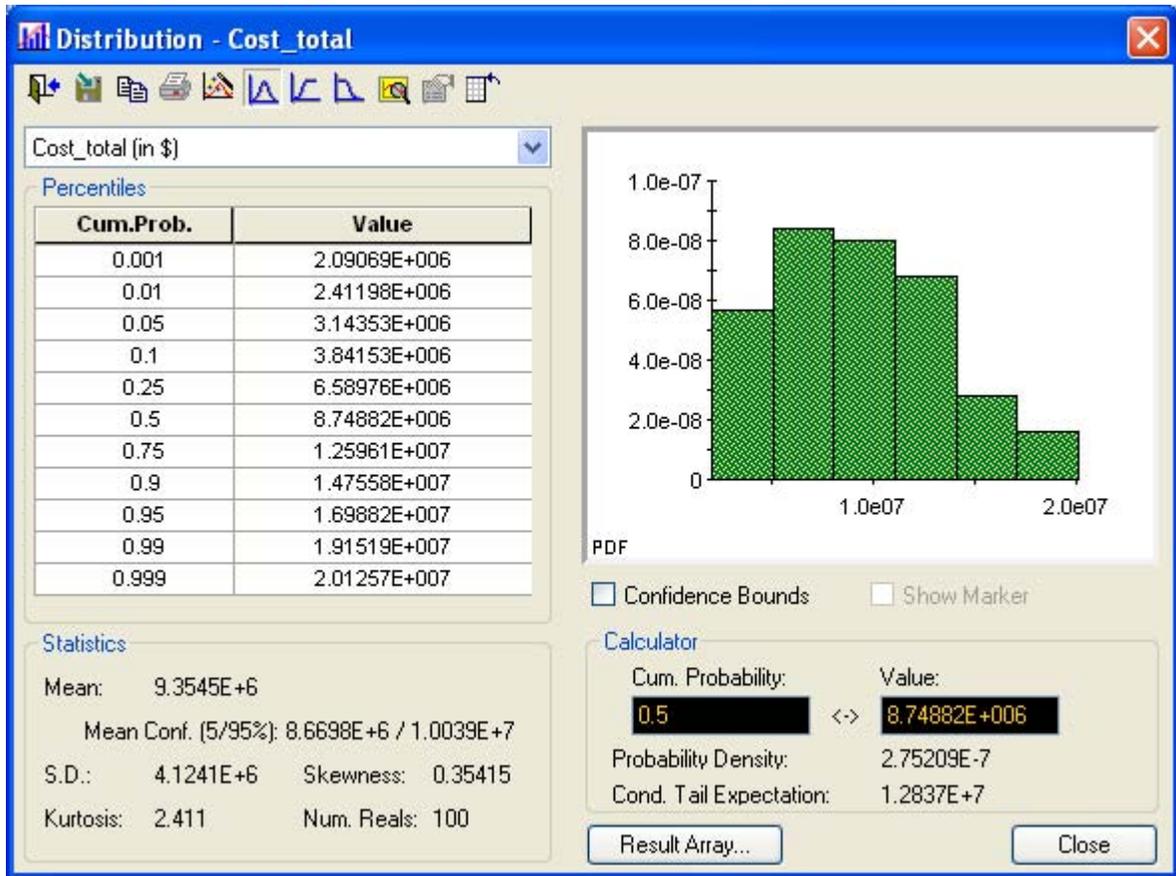
Time (yr)	1	2	3	4	5	6	7
0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0
4	3421.3	3419.5	3437.9	3398.7	3160	3366	3438.1
6	3444.1	3438.1	3502.6	3362.9	2605	3251.6	3503.2
8	3152.2	3143	3245.4	3020.3	1935.2	2849	3246.4
10	2885.3	2873.7	3006.3	2710.6	1440.3	2496.1	3007.8
12	2642.3	2628.8	2785.3	2431.8	1074.2	2187.5	2787.1
14	2420.8	2406.1	2580.8	2180.9	802.5	1917.7	2582.9
16	2218.8	2203.3	2391.7	1955.2	600.35	1681.6	2394.1
18	2034.5	2018.6	2216.7	1752.1	449.63	1475.1	2219.5
20	1866.3	1850.1	2054.8	1569.5	337.07	1294.2	2057.8
22	1712.6	1696.5	1905	1405.3	252.89	1135.9	1908.2
24	1572.1	1556.2	1766.3	1257.6	189.86	997.12	1769.8
26	1443.7	1428.1	1637.9	1124.9	142.61	875.54	1641.5
28	1326.2	1311.1	1519.1	1005.6	107.17	768.97	1522.8
30	1218.6	1204	1409	898.46	80.57	675.52	1412.9
32	1120.2	1106.1	1307	802.24	60.591	593.56	1311.1
34	275.36	268.41	398.74	373.73	10.604	168.72	400.72
36	1.1987	2.1463	4.0944	107.49	0.04235	1.9696	8.2337
38	0.030536	0.94169	2.1242	92.732	0.00042278	1.0721	5.9987
40	0.025787	0.86944	1.9765	80.753	0.00027067	0.94496	5.5913
42	0.023888	0.80494	1.8438	70.135	0.00020387	0.8346	5.2162
44	0.022129	0.74524	1.7201	60.73	0.00015356	0.73715	4.8665
46	0.0205	0.68996	1.6047	52.414	0.00011567	0.65111	4.5404
48	0.018991	0.6388	1.497	45.072	8.7121e-05	0.57512	4.2363
50	0.017593	0.59143	1.3967	38.602	6.5621e-05	0.50802	3.9527
52	0.016297	0.54758	1.3031	32.911	4.9427e-05	0.44877	3.6882
54	0.015098	0.50698	1.2158	27.918	3.7229e-05	0.39643	3.4415
56	0.013986	0.4694	1.1344	23.548	2.8042e-05	0.35021	3.2114
58	0.012957	0.4346	1.0584	19.735	2.1121e-05	0.30939	2.9967
60	0.012003	0.40239	0.98758	16.417	1.5909e-05	0.27333	2.7965
62	0.011119	0.37257	0.92151	13.542	1.1983e-05	0.24148	2.6098
64	0.010301	0.34496	0.85988	11.061	9.0258e-06	0.21335	2.4356
66	0.0095424	0.31939	0.80239	8.9314	6.7984e-06	0.1885	2.2731
68	0.00884	0.29573	0.74876	7.1137	5.1207e-06	0.16655	2.1215
70	0.0081893	0.27382	0.69873	5.5734	3.857e-06	0.14716	1.98
72	0.0075865	0.25353	0.65206	4.2705	2.9051e-06	0.13002	1.848

16. Click on the tab of **Probability Histories** from the table view to view the probability history table. The columns correspond to the statistic of the all realizations, including the mean, median, lower/upper bounds, 5%/95% percentiles and 25%/75% percentiles.

Time (yr)	Mean	Lower Bound	5%	25%	Median	75%	95%
0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0
4	3427.5	3160	3268.2	3397.7	3444.2	3486.8	3514.3
6	3472.2	2605	2930.3	3360.3	3524.7	3680.5	3783.4
8	3207.5	1935.2	2373.6	3017.4	3280.4	3539	3714.4
10	2970.5	1440.3	1922.6	2707.6	3051.6	3401.3	3645.1
12	2758.5	1074.2	1558	2429.1	2838.4	3268.7	3576.9
14	2568	802.5	1263.1	2178.7	2639.8	3140.9	3509.8
16	2396.2	600.35	1024.4	1953.8	2454.8	3017.9	3443.7
18	2240.8	449.63	831.12	1751.7	2282.6	2899.4	3378.8
20	2099.6	337.07	674.55	1570.1	2122.8	2785.2	3314.9
22	1970.9	252.89	547.65	1407	1975.6	2675.3	3252.1
24	1853.3	189.86	444.76	1261.2	1838.9	2569.4	3190.3
26	1745.6	142.61	361.3	1131.5	1711.8	2467.4	3129.5
28	1646.6	107.17	293.59	1015.3	1593.7	2369.2	3069.6
30	1555.4	80.57	238.62	911.02	1483.9	2274.7	3010.8
32	1471.3	60.591	193.99	817.51	1381.7	2183.6	2952.9
34	567.06	10.604	53.88	268.93	504.26	813.12	1300.4
36	70.978	0.04235	0.59018	6.2405	23.593	100.48	255.22
38	64.314	0.00042278	0.11246	4.1643	19.582	90.456	240.7
40	60.295	0.00027067	0.09304	3.8166	17.077	82.272	225.61
42	56.509	0.00020387	0.077411	3.4627	14.896	78.236	217.69
44	52.926	0.00015356	0.064409	3.1193	12.993	73.56	209.99
46	49.526	0.00011567	0.053591	2.825	11.584	64.958	202.5
48	46.281	8.7121e-05	0.044591	2.6418	10.585	57.83	195.21
50	43.134	6.5621e-05	0.037103	2.4137	10.033	54.28	189.7
52	40.495	4.9427e-05	0.030872	2.1657	9.3059	48.833	185.12
54	38.094	3.7229e-05	0.017949	2.0139	8.0878	45.799	180.65
56	35.85	0	0.015628	1.7306	6.4177	42.39	174.39
58	33.879	0	0.0082967	1.4775	5.7385	38.903	167.6
60	32.049	0	0.0052442	1.3663	4.7082	35.329	161.02
62	30.363	0	0.00086029	1.0691	4.3578	32.73	153.66
64	28.786	0	0.0003031	0.98009	3.8475	30.004	142.49
66	27.289	0	0.00021459	0.77698	3.3655	28.216	131.55
68	25.867	0	0.00017231	0.71443	3.0355	26.646	126.77
70	24.517	0	0.00013837	0.65708	2.796	25.176	120.82
72	23.235	0	0.00010905	0.58524	2.5749	23.798	115.07

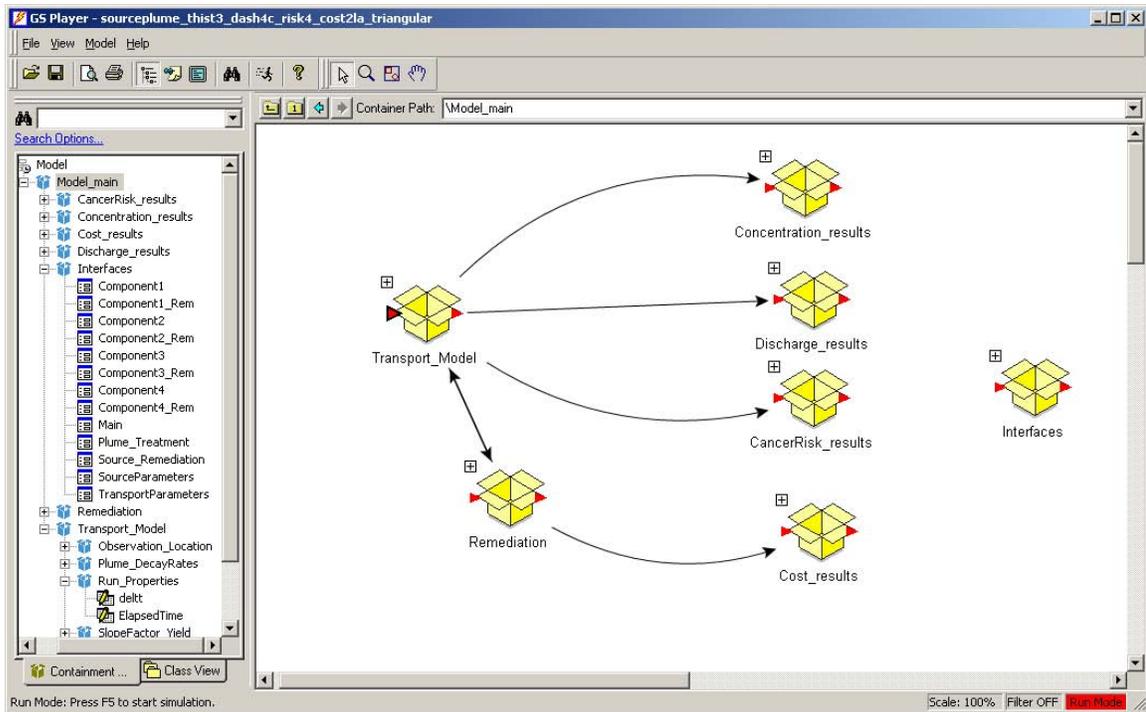
Steps 11 ~ 16 are for viewing the **Total Concentration**. Steps 11~16 can be used to view the **Total Discharge** and **Total Cancer Risk**, respectively.

17. Click the **Total Cost** tab from the main interface to show the probability distribution summary screen:

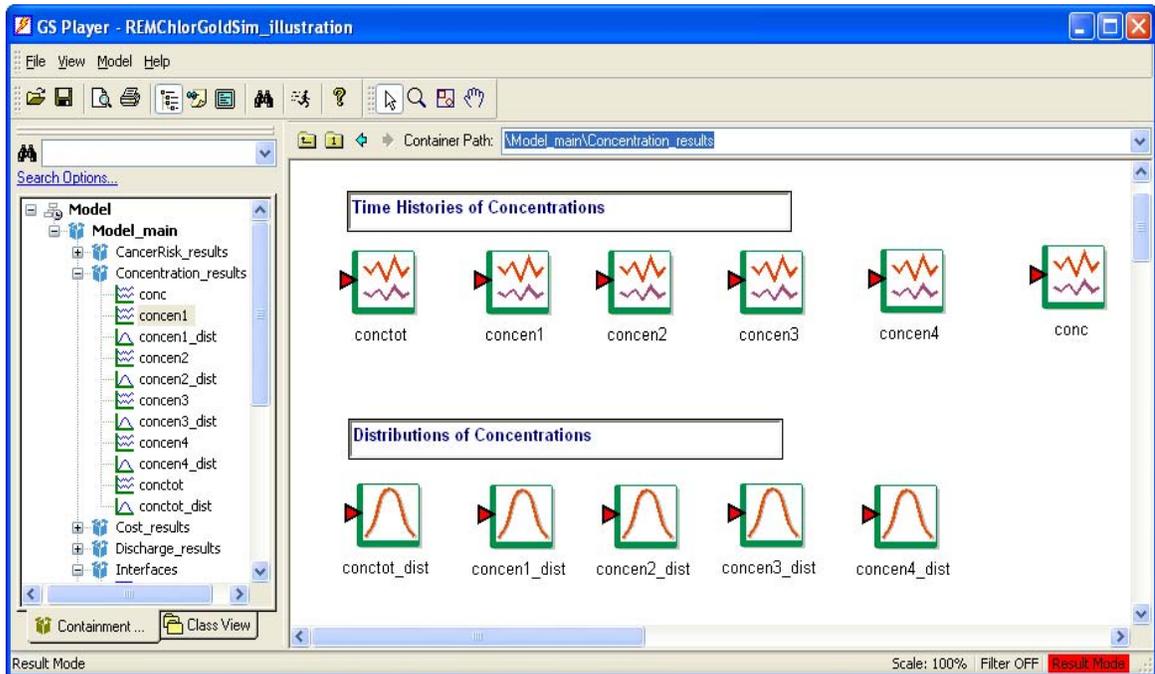


This screen shows the distribution statistics, including the mean, standard deviation, skewness and kurtosis, and the histogram of the PDF for the total remediation cost. Click the **Source Cost** tab and the **Plume Cost** tab from the main interface to view the source remediation cost and plume remediation cost.

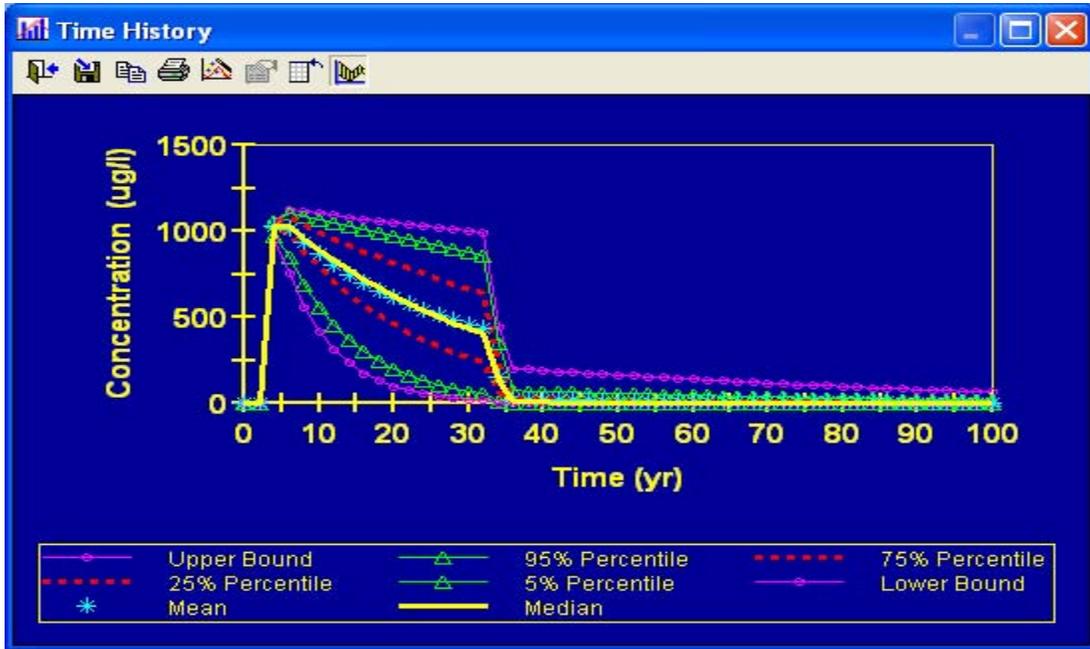
18. The concentration, mass discharge and cancer risk of each individual component also can be viewed. To do this, click the **Explore Model** tab from the main interface and the following screen showing the top level of the model stucture will appear:



To view the concentration of each individual component, click the plus sign on the top left side of the **Concentration_results** container and the following window will appear:

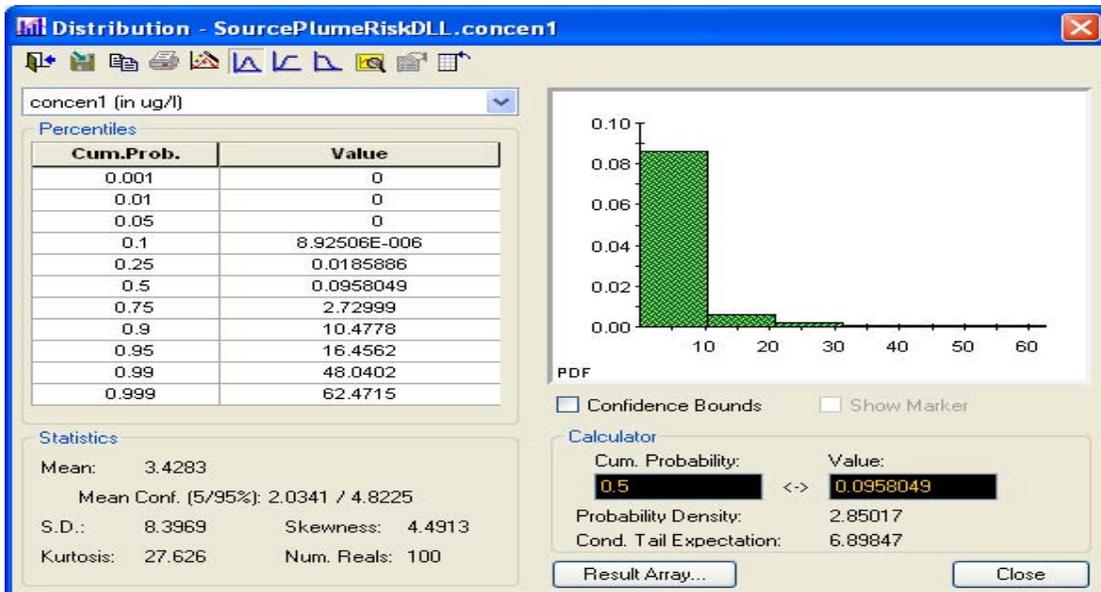


The top row elements are the time histories of concentrations for the total (**conctot**), component 1 (**concen1**), component 2 (**concen2**), component 3 (**concen3**), component 4 (**concen4**), and all four components (**concc**). Double click the element **concen1** to show the probabilistic time history of the component 1:



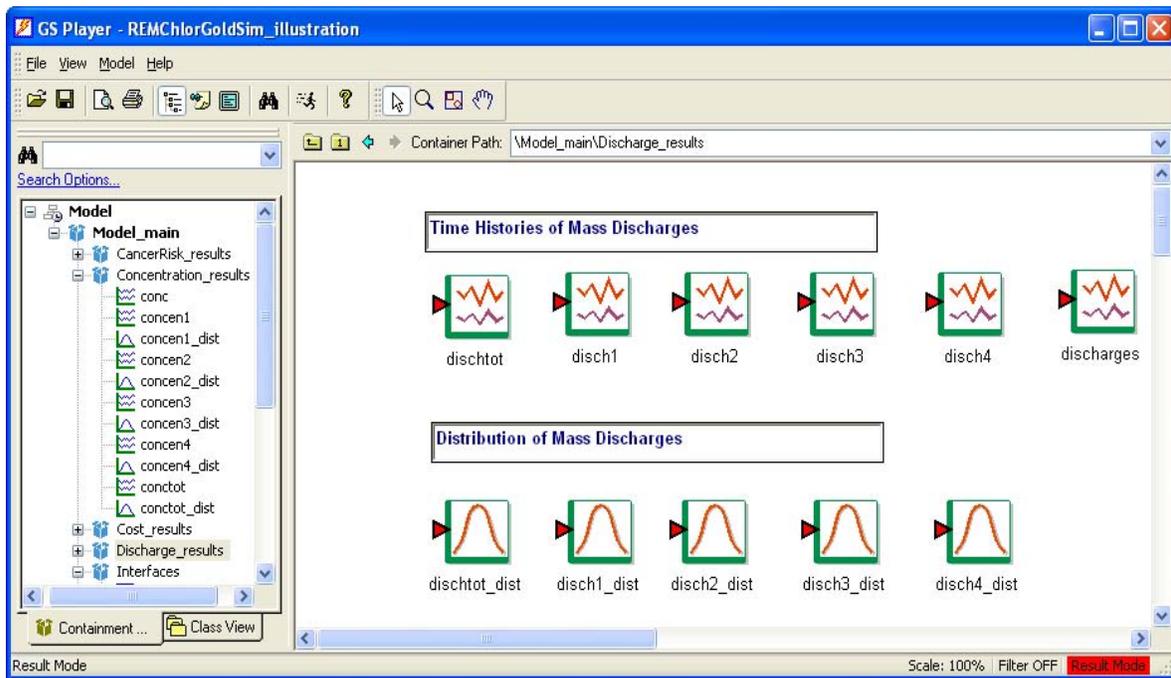
Repeat steps 11 ~ 16 to view other displays for the concentration of the component 1.

The bottom row elements are the distributions of concentrations for the total (**conctot_dist**), component 1 (**concen1_dist**), component 2 (**concen2_dist**), component 3 (**concen3_dist**), and component 4 (**concen4_dist**). Double click the element **concen1_dist** to view the distribution of the component 1:



Click a different result element to view the concentration of other single component. To go back to the main interface, click the **Go** tab on the Run Controller and select **Main**.

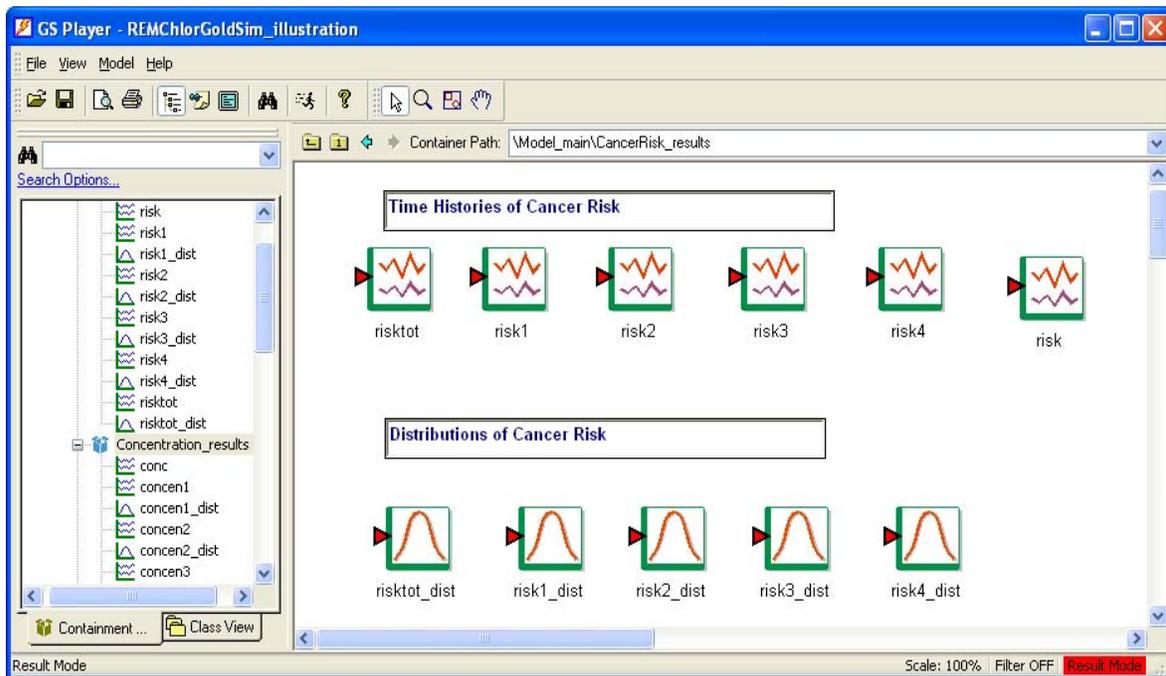
19. To view the mass discharge of each individual component, click the plus sign on the top left side of the **Discharge_results** container from the top level of model structure window (shown in step 18), and the following window will appear:



The top row elements are the time histories of mass discharges for the total (**dischtot**), component 1 (**disch1**), component 2 (**disch2**), component 3 (**disch3**), component 4 (**disch4**), and all four components (**discharges**). The bottom row elements are the distributions of mass discharges for the total (**dischtot_dist**), component 1 (**disch1_dist**), component 2 (**disch2_dist**), component 3 (**disch3_dist**), and component 4 (**disch4_dist**). Click an element to view the mass discharge for a single component.

To go back to the main interface, click the **Go** tab on the Run Controller and select **Main**.

20. To view the cancer risk for each component, click the plus sign on the top left side of the **CancerRisk_results** container from the top level of model structure window (shown in step 18), and the following window will appear:



The top row elements are the time histories of mass discharges for the total (**risktot**), component 1 (**risk1**), component 2 (**risk2**), component 3 (**risk3**), component 4 (**risk4**), and all four components (**risk**). The bottom row elements are the distributions of mass discharges for the total (**risktot_dist**), component 1 (**risk1_dist**), component 2 (**risk2_dist**), component 3 (**risk3_dist**), and component 4 (**risk4_dist**). Click an element to view the cancer risk for a single component.

To go back to the main interface, click the **Go** tab on the Run Controller and select **Main**.

Model Input Variables

DNAPL Source Parameters and Dimensions

Source Parameters – Initial Time of DNAPL Release ($t=0$)

The screenshot shows a software interface for defining source parameters. It is divided into two main sections: 'Source Parameters' and 'Source Dimensions'. Each section contains three columns of input fields. In the 'Source Parameters' section, the first column is for 'Initial Concentration (g/L)', the second for 'Initial Mass (kg)', and the third for 'Power Function Exponent'. In the 'Source Dimensions' section, the first column is for 'Source Width (m)', the second for 'Source Depth (m)', and the third for 'Source Length (m)'. Each input field has a 'Min', 'Likely', and 'Max' value. Below each set of three fields is a checkbox labeled 'If checked, use Deterministic Value' and a corresponding input field for the deterministic value.

Initial Concentration = Initial source zone concentration; C_0 , flow averaged concentration of dissolved chlorinated solvent leaving the source zone, g/l

The initial concentration is assumed to have a triangular distribution. The triangular PDF is defined by a minimum value, a most likely value and a maximum value. This variable is site-dependent; do not use the default value. The model uses the probabilistic value unless the deterministic value is checked.

Initial Mass = Initial source zone contaminant mass, M_0 , kg

The initial mass is assumed to have a triangular distribution. The triangular PDF is defined by a minimum value, a most likely value and

a maximum value. This variable is site-dependent; do not use the default value. The model uses the probabilistic value unless the deterministic value is checked.

Power Function Exponent = Exponent Γ in source concentration versus mass power function (Equation (2))

The exponent is assumed to have a log-normal distribution. The log-normal PDF is defined by a geometric mean and a geometric standard deviation. This variable is site-dependent; do not use the default value. The suggested value for this variable is ranging from 0.5 to 2 [Rao and Jawitz, 2003; Falta et al., 2005a; Newell and Adamson, 2005; Fure et al., 2005; Jawitz et al., 2005; McGuire et al., 2006; Newell et al., 2006]. The model uses the probabilistic value unless the deterministic value is checked.

Source Width = Source zone width, Y , m

The source width is assumed to have a triangular distribution. The triangular PDF is defined by a minimum value, a most likely value and a maximum value. This variable is site-dependent; do not use the default value. The model uses the probabilistic value unless the deterministic value is checked.

Source Depth = Vertical thickness of source zone, Z , m

The source depth is assumed to have a triangular distribution. The triangular PDF is defined by a minimum value, a most likely value and a maximum value. This variable is site-dependent; do not use the default value. The model uses the probabilistic value unless the deterministic value is checked.

Source Length = Source zone length, X , m

The source length is assumed to have a triangular distribution. The triangular PDF is defined by a minimum value, a most likely value and a maximum value. This variable is site-dependent; do not use the default value. The model uses the probabilistic value unless the deterministic value is checked.

Source Remediation

Start Time		End Time		Min	Likely	Max	If checked, use Deterministic Value	
Remediation Time (yr)	30		31	0	0.01	0.1	<input type="checkbox"/>	0.01

Start Time = Time when source remediation begins, t_1 , yr

The start time is a deterministic parameter.

End Time = Time when source remediation ends, t_2 , yr

The end time is a deterministic parameter.

Aqueous Phase Source Decay = First order aqueous phase source decay rate by processes other than dissolution and flushing, λ_s . This might include biological or chemical reactions in the source zone that destroy source mass, yr^{-1}

The aqueous source decay is assumed to have a triangular distribution. The triangular PDF is defined by a minimum value, a most likely value and a maximum value. The model uses the probabilistic value unless the deterministic value is checked.

The screenshot shows a software dialog box titled "source plume function - SourceRemediation". The main heading is "Source Remediation". The interface includes the following fields and options:

- Remediation Time (yr):** Start Time: 30, End Time: 31.
- Aqueous Phase Source Decay (1/yr):** Min: 0, Likely: 0.01, Max: 0.1. There is a checkbox "If checked, use Deterministic Value" which is unchecked, with a value of 0.01.
- Percent Removed:** A table with columns for Mean, Stdv, Min, and Max.

	Mean	Stdv	Min	Max
<input checked="" type="checkbox"/> Thermal Methods	0.97	0.025	0.56	1
<input type="checkbox"/> Surfactant Flooding	0.95	0.01	0.91	1
<input type="checkbox"/> Chemical Oxidation/Reduction	0.88	0.05	0	1
<input type="checkbox"/> Bioremediation	0.95	0.02	0.29	1
<input type="checkbox"/> If checked, use enhanced aqueous phase decay rate for remediation efficiency (1/yr)	0.8	0.6	0.95	
- Unit Cost (\$/cubic meter):** A table with columns for Mean, Stdv, Min, and Max.

	Mean	Stdv	Min	Max
<input checked="" type="checkbox"/> Thermal Methods	115.1	50	41.85	392.39
<input type="checkbox"/> Surfactant Flooding	503.56	375	86.32	7193.7
<input type="checkbox"/> Chemical Oxidation/Reduction	163.49	65	26.16	667.52
<input type="checkbox"/> Bioremediation	37.93	25	2.62	294.29
- Deterministic Values:** For each technology, there is a checkbox "If checked, use Deterministic Value" and a corresponding input field.
 - Thermal Methods: 115.1
 - Surfactant Flooding: 503.56
 - Chemical Oxidation/Reduction: 163.49
 - Bioremediation: 37.93
 - Enhanced aqueous phase decay rate: 0.8

Percent Removed = Fraction of source mass at time t_1 that is removed by source remediation technologies, X . $0 \leq X \leq 1$

The percent removed is assumed to have a beta distribution based on the data by McGuire et al. [2006] [Liang, 2009]. The beta PDF is defined by a mean, a standard deviation, a minimum value, and a maximum value. Currently four technologies are functional. To simulate a specific technology, select the corresponding technology check box. The model uses the probabilistic value unless both the specific technology and the corresponding deterministic value are checked. For each run, only one type of the technology can be selected.

Note: for enhanced bioremediation technology, remediation efficiency can be measured by the enhanced aqueous phase decay rate (yr^{-1}), in addition to the percent removed. The enhanced aqueous phase decay rate is assumed as a triangular distribution. The triangular PDF is defined by a minimum value, a most likely value and a maximum value. In order to run the model with the enhanced aqueous phase decay rate option for bioremediation technology, select both bioremediation technology and enhanced aqueous phase decay rate.

The model uses the probabilistic value for the enhanced decay rate unless the deterministic value is checked.

If the enhanced aqueous phase decay rate is selected, it overrides the aqueous phase source decay rate; otherwise, the natural source decay rate is applied.

Unit Cost = Unit cost of source remediation technologies, \$/cubic meter

The unit cost is assumed to have a beta distribution based on the data by McDade et al. [2005] [Liang, 2009]. The beta PDF is defined by a mean, a standard deviation, a minimum value, and a maximum value. Currently four technologies are functional. To compute the remediation cost for a specific technology, select the corresponding technology check box. The model uses the probabilistic value unless both the specific technology and the corresponding deterministic value are checked. For each run, only one type of the technology can be selected.

Transport Parameters

Darcy Velocity = Darcy flux (velocity) in the flow system, V . The unretarded chemical velocity, (pore velocity, v) is the Darcy velocity divided by the porosity. The total flow rate through the source zone, $Q = VYZ = \phi vYZ$. Darcy velocity unit is m/yr

The Darcy velocity is assumed to have a normal distribution. The normal PDF is defined by a mean and a standard deviation. This variable is site-dependent; do not use the default value. The model uses the probabilistic value unless the deterministic value is checked.

Porosity = Effective porosity, ϕ

The porosity is assumed to have a triangular distribution. The triangular PDF is defined by a minimum value, a most likely value and a maximum value. This variable is site-dependent; do not use the default value. The model uses the probabilistic value unless the deterministic value is checked.

Retardation Factor = Retardation factor for all dissolved species (must be equal to each other), *R*. Typically estimated from organic carbon partition coefficient and soil fraction of organic carbon

The retardation factor is assumed to have a triangular distribution. The triangular PDF is defined by a minimum value, a most likely value and a maximum value. This variable is site-dependent; do not use the default value. The model uses the probabilistic value unless the deterministic value is checked.

Scale-dependent Dispersivity Parameters					
	Min	Likely	Max	If checked, use Deterministic Value	
Longitudinal	0.001	0.01	0.1	<input checked="" type="checkbox"/>	0.01
Transverse	0.0001	0.001	0.01	<input checked="" type="checkbox"/>	0.001
Vertical	1e-5	0.0001	0.001	<input checked="" type="checkbox"/>	0.0001

Longitudinal Dispersivity Parameter = Scale-dependent longitudinal dispersivity parameter. The product of this parameter and the flow distance is the longitudinal dispersivity.

The longitudinal dispersivity parameter is assumed to have a triangular distribution. The triangular PDF is defined by a minimum value, a most likely value and a maximum value. The model uses the probabilistic value unless the deterministic value is checked.

Transverse Dispersivity Parameter = Scale-dependent transverse dispersivity parameter. The product of this parameter and the flow distance is the transverse dispersivity. This is generally 1/10 or less of the longitudinal dispersivity parameter value.

The transverse dispersivity parameter is assumed to have a triangular distribution. The triangular PDF is defined by a minimum value, a most likely value and a maximum value. The model uses the probabilistic value unless the deterministic value is checked.

Vertical Dispersivity Parameter = Scale-dependent vertical dispersivity parameter. The product of this parameter and the flow distance is the vertical dispersivity. This is generally 1/100 or less of the longitudinal dispersivity parameter value.

The vertical dispersivity parameter is assumed to have a triangular distribution. The triangular PDF is defined by a minimum value, a most likely value and a maximum value. The model uses the probabilistic value unless the deterministic value is checked.

Number of Stream Tubes = Number of streamtubes used to simulate longitudinal dispersion. The more tubes used, the smoother the solution will look, but the longer it will take to compute; problem execution time is directly proportional to the number of streamtubes used. A solution calculated with only 10 streamtubes will still represent the dispersion

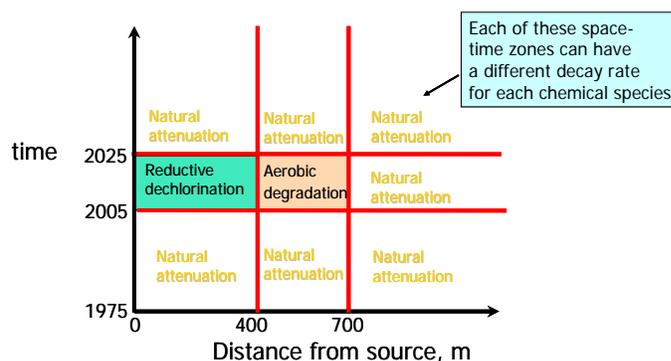
reasonably well, but it will not be “smooth”. A solution calculated with 500 streamtubes will be smooth, but it will take 50 times longer to compute.

The number of stream tubes is a deterministic parameter.

Plume Decay Rates and Yield Coefficients

The plume reaction parameters are entered using a table that mimics the distance-time reaction graph. Note that in the model, time starts at zero, when the DNAPL spill occurs, at location $x=0$. The 9 different reaction rates must be entered sUSEPARately for each of the 4 chemical species using the “Component #” tabs.

Component 1 is always the ultimate parent compound, and it is the component that is released from the DNAPL source zone. Component 2 is produced from the decay of component 1, and it decays to produce component 3, Component 3 decays to produce component 4. Component 4 is assumed to decay into a harmless species.



Yield Coefficients

Function - Component2

Component 2

Component Name: 2

Yield 2 From 1:

Min Likely Max

If checked, use Deterministic Value

Yield 2 From 1 = Mass of component 2 created by first order decay of component 1, y_{21} . Typically, for reductive dechlorination, this would be the molecular weight of component 2 divided by the molecular

weight of component 1. If component 1 decays without producing any important daughter products, this yield coefficient would be zero.

The yield 2 from 1 is assumed to have a triangular distribution. The triangular PDF is defined by a minimum value, a most likely value and a maximum value. The model uses the probabilistic value unless the deterministic value is checked.

Reaction - Component3

Component 3

Component Name: 3

Yield 3 From 2: Min 0.01, Likely 0.74, Max 1

If checked, use Deterministic Value: 0.74

Yield 3 From 2 = Mass of component 3 created by first order decay of component 2, y_{32} . Typically, for reductive dechlorination, this would be the molecular weight of component 3 divided by the molecular weight of component 2. If component 2 decays without producing any important daughter products, this yield coefficient would be zero.

The yield 3 from 2 is assumed to have a triangular distribution. The triangular PDF is defined by a minimum value, a most likely value and a maximum value. The model uses the probabilistic value unless the deterministic value is checked.

Reaction - Component4

Component 4

Component Name: 4

Yield 4 From 3: Min 0.01, Likely 0.32, Max 1

If checked, use Deterministic Value: 0.32

Yield 4 From 3 = Mass of component 4 created by first order decay of component 3, y_{43} . Typically, for reductive dechlorination, this would be the molecular weight of component 4 divided by the molecular weight of component 3. If component 3 decays without producing any important daughter products, this yield coefficient would be zero.

The yield 4 from 3 is assumed to have a triangular distribution. The triangular PDF is defined by a minimum value, a most likely value and a maximum value. The model uses the probabilistic value unless the deterministic value is checked.

Plume Reaction Zones

The nine possible plume reaction zones are defined by entering two times, and two distances.

Time Period 1 = Defines the time, *tplume 1* when plume reaction rates change from their initial value (which started at $t=0$). Note that this time is unrelated to the time of source remediation. Units are years.

Time Period 2 = Defines the time, *tplume 2* when plume reaction rates change from their previous value (which started at $t=tplume 1$). Note that this time is also unrelated to the time of source remediation. Units are years. The third time period occurs after *tplume 2*.

X1 = Defines the first distance zone for reaction rates, m.

X2 = Defines the second distance zone for reaction rates, m. The third zone occurs beyond *X2*.

The time period 1, time period 2, *X1*, and *X2* are deterministic parameters.

Plume Species First Order Decay Rates

A total of 36 first order reaction rates are entered in the model: 9 for each species. The plume treatment efficiency is measured by reaction rate. For each component, two of nine reaction zones, Zone 1 and Zone 2 in Period 2, can be used for plume treatment and other seven zones are used for natural attenuation.

The user specifies the seven natural attenuation rates for each component in the **Component #** interface. A sUSEPARate interface for each individual species is pulled up by clicking on the appropriate **Component #** tab. The user specifies the two treatment rates in the **component #_Rem** interface, which is pulled up

by clicking on **Treatment Rate** tab. A sUSEPARate interface for each species is pulled up by clicking the appropriate **Component#_Rem** tab. If all nine zones are natural attenuation, then use natural attenuation rates for treatment rates.

All decay rates have units of yr^{-1} . All rates are assumed to have triangular distributions. The triangular PDF of each decay rate is defined by a minimum value, a most likely value and a maximum value. These decay rates are site-dependent variables; do not use the default values. The model uses the probabilistic values sampled from PDFs for the decay rates unless the deterministic values are checked.

Plume Treatment Dimensions and Costs

The plume treatment dimensions and costs interface is pulled up by clicking on the **Treatment Dimensions/Costs** tab from the treatment rate interface. Two treatment zones have different lengths, widths and depths. The length for the first treatment zone is X1 and the length for the second zone is X2-X1. All dimensions have units of m.

Generally, the costs of plume treatment include the capital cost (treatment volume multiply by the unit cost) and the annual operation & Management (O&M) cost. To calculate the net present value (NPV) of the O&M cost for a certain treatment period, an annual inflation rate and an interest rate are also included in the model.

The screenshot shows the 'Plume Treatment' interface with the following details:

- Title Bar:** source plume function - Plume_Treatment
- Grid Structure:**
 - Vertical Axis (Time, Years):** Period 3 (top), Period 2 (middle), Period 1 (bottom).
 - tpume 2:** 50
 - tpume 1:** 30
 - Horizontal Axis (Distance From Source, Meters):**
 - X1:** 400
 - X2:** 700
- Zone 1 (Distance 0-400m):**
 - Period 3: Natural Attenuation
 - Period 2: Treatment Zone
 - Treatment Width (m): 5
 - Treatment Depth (m): 5
 - Unit Cost (\$/cubic meter):

Min	Likely	Max	If checked, use Deterministic Value
1	10	100	<input type="checkbox"/> 10
 - Period 1: Natural Attenuation
- Zone 2 (Distance 400-700m):**
 - Period 3: Natural Attenuation
 - Period 2: Treatment Zone
 - Treatment Width (m): 50
 - Treatment Depth (m): 5
 - Unit Cost (\$/cubic meter):

Min	Likely	Max	If checked, use Deterministic Value
1	10	100	<input type="checkbox"/> 10
 - Period 1: Natural Attenuation
- Zone 3 (Distance >700m):** Natural Attenuation in all periods.

- Summary Parameters:**
- Present Annual O&M Cost (\$):**

Min	Likely	Max	If checked, use Deterministic Value
1000	100000	1e6	<input type="checkbox"/> 180000
- Treatment Period (tpume2-tpume1, yr):** 20
- Inflation Rate (%):** 4
- Interest Rate (%):** 6
- Buttons:** Treatment Rate, Main Interface

Treatment Width = Plume treatment zone width, m

Two plume treatment zones have different widths. The treatment widths are deterministic parameters.

Treatment Depth = Vertical thickness of the plume treatment zone, m

Two plume treatment zones have different treatment depths. The treatment depths are deterministic parameters.

Unit Cost = Unit cost of plume treatment, \$/cubic meter

Two plume treatment zones may use different methods and have different unit costs. The unit costs of the plume treatment are assumed to have triangular distributions. The triangular PDF is defined by a minimum value, a most likely value and a maximum value. These unit costs are site-dependent variables; do not use the default values. The model use the probabilistic values sampled from PDFs unless the deterministic value is checked.

Present Annual O&M Cost = Present annual O&M cost of the plume treatment, \$

The present annual O&M cost is assumed to have a have triangular distributions. The triangular PDF is defined by a minimum value, a most likely value and a maximum value. The present annual O&M cost a site-dependent variable; do not use the default values. The model use the probabilistic values sampled from PDFs unless the deterministic value is checked.

Treatment Period = Defines the time for plume treatment operation and management, starting from tplume1 and ending at tplume2, yr

The treatment period is a deterministic parameter.

Inflation Rate = Annual inflation rate, %

The inflation rate is a deterministic parameter.

Interest Rate = Annual interest rate, %

The interest rate is a deterministic parameter.

Cancer Risk Parameters

Cancer Risk Slope Factor			If checked, use Deterministic Value	
Oral	<input type="text" value="0.1"/>	<input type="text" value="0.54"/>	<input checked="" type="checkbox"/>	<input type="text" value="0.54"/>
Inhalation	<input type="text" value="0.001"/>	<input type="text" value="0.021"/>	<input checked="" type="checkbox"/>	<input type="text" value="0.021"/>
	Min	Most		Max

Two sets of excess cancer risk slope factors are entered for each component in **Component #** interface: one for ingestion (drinking the water), and one for inhalation (breathing vapors in the shower, bathroom, and house). Note that direct vapor transport through the vadose zone is not included here. The units for the slope factors are risk per mg contaminant per kg body weight per day.

Oral Cancer Risk Slope Factor = Lifetime oral cancer risk slope factor, risk per mg contaminant per kg body weight per day

The oral cancer risk slope factor is assumed to have a triangular distribution. The triangular PDF is defined by a minimum value, a most likely value and a maximum value. The oral cancer risk slope factor is a site-dependent variable; do not use the default values. The model use the probabilistic values sampled from PDFs unless the deterministic value is checked.

Inhalation Cancer Risk Slope Factor = Lifetime inhalation cancer risk slope factor, risk per mg contaminant per kg body weight per day

The inhalation cancer risk slope factor is assumed to have a triangular distribution. The triangular PDF is defined by a minimum value, a most likely value and a maximum value. The inhalation cancer risk slope factor is a site-dependent variable; do not use the default values. The model use the probabilistic values sampled from PDFs unless the deterministic value is checked.

Tutorials

Getting Started

In this manual, four tutorial examples are included.

In order to run the tutorial, tutorial model files (with the extension name of .gsp) and the DLL file (with the extension name of .dll) need to be under the same directory.

To open a model file, double click a tutorial model file.

To run a model file, click the **Run Model** tab on the main interface.

To save a model file, click the **Explore Model** tab on the main interface, then click the **File** menu on the top tool bar and select **Save** or **Save As**

To reset a model file, after a simulation is finished, click on **Reset** from the **GoldSim Run Controller** to reset the model in order to edit the parameter values and run a new simulation.

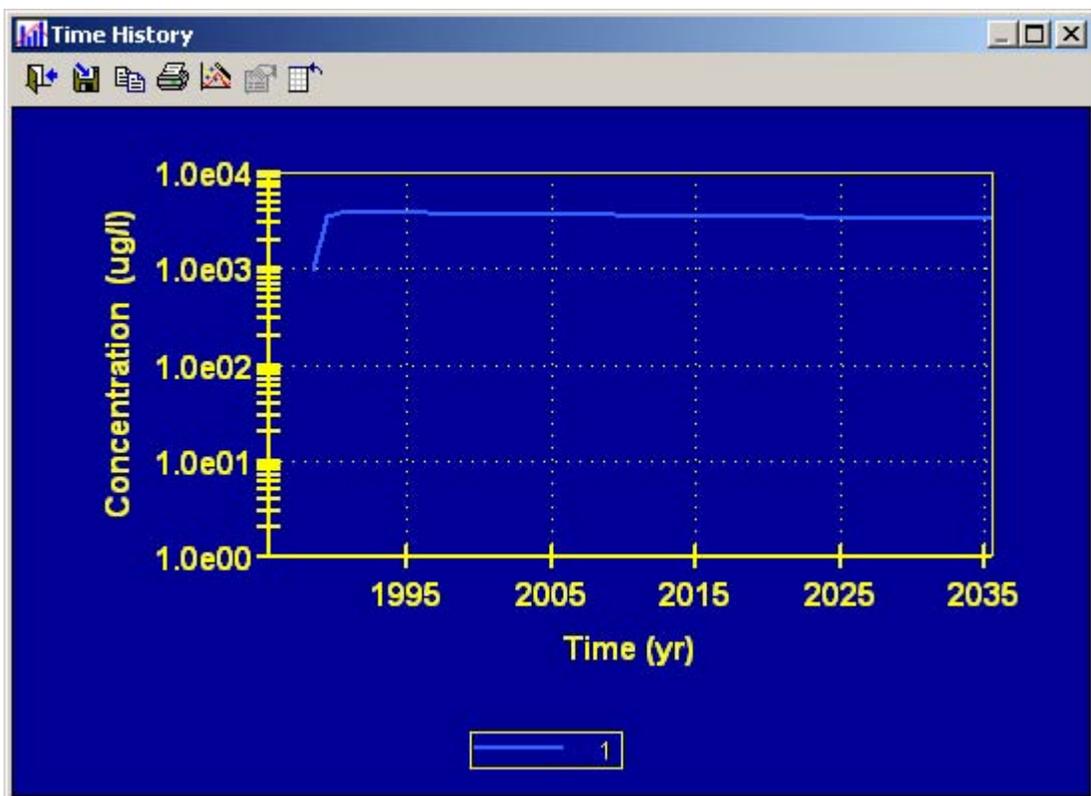
To close a model file, after a simulation is finished, close the model file from the main interface or click the **Explore Model** tab on the main interface, then click the **File** menu on the top tool bar and select **Exit**.

Tutorial 1: Deterministic Thermal Remediation of a PCE Source.

This hypothetical problem starts from a deterministic setup, involving a 1620 kg release of tetrachloroethylene (PCE) from the source zone, with a groundwater darcy velocity of 20m/yr, and an average porosity of 0.33. The source zone has dimensions of X=10 m, Y=10 m and Z=3 m. The source is assumed to behave according to Equation (2), with an exponent, Γ , of 1. This type of source behavior gives an exponential decay of the source mass and concentration with time [Newell et al., 1996; Parker and Park, 2004; Zhu and Sykes, 2004; Newell and Adamson, 2005]. The release was assumed to have occurred in 1985, and the initial source concentration was 10 mg/l, leading to an initial source discharge of 6 kg of PCE per year.

Initially, PCE and its daughter products, trichloroethylene (TCE), dichloroethylene (DCE) and vinyl chloride (VC) were assumed to undergo natural attenuation. The medians of the decay rates from BIOCHLOR database [Aziz et al., 2000] were assigned to PCE, TCE, DCE, and VC as 1.1 yr^{-1} , 1.2 yr^{-1} , 1.2 yr^{-1} , and 1.7 yr^{-1} , respectively. The compounds were specified a retardation factor of 2, the longitudinal dispersivity is equal to 0.01 times the travel distance, the transverse dispersivity is 1/10 of the longitudinal dispersivity, and the vertical dispersivity is 1/10 of the transverse dispersivity.

It is assumed that the compliance plane is located at the 100 meters downstream from the source. In the absence of any type of remediation, this release would result in a deterministic total concentration around 3600 ug/l at the compliance plane in 2010, and 3400 ug/l in 2025 due to flushing process:



Suppose some remediation effort is proposed in 2010, and the remediation goal is to reduce the total concentration to less than 200 ug/l in 15 years following the remediation (year 2025) at the compliance plane.

This tutorial is set up to simulate a very effective thermal remediation of the source that removes **97%** of the source mass in 2010, with a period of **0.2** years. Double click the tutorial file (Tutorial1.gsp) to open it and then click on the different tabs from left side of the main interface to view the simulation settings and the input parameters.

Source Remediation

Remediation Time (yr) Start Time End Time

 25 25.2 Aqueous Phase Source

Percent Removed

Thermal Methods Mean Stdv Min Max If checked, use Deterministic Value

 0.94 0.03 0.56 1 0.97

This tutorial is run under the deterministic simulation mode. To view this, click the **Simulation Settings** tab from the main interface, then click the **Monte Carlo** tab, and the simulation option window shows that the **Deterministic Simulation** mode is selected. Under the **Time** tab, the time settings show the simulation duration is set as from **1985** to **2085** with a time step of **1** year.

Simulation Settings...

Time Monte Carlo Globals Information

Define Monte Carlo options to carry out a probabilistic simulation, and specify the sampling method for Stochastic variables.

Probabilistic Simulation

Realizations: 100 # Histories to save: 100

Run the following Realization only: Realization: 89

Use Latin Hypercube Sampling

Repeat Sampling Sequences Random Seed: 1

Deterministic Simulation

Solve Simulation deterministically using:

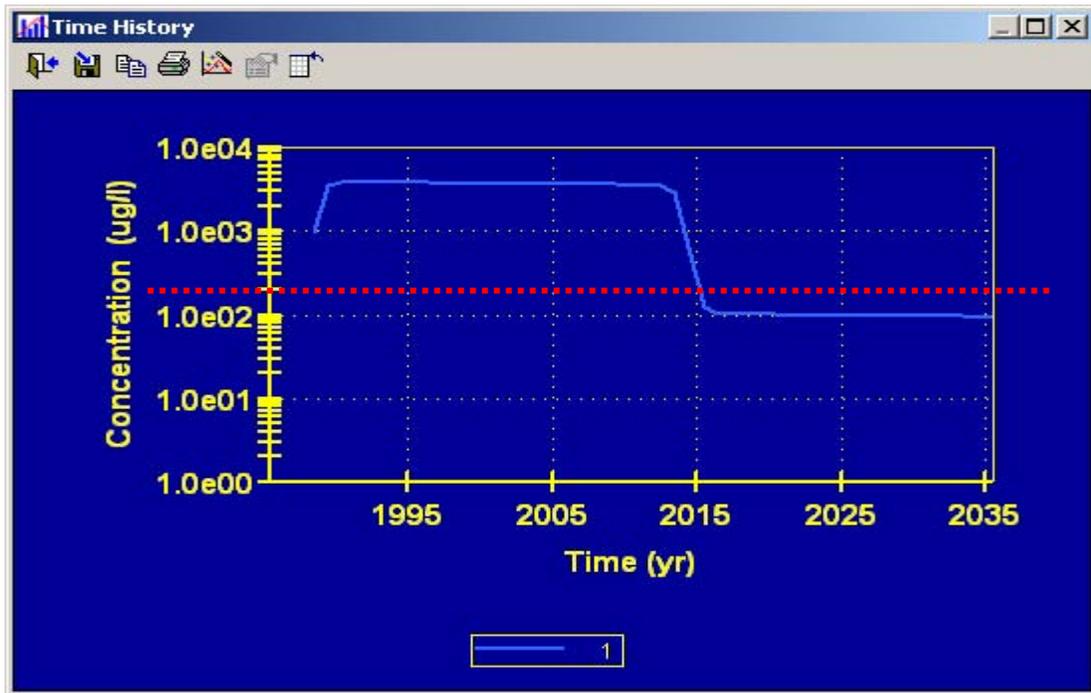
Element Deterministic Values

Element Mean Values

Specified Quantile: 0.5

OK Cancel Help

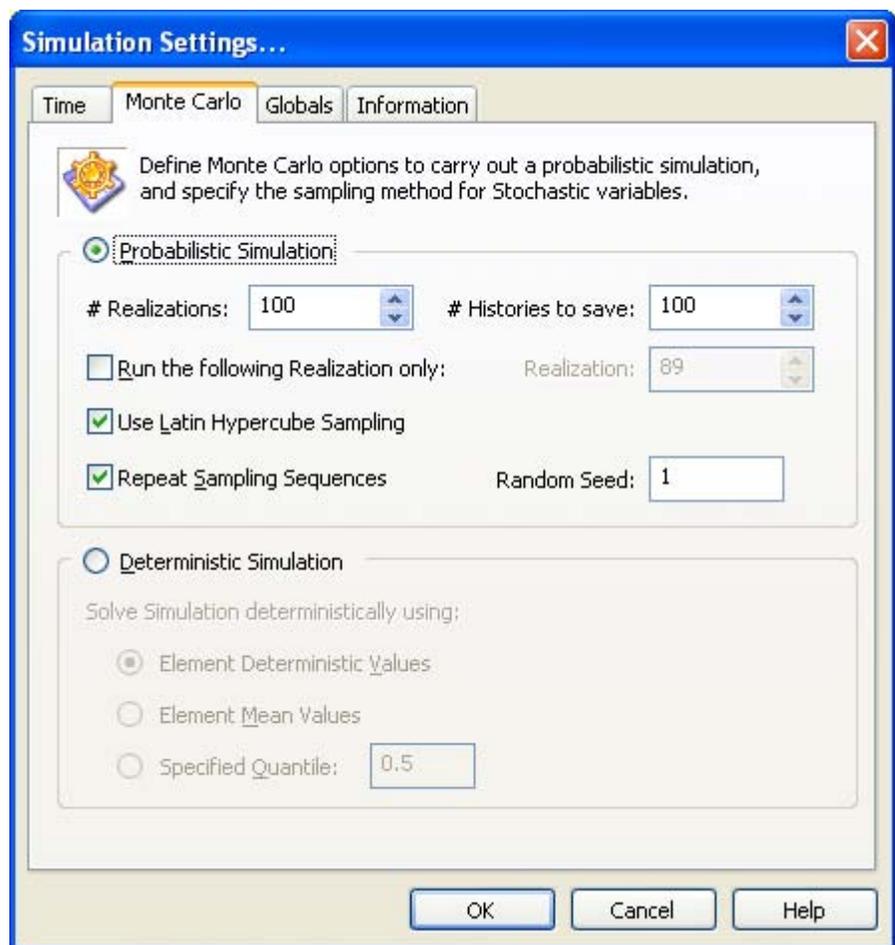
After viewing the simulation settings, click **OK** to go back the main interface and click the **Run Model** tab to run the model. After the simulation is completed, select **Total Concentration** from the main interface to view the deterministic result of the concentration 100 meters downgradient from the source. The total concentration in 2025 is about 98 ug/l, which meets the remediation goal (red dotted line). Based on this simulation, it appears that the remediation should work, but it does not include any uncertainty.



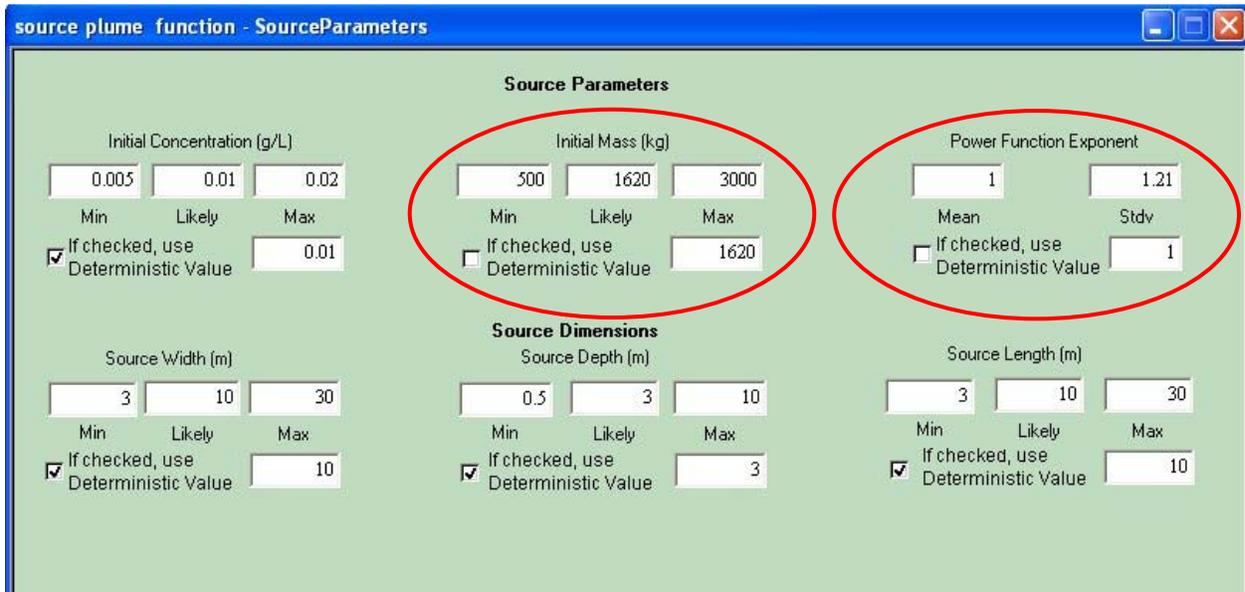
Tutorial 2: Thermal Remediation of a PCE Source Considering Uncertainties in Source Parameters.

This tutorial example is identical to the previous deterministic source remediation case except that we will now make two source parameters (initial source mass and power function exponent in Equation 2) uncertain and run a probabilistic simulation of a source remediation. The remediation concentration goal remains same.

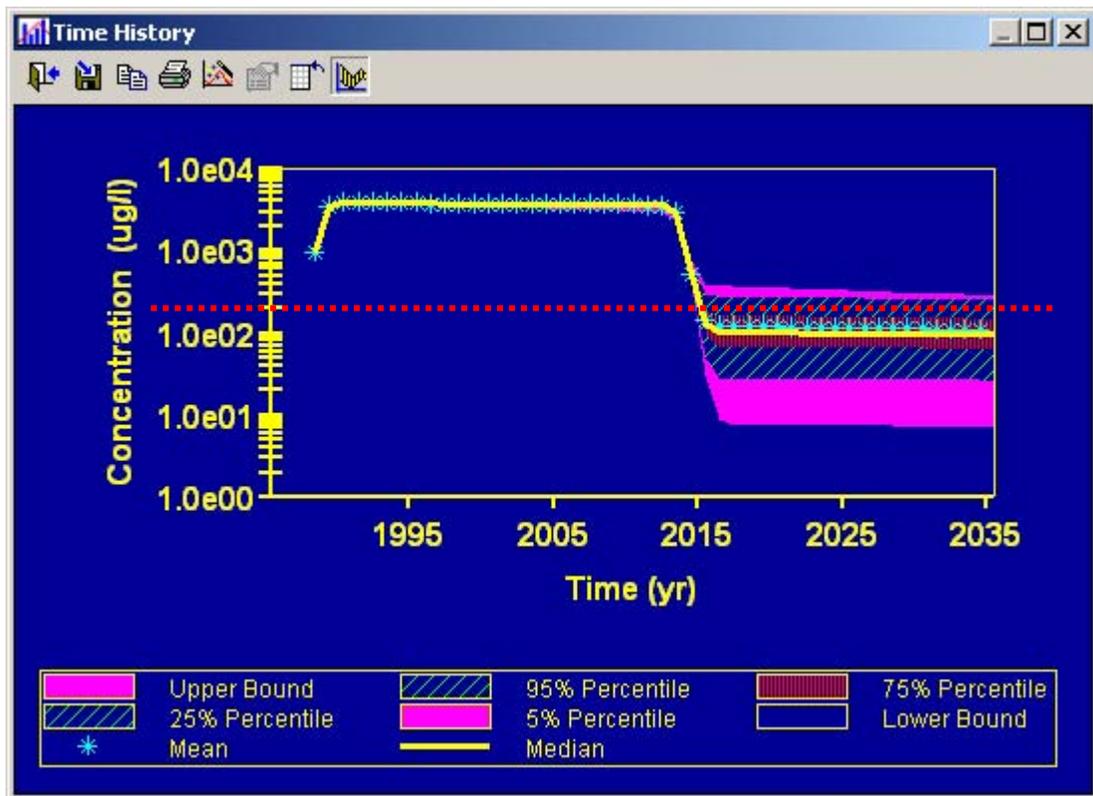
Double click the tutorial file (Tutorial2.gsp) to open it. Then click on the **Simulation Settings** tab from the main interface, under the **Monte Carlo** tab, the simulation options show that the **Probabilistic Simulation** mode is selected and the number of Monte Carlo realizations is **100**. Click **OK** to go back the main interface.



Click on the **Source Zone Parameters** tab from the main interface to view the settings of source zone parameters. The **Initial Mass** and **Power Function Exponent** are set as the stochastic parameters as the check boxes of deterministic values unselected. Put the cursor on **Initial Mass (kg)**, a tool box will appear and show that the initial source mass has a triangular distribution. This triangular distribution is defined by a minimum value (**Min**) of **500** kg, a most likely value (**Likely**) of **1620** kg, and a maximum value (**Max**) of **3000** kg. Put the cursor on **Power Function Exponent**, a tool box will appear and show that power function exponent has a log-normal distribution. This log-normal distribution is defined by a geometric mean of **1** and a geometric standard deviation of **1.21**.



After viewing the uncertain source parameters settings, go back to the main interface and click the **Run Model** tab. Once the probabilistic simulation is completed, select the **Total Concentration** from the main interface to view the probabilistic result of the concentration 100 meters downgradient from the source. The remediation goal (red dotted line) falls between the 75th percentile and 95th percentile. The 75th percentile concentration at 100m in 2025 is about **154** ug/l and the upper bound concentration is **324** ug/l. Given the uncertainties in the initial source mass and the power function exponent, the model predicts more than 75% probability of meeting the remediation concentration goal.



Time History

Date/Time	Mean	Lower Bound	5%	25%	Median	75%	95%	Upper Bound
Jul 01, 2016	122.41	8.6469	28.477	67.259	103.05	161.94	275.21	369.72
Jul 02, 2017	120.43	7.3844	27.159	65.742	101.39	159.92	271.95	363.37
Jul 02, 2018	119.69	7.2866	27.013	65.491	101.02	159.2	269.95	358.24
Jul 02, 2019	119.06	7.2836	26.963	65.366	100.7	158.6	268.07	353.25
Jul 01, 2020	118.43	7.2807	26.913	65.242	100.38	157.99	266.69	348.28
Jul 02, 2021	117.81	7.2777	26.864	65.117	100.05	157.39	265.47	343.35
Jul 02, 2022	117.18	7.2747	26.814	64.994	99.729	156.79	264.25	338.45
Jul 02, 2023	116.57	7.2717	26.765	64.87	99.407	156.19	263.03	333.57
Jul 01, 2024	115.95	7.2687	26.716	64.747	99.085	155.05	261.82	328.73
Jul 02, 2025	115.34	7.2657	26.667	64.624	98.765	153.87	260.62	323.92
Jul 02, 2026	114.73	7.2628	26.618	64.501	98.446	152.71	259.41	319.14
Jul 02, 2027	114.12	7.2598	26.57	64.378	98.127	151.7	258.21	314.39
Jul 01, 2028	113.52	7.2568	26.521	64.256	97.81	151.08	257.02	309.67

Tutorial 3: Probabilistic Thermal Remediation of a PCE Source.

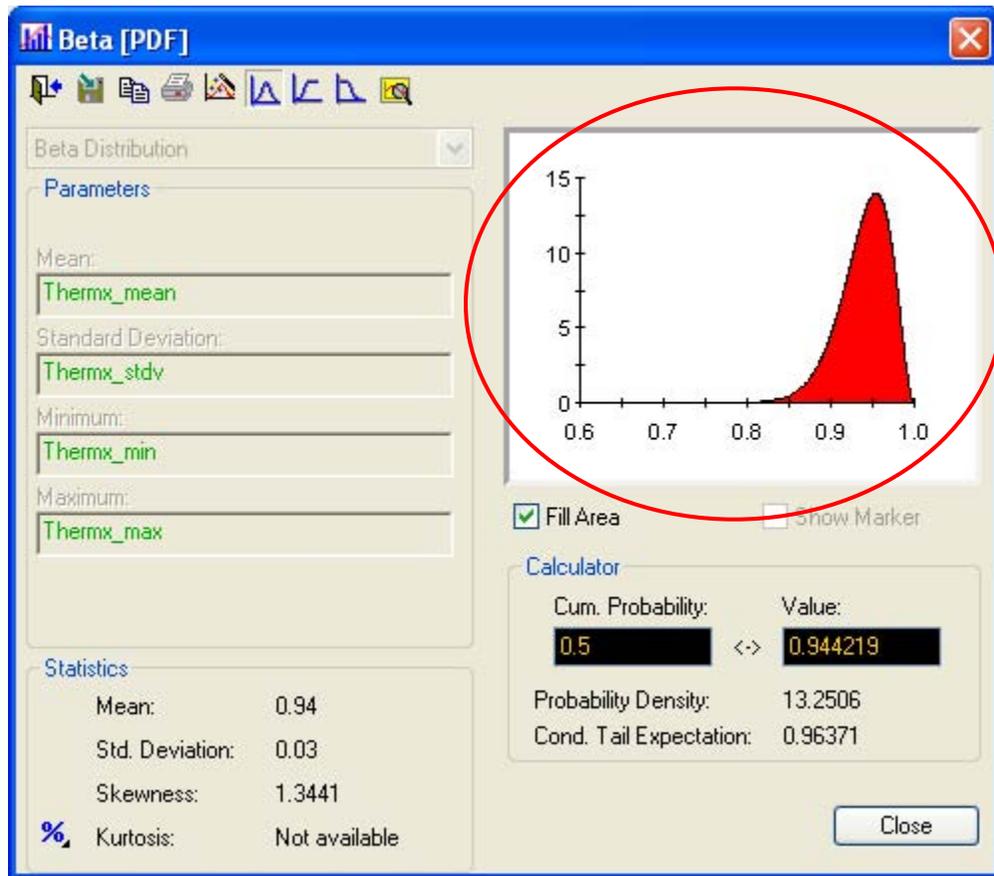
This tutorial example is identical to the previous source remediation case except that we will now make one more parameter (source removal fraction) uncertain and run a probabilistic simulation of a source remediation. The remediation concentration goal remains same.

Double click the tutorial file (Tutorial3.gsp) to open it and then click on the **Simulation Settings** tab from the main interface. Under the **Time** tab, the time settings show the simulation duration time is set as from **1985** to **2085** with a time step of 1 year; under the **Monte Carlo** tab, the simulation options show that the **Probabilistic Simulation** mode is selected and the number of Monte Carlo realizations is **100**. Click **OK** to go back the main interface.

Click on the **Source Zone Parameters** tab from the main interface to view the settings of source zone parameters. The **Initial Mass** and **Power Function Exponent** are set as the stochastic parameters as discussed in the previous case. Click on the **Source Remediation** tab from the main interface to view the settings of source remediation parameters. The **Thermal Methods** is selected and the fraction of source mass removal is set as the stochastic parameter as the check box of the deterministic values remains unselected. Put the cursor on **Percent Removed**, a tool box will appear and show that the fraction of source mass removal has a beta distribution. This beta distribution is defined by a mean (Mean) of **0.94**, a standard deviation (Stdv) of **0.03**, a minimum value (**Min**) of **0.56**, and a maximum value (**Max**) of **1**.

Source Remediation						
Remediation Time (yr)	Start Time	End Time	Aqueous Phase Source			
	25	25.2				
Percent Removed						
<input checked="" type="checkbox"/> Thermal Methods	Mean	Stdv	Min	Max	<input type="checkbox"/> If checked, use Deterministic Value	
	0.94	0.03	0.56	1		0.97

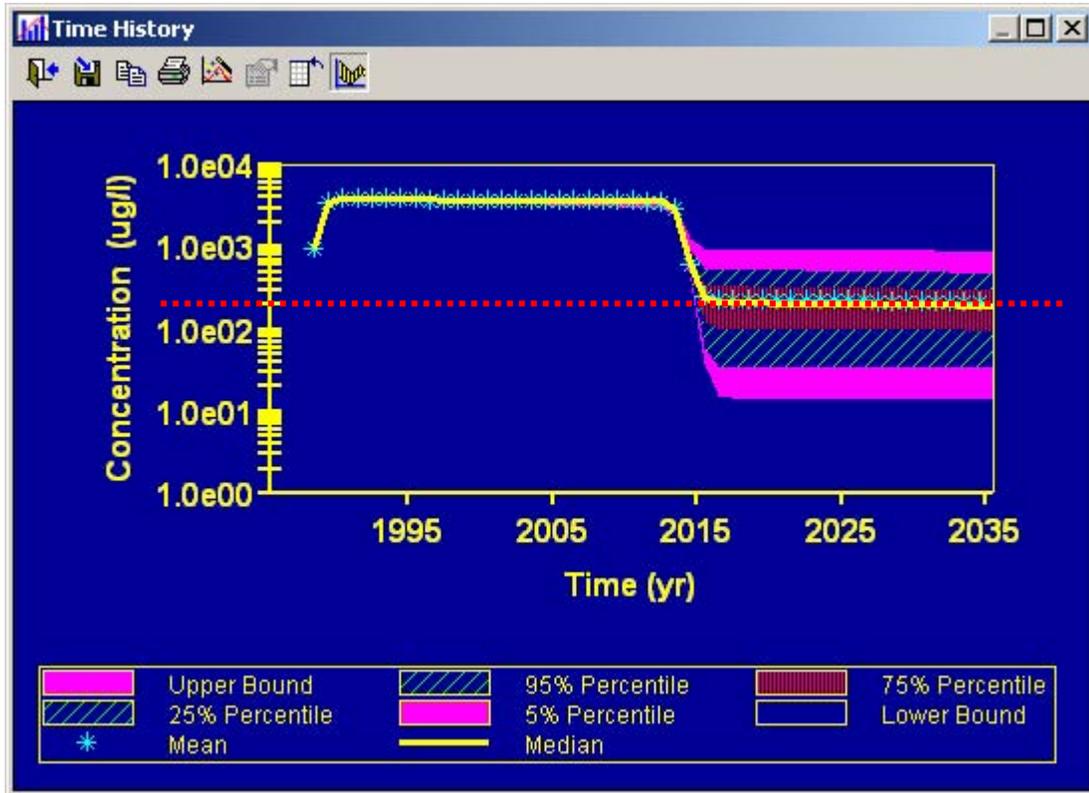
To view the actual beta PDF of the **Percent Removed** parameter, go back the main interface and click the **Explore Model** tab, click the plus sign of the **Remediation** container, then click the plus sign of the **SourceRem_Parameters** container, continuously click the plus sign of the **Remediation_Efficiency** container, double click the **Thermx_prob** element, under the **Definition** window, click the **Edit** tab, and the beta PDF window will appear.



Close the **Beta[PDF]** window and **Definition** window and then go back to the main interface by clicking **Go** from the **GoldSim Run Controller** and select **Main**. After viewing the three uncertain parameters, the initial source mass, the power function exponent and the fraction of source mass removal of the thermal remediation, click the **Run Model** tab from the main interface.

After the probabilistic simulation is completed, select the **Total Concentration** from the main interface to view the probabilistic result of the concentration 100 meters downgradient from the source.

From the chart view, the remediation goal (red dotted line) is close to the median. From the table view, the median concentration at 100m in 2025 is about **203 ug/l** and the upper bound concentration 2025 is about 900 ug/l. The remediation effort is predicted to meet the goal approximately 50% of the time given uncertainties in the initial source mass, the power function exponent, and the source remediation efficiency. The model predicts a likely failure of the original design. Compared to the previous case, the uncertainty of the source remediation efficiency resulted in a lower chance of meeting the remediation goal.

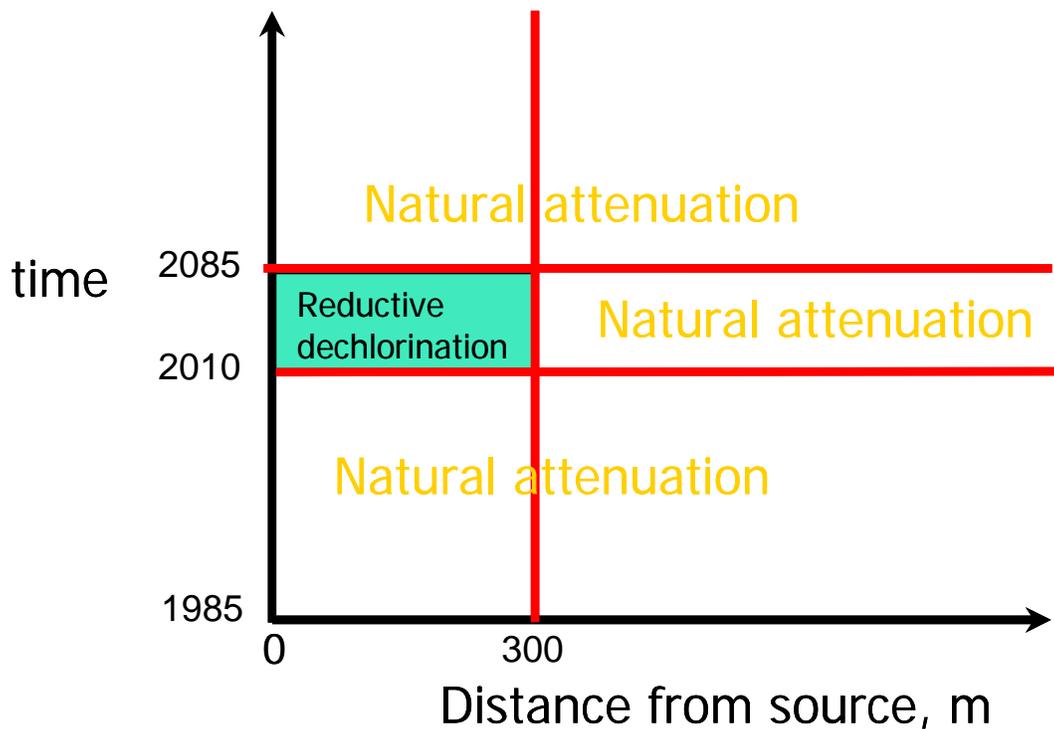


Time History

Date/Time	Mean	Lower Bound	5%	25%	Median	75%	95%	Upper Bound
Jul 02, 2010	3562.1	3003.9	3315.2	3519.7	3588.2	3644.2	3705.3	3742.7
Jul 02, 2011	3548.2	2969.4	3291.4	3504	3575.3	3633.6	3697.4	3736.4
Jul 01, 2012	3534.4	2935.3	3267.8	3488.4	3562.5	3623.1	3689.5	3730.1
Jul 02, 2013	2953.3	2416.9	2705.1	2885.6	2973.3	3043.6	3138.3	3243.4
Jul 02, 2014	629.13	393.86	442.66	506.42	608.37	728.53	899.96	1273.6
Jul 02, 2015	253.63	37.233	58.393	123.95	232.92	352.38	548.33	947.91
Jul 01, 2016	230.66	15.568	35.316	100.41	210.28	328.97	524.7	926.12
Jul 02, 2017	228.31	14.188	33.886	98.759	208.26	325.97	520.55	922.17
Jul 02, 2018	227.17	14.064	33.735	98.393	207.46	324.16	517.55	919.25
Jul 02, 2019	226.13	14.044	33.69	98.135	206.76	322.45	514.66	916.43
Jul 01, 2020	225.1	14.024	33.645	97.878	206.07	320.76	511.77	913.62
Jul 02, 2021	224.07	14.005	33.6	97.622	205.37	319.07	508.9	910.81
Jul 02, 2022	223.05	13.985	33.555	97.366	204.68	317.4	506.03	908
Jul 02, 2023	222.03	13.965	33.51	97.111	204	315.73	503.18	905.2
Jul 01, 2024	221.02	13.945	33.465	96.857	203.31	314.07	500.34	902.41
Jul 02, 2025	220.01	13.926	33.42	96.604	202.63	312.42	497.51	899.62
Jul 02, 2026	219	13.906	33.375	96.351	201.95	310.77	494.69	896.84
Jul 02, 2027	218	13.887	33.331	96.099	201.27	309.14	491.88	894.06
Jul 01, 2028	217	13.867	33.286	95.847	200.59	307.51	489.09	891.29
Jul 02, 2029	216.01	13.848	33.241	95.596	199.48	305.89	486.3	888.52
Jul 02, 2030	215.02	13.828	33.197	95.346	198.7	304.28	483.52	885.76

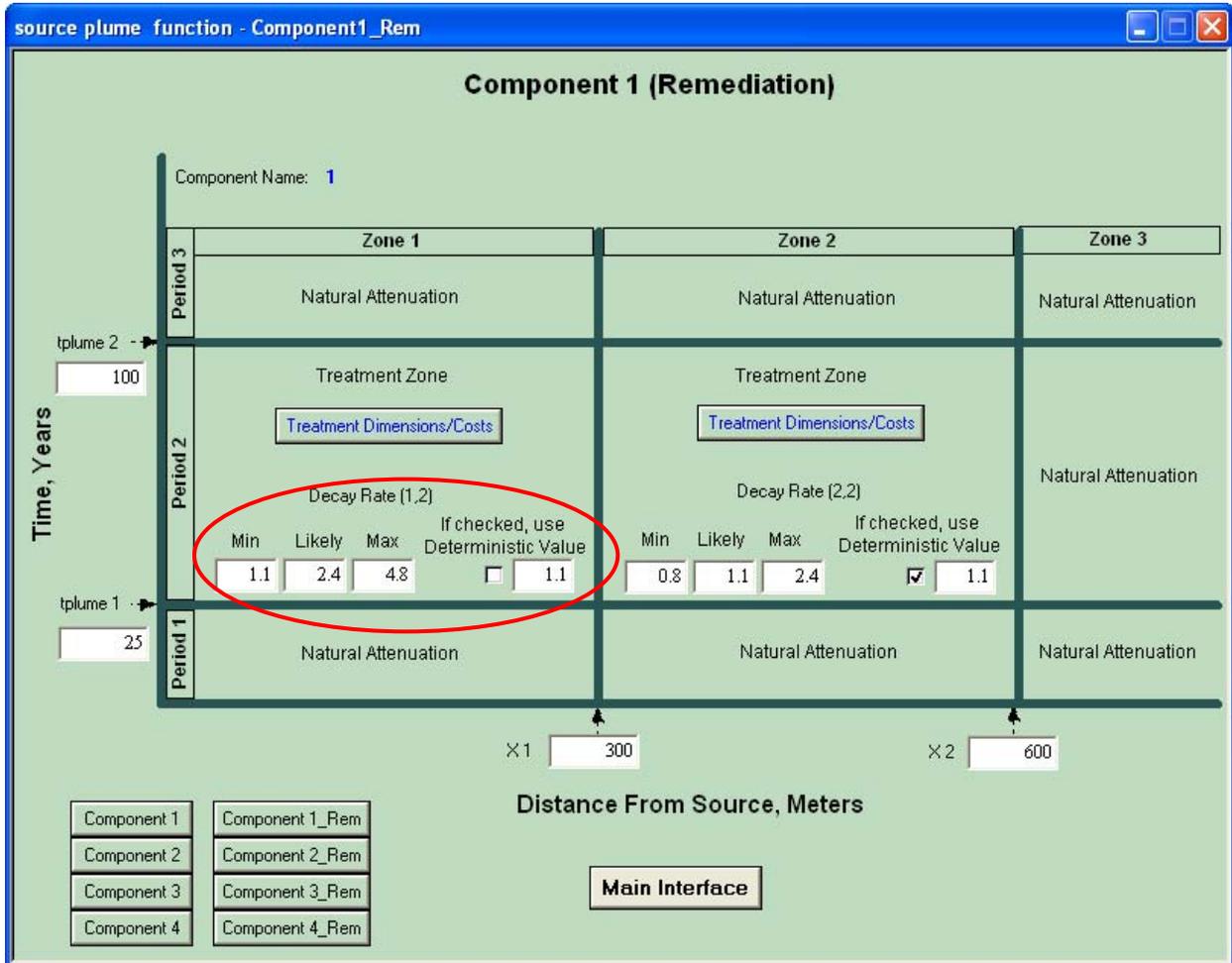
Tutorial 4: Probabilistic Thermal Remediation of PCE Source with Enhanced Plume Degradation.

This tutorial example is based on the previous source remediation case, but we will now add an enhanced bioremediation of PCE and TCE in the dissolved plume. Here, the reductive dechlorination of PCE and TCE will be enhanced for the first 300 m, sustained indefinitely, from 2010 to 2085 (years 25 to 100). This is illustrated graphically using a distance-time reaction zone plot (that corresponds to the REMChlor plume reaction matrix):

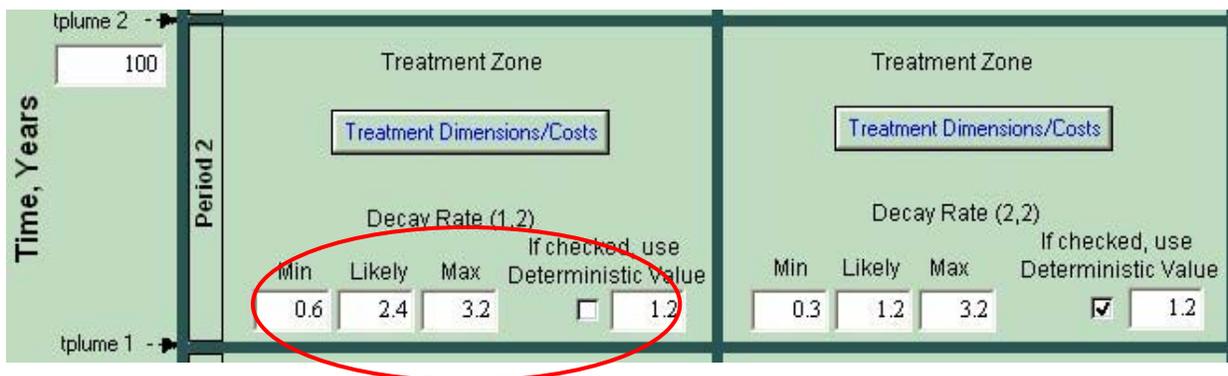


In the first 300 m, the enhanced biodegradation rates of PCE and TCE from 2010 to 2085 are treated as the stochastic variables. In the first 300 m, the natural attenuation rates of DCE and VC from 2010 to 2085 are also treated as the stochastic variables. The natural attenuation rates of PCE, TCE, DCE and VC in other reaction zones keep unchanged and use deterministic values.

Double click the tutorial file (Tutorial4.gsp) to open it and then click on the **Plume Decay Rates** tab from the main interface to view the settings of plume parameters for the first component (PCE). Click the **Treatment Rate** tab from the **Component 1** interface to view the **Component 1 (Remediation)** interface, which shows the two treatment zones. Here the reductive dechlorination of PCE only occurs in the first zone (Zone 1 in Period 2) and the second zone (Zone 2 in Period 2) keeps unchanged as the natural attenuation zone. The enhanced biodegradation rate of PCE in the first treatment zone has a triangular distribution with a **Min** of 1.1 yr^{-1} , a **Likely** of 2.4 yr^{-1} , and a **Max** of 4.8 yr^{-1} .



Click the **Component 2_Rem** tab from the **Component 1 (Remediation)** interface to view the plume remediation interface for component 2 (TCE), the **Component 2 (Remediation)** interface. Here the reductive dechlorination of TCE only occurs in the first zone and the second zone keeps unchanged as the natural attenuation zone. The enhanced biodegradation rate of TCE in the first treatment zone has a triangular distribution with a **Min** of 0.6 yr^{-1} , a **Likely** of 2.4 yr^{-1} , and a **Max** of 3.2 yr^{-1} .



Click the **Component 3_Rem** tab from the **Component 2 (Remediation)** interface to view the plume remediation interface for component 3 (DCE), the **Component 3 (Remediation)** interface. Here DCE keeps the natural attenuation process in both zones. The decay rate of DCE in the first zone has a triangular distribution with a **Min** of 0.1 yr^{-1} , a **Likely** of 1.2 yr^{-1} , and a **Max** of 20.9 yr^{-1} .

Decay Rate (1,2)		Decay Rate (2,2)	
Min	Likely	Max	If checked, use Deterministic Value
0.1	1.2	20.9	<input type="checkbox"/>
			<input checked="" type="checkbox"/>

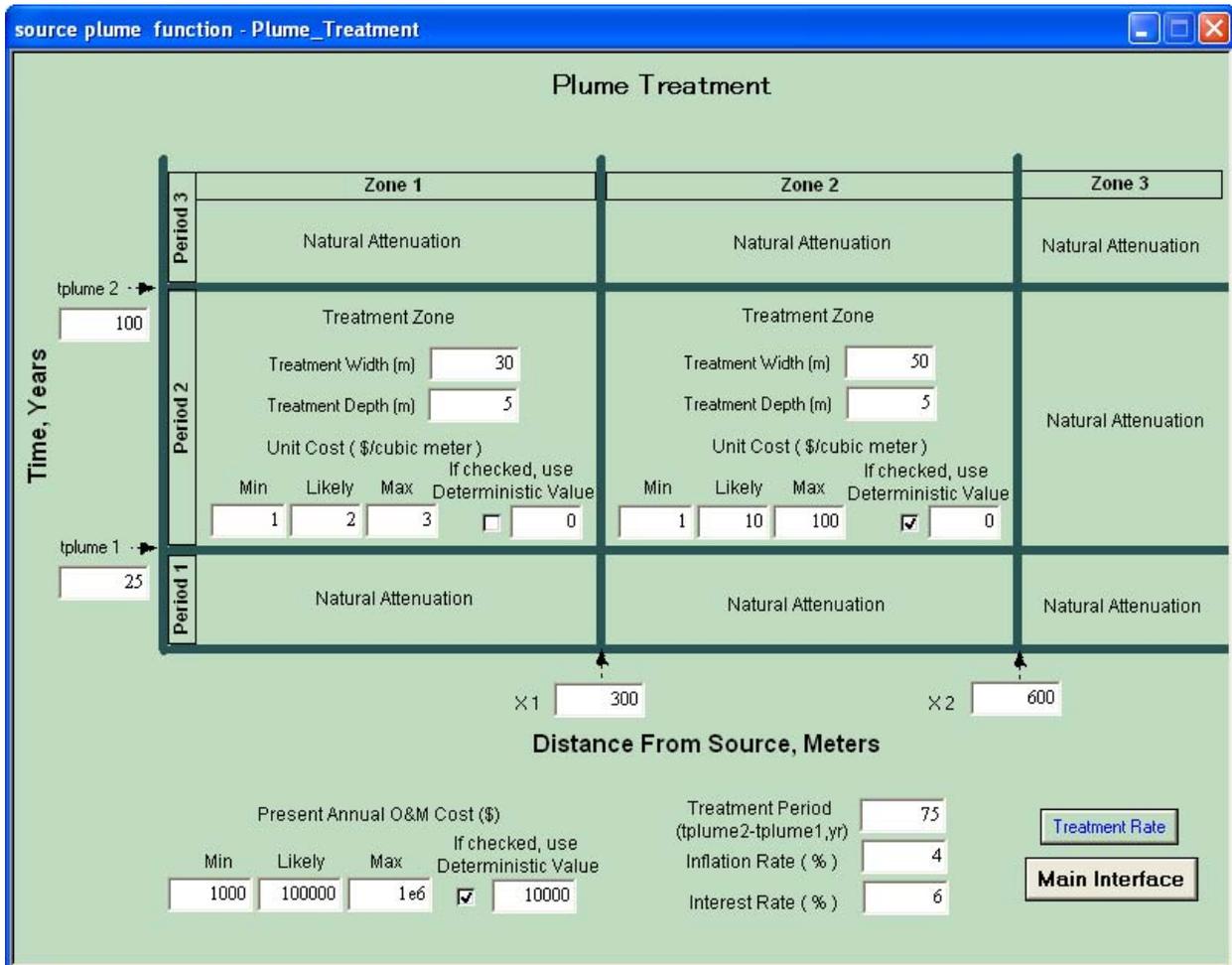
Click the **Component 4_Rem** tab from the **Component 3 (Remediation)** interface to view the plume remediation interface for component 4 (VC), the **Component 4 (Remediation)** interface. Here VC keeps the natural attenuation process in both zones. The decay rate of VC in the first zone has a triangular distribution with a **Min** of 0.4 yr^{-1} , a **Likely** of 1.7 yr^{-1} , and a **Max** of 12.2 yr^{-1} .

Decay Rate (1,2)		Decay Rate (2,2)	
Min	Likely	Max	If checked, use Deterministic Value
0.4	1.7	12.2	<input type="checkbox"/>
			<input checked="" type="checkbox"/>

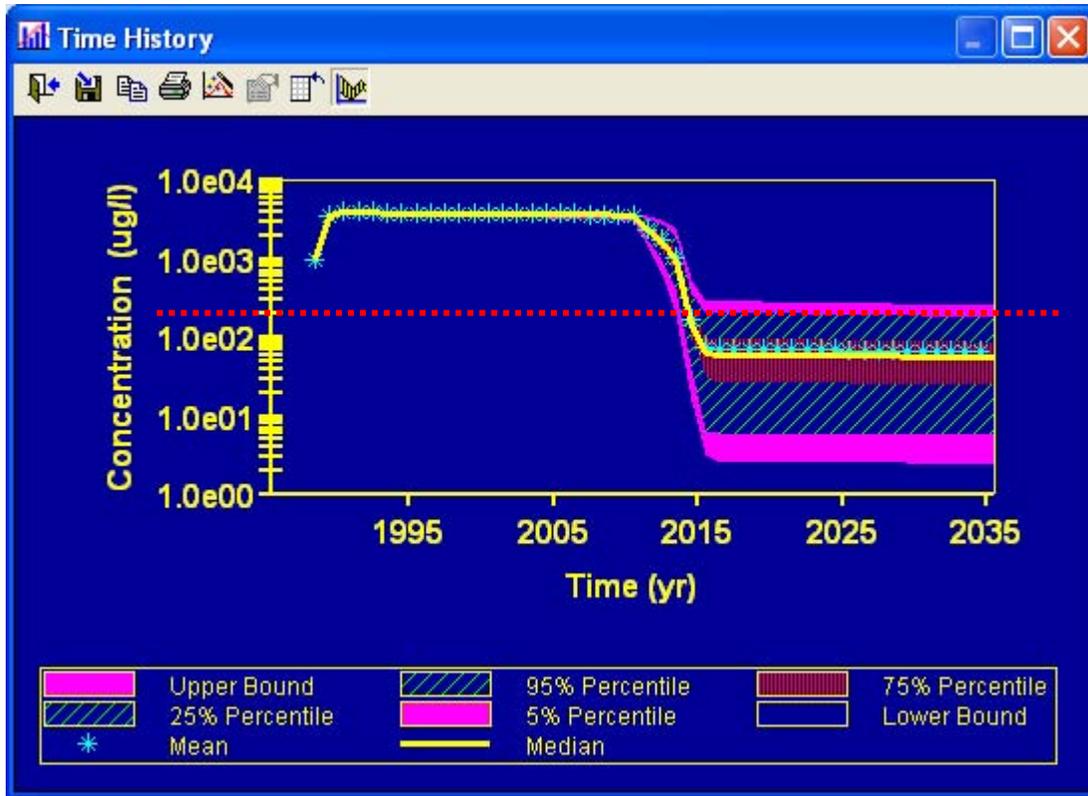
Costs for both source remediation and plume treatment will be computed in this problem. The source remediation unit cost is made uncertain by unselecting the deterministic value check box. The **Source Remediation** interface shows that the unit cost of thermal treatment has a beta distribution with a **Mean** of $115.1 \text{ \$/m}^3$, a **Stdv** of $50 \text{ \$/m}^3$, a **Min** of $41.85 \text{ \$/m}^3$, and a **Max** of $392.39 \text{ \$/m}^3$.

	Percent Removed				If checked, use Deterministic Value	Unit Cost (\$/cubic meter)				If checked, use Deterministic Value	
	Mean	Stdv	Min	Max		Mean	Stdv	Min	Max		
<input checked="" type="checkbox"/> Thermal Methods	0.94	0.03	0.56	1	<input type="checkbox"/>	115.1	50	41.85	392.39	<input type="checkbox"/>	115.1

To view the plume treatment dimensions and costs parameters, in any **Component # (Remediation)** interface, click the **Treatment Dimensions/Costs** tab and the **Plume Treatment** interface will appear. The **Plume Treatment** interface shows that the treatment zone (Zone 1 in Period 2) has a **Treatment Width** of 30 m and a **Treatment Depth** of 5 m. The **Unit Cost** in the treatment zone (Zone 1 in Period 2) is made uncertain and has a triangular distribution with a **Min** of 1 \$/m³, a **Likely** of 2 \$/m³, and a **Max** of 3 \$/m³. The another treatment zone (Zone 2 in Period 2) is remaining the natural attenuation condition, so dimensions and the unit cost for this zone does contribute to the remediation cost. The **Present Annual O&M Cost** has a deterministic value of \$ 10,000. The **Inflation Rate** is 4% and the **Interest Rate** is 6%. The **Treatment Period** is 75 years.



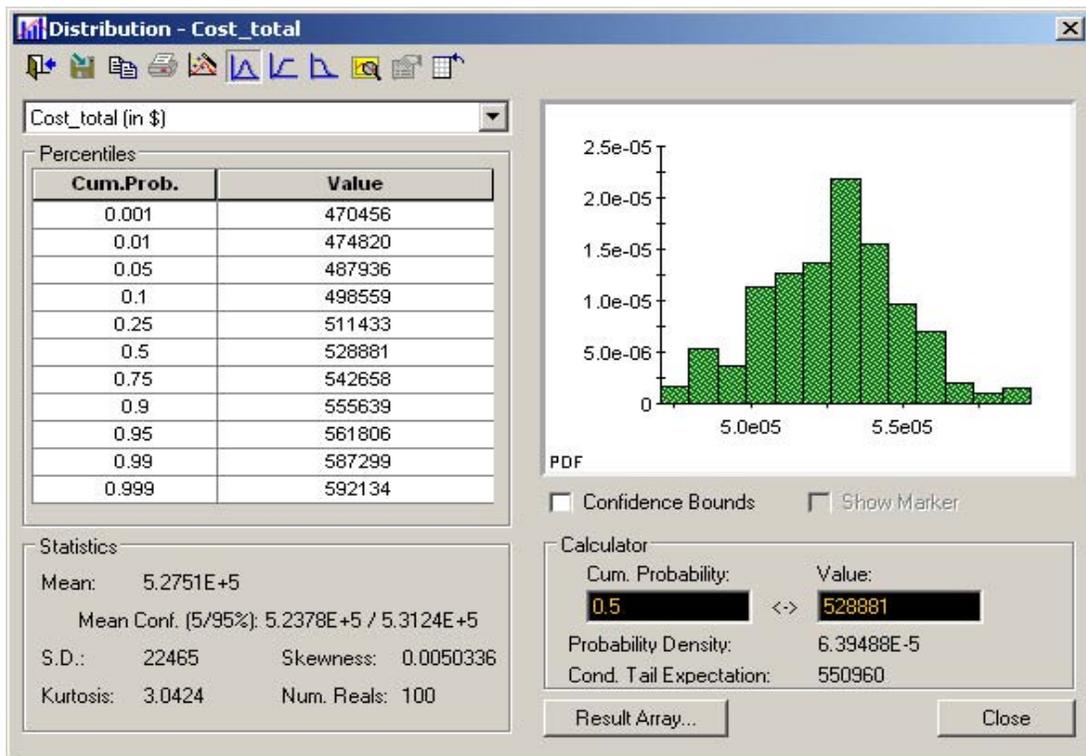
After viewing the parameter settings, go back to the main interface and click the **Run Model** tab. After simulation is completed, select **Total Concentration** from the main interface to view the probabilistic result of the concentration 100 meters downgradient from the source.

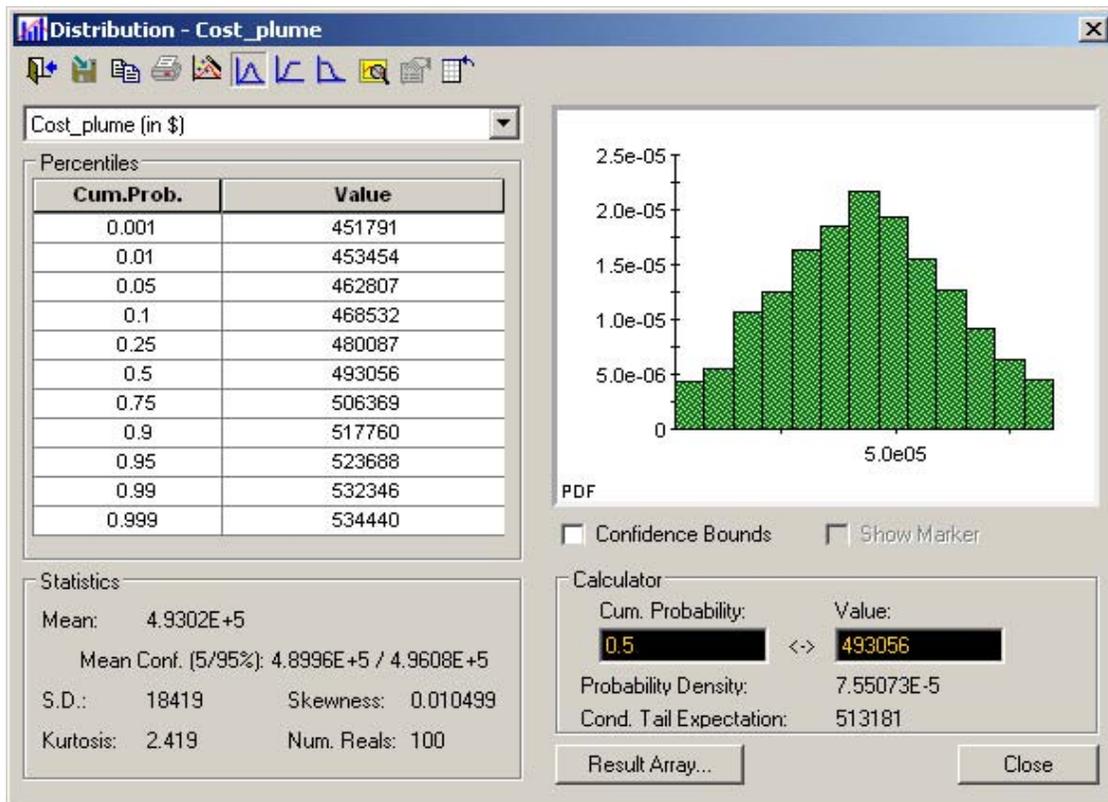
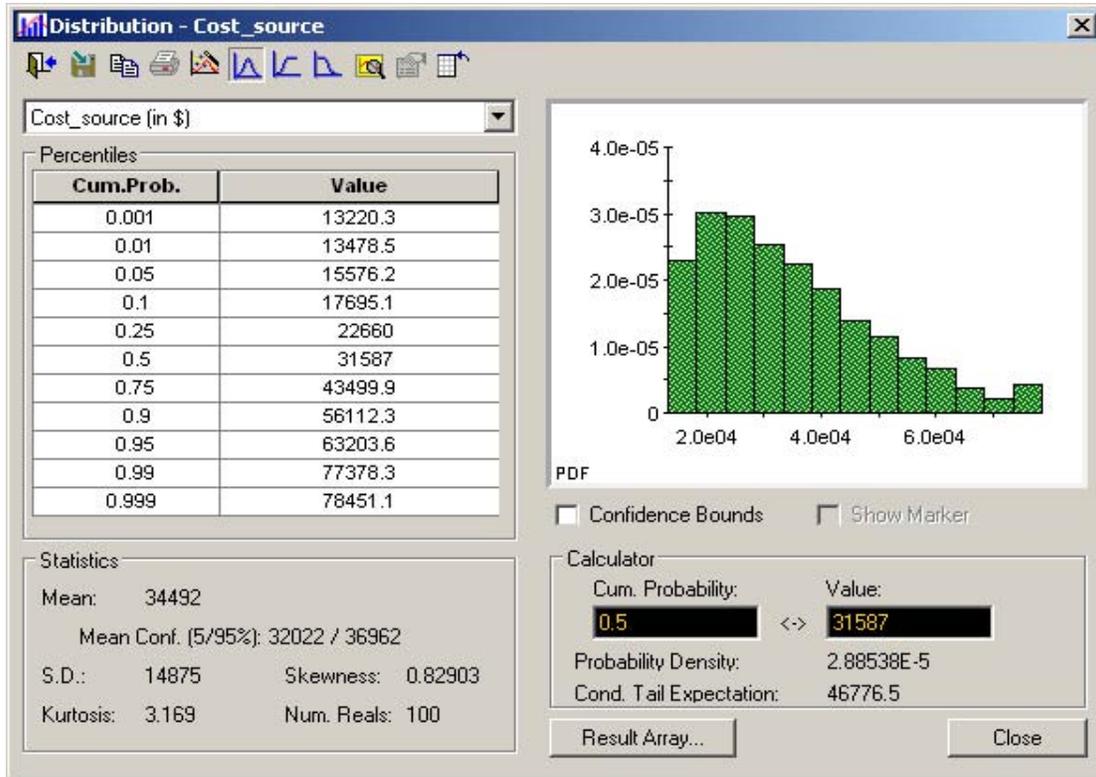


Date/Time	Mean	Lower Bound	5%	25%	Median	75%	95%	Upper Bound
Jul 02, 2014	171.7	15.341	40.473	95.89	141.48	226.18	370.21	537.05
Jul 02, 2015	75.761	3.1197	6.5392	31.072	62.611	99.103	207.12	292.92
Jul 01, 2016	71.389	2.5541	6.0057	26.673	60.302	94.093	201.86	283.57
Jul 02, 2017	70.876	2.5345	5.8697	26.424	59.963	93.738	200.29	281.42
Jul 02, 2018	70.537	2.5285	5.8529	26.3	59.782	93.449	199.33	279.58
Jul 02, 2019	70.211	2.523	5.8431	26.18	59.605	93.163	198.42	277.78
Jul 01, 2020	69.886	2.5175	5.8333	26.06	59.41	92.877	197.51	275.98
Jul 02, 2021	69.563	2.512	5.8236	25.941	59.191	92.593	196.61	274.19
Jul 02, 2022	69.241	2.5065	5.8138	25.823	58.974	92.309	195.71	272.4
Jul 02, 2023	68.921	2.5011	5.8041	25.705	58.726	91.783	194.82	270.62
Jul 01, 2024	68.602	2.4956	5.7945	25.588	58.477	91.245	193.93	268.85
Jul 02, 2025	68.284	2.4902	5.7848	25.472	58.229	90.71	193.04	267.08
Jul 02, 2026	67.968	2.4848	5.7751	25.372	57.983	90.177	191.4	265.32
Jul 02, 2027	67.653	2.4794	5.7655	25.288	57.737	89.647	189.78	263.56
Jul 01, 2028	67.339	2.474	5.7559	25.205	57.492	89.12	188.16	261.81
Jul 02, 2029	67.027	2.4687	5.7463	25.122	57.248	88.595	186.55	260.07

From the chart view, the remediation goal (red dotted line) is close to the 95th percentile. From the table view, the 95th percentile concentration at 100m in 2025 is about **193 ug/l** and the upper bound concentration 2025 is about 267 ug/l. The remediation effort would meet the goal with about 95% certainty. Compared to the previous case, the addition of the plume bioremediation along with the original source remediation increased the chance of meeting the remediation goal. The new design including the source remediation and the enhanced plume biodegradation appears to be robust.

A remediation cost analysis is also conducted during the simulation. Select **Total Cost** from the main interface to view the statistics and the distribution of the total remediation cost. The mean total cost is **\$527,500**. Select **Source Cost** from the main interface to view the statistics and the distribution of the source remediation cost. The mean total cost is **\$34,500**. Select **Plume Cost** from the main interface to view the statistics and the distribution of the plume remediation cost. The mean total cost is **\$493,000**.





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