DG>Plume

User Manual

(Release 1.7, October 2002)

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About DG>Plume

This is DG>Plume version 1.7 DG>Plume is a dedicated tool for calculating the transport of contaminants in an uniform flowfield. GeoDelft started developing DG>Plume in 2001. DG>Plume is a graphical user interface around the existing programs AT123D (for the calculation of transport of contaminants) and PRISM (for making probabilistic calculations) See the Introduction [Chapter 1] for more information about DG>Plume.

History

AT123D. AT123D, analytical, transient One-, Two-, and Three-Dimensional Model, is an analytical groundwater transport model. AT123D computes the spatial-temporal concentration distribution of contaminants in the aquifer system and predicts the transient spread of a contaminant plume through a groundwater aquifer**.** AT123D was originally developed at Oak Ridge National Laboratory, Oak Ridge, Tennessee. The first relase was in 1981 by Dr Yeh, who is currently at Pennsylvania State University, Dept. of Civil Engineering, University Park, PA 16802. The International Ground Water Modeling Center (IGWMC) has made some improvements and corrections. GeoDelft has used the IGWMC AT123D version 1.31 (November 1996) as a base version for the development of DG>Plume (Yeh, 1996).

PRISM. PRISM is a system of programs designed to efficiently evaluate the uncertainity associated with modelpredictions as a result of uncertainities associated with model parameters. The PRISM has been developed by the Studsvik Energteknik. The program was released in 1983 and is best known for studies on the risks of nuclear waste. [Gardner, R.H., B. Rojder and U. Bergstrom. 1983}

DG>Plume. DG>Plume is a graphical user interface for the combined use of AT123D and PRISM. The development of the program started in 2001.

About this manual

This manual describes how to use DG>Plume [Chapter 3],], with an explanation about the stochastic options [Chapter 4] and includes examples and a tutorial [Chapter 5] and background information to the program [Chapter 6]. This information is also available using DG>Plume's online Help function.

About GeoDelft

GeoDelft is one of the world's most renowned institutes for geotechnical and environmental research. GeoDelft is continuously applying its growing knowledge through consultancy, measurements and predictions – to projects that are often very challenging. GeoDelft actively stimulates the dissemination and utilization of its knowledge, especially through dedicated software such as DG>Plume.
For more information on GeoDelft, you can visit the GeoDelft website: http://www.geodelft.nl. For more information about geotechnical and geo-environmental software, including download options, visit http://www.delftgeosystems.nl.
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Definitions

Adsorption Distribution Coefficient. (K_d) Also called: Partition coefficient	the ratio of the concentration of a chemical species adsorbed on a soil to the concentration of the species in the soil solution.
Analytical model	Exact mathematical solutions of the flow and/or transport equation for all points in time and space. In order to produce these exact solutions, the flow/transport equations have to be simplified (e.g. very limited, if any, representation of the spatial and temporal variation of the real system).
Aquifer	A bed of saturated underground soil or rock that provides vast amounts of water
Bulk density	the ratio of the mass of dried soil to its total bulk volume (solids and pores together).
Cumulative distribution (CDF)	Mathematical function of a parameter representing the probability distribution, usually conceptualised as a graph showing the percentage of values less than or equal to a given value.function
Decay halflife time (λ)	the rate coefficient describing the first-order decay process for dissolved constituent
Dependent parameter	Two parameters are dependent if knowledge of the value of one of them alters the probability distribution of the other.
Deterministic model	A model where all elements and parameters of the model are assigned unique values.
Diffusion	the movement of a particle or substance from an area of high concentration to an area of low concentration
Dispersivity	A property that quantifies the physical dispersion of a solute being transported in a porous medium.
Distribution	Description of the frequency of observations.
Eigen value	a central concept in linear algebra (i.e. matrix algebra). The number of eigenvalues is used in DG>Plume to solve the series evaluation of the transport equation
Event	Single occurrence.
Flow gradient (also hydraulic gradient)	A coefficient of proportionality describing the rate at which water can move through a permeable medium
Flexible Emission Control (FEC)	Systematic monitoring strategy developed by GeoDelft. The contamination is controlled within 4 predefined borders. Intervention schemes are defined in the event that control levels are exceeded.
Geometric mean	Exponential of mean of logarithms, the n^{th} root of the product of n values.
Harmonic mean	Reciprocal of the arithmetic mean of the reciprocals of the observations.
Heterogeneity	Variability in space.
Histogram	A column graph showing numbers of measured values occurring within equally-spaced intervals.
Hydraulic gradient	The rate change in total hydraulic head with change in distance in a given direction. (dimensionless).

Latin Hypercube method	A sampling technique used in stochastic calculations by DG>Plume where the parameter space is sub-divided and parameter values are then picked from each interval as a way of ensuring that values are taken from the entire probability distribution.
Limit border points (also callled fail safe limit)	Imaginary points where the concentration must not exceed a predefined trigger concentration in order to protect targets in the vicinity
Log-normal distribution	A probability distribution whose logarithms are distributed normally.
Mean (arithmetic)	Arithmetic average of a set of values, $1/n^{th}$ of the sum of n values.
Median	Value for which there is a 50% probability of the actual value from a distribution being greater.
Mode	Most likely value of a set of observations.
Model	A simplification of reality in order to aid in the understanding of and/or predict the outcomes of the real system. In this report the term `model' is used to describe the code or equations plus the data.
Monte-Carlo analysis	A method of carrying out a calculation using probability distributions rather than numbers. It is simple and powerful and involves repeated sampling from the input distributions.
Normal distribution	A probability distribution characterised by a mean and standard deviation.
Numerical model	Solution of the flow and/or transport equation using numerical approximations, i.e. inputs are specified at certain points in time and space which allows for a more realistic variation of parameters than in analytical models. However, outputs are also produced only at these same specified points in time and space.
Observation points	Monitoring points where ground water samples can be taken to check the calculated concentration.
Organic carbon partition coefficient: (Koc)	Organic carbon partition coefficient is the partition coefficient in a soil divided by the organic carbon content of the soil.
Parameter (hydrogeological)	Physical property of the system under investigation (e.g. hydraulic conductivity).
Parameter (distribution)	Characteristic of a theoretical probability distribution (e.g. mean, standard deviation).
Percentile	The value below which occur a specified proportion of observations (in an ordered set of observations).
Plume	A well-defined, usually mobile, area of contamination found in surface water or groundwater.
Population	All the possible outcomes of an event, e.g. hydraulic conductivity of all possible l cm^3 of an aquifer.
Porosity	The ratio of the volume of void spaces in a rock or sediment to the total volume of the rock or sediment. (dimensionless).
Probability	Any outcome of an event can be allocated a probability p (with $0 \leq p \leq 1$) such that, if the event happened an infinite number of times, the proportion of times that this outcome occurred would be p. If p=0 then the event never occurs, and if p=1 the event always occurs.
Probability density function	Mathematical function representing the probability (PDF) distribution of a parameter, i.e. the likelihood that a given value will occur.

Probability distribution	The probabilities associated with the possible outcomes of an event. The 'event' in the context of this document is usually the value of a parameter.
Parameter of distribution	Characteristic of a theoretical distribution (e.g. mean, standard deviation).
Probabilistic model	An aggregation of model realisations, where the input parameters to each realisation are characterised by probability distributions.
Realisation	Single calculation with a single set of parameter values (in the context of repeated parameter sampling in a stochastic calculation).
Retardation	A measure of the reduction in solute velocity relative to the velocity of the advecting groundwater caused by processes such as adsorption. Mathematically, the retardation factor, R, is defined as $R=1+\rho K_d/\theta$, where ρ is bulk density, K_d is partition coefficient, and θ is volumetric water content.
Sample	A sub-set of the population.
Saturated zone	The zone of geological material that occurs below the water table, the pores of which are filled with water (soil moisture equals porosity), and the fluid pressure exceeds atmospheric
Scale dependency	The tendency of a parameter to take different values depending on the scale over which it is being measured.
Sensitivity analysis	A process of identifying the model parameters that have most effect on the model output.
Skewed distribution	A distribution which has a degree of asymmetry about the centre value of the distribution.
Stable plume (also called steady state situation)	The situation in which a groundwater plume margin is stationary and concentrations at points within the plume do not change over time. Usually defined at the front of the plume
Standard deviation	Measurement of the variability of a distribution. Square root of the variance.
Stochastic field	Used to describe the uncertainty of a parameter which varies in space.
Triangular distribution	A simple probability distribution with a PDF graph that looks like a triangle and is defined by a minimum, most likely and maximum value.
Uncertainty	The degree to which a well-defined and located parameter (e.g. the horizontal hydraulic conductivity of a 1 cm cube of rock at a defined location) is unknown.
Uniform distribution	A simple probability distribution giving equal chance for a range of values given a minimum and maximum value.
Upscaling	The process of deriving an effective value for a parameter applicable to the scale of interest, using information about the value of the parameter at a smaller scale, its variability, and the process of interest.
Trigger concentration	A concentration of a contaminant which, if exceeded, will trigger an action (e.g. the model output in DG>Plume)
Variability	The degree to which a well defined parameter varies in space and/or time, e.g. the hydraulic conductivity of all possible 1 cm cubes of rock from a particular aquifer horizon.
Variance	Measurement of the variability of a distribution. Square of the standard deviation

1 Introduction

DG>Plume is a tool used to predict the transport of contaminants. The program determines when a steady state situation is reached and how a monitoring system can be optimised. For these calculatios a probabilistic aproach is used. For a more detailed introduction too DG>Plume, see:

- For whom is DG>Plume intended? [§ 1.1]
- Why choose DG>Plume? [§ 1.2]
- Features [§ 1.3]
- System requirements [§ 1.4].

You can also switch directly to the descriptions of:

- Getting started [Chapter 2]
- Working with DG>Plume [Chapter 3]
- Tutorial with examples [Chapter 5]
- Background information [Chapter 6].

1.1 For whom is DG>Plume intended?

DG>Plume was developed especially for engineers working on projects with contaminated groundwater. With DG>Plume you can make predictions about the transport of contaminants. With special options in DG>Plume a steady state situation or a Flexible Emission Control (FEC) option can be checked. DG>Plume's graphical interactive interface requires just a short training period for novice users. This means that you can focus your skills directly on the input of the data and on the subsequent calculations.

1.2 Why choose DG>Plume?

- DG>Plume enables you to calculate the transport of contaminants efficiently and quickly. It uses powerful analytical algorithms, thereby requiring no difficult boundary conditions to be entered.
- All major transport processes are included in the model: source strength, dispersivity (horizontal and vertical), diffusion, adsorption (retardation) and decay (first order).
- With DG>Plume you can check if and when a steady state situation will be reached
- DG>Plume is especially made to quantify FEC (Flexible Emission Control) options. In the program the reliability of the designed monitoring system can be checked
- The most simple solution is to calculate contaminant transport using fixed parameters: a deterministic calculation. But in real problems the parameters vary in a wide range. This uncertainty may be quantified: each parameter can be defined stochastically, e.g. with a uniform or log normal distribution function. The easy to enter stochastic option makes this an unique transport modelling program.

- The functionality of DG>Plume will keep in step with future demands as a consequence of continuous further development.
- GeoDelft's expertise in transport of contaminants guarantees optimal usability and high-quality support.

1.3 Features

This section contains an overview of DG>Plume's options and limitations [§ 1.3.3]. For more information, see Working with DG>Plume [Chapter 3] and Background information [Chapter 6].

1.3.1 The four main options

DG>Plume offers four main options presented in Figure 1. All four options can be calculated in a deterministic as well in a stochastic way. In the stochastic mode the distribution of probability can be calculated, for example the detection of a plume by the monitoring network.

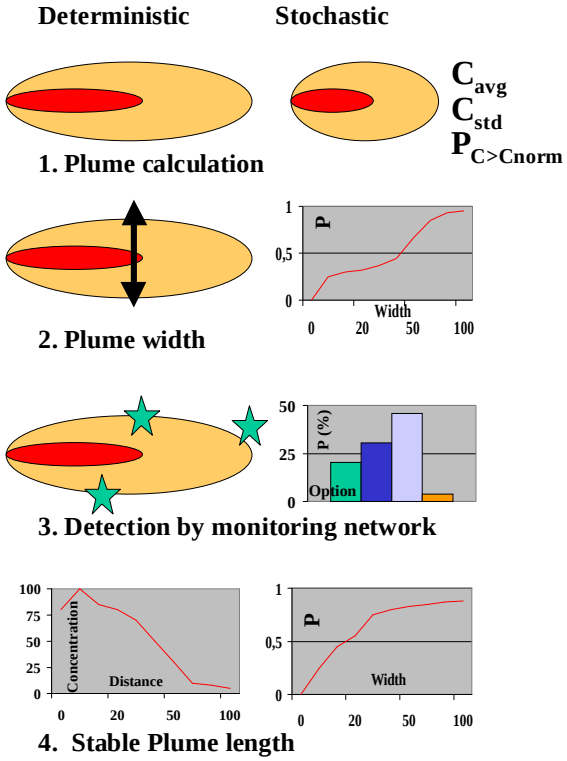


Figure 1 The four main options

1. Plume calculation

With this option concentrations of a contaminant can be calculated for different time steps and for different depths

2. Plume width

The plume width option is a useful tool for a first design of a monitoring system. With the calculated maximum width of the plume an indication of the distance of the monitoring points is given.

3. Detection by monitoring network

For the third option, the detection by the monitoring network, the probabilistic options become very useful. By making automatically calculations with different input parameters the chance of detection of the plume by the monitoring network can be quantified

4. Steady state situation

In the Netherlands a steady state situation can be an acceptable remediation option, if this situation is reached within 30 years. This can be checked with the fourth option.

1.3.2 Results

Analysis results are presented in a report, and in graphical form. The report contains a summary of the input data and the results of the calculated concentrations. You can also view graphical output of the calculated concentrations in the form of graphs or contour maps..

1.3.3 Limitations

When you work with DG>Plume, the following limitations apply:

- Uniform horizontal flowfield
- Only 1 layer
- Only 1 contaminant at a time.
- No variations of input in time

1.4 System requirements

You will need the following configuration to run DG>Plume:

- IBM-compatible PC with Pentium processor
- Windows 95/98/2000 or Windows NT 4.0 (Intel) operating system
- A minimum of 32 Mb RAM
- A minimum of 10 Mb free hard disk space
- SVGA monitor.

The following display settings are supported for DG>Plume:

- color: + 65536 colors / high color 16 bits
- resolution: 800 x 600 with small fonts
  1024x768 with small fonts
  1024x768 with large fonts

To display the DG>Plume Help texts properly, the Symbol TrueType font must be installed on your system. To be sure of a correct display on screen and paper, the font MS Sans Serif and the TrueType font Arial should be installed also.

1.5 Installation

The installation procedure for DG>Plume will vary according to the system configuration and type of license. GeoDelft will provide the proper installation instructions, together with the installation software.
If you have questions about installing DG>Plume, please contact the support team at GeoDelft: support@geodelft.nl.

2 Getting Started

This section deals with the following topics:

- Files used by DG>Plume [§ 2.1]
- How to start DG>Plume [§ 2.2]
- How the main window of DG>Plume is organized [§ 2.3]
- How to display online Help [§ 2.4]
- How to obtain support [§ 2.5]
- Program options [§ 2.6]
- File menu [§ 2.7]

2.1 Files

*.pui	Input file (ASCII): Contains the input with the problem definition. After interactive generation, this file can be reused in subsequent DG>Plume analyses.
*.pud	Output file (ASCII): After a calculation has been performed, all output is written to this file. If there are any errors in the input, they are described in this file.
*.set	Settings file (ASCII): Working file with settings data.

2.2 Starting DG>Plume

To start DG>Plume, click Start on the Windows menubar, or double-click a DG>Plume input file that was generated during a previous session. When you start DG>Plume from the Windows Menubar, the last project you worked on will open automatically, unless configured otherwise in the Program Options. DG>Plume will display the main window.

2.3 Main Window

When you start DG>Plume, the main window is displayed. This window contains a menubar [§ 2.3.1], an icon bar [§ 2.3.2] and an Input View.

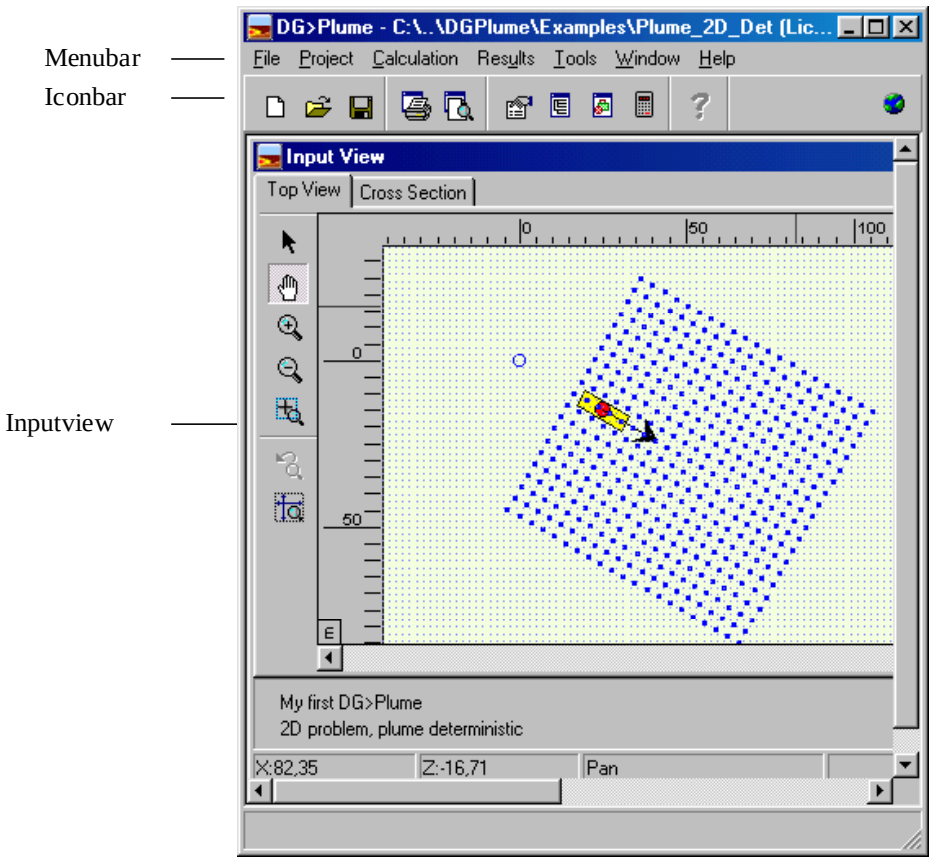


Figure 2 - DG>Plume main window

2.3.1 The Menubar

To access the DG>Plume menus, click the menu names on the Menubar.

Figure 3 - DG>Plume Menubar

The menus contain the following functions:

File	Standard Windows options for opening and saving files as well as several DG>Plume options for exporting and printing the contents of the Output View data.
Project	Options for defining Project Properties [§ 3.2], Model input [§ 3.2 and further] and the Input View.
Calculation	To start a calculation
Results	Options for presenting the results in a report, dump file, contour plot or a graph [§ 3.8].
Tools	Options for editing DG>Plume program defaults [§ 2.6].
Window	Default Windows options for arranging the DG>Plume windows and choosing the active window.
Help	Online Help [§ 2.4].

2.3.2 The icon bar

You can use the buttons on the icon bar to quickly access frequently used functions (see below).

Figure 4 - DG>Plume icon bar

Click on the following buttons to activate the corresponding functions:

 Start a new DG>Plume project.

 Open the input file of an existing project.

 Save the input file of the current project.

 Print the contents of the currently active window.

 Display a print preview of the current contents of the *Results* window.

 Open the *Project Properties* window. Here you can enter the project title and other identification data, the Graph Settings, and Contourplot settings for your project.

 Open the tree view Input window. In this window all input data is entered.

Open the Input View window

 Start the DG>Plume calculation.

 Display the contents of online Help.

2.4 Getting Help

There are a number of ways you can find the Help topic you are looking for:

Screen Help	F1	Press F1 for Help about the window in which you are working.
Contents	Help Topics	Click this button in the Help window for an overview of the available Help topics. You can search in a Table of Contents or an Index or you can use *Find* to search for specific words.
Searching by word	Search	Click this button to search for Help topics on the basis of a specific word.
Browsing through Help	<< >>	Use these buttons to browse through a series of Help topics that follow each other logically.
Extra information		When a hand is being displayed as you move the mouse over text marked in green or over an illustration, you just have to click for more information.

There are two options for printing Help topics:

In a Help window, click Print to print the contents of the window.

Mark a line in the Contents tab of the Help Topics window and click Print.
If you mark a line preceded by ?, only this topic will be printed.
If you mark a line preceded by or , all corresponding topics will be printed.

To display and print the Help texts properly, the Symbol TrueType font must be installed on your system.

2.5 Getting Support

If you encounter any problems, you should first consult the online Help and the frequently asked questions (FAQ's) at http://www.delftgeosystems.nl. If you do not find the answers you are looking for, you can e-mail (preferred) or fax your problem descriptions to GeoDelft's support team.
When you send a problem description, please add a full description of your working environment. To do this conveniently, choose the Support option in the Help menu.
The System Info tab contains all relevant information about your system and the DG>Plume software. The Problem description tab enables you to add a description of the problem you may have encountered.
You can either save your problem report to a file or send it to your printer or PC fax. You can email the document to support@geodelft.nl or alternatively fax it to (+31)(+15) 2610821.

2.6 Tools: options

On the Menubar, click Tools and then choose Options to open the corresponding input window. In this window, you can optionally define your own preferences for some of the program's default values.

View Tab

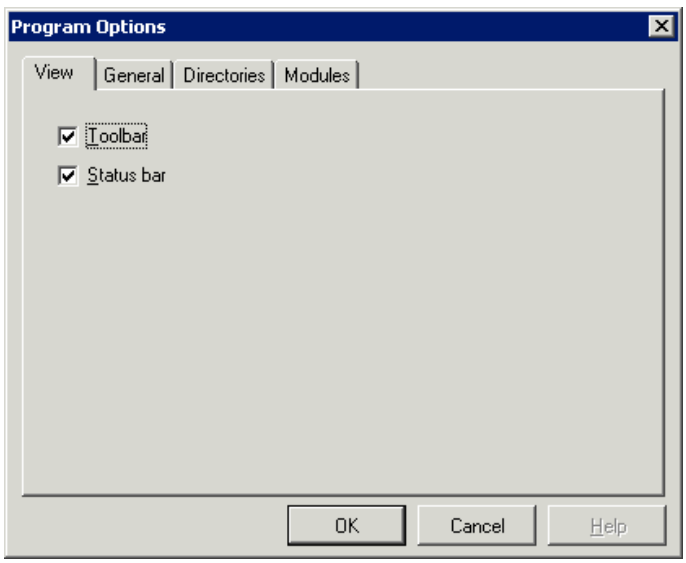


Figure 5 - Program Options window, View tab

Toolbar & Statusbar Indicate whether the toolbar and/or status bar must be displayed each time you start DG>Plume.

General tab

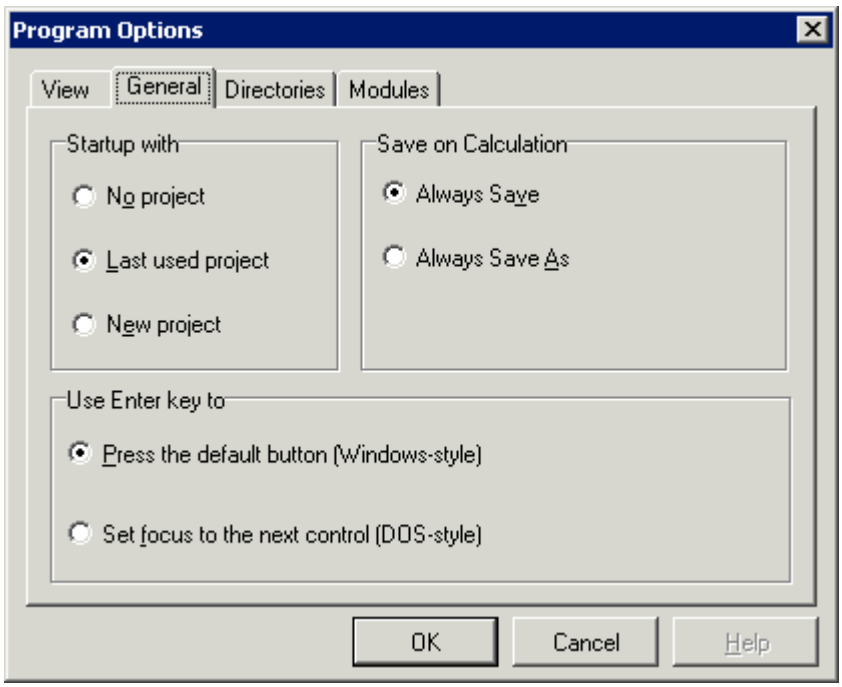


Figure 6 - Program Options window, General tab

Startup with Click one of these toggle buttons to determine whether or not a project should be opened or initiated when you start DG>Plume.

No project: Each time you start DG>Plume, you must use the buttons in the toolbar or the options in the File menu to open an existing project or start a new one.

Last used project: Each time you start DG>Plume, the last project you worked on is opened automatically.

New project: When you start DG>Plume, a new project is created. All parameters are set to 0-values.

Note that this program option is ignored when DG>Plume is being started by double-clicking an input file.

Use Enter key to The toggle buttons allow you to determine the way the Enter key is used in DG>Plume, either as an equivalent of pressing the default button (Windows-style) or to shift the focus to the next item in a window. The Enter key does not have a function in the Tree Input.

Save on calculation The toggle buttons determine how input data is saved prior to calculation. You can either save the input data automatically, using the same file name each time, or you can specify a file name each time the data is saved.

Directories tab

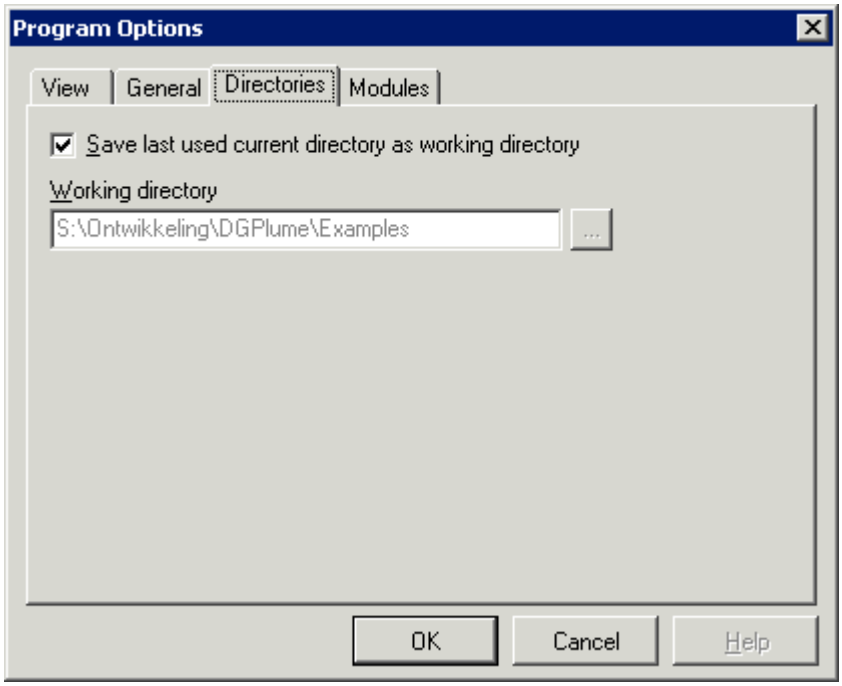


Figure 7 - Program Options window, Directories tab

Working directory

You can either automatically make the last used directory your working directory, or you can specify a default path.
This working directory is automatically set when DG>Plume is started.

Modules tab

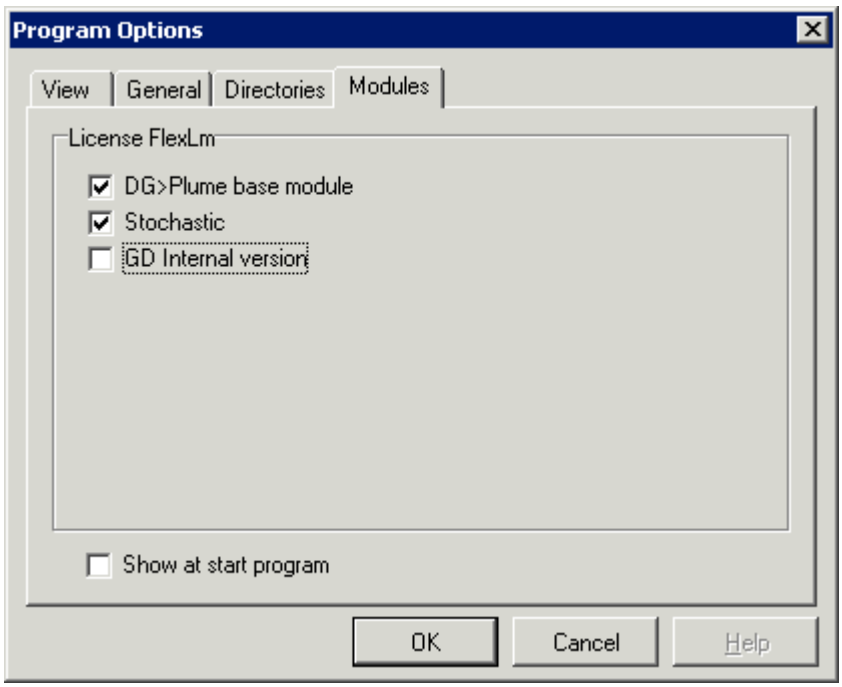


Figure 8 - Program Options window, Modules tab

Different modules can be selected. Only a module for which a licencse is obtained can be activated. When no license is obtained the model will run in demo mode (visible with the text DEMO MODE in the upper right corner of the screen). After selecting a new module you have to close and restart DG>Plume to activate the new module.

DG>Plume Base version	Base version of DG>Plume. Stochastic calculations are not possible
Stochastic	Extended version with stochastic options
GD internal version	Enable this checkbox for use of GeoDelft users of DG>Plume
Show at start program	Enable this checkbox to start DG>Plume with modules tab page

2.7 File menu

Besides the familiar Windows options for opening and saving files, the *File* menu contains a number of options specific to DG>Plume:

Copy Active Window to Clipboard
Use this option to copy the contents of the active window to the Windows clipboard so that you can paste them into another application. The contents are being pasted either in text format or Windows Meta File format.

Export Active Window
Use this option to export the contents of the active window as a Windows Meta File (*.wmf), a Drawing Exchange File (*.dxf) or a text file (*.txt).

Page Setup
The Page Setup option in the File menu allows you to define the way you want to print DG>Plume plots and reports. Here you can define the printer, paper size, orientation and margins. For plots, you can also specify whether and where axes are required.

Click 

to get DG>Plume to define how the data can best fit on the page.

Print Preview Active Window
Display a preview of the printout of the current contents of the *Outline View* window or *Result* window.

Print Active Window
Print the current contents of the *Outline View* window or *Results* window.

Print Preview Report
Display a preview of the printout of the *Report File* with all the used input parameters

Print Active Window
Print the current contents of the *Report File* with all the used input parameters

3 Working with DG>Plume

If you are a novice user, the tutorial and example files [Chapter 5] will help find your way quickly. There are reference descriptions available for the following subjects:

- Getting Started [Chapter 2]
- Input Menus [§ 3.1]
- Project Menu [§ 3.2]
- Tree Input Menu [§ 3.3 and further]
- Calculation [§ 3.7]
- View Results Menu [§ 3.8].

You can use the examples [Chapter 5] as a convenient starting point for your own project.

3.1 Input menus

Before you can start a calculation, you must enter the input data. You can do this using the following input windows:

- Project Menu [§ 3.2]
- Tree Input Menu [§ 3.3]

After entering the data, you can start the actual calculation [§ 3.7].

3.2 Project menu

The project menu can be entered on two different ways:

- On the Menubar, click *Project* and choose *Properties*:
- Click on the Properties Icon: 

The *Project Properties* window contains three tabs, on which you can change the settings for the current project:

- Identification [§ 3.2.1]
- Input View [§ 3.2.2]
- Contour Settings [§ 3.2.3]

3.2.1 Project Properties - Identification

The *Identification* tab is used to specify the project identification data:

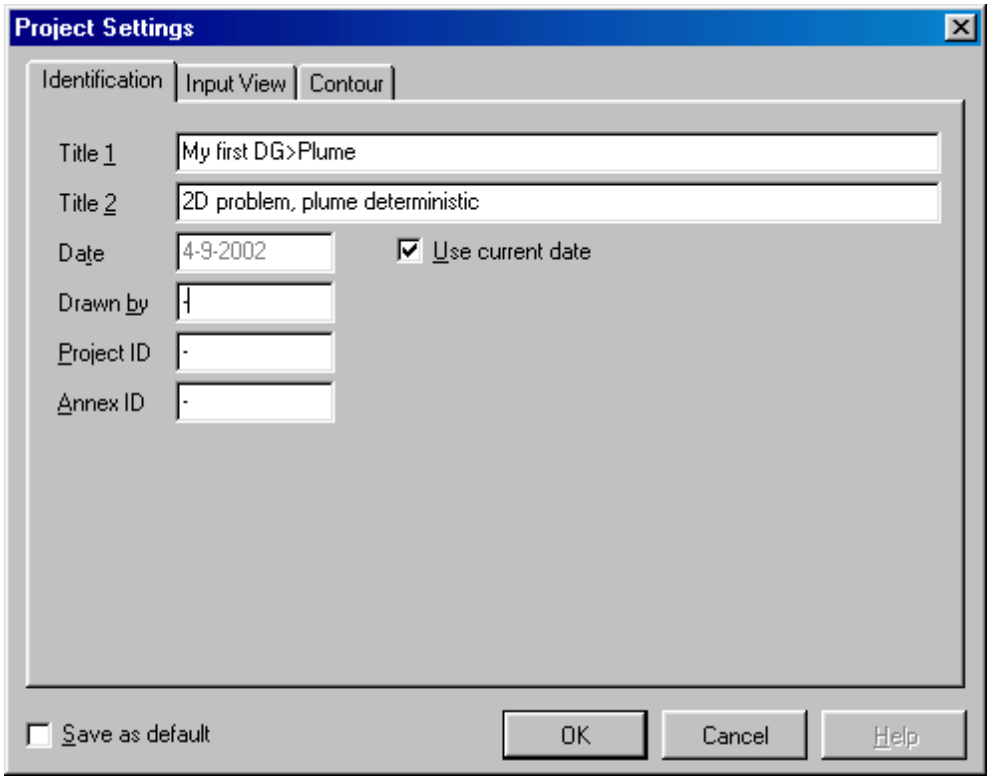


Figure 9 - Project Properties window, Identification tab

Titles	Use *Title 1* to give the calculation a unique, easily recognizable name. *Title 2* can be added to indicate specific characteristics of the calculation. Both titles will be included on printed output.
Date	The date entered here will be used on printouts and graphic plots for this project. You can either use the current date on each printout or enter a specific date.
Drawn by	Enter the name of the user performing the calculation or generating the printout.
Project ID	Enter your project identification number.
Annex ID	Specify the annex number of the printout.

Enable the checkbox Save as default if you want to use the current settings every time you start DG>Plume, or create a new project.

3.2.2 Project Properties – Input View

Use the *Input View* tab to specify the settings in the input View.

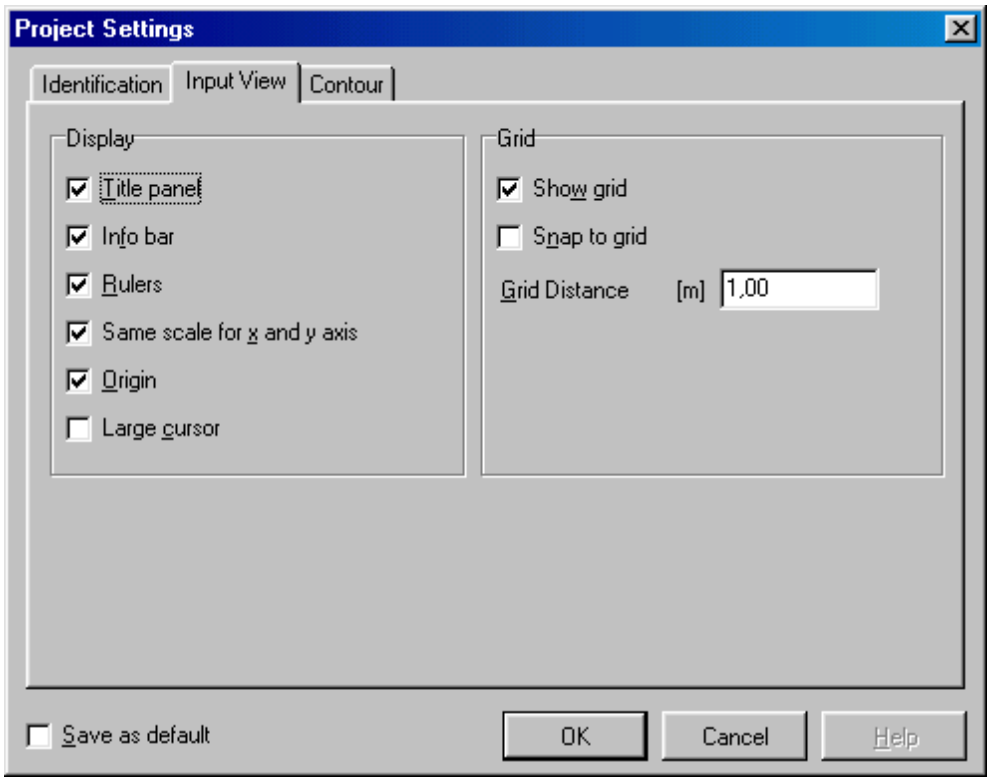


Figure 10 - Project Properties window, Input View tab

Grid

Show Grid	Enable this checkbox to display the grid points.
Snap to Grid	Enable this checkbox to ensure that objects align to the grid automatically when they are moved or positioned in a graph.
Grid Distance	Enter the distance between two grid points.

Display

Title panel	Enable this checkbox to display the title panel with the project titles at the bottom of the *Input View* window.
Infobar	Enable this checkbox to display the information bar at the bottom of the *Input View* window.
Rulers	Enable this checkbox to display the rulers.
Same scale for x and y axis	Enable this checkbox to display the x and y axis with the same scale.
Origin	Enable this checkbox to draw a circle at the origin.
Large cursor	Enable this checkbox to use the large cursor instead of the small one.

Mark the checkbox Save as default if you want to use the current settings every time you start DG>Plume.

3.2.3 Project Properties - Contour Settings

Use the *Contour Settings* tab to specify the settings for the graphic representation of calculation results in a contour plot [§ 3.8.3].

Figure 11 - Project Properties window, Contour Plot Settings tab

Display

Title panel	Enable this checkbox to display the title panel with the project titles at the bottom of the Contour Plot window.
Infobar	Enable this checkbox to display the information bar at the bottom of the Contour Plot window.
Legend	Enable this checkbox to display the legend
Options panel	Enable this checkbox to display the options panel at the top of the Contour plot window. With the options panel the number of colors can be adjusted within the contour plot window
Same scale for x and y axis	Enable this checkbox to display the x and y axis with the same scale.
Rulers	Enable this checkbox to display the rulers
Mesh	Enable this checkbox to display the contour mesh.

Contour options

Shades visible	Enable this checkbox to display the colour shades
Lines visible	Enable this checkbox to display the contour lines
Autorefresh	Enable this checkbox to refresh the contour plot automatically every time an option has been changed in the Contour Properties
Palette	Choose the desired colour scheme
Legend decimals	Enter the desired number of decimals in the legend

Contour range

Autorange	Choose this option for automatic display of the contours within the minimum and maximum calculated values
Manual range	Choose this option for display of the contours within the chosen range of concentration values

Mark the checkbox Save as default if you want to use the current settings every time you start DG>Plume

3.3 Tree input menu

The project menu can be entered on two different ways:

- On the Menubar, click Project and choose Input:
- Click on the Properties Icon: 

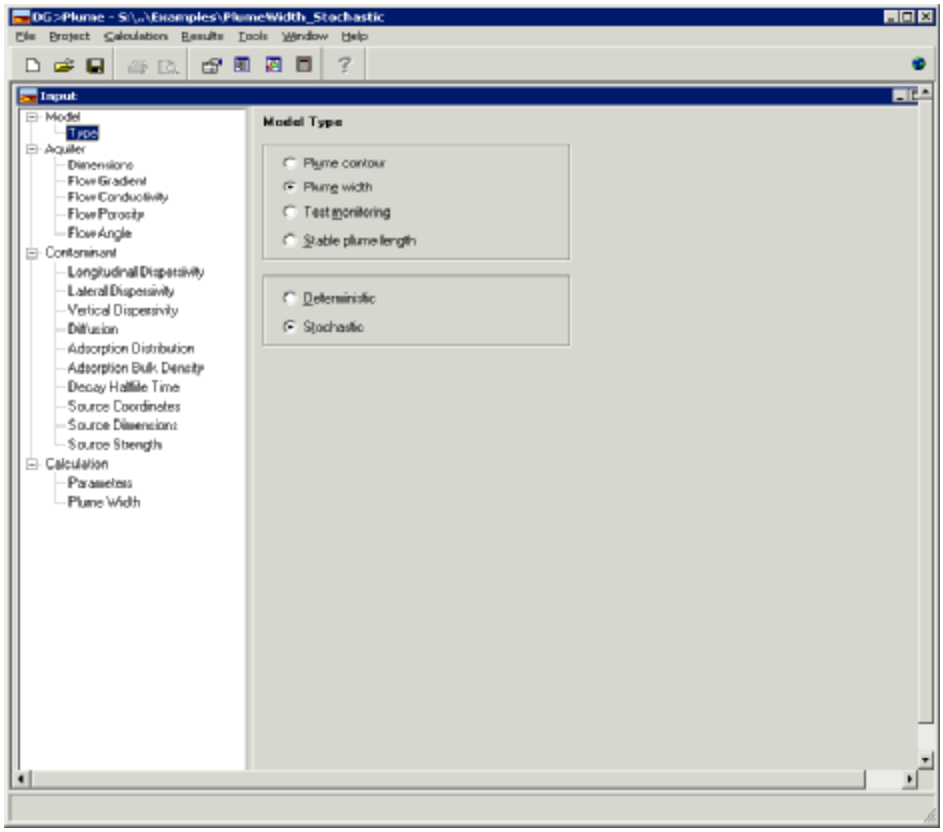


Figure 12 Tree Input Menu; Model Type

3.3.1 Tree input Menu: Model Type

With DG>Plume four types of calculation can be made. The input starts with a choice of one of these calculation types.

1. Plume calculation

With this option concentrations of a contaminant can be calculated for different time steps and for different depths

2. Plume width

The plume width option is a useful tool for a first design of a monitoring system. With the calculated maximum width of the plume an indication of the distance of the monitoring points is obtained.

3. Detection by monitoring network

For the third option, the detection by the monitoring network, the probabilistic options become very useful. With different input parameters the chance of detection of the plume by the monitoring network can be quantified

4. Steady state situation

In the Netherlands a steady state situation can be an acceptable remediation option, if this situation is reached within 30 years. This can be checked with the fourth option.

The backgrounds of the four options are described in more detail with examples of all four options in the tutorial [Chapter 5].

Secondly a choice has to be made between a deterministic and a stochastic calculation. It is advised to start with a deterministic calculation. Later the calculation can be done stochastically. Backgrounds about stochastic calculations are presented in Chapter 4.

3.4 Tree input menu: Aquifer

The text for this paragraph is partly extracted from the BIOCHLOR user manual [Aziz, C.E. et al, 2000].

3.4.1 Aquifer dimensions

DG>Plume calculates a semi-analytical solution for a indefinite flow field. The user can limit the aquifer boundaries by enabling the checkboxes *Finite Height* and *Finite Width* and entering the co-ordinates between the desired limits (Y1,Y2,Z1,Z2).

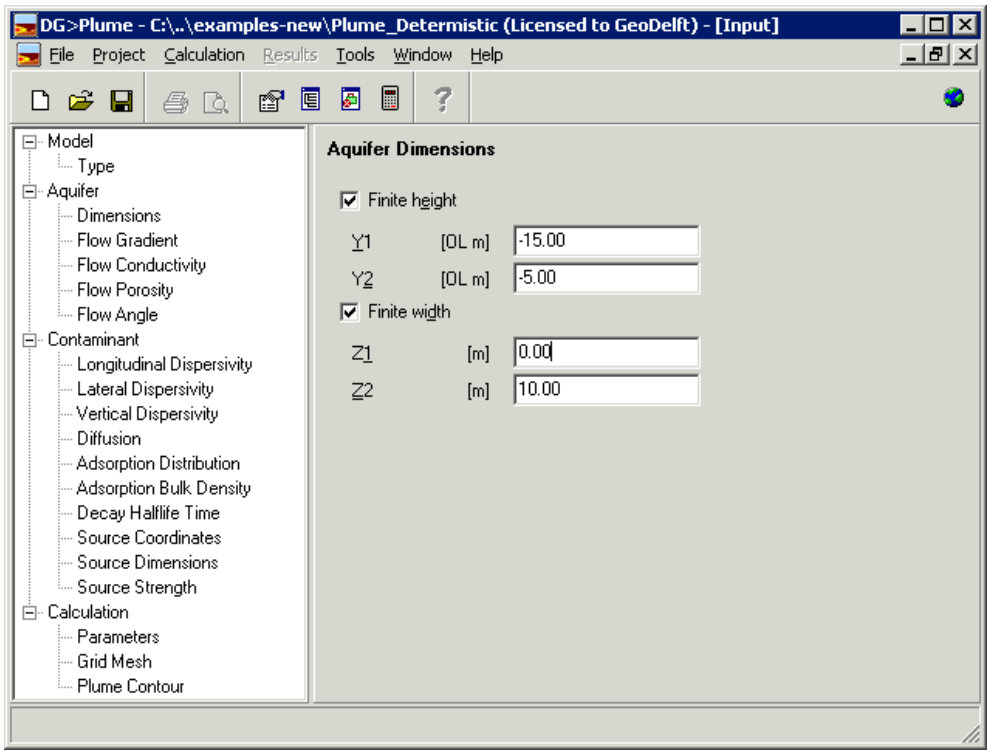


Figure 13 – Tree Input Menu, Aquifer

Note: the height of the co-ordinates is defined in the Y-direction (see Figure 14).

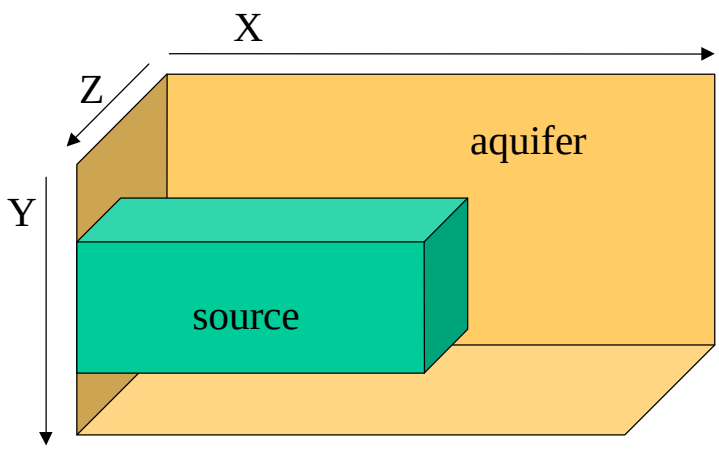


Figure 14 – Definition of dimensions of the aquifer and the source

3.4.2 Flow gradient

Parameter	**Flow gradient (i)**
Units	m/m
Description	The slope of the potentiometric surface. In unconfined aquifers, this is equivalent to the slope of the water table.
Typical values	0.0001 - 0.02 m/m
Preferable probabilistic distribution	Uniform
Source of data	Calculated by constructing potentiometric surface maps using static water level data from monitoring wells and estimating the slope of the potentiometric surface.

3.4.3 Flow conductivity

Parameter	**Flow conductivity (k)**
Units	m/d
Description	Horizontal hydraulic conductivity of the saturated porous medium; a coefficient of proportionality describing the rate at which water can move through a permeable medium.
Typical values	Clays: < 0.001 m/d Silts: 0.001 – 1 m/d Silty sands: 0.01 – 100 m/d Clean sands: 0.1 – 100 m/d Gravels: > 100 m/d Note: DG>Plume is intended for horizontal flow only. Therefore it is advised not to enter low conductivity values (e.g. for clay)
Preferable probabilistic distribution function	Log-normal
Source of data	Pump tests or slug tests at the site

3.4.4 Flow porosity

Parameter	**Flow porosity (n)**
Units	m^3/m^3
Description	Dimensionless ratio of the volume of interconnected voids to the bulk volume of the aquifer matrix. Note that "total porosity" is the ratio of all voids (included non-connected voids) to the bulk volume of the aquifer matrix. Differences between total and effective porosity reflect lithologic controls on pore structure. In unconsolidated sediments coarser than silt size, effective porosity can be less than total porosity by 2-5% (Smith and Wheatcraft, 1993).
Typical values	Values for Effective Porosity: Clay 0.01 -0.20 Sandstone 0.005 -0.10 Silt 0.01 -0.30 Unfractioned Limestone 0.001 -0.05 Fine Sand 0.10-0.30 Fractured Granite 0.00005 - 0.01 Medium Sand 0.15-0.30 Coarse Sand 0.20-0.35 Gravel 0.10-0.35 (From Wiedemeier et al., 1995; originally from Domenico and Schwartz, 1990 and Walton, 1988).
Preferable probabilistic distribution	Uniform, Normal
Source of data	Typically estimated. One commonly used value for silts and sands is an effective porosity of 0.25.

3.4.5 Flow angle

Parameter	**Flow angle (α)**
Units	Degrees
Description	Direction of the groundwater flow (clock-wise with the x-direction)
Typical values	All values between - 180 ^{0} and 180^0 è 0^0 ç 180^0 ↑ -90^0 ↓90
Preferable probabilistic distribution	Uniform, Triangular
Source of data	Calculated by constructing potentiometric surface maps using static water level data from monitoring wells

3.5 Tree input menu: Contaminant

The text for this paragraph is partly extracted from the BIOCHLOR user manual [Aziz, C.E. et al, 2000].

3.5.1 Longitudinal dispersivity

Parameter	**Longitudinal dispersivity (alpha x)**
Units	m
Description	Dispersion refers to the process whereby a dissolved solvent will be spatially distributed longitudinally (along the direction of ground-water flow), laterally (perpendicular to ground-water flow), and vertically (downward) because of mechanical mixing and chemical diffusion in the aquifer. These processes develop the "plume" shape that is the spatial distribution of the dissolved solvent mass in the aquifer. Selection of dispersivity values is a difficult process, given the impracticability of measuring dispersion in the field. However, simple estimation techniques based on the length of the plume or distance to the measurement point ("scale") are available from a compilation of field test data. Researchers indicate that dispersivity values can range over 2-3 orders of magnitude for a given value of plume length or distance to measurement point [Gelhar et al., 1992].
Typical values	One commonly used relation is to assume that alpha x is 10% of the estimated plume length.
Preferable probabilistic	Uniform, Triangular

distribution	
Source of data	Typically estimated using the relations provided above More information in literature [i.e. Gelhar et al., 1992]

3.5.2 Lateral dispersivity

Parameter	**Lateral dispersivity (alpha z)**
Units	m
Description	Dispersion refers to the process whereby a dissolved solvent will be spatially distributed longitudinally (along the direction of ground-water flow), laterally (perpendicular to ground-water flow), and vertically (downward) because of mechanical mixing and chemical diffusion in the aquifer. These processes develop the "plume" shape that is the spatial distribution of the dissolved solvent mass in the aquifer. Selection of dispersivity values is a difficult process, given the impracticability of measuring dispersion in the field. However, simple estimation techniques based on the length of the plume or distance to the measurement point ("scale") are available from a compilation of field test data. Researchers indicate that dispersivity values can range over 2-3 orders of magnitude for a given value of plume length or distance to measurement point [Gelhar et al., 1992].
Typical values	One commonly used ratio is: Alpha z: alpha x = 0.10 Based on high reliability points from [Gelhar et al., 1992]
Preferable probabilistic distribution	Uniform, Triangular
Source of data	Typically estimated using the relations provided above more information in literature [i.e. Gelhar et al., 1992]

3.5.3 Vertical dispersivity

Parameter	**Vertical dispersivity (alpha y)**
Units	m
Description	Dispersion refers to the process whereby a dissolved solvent will be spatially distributed longitudinally (along the direction of ground-water flow), laterally (perpendicular to ground-water flow), and vertically (downward) because of mechanical mixing and chemical diffusion in the aquifer. These processes develop the "plume" shape that is the spatial distribution of the dissolved solvent mass in the aquifer. Selection of dispersivity values is a difficult process, given the impracticability of measuring dispersion in the field. However, simple estimation techniques based on the length of the plume or distance to the measurement point ("scale") are available from a compilation of field test data. Researchers indicate that dispersivity values can range over 2-3 orders of magnitude for a given value of plume length or distance to measurement Point [Gelhar et al., 1992].
Typical values	One commonly used ratio is: Alpha y : alpha x = 0.05 (ASTM, 1995) Alternatively, alpha y :alpha x can be set to a very low number (e.g., E-99) to yield a conservative estimate of vertical dispersion.
Preferable probabilistic distribution	Uniform, Triangular
Source of data	Typically estimated using the relations provided above more information in literature [Gelhar et al., 1992]

3.5.4 Diffusion

Parameter	**Diffusion coefficient (D)**
Units	m^2/d
Description	Diffusion is the process of transport of contaminants due to concentration differences. The diffusion coefficient is defined as the amount of solute that passes across a unit cross section in a porous medium in unit time under the influence of a unit concentration gradient. Note that in various other transport programs this factor is included in the advective dispersion equation. In these programs the hydrodynamic dispersion is defined as the sum of the mechanical dispersion and the molecular diffusion
Typical values	This value varies somewhat for different chemicals and characteristics of the porous mediums, but a typical value to use is 8.5×10^{-5} m^2/d.
Preferable probabilistic distribution	Uniform, Triangular
Source of data	Chemical and physical reference books

3.5.5 Adsorption distribution

Parameter	**Adsorption distribution coefficient (K_d)**
Units	m^3/kg
Description	Adsorption to the soil matrix can reduce the concentration of dissolved contaminants moving through the ground water. Especially organic humus material is capable of adsorption of hydrocarbons (the longer the carbon chains the better adsorption takes place). Heavy metals are adsorbed by clays and (Fe)oxide coatings of sand grains. DG>Plume calculates the linear isotherm: the proportion between the concentration of the contaminant dissolved in water phase and the one adsorbed onto the solid phase: $K_d = S / C$ and $K_d = f_{oc} * K_{oc}$ With: C concentration of the contaminant dissolved in the water phase (kg/m^3) S concentration of the contaminant adsorbed onto the solid phase (kg/kg) K_d distribution coefficient (m^3/kg) f_{oc} fraction organic carbon on uncontaminated soil (kg/kg) K_{oc} organic carbon-water partition coefficient (m^3/kg) The distribution coefficient is used to calculate the retardation factor: $R = 1 + K_d \ r_b / n$ With: R retardation factor of the contaminant (-) ρ_b bulk density of solid soil material (kg/m^3) n porosity (m^3/m^3) the retardation factor can be seen as the ratio between the average pore water velocity and the rate of migration of the specific contaminant. A retardation factor of 5 means that the pore water is moving five times as fast as the contaminant. On the contrary, when a site is polluted it takes at least 5 pore volumes of clean water to desorp the contaminant. A retardation factor can be defined crafty by: - Setting the Kd value to: R –1 - Setting the ρ_b value (adsorption bulk density) to the same as the porosity value (the ρ_b value is only used for the calculation of the adsorption)

Typical values	Reported values for K_d cover a wide range of values for different contaminants and the values are temperature dependent: The following range of K_{oc} are reported: Benzene 0.02 - 0.4 m^3/kg Pyrene 2 - 200 m^3/g Ethyl Benzene 0.09 – 1.5 m3/kg Tetrachloroethylene 0.1- 3 m3/kg Dichloroethane 0.01 - 0.25 m3/kg Trichloroethylene 0.02 – 0.5 m3/kg Naphthalene 0.1 - 2.5 m3/kg A typical f_{oc} range is 0.0002 - 0.02 (kg/kg)
Preferable probabilistic distribution	Uniform, Triangular
Source of data	Either from an analysis of soil samples at a geotechnical lab or, more commonly estimated with the given relations above.

3.5.6 Adsorption bulk density

Parameter	**Adsorption bulk density (ρ_b)**
Units	kg/m^3
Description	the ratio of the mass of dried soil to its total bulk volume (solids and pores together).
Typical values	Although this value can be measured in the lab, in most cases estimated values are used. A value of 1650 kg/m^3 is used frequently. The following ranges are reported: Clay 1200 – 1800 kg/m^3 Silt 1100 – 1800 kg/m^3 Sand 1300 – 1900 kg/m^3 Gravel 1600 – 2100 kg/m^3
Preferable probabilistic distribution	Uniform, Normal
Source of data	Typically estimated using the relations provided above

3.5.7 Decay halflife time

Parameter	**Decay halflife time (λ)**
Units	1/yr
Description	the rate coefficient describing the first-order decay process for dissolved constituents. The first-order decay coefficient equals 0.693 divided by the half-life of the contaminant in ground water. If a dissolved solvent is undergoing first order decay only, the rate of biotransformation depends on the concentration of the contaminant and the rate coefficient. In the case of sequential first order decay, the solvent is assumed to degrade by first order kinetics. But also simultaneously it can be produced by the first order decay of the preceding compound. This can only be simulated in DG>Plume with a different model run. Considerable care must be exercised in the selection of a first-order decay coefficient for each constituent to avoid significantly over-predicting or underpredicting actual decay rates.
Typical values	Perchloroethylene 0.07 to1.20 yr^{-1} Trichloroethylene 0.05 to 0.9 yr^{-1} cis-1,2-Dichloroethylene 0.18 to 3.3 yr^{-1} Vinyl Chloride 0.12 to 2.6 yr^{-1} DDT 15 yr^{-1} Radium 1580 yr^{-1} *(from Wiedemeier et al., 1999)*
Preferable probabilistic distribution	Uniform, Triangular
Source of data	One may adopt a trial-and-error procedure to derive a best-fit decay coefficient for the contaminant by varying the decay coefficient until predicted concentrations match measured concentrations. Literature Values: Various published references are available listing biotransformation rate coefficients (e.g., USEPA, 1998; Howard et al., 1991). Many references report the half-lives; these values can be converted to the first order decay coefficients using k = 0.693 / (dissolved solvent half-life time). Other Methods: The "Technical Protocol for Evaluating Natural Attenuation of Chlorinated Solvents in Ground Water" (USEPA, 1998) describes other methods for obtaining rate coefficients, including the use of microcosm data and use of field tracer tests

3.5.8 Source co-ordinates and source dimensions

The extent of the source of the contamination can be entered in the menus *Source Co*-ordinates and Source Dimension. First the origin (X,Y,Z co-ordinate) of the source is entered in the menu Source co-ordinates. From this point the extent of the contamination is defined with the Source dimensions menu.

Note: the height of the co-ordinates is defined in the Y-direction (Figure 14)

Depending on the source co-ordinates the source can be:

- A point ($x_1 = x_2$, $y_1 = y_2$, $z_1 = z_2$)
- A line (e.g. $y_1 = y_2$, $z_1 = z_2$)
- An area (e.g. $y_1 = y_2$)
- A volume

The calculation will be one dimensional if y_1 and y_2 corresponds with the aquifer dimensions (height) and z_1 and z_2 corresponds with the aquifer width. The calculation will be two dimensional if either (y_1, y_2) or (z_1, z_2) corresponds with the aquifer dimensions.

3.5.9 Source strength

The source strength is entered in the menu *Source Strength.*

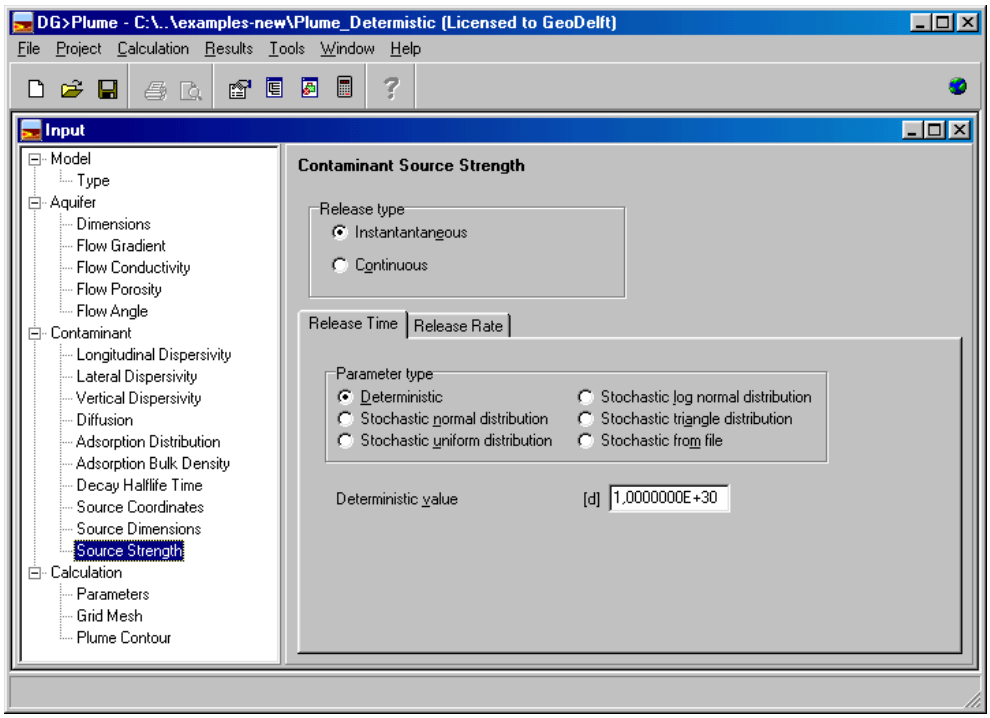


Figure 15 Contaminant source strength

Release type Instantaneous	Enable this checkbox to choose a source which releases instantaneous (eg. in case of a temporary emergency, like a suddenly emptying tank)
Release type Continuous	Enable this checkbox to choose a source which releases a continuous contamination (for a sequence of days or years; e.g. a slowly leaking tank). The source strength is defined in a release per day (kg/d). This means no concentrations are defined as input value
Release time	For a *continuous* source: Time in days when the contamination ends (the contamination starts spreading at day1). For an *instantaneous* source: Time in days of the 'accident'
Release rate	For a *continuous* source: Emission in kg/d of the contamination For an *instantaneous* source: Total amount of contamination in kg

3.6 Tree input menu: Calculation

The calculation parameters are dependent on the choice of one the four options [see § 3.3.1]. Therefore the calculation options are described separately for the four model types. First the general calculation parameters are described [see § 3.6.1]

3.6.1 Calculation: Parameters

Dependent on the choice of calculation type the calculation parameters are defined:

- Deterministic (with one fixed value per parameter)
- Stochastic (with a Probability Distribution Function per parameter

It is advised to start with a deterministic calculation.

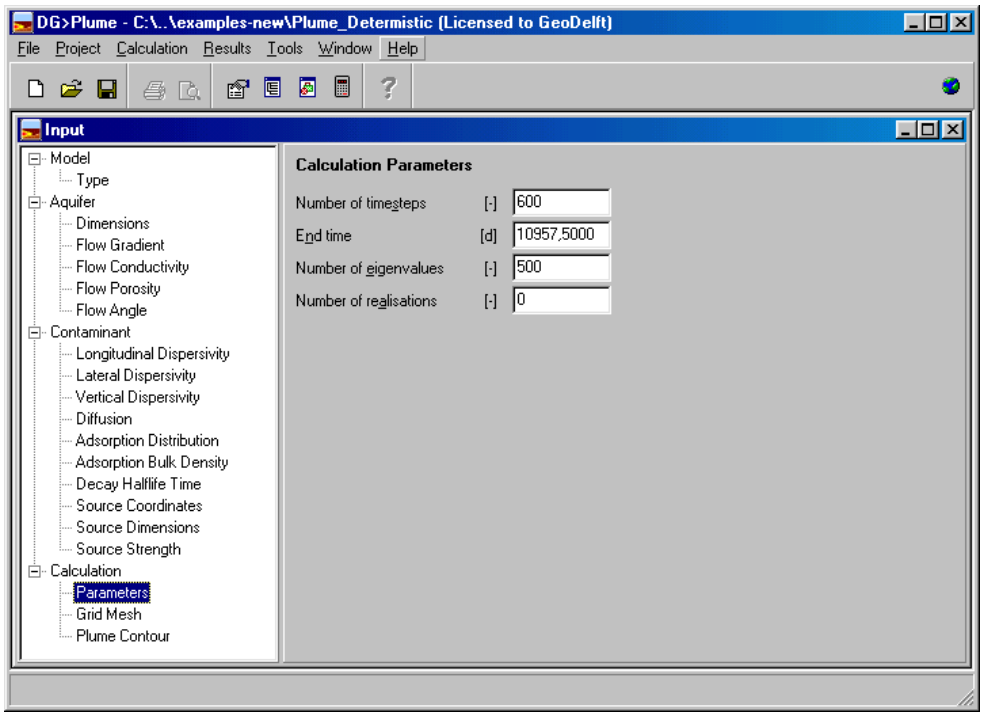


Figure 16 Calculation parameters

The general calculation parameters for all four models are:

Number of timesteps (-)	Number of (unitless) time steps used in the calculation. Note: the chosen time steps to present in a contour plot or graph are entered later
End time (d)	End time of the calculation
Eigenvalues (-)	Number of eigenvalues used for series solution of the transport equation. The default value is set to 500. Increasing this number will improve the accuracy of the results. Decreasing this number will increase the speed of the calculation.
Number of realisations (-)	Number of calculations made with a single set of parameters. In the deterministic mode this option is not visible (and automatically set to a value of 1). With values larger than 1 a stochastic calculation is made. A minimum value of 10 is recommended. Increasing this number will improve the accuracy of the stochastic calculations.

3.6.2 Plume Contour model

With this option concentrations of a contaminant can be calculated for different time steps and for different depths. For the general calculation parameters see § 3.6.1.

3.6.2.1 Calculation Grid mesh for Plume Contour

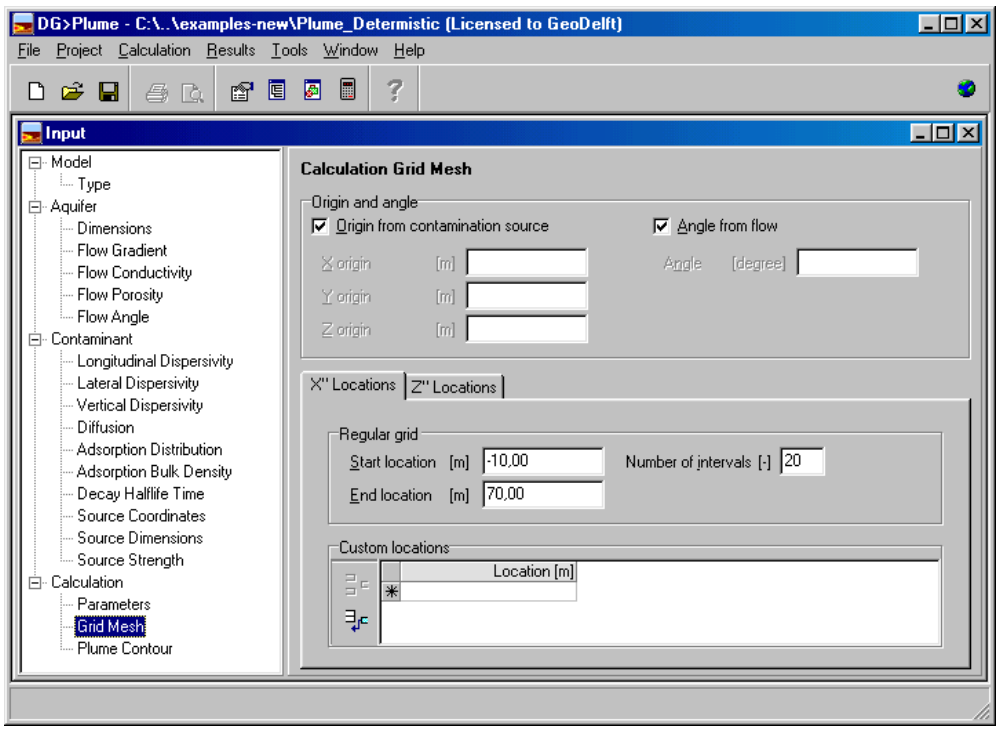


Figure 17 Grid mesh parameters for Plume contour model

Origin and Angle

Origin from contamination source	When this checkbox is enabled the origin of the grid mesh is automatically the same as the chosen origin (centre) of the contamination source. When this option is not chosen the co-ordinates have to be entered manually
Angle from flow	When this checkbox is enabled the angle of the grid mesh is automatically the same as the chosen angle of flow. When this option is not chosen the angle of flow has to be entered manually

Grid Mesh

The grid is defined in the X direction (length of the plume) and the Z-direction (width of the plume) by selecting a starting location, an end location and a number of intervals. On this grid a concentration is calculated for the presentation on a contour plot. Each grid point of the mesh can be seen on the *Input View* as a blue dot.

3.6.2.2 Calculation Plume Contour

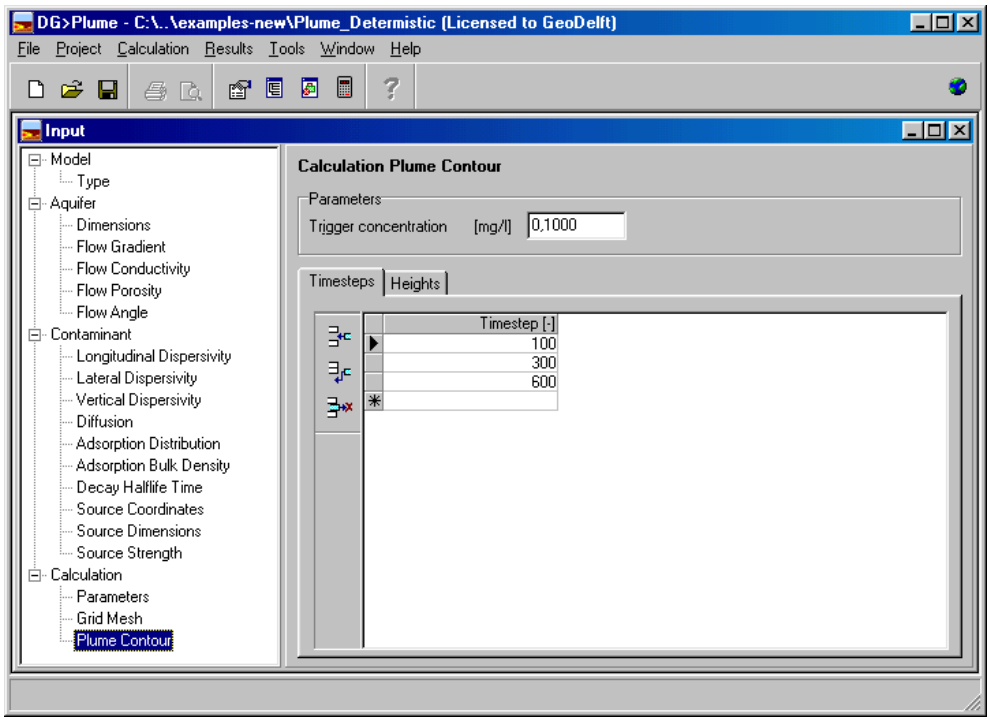


Figure 18 Plume contour: calculation parameters for Plume contour model

Trigger concentration (mg/l) This option is only used when a stochastic calculation is made. In this case the chance (%) of exceeding the trigger concentration is presented on the contour plot.

Timesteps(-) Timesteps for which a contour plot can be presented on the contour plot. The timesteps are (unitless) steps within the interval defined in *Calculation Parameters*[§ 3.6.1]

Rows can be added or deleted with the icons besides the rows:  and 

Heights Height relative to the defined origin for which a contour plot can be presented on the contour plot.

Rows can be added or deleted with the icons besides the rows:  and 

3.6.2 Plume Width model

The Plume Width option is an useful tool for a first design of a monitoring system. The calculated maximum width of the plume can be used as a first guess for the distance between the monitoring points. For a good understanding of the concept see the chapter about Flexible Emission Control [§ 6.1] and the tutorial [§ 5.4]

In the Plume Width option the observation points and intervention point can be defined. The location of the points can be checked in the Input View Window (see Figure 19). For the general calculation parameters see § 3.6.1.

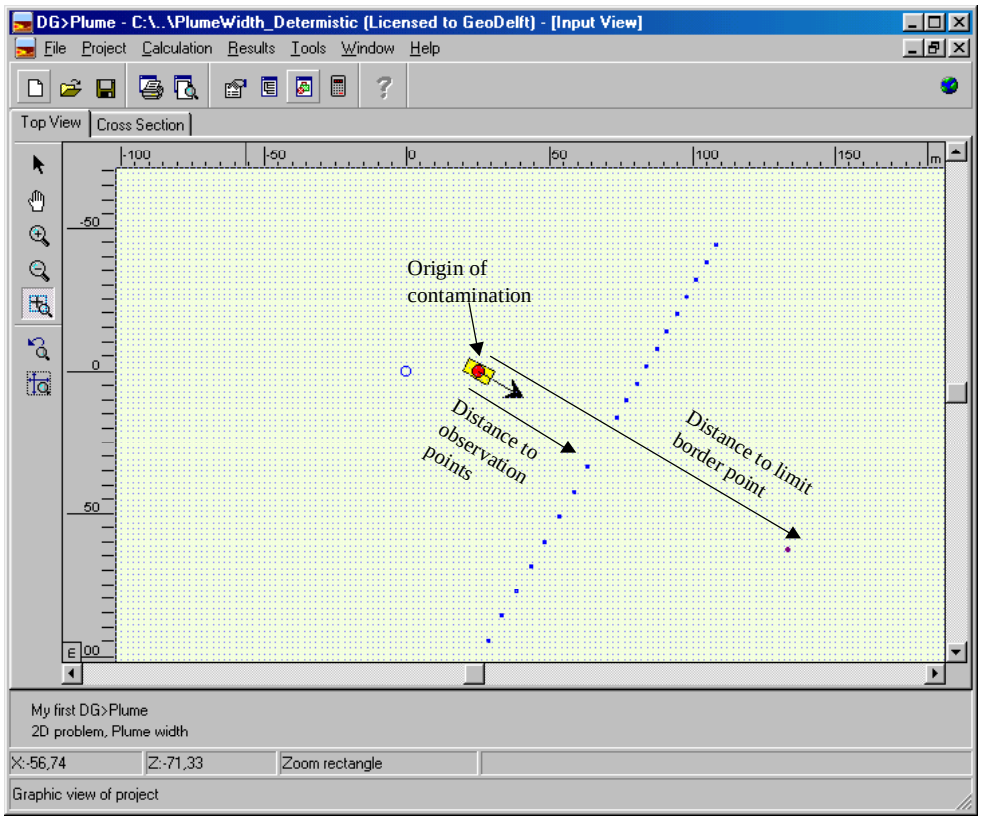


Figure 19 Input view: Plume width model

3.6.3 Plume width: parameters

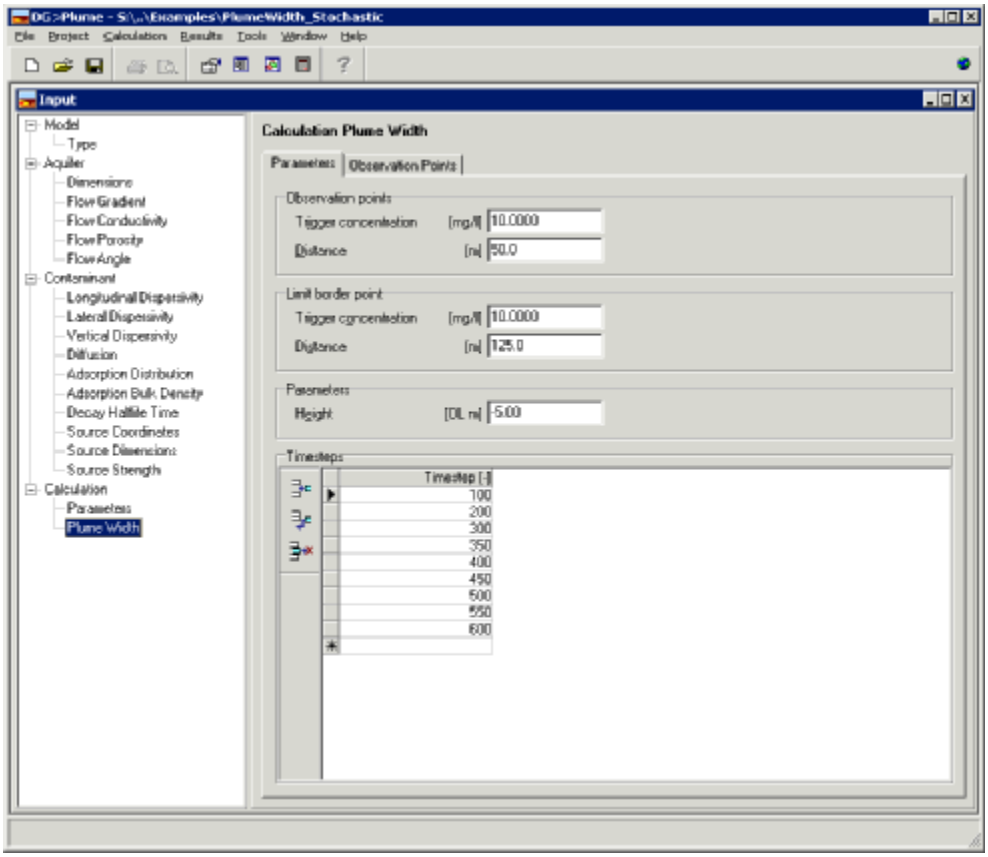


Figure 20 Calculation parameters for Plume Width model

General Parameters

Trigger concentration of observation points (mg/l)	Trigger concentration for exceedence in one of the observation points
Distance of observation points (m)	Distance of the row of observation points from the origin of the source of contamination in the direction of the ground water flow (see Figure 19). The distance is derived from the observation point nearest to the origin. The location of the observation points is defined under the Tab *Observation Points* [§ 3.6.3.1]
Trigger concentration of intervention points (mg/l)	Trigger concentration for exceedence in the intervention point
Distance of intervention	Distance of the intervention point from the origin of the source of contamination in the direction of the ground water

point (m) flow (see Figure 17).

Height Height relative to the origin for calculating the concentrations

Timesteps(-) Timesteps for which the concentrations are calculated. The timesteps are (unitless) steps within the interval defined in *Calculation Parameters.*Rows can be added or deleted with the icons besides the rows:

 and 

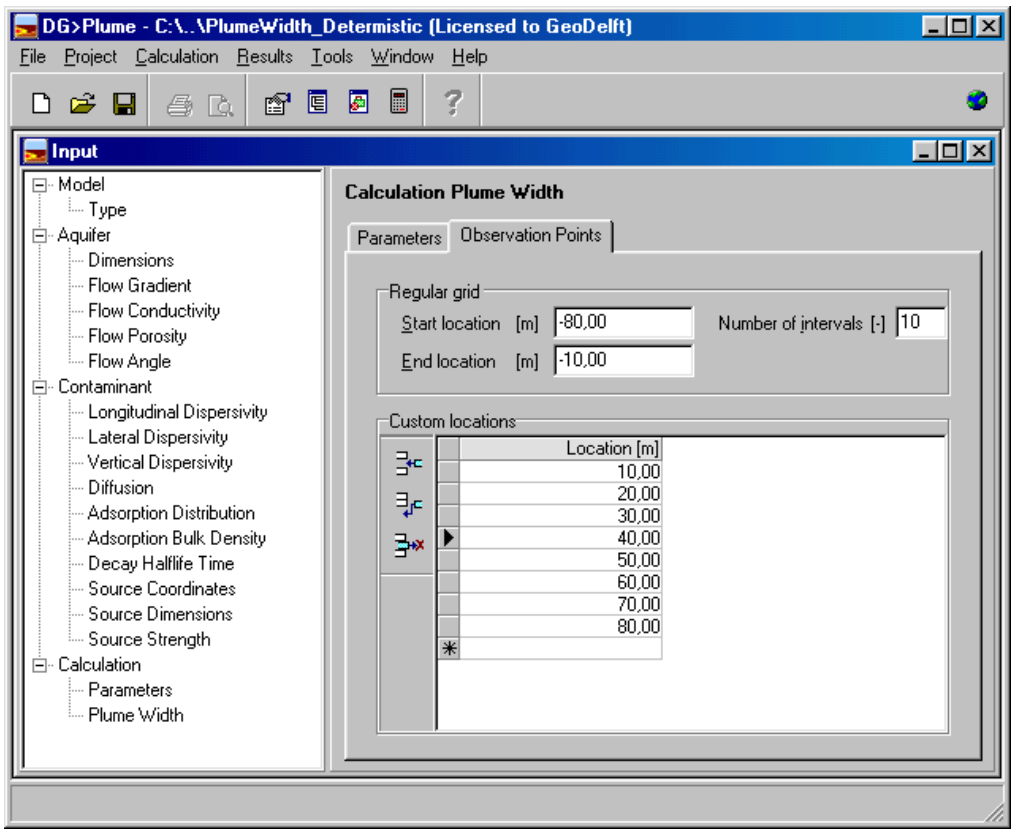


Figure 21 Observation points parameters for Plume Width model

The location of the observation points can be entered in two different ways: with a regular Grid or with Custom locations. Both ways can be combined as well. The observation points are placed on a row perpendicular to the direction of the ground water flow.

3.6.3.1 Plume width: Observation points

Observation points

Regular grid	Observation points are entered in a regular grid on a row in a fixed *Number of Intervals* between a *Start Location* and *End Location.*
Custom Locations	Custom locations can be entered per row. Rows can be added or deleted with the icons besides the rows:  and 

3.6.4 Test Monitoring model

The Test Monitoring option is an useful tool for a the design of a monitoring system.

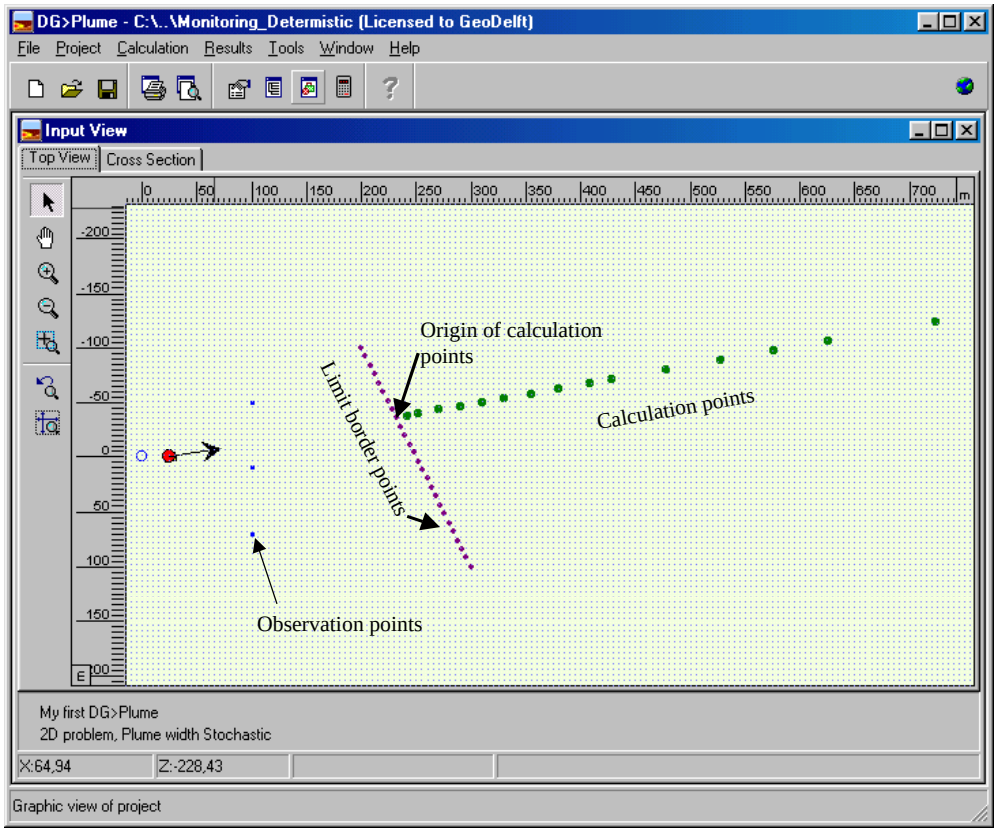


Figure 22 Input View of the Test Monitoring option

In the Test Monitoring option the observation points, the limit border point and the calculation points can be defined. DG>Plume checks whether calculated concentrations will be exceeded above a defined trigger concentration behind the limit border points (‘fail safe limit’). In that case the area of the polluted area can be calculated. Besides there is an option to check if the monitoring network is set up well for protecting the fail safe limit. The location of the points can be checked in the Input View Window (see Figure 22). For a good understanding of the FEC concept see the chapter about Flexible Emission Control [§ 6.1]. For the general calculation parameters see § 3.6.1.

3.6.4.1 Test Monitoring Parameters

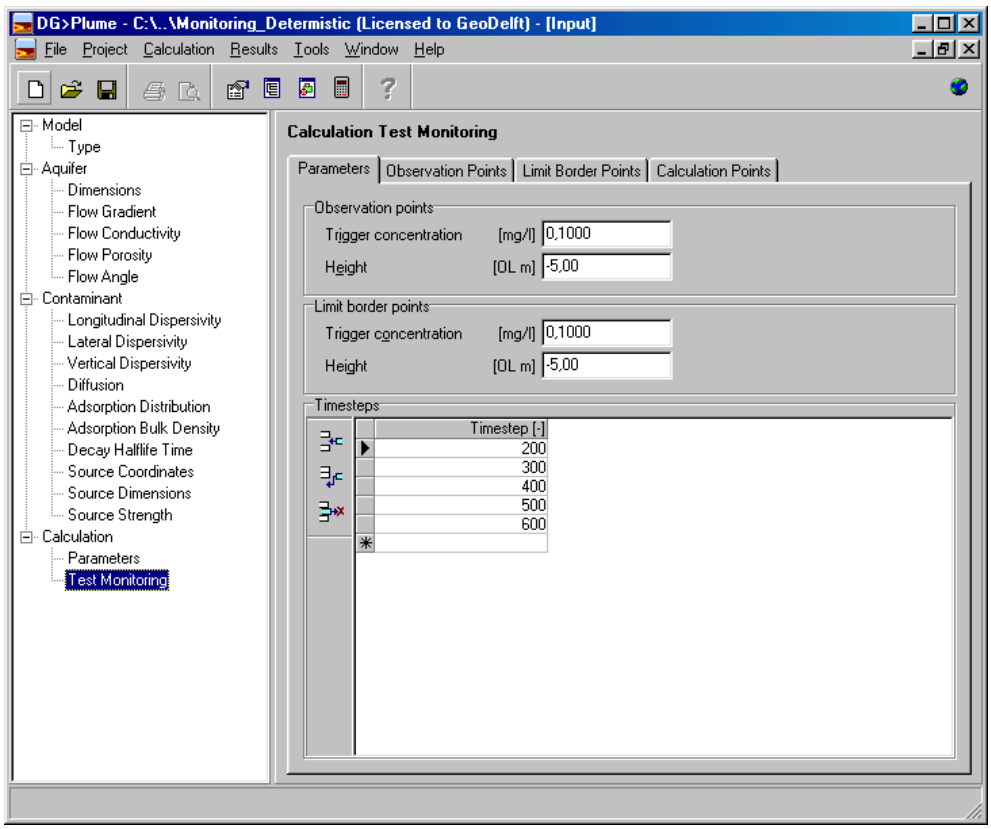


Figure 23 General Parameters for Test Monitoring model

Parameters

Trigger concentration of observation points (mg/l)	Trigger concentration for exceedence in one of the observation points
Height observation point(m)	Height relative to the origin where the exceedence of the trigger concentration in the observation points is checked
Trigger concentration of limit border (mg/l)	Trigger concentration for exceedence in the limit border points

Height limit border point(m) Height relative to the origin where the exceedence of the trigger concentration in the limit border points is checked

Timesteps Timesteps for which the concentrations are calculated. The timesteps are (unitless) steps within the interval defined in *Calculation Parameters.* Rows can be added or deleted with the icons besides the rows:

 and 

3.6.4.2 Test Monitoring: Observation points

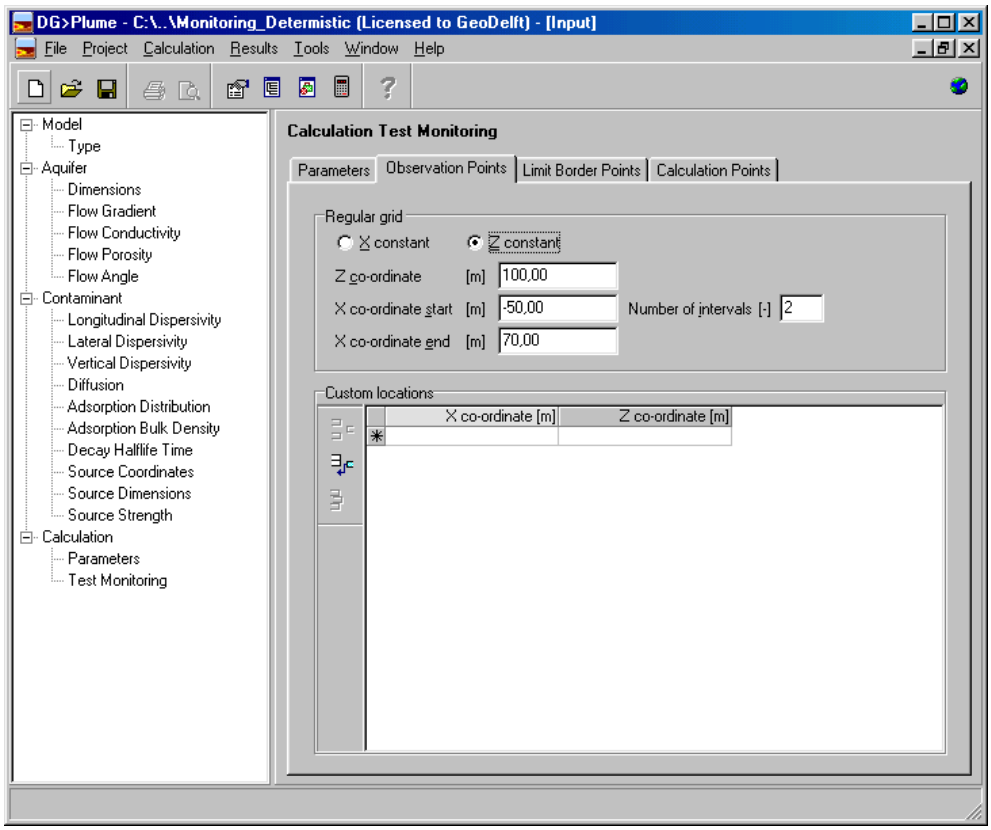


Figure 24 Observation points parameters for Test monitoring model

The location of the observation points can be entered in two different ways: with a *Regular Grid* or with *Custom locations*. Both ways can be combined as well.

Observation points

Regular grid Observation points are entered in a regular grid with either a fixed X co-ordinate or a fixed Z-co-ordinate.

Custom Locations Custom X,Z locations can be entered per row. Rows can be added or deleted with the icons besides the rows:

 and 

3.6.4.3 Test Monitoring: Limit Border points

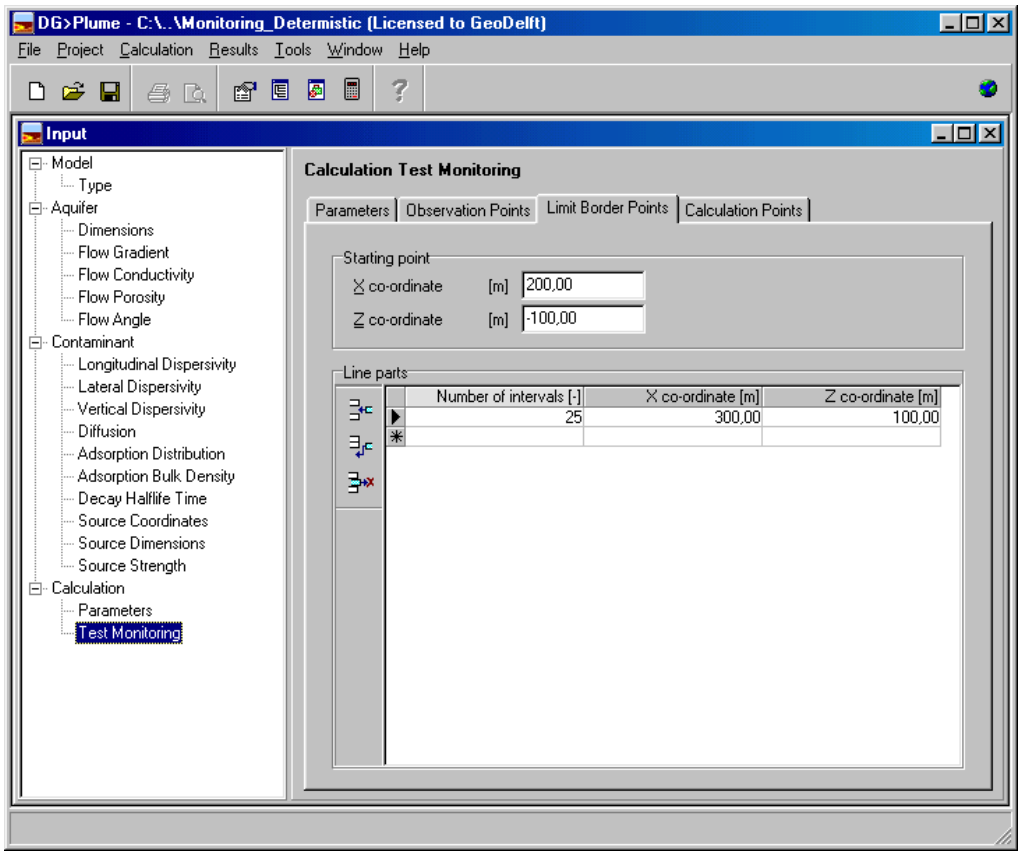


Figure 25 Test monitoring model: Limit border points parameters for

Limit border points

Starting point	X and Z co-ordinate of first limit border point
Line parts	Limit border line between the defined Starting Point and the entered X and Z co-ordinate. The number of points are defined in the *Number of Intervals.* More lines of limit borders can be added of removed with the icons besides the rows:  and 

3.6.4.4 Test Monitoring: Calculation Points

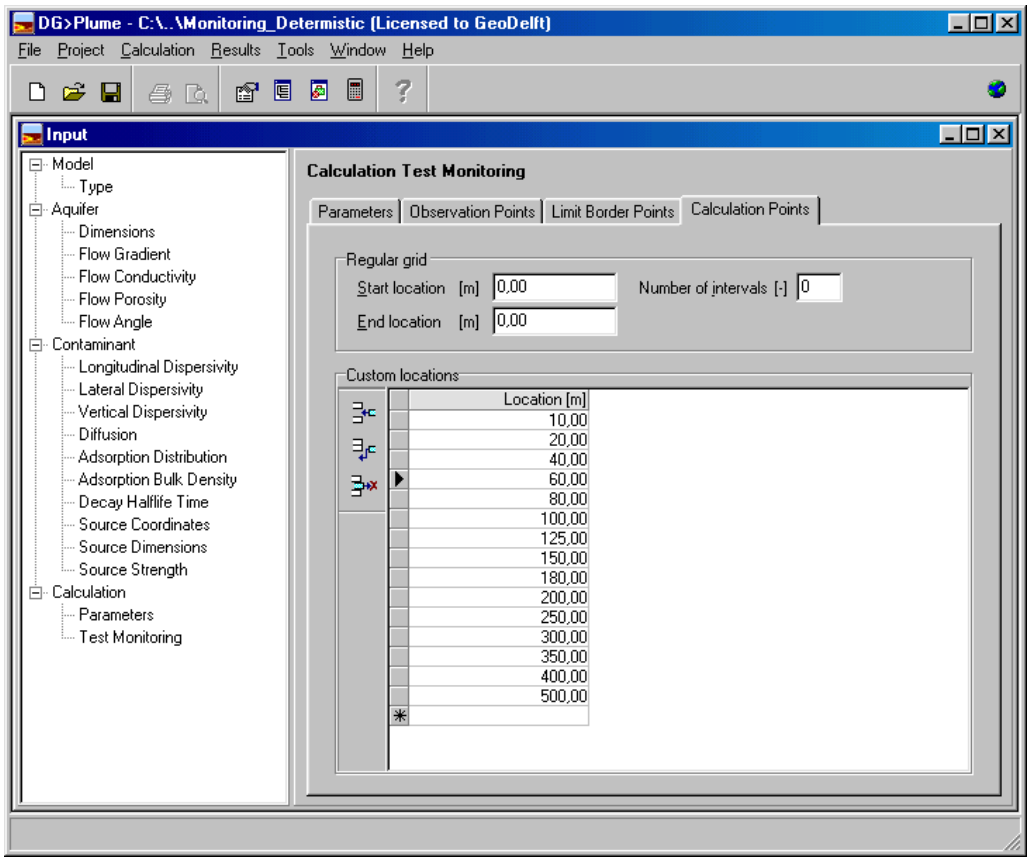


Figure 26 Test monitoring model: Calculation points

Calculation points are used for the calculation of the polluted area. Therefore the origin (0,0) of the calculation poins is located in the centre of the limit border. Negative co-ordinates for the calculation points can not be entered.

The program checks if the calculated concentration exceeds the defined trigger value for the limit border points. Calculation points can be entered in a regular grid or at customs locations. A combination of the two is possible as well. The last calculation point should be placed far enough for the the calculation of the polluted area. Else DG>Plume will give a warning in the dump file.

Calculation points

Regular grid	Calculation points are entered in a regular grid in a regular *Number of Intervals* between a *Start Location* and *End Location*
Custom Locations	Custom X,Z locations can be entered per row. Rows can be added or deleted with the icons besides the rows:  and 

3.6.5 Stable Plume Length Model

With the Stable Plume Length option it can be checked if and when a steady state situation is reached in the calculation points (located on row in the direction of the groundwater flow). For the general calculation parameters see § 3.6.1.

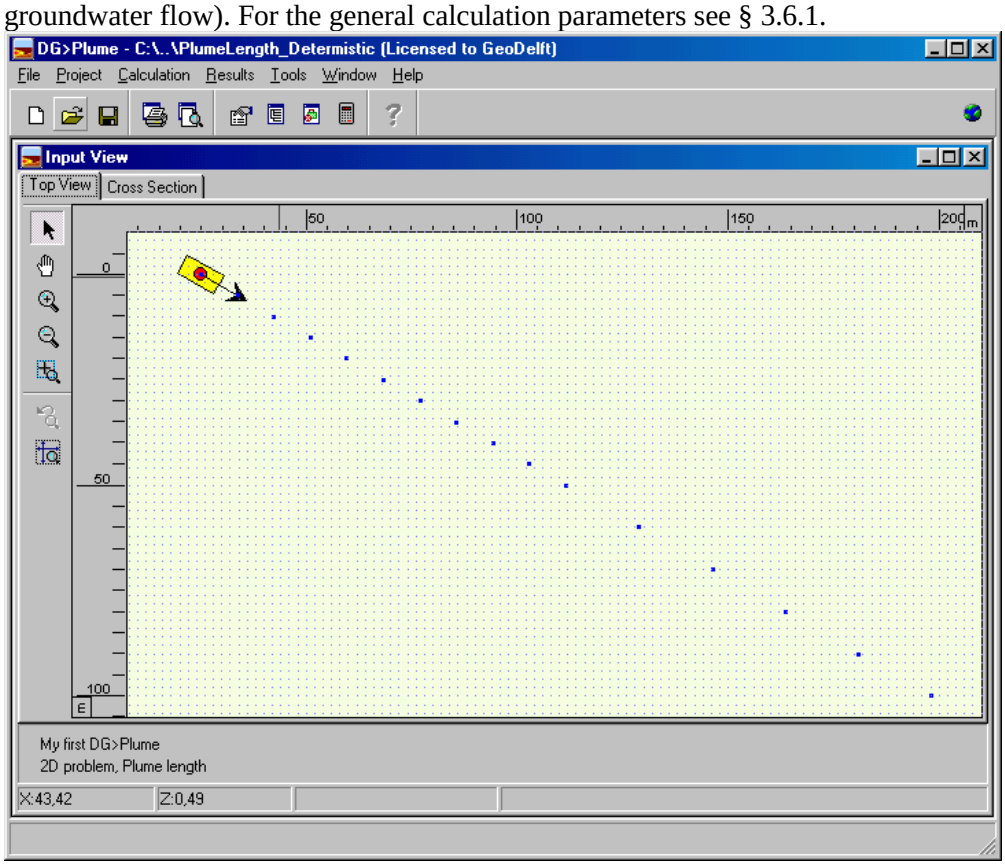


Figure 27 Input View of the Stable Plume Length option

3.6.6 General parameters

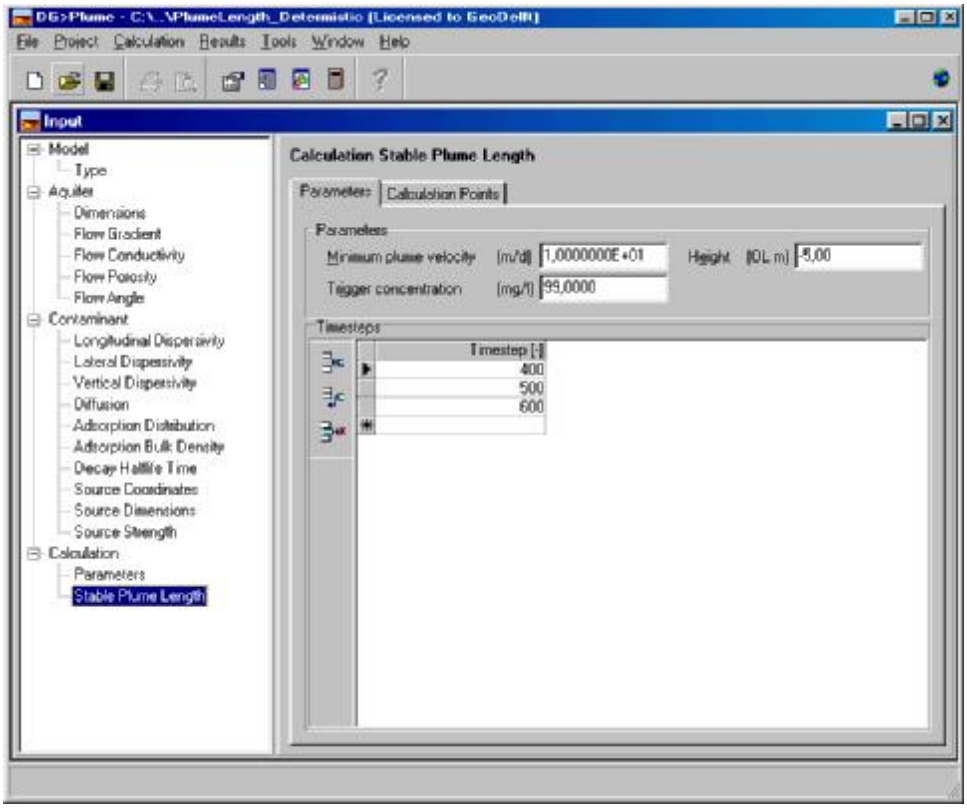


Figure 28 Calculation parameters for Stable Plume Length model

General Parameters

Minimum Plume velocity (m/d)	This option is only used for the stochastic option. When the trigger concentration in the plume is spreading less than the minimum velocity it is assumed that a Stable Plume Length is reached
Trigger concentration of limit border (mg/l)	This option is only used for the stochastic option. When the trigger concentration in the plume is spreading less than the minimum velocity it is assumed that a Stable Plume Length is reached
Height (Y co-ordinate)	Height relative to the origin (Y direction)
Timesteps(-)	Timesteps for which the concentrations are calculated. The timesteps are (unitless) steps within the interval defined in *Calculation Parameters.* Rows can be added or deleted with the icons besides the rows:  and 

3.6.6.1 Calculation points

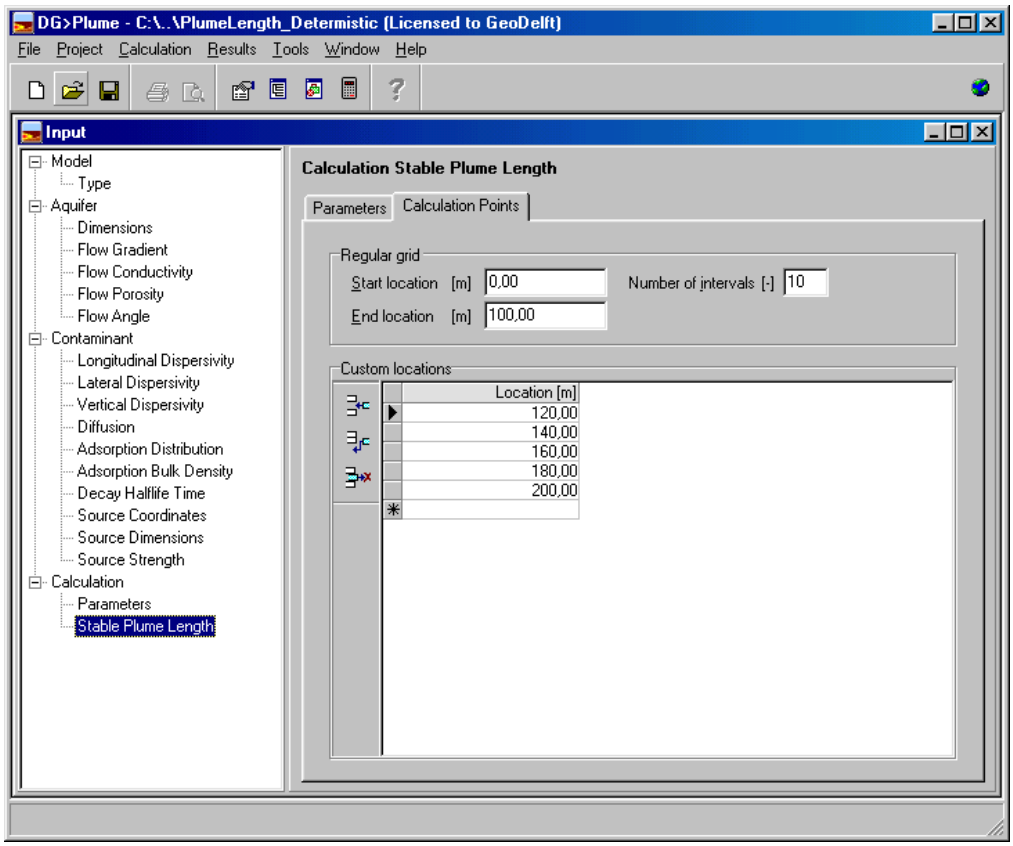


Figure 29 Calculation Points parameters for Stable Plume Length model

The location of the observation points can be entered in two different ways: with a *Regular Grid* or with *Custom locations*. Both ways can be combined as well.

The observation points are always located on a row in the direction of the groundwater flow. Therefore only one co-ordinate for the distance from the source has to be defined.

Calculation points

Regular grid	Calculation points are entered in a regular grid on a row in a *Number of Intervals* between a *Start Location* and *End Location*
Custom Locations	Custom locations for calculation points. Rows can be added or deleted with the icons besides the rows:  and 

3.7 Calculation

On the Menubar, click *Calculation, Start* to start the calculation. The calculation can be started as well with the Calculation icon: 

3.8 View results Menu

On the Menubar, click *Results* to display the following menu options:

- Report [§ 3.8.1]
- View dump file [§ 3.8.2]
- Plume contour [§ 3.8.3]
- Plume Width [§ 3.8.4
- Test Monitoring [§ 3.8.5]
- Stable Plume Length [§ 3.8.6]

3.8.1 Report

On the Menubar, click *Results* and then choose *Report* to view a window displaying a report of the analysis results. Click  to print the report. The report can be saved in Acrobat Reader (PDF) format, Internet format (HTML) or in Rave Snapshot File (NDR) format.

- The report contains the following elements:
- Header with general data.
- Overview of all the input data

3.8.2 Dump File

On the Menubar, click *Results* and then choose View *DumpFile* to view a window displaying the contents of the ASCII dump file. The report contains the following elements:

- Header with general data.
- Overview of all the input data
- Overview of all the output data

The dump file can only be saved as ASCII text with *Copy* and *Paste* commands into another text editor (eg. WORD).

3.8.3 Plume Contour

On the Menubar, click *Results* and then choose *Plume Contour* to view a window displaying the calculated plume contours. This option will only be shown when the option *Plume Contour* in the *Input Menu: Type* [§ 3.3.1] has been chosen.

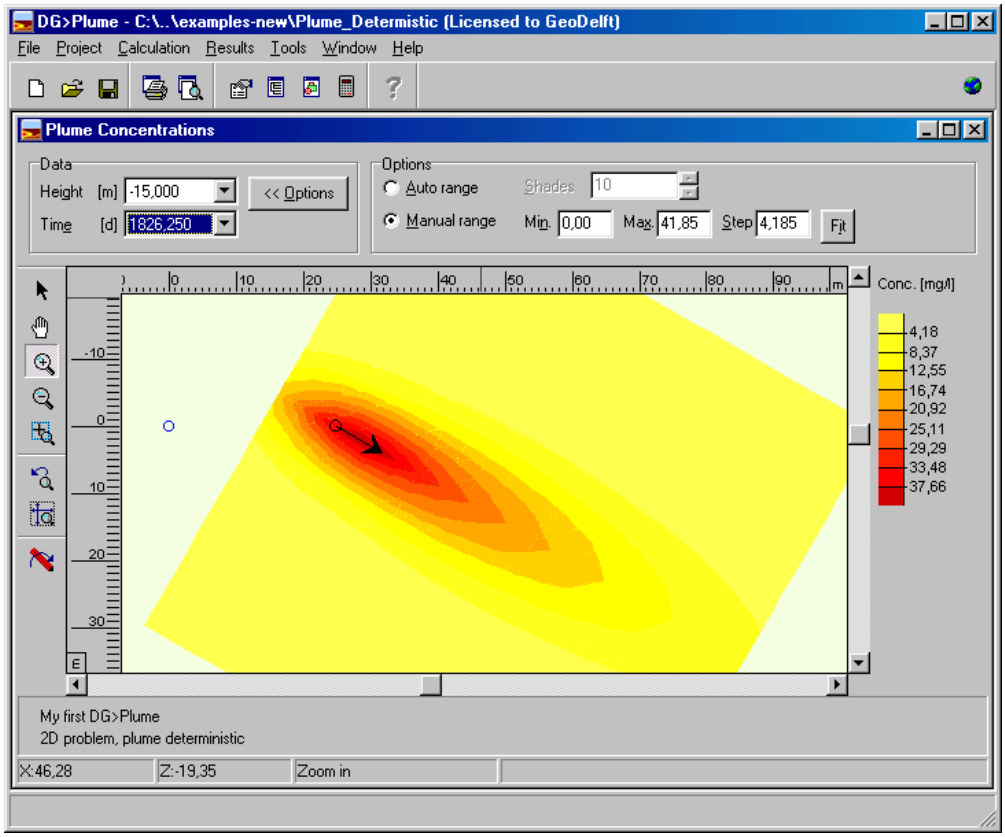


Figure 30 Output window of Plume Contours

In the output window the desired contours can be chosen out of the defined *Calculation Parameters* (see § 3.6.1 and 3.6.2.2)

- On the desired height with the button *Height*
- On the desired timestep with the button *Time*

For the deterministic option only one contour plot (for the calculated concentration) is presented. In the stochastic mode different calculations are made with a stochastic field (see Chapter 4). For the stochastic option three tab pages are available:

- *Average (mg/l)*: the average calculated concentration.
- *Variation (-)*: the variation coefficient defined as: standard deviation / mean concentration. This parameter gives insight in the relative uncertainity in the calculated results. The variation coefficient will increase on the edges of the flow field
- *Chance (%)*: the chance that the defined trigger concentration will be exceeded

3.8.4 Plume Width

On the Menubar, click *Results* and then choose *Plume Window* to view a window displaying the graph of the plume width. This option will only be shown when the option *Plume Width* in the *Input Menu: Type* (see § 3.3.1) has been chosen.

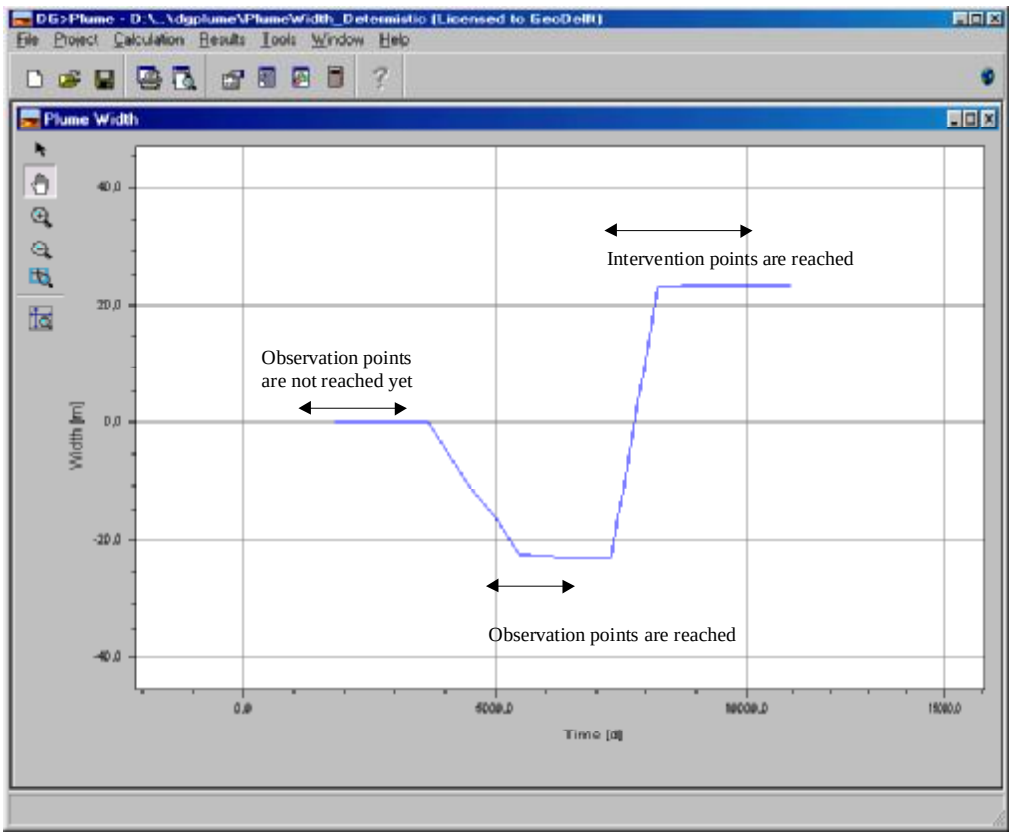


Figure 31 Output window of Plume Width Deterministic

3.8.4.1 Deterministic

In the output window a graph is shown with the calculated maximum plume width versus time. In the graph three intervals can be seen (Figure 31).

- The plume width equals 0 meters. This means the defined trigger concentration is not exceeded at the observation points
- The plume width has a negative value. The absolute value equals the plume width when the defined trigger concentration is exceeded in the observation points, but not in the intervention points
- The plume width has a positive value. This value equals the plume width when the defined trigger concentration is exceeded in the intervention point

Best results are obtained when the trigger concentrations for the observation points and the intervention point are set to an equal value. When no valid solution is obtained (e.g. when the trigger concentration is not exceeded) no graph is shown. In this case look with *Results View Dumpfile* in the generated dumpfile.

3.8.4.2 Stochastic

When the stochastic option is chosen a chance distribution graph is shown. In the output window two tab pages can be chosen:

- Width: chance distribution of the calculated plume width.
- Time: chance distribution of the exceedence of the trigger concentration in the intervention point

3.8.5 Test Monitoring

On the Menubar, click *Results* and then choose *Test Monitoring* to view a window displaying the results of the hits by the monitoring wells. This option will only be shown when the option *Test Monitoring* in the *Input Menu: Type* (see § 3.3.1) has been chosen.

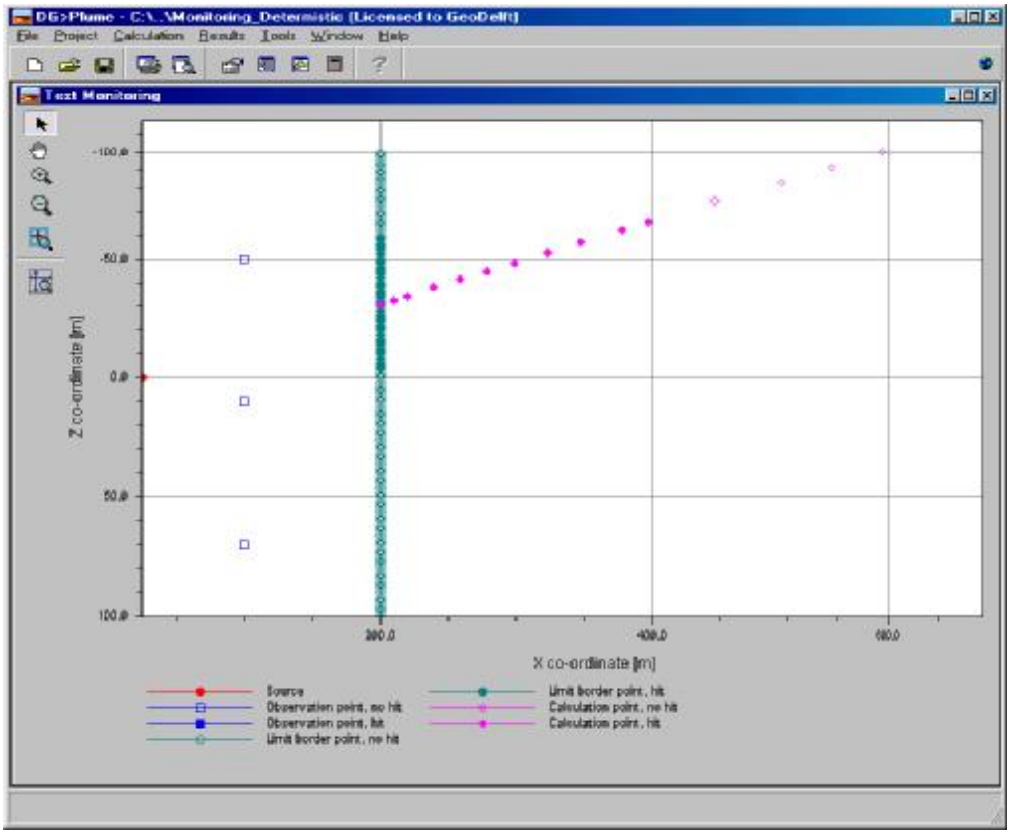


Figure 32 Output window of test Monitoring Deterministic

3.8.5.1 Deterministic

In the output window a map is shown with the results of the hits and no hits by the different monitoring points. The meaning of the coloured symbols is explained below in Figure 34. For a good understanding of the meaning of the limit border, the observation points and the calculation points see § 6.1 about the FEC concept and § 3.5.8 in the tutorial.

3.8.5.2 Stochastic

When the stochastic option is chosen in the output window three tab pages can be chosen:

- Surface: The cumulative chance versus the surface that will be contaminated above the defined trigger concentration in the intervention point
- Time: The cumulative chance versus the time that the defined trigger concentration in the intervention point will be exceeded
- Detection: the chance that a contamination will be detected by the observation points and/or the limit border points. With this option it can be checked whether the monitoring network is functioning properly (see Figure 33)

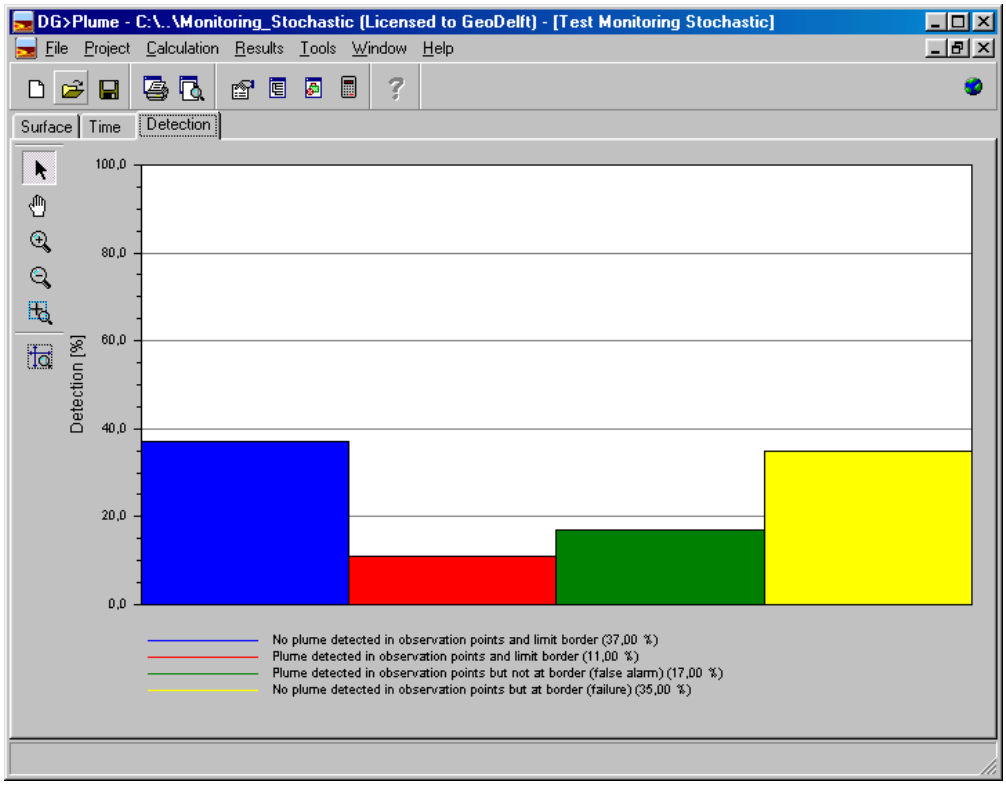
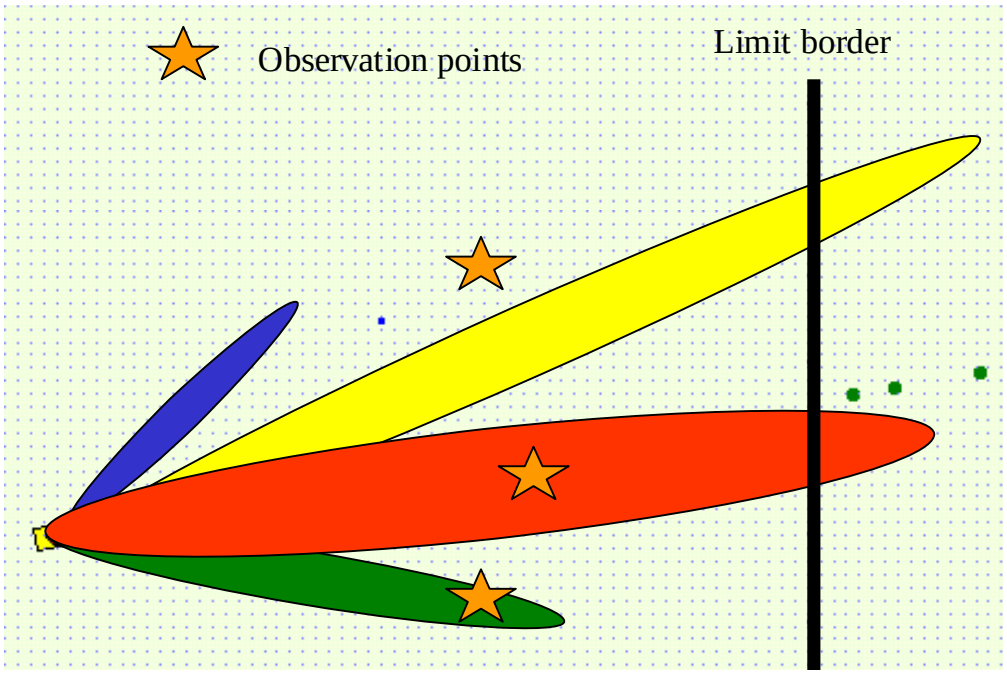


Figure 33 Output window of Test Monitoring Stochastic: Detection

In Figure 33 the output window of the detection option is shown. In this window the four main results of the monitoring network are presented. This is explained schematicly in Figure 34.



Detection by observation points	Detection by limit border points	Meaning	Color
No	No	No critical situation	
Yes	No	False alarm	
Yes	Yes	Good working system	
No	Yes	Failure of system	

Figure 34 Schematic presentation of the output options: Monitoring Stochastic: Detection

3.8.6 Stable Plume Length

On the Menubar, click *Results* and then choose *Stable Plume Length* to view a window displaying the results of the hits by the monitoring wells. This option will only be shown when the option *Stable Plume Length* in the *Input Menu: Type* (see § 3.3.1) has been chosen.
A stable plume is defined as a situation where the defined trigger concentration is moving with a velocity smaller than the defined plume velocity. The plume velocity and trigger concentration are defined in the Calculation Stable Plume Length menu (see § 3.6.6).

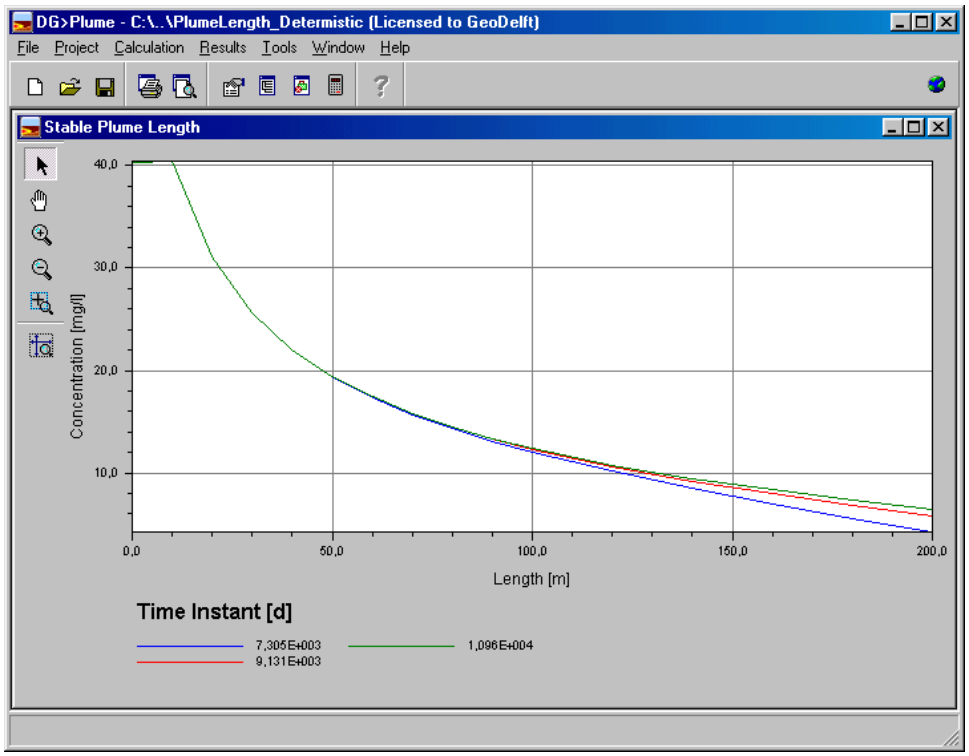


Figure 35 Output window of Stable Plume Length Deterministic

Deterministic

In the output window a graph is shown of the calculated plume length versus the concentration. For each defined time step a graph is presented. In the example shown in Figure 35 it can be seen that for concentrations higher than 10 mg/l a stable state situation will be reached. For concentrations lower than 10 mg/l the graphs differ for the three timesteps.

Stochastic

When the stochastic option is chosen in the output window three tab pages can be chosen:

- Length: The cumulative chance versus the calculated length of the stable plume. A negative plume length means that no stable plume length has been reached.
- Time: The cumulative chance versus the time that a stable plume length will be reached

4 Stochastic calculations

The text for this chapter is partly extracted from the Guidance on Assigning Values to Uncertain Parameters in Subsurface Contaminant Fate and Transport Modelling [McMahon et al., 2001]

4.1 General background

Risks may be assessed qualitatively (e.g. a high, medium or low risk of pollution) or quantitatively (e.g. by predicting the concentration and consequences of a contaminant at a specified location at a certain time). This report deals specifically with quantitative approaches for contaminant transport modelling in groundwater, as part of quantitative risk assessment, which can be divided into two categories: deterministic and probabilistic. Deterministic assessments involve the assignment of a single value to each parameter, and the calculation results in a single number. This approach implies a high degree of certainty in the input data, e.g. the input parameter can be defined by a single value or its variability is known everywhere. A high proportion of environmental risk assessments involve studies of the subsurface where such a level of certainty is not present.

Probabilistic approaches provide methods of addressing uncertainty or variability in a known and structured way using probability distributions of values; as knowledge increases the corresponding reduction in uncertainty can be incorporated. A range of possible outcomes, which can be described by a probability distribution, will be generated by a probabilistic model as a result of the combination of different input parameter values (e.g. by calculating the percentage chance that a specified concentration will be exceeded at a specified location at a certain time).

4.2 Uncertainty and variability

In theory, if the values of all the relevant hydrogeological parameters are known, and the contaminant release history is known, it is possible to calculate the expected concentration of a contaminant at any subsequent time and location of interest. In practice, such precise calculations are rarely possible because of lack of knowledge in key parameters. Two basic kinds of lack of knowledge can be distinguished: uncertainty in a parameter that clearly has a single value (e.g. the catastrophic failure of a storage tank is a discrete event, even though the precise date of failure may not be known), and variability in a parameter that is a function of location or time (e.g. the hydraulic conductivity of the material comprising an aquifer).

A parameter having a single, albeit uncertain, value can be described by a probability density function or PDF. The PDF describes how likely it is that the parameter has any particular value.

A parameter that varies in space, for example hydraulic conductivity, could be defined if sufficient data were available. However, this will seldom be the case. As a result our knowledge of the hydraulic conductivity at every point, other than at the point of measurement, is uncertain. This is what is known as a stochastic field.

In practice, there will usually be some relationship between the hydraulic conductivities at adjacent points. It may be possible to derive a statistical description of the spatial variability of a parameter, for example using geostatistics. From this description, it is possible to generate realisations of the spatial distribution of a parameter value. The generation of these realisations is a very large subject, beyond the scope of this guidance.

In practice for many models, stochastic fields will be simplified into single parameters. For example, rather than modelling the spatial variation of hydraulic conductivity between contaminant source and receptor, a single appropriate average value of hydraulic conductivity may be used. Because the detailed distribution of hydraulic conductivity is unknown, this overall average value is uncertain. An uncertain single value can be described by a PDF. There are statistical techniques that can be used to derive the PDF of the appropriate average, given measurements of point values.

4.3 Probability Distribution Functions (PDF)

This section explains and defines the probability distributions used in DG>Plume. Figure 36 gives the mathematical and graphical representation of four distribution functions. Figure 36 has been drawn so that each of the distributions presented have been derived using the same mean (10), standard deviation (3) and ensuring that the area under the curve is always 1.

Probability density functions require different numbers of parameters to be defined. For example, the Uniform distribution requires a minimum and maximum value to be defined, whereas the Triangular distribution requires a minimum, most likely and a maximum value. Thus the definition of a PDF is not necessarily the answer for all data shortage problems as an uncertain hydrogeological parameter value is described in terms of two or more uncertain statistical parameters. This may not represent an increase in knowledge!

Distribution	PDF	Mean	Variance	Mode	Median	Parameters
Uniform	$0 \quad x<a$ $1/(b-a) \quad a<x<b$ $0 \quad b<x$	$(a+b)/2$	$(b-a)^2/12$	None	$(a+b)/2$	a (minimum), b (maximum)
Normal	$\frac{1}{\sigma\sqrt{2\pi}}\exp\left(\frac{-(x-\mu)^2}{2\sigma^2}\right)$	μ	σ^2	μ	μ	μ, σ
Log-normal	$\frac{1}{x\sigma\sqrt{2\pi}}\exp\left(\frac{-(\ln x-\mu)^2}{2\sigma^2}\right)$	$\exp(\mu+½\sigma^2)$	$\exp(2\mu+\sigma^2).(\exp(\sigma^2)-1)$	$\exp(\mu-\sigma^2)$	$\exp(\mu)$	μ, σ
Triangular	$0 \quad x<a$ $2(x-a)/(b-a)(c-a) \quad a<x<b$ $2(c-x)/(c-b)(c-a) \quad b<x<c$ $0 \quad x>c$	$(a+b+c)/3$	$(a^2+b^2+c^2-ab-ac-bc)/18$	b	$a+\sqrt{[½(c-a)(b-a)]} \quad b>(a+c)/2$ $c-\sqrt{[½(c-a)(c-b)]} \quad b<(a+c)/2$	a (minimum), b (most likely), c (maximum)

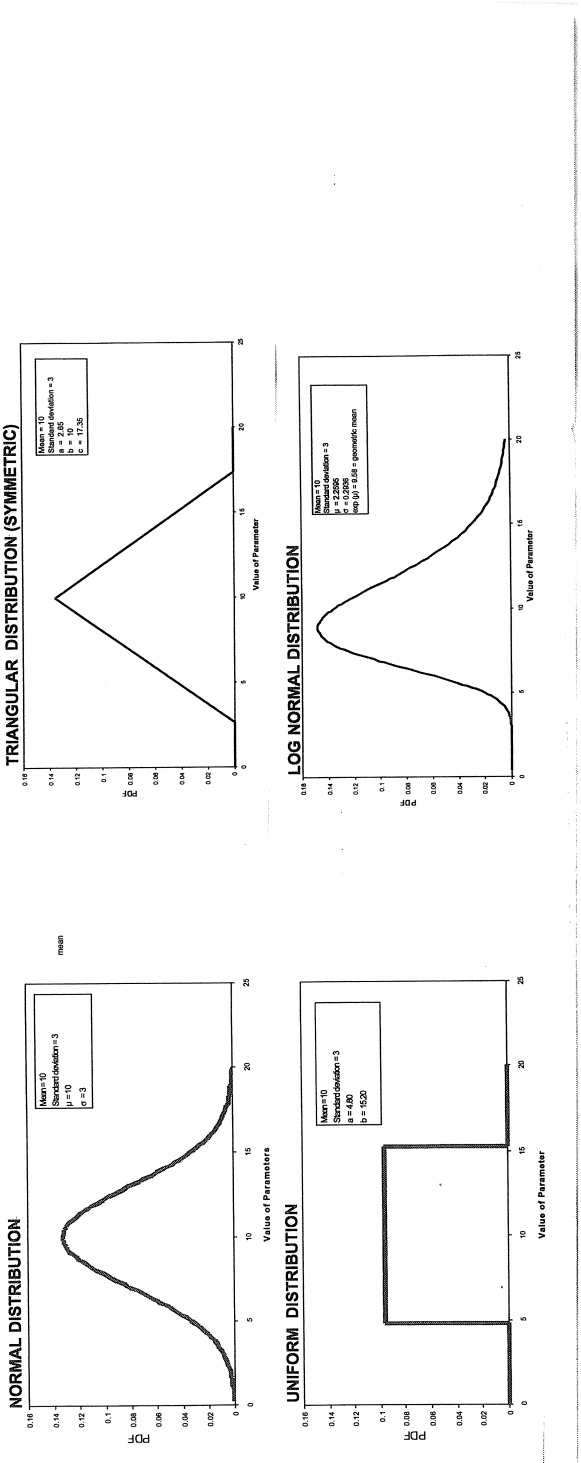


Figure 36 Mathematical and graphical representation of four PDF's

4.3.1 Normal Distribution

The most common observed distribution is the Normal distribution (also called the Gaussian distribution). The Normal distribution implies a symmetrical grouping of the sample around a specific value (mean) with less chance of a sample further away from this value. The graph of the PDF is often referred to as the "bell-curve". An example of a normally distributed parameter is the distribution of the porosity in a certain geological unit.

Probabilities from Normal distributions can be described as either a one-tailed or two-tailed distributions. DG>Plume is using only a two-tailed distribution where with both high and low extreme values (i.e. the range in values across the mean). A one-tailed probability is used when outcomes above or below a certain value are of concern.

It is useful to note that 68.3% of a Normal distribution occurs within one standard deviation on either side of the mean (two-tailed probability), 95.4% within two standard deviations and 99.7% within three standard deviations.

The Normal distribution function can theoretically take any value from minus infinity to plus infinity (i.e. it is unbounded). In principle, therefore, any parameter known always to be positive cannot be perfectly normal because there is zero probability that a negative number will occur. In practice, the Normal distribution is the best distribution for very many observations in nature and as long as the mean is more than three standard deviations away from zero (in which case the distribution produces a probability of a negative number of only 0.15%), it can be safely used.

The Normal distribution is symmetrical about its mean. If there is evidence that a distribution is skewed, then the Normal distribution should not be used.

The Normal distribution can usually be used to describe the variation in porosity measurements

4.3.2 Uniform Distribution

The Uniform distribution distributes probability equally between two extreme values. Example: If monitoring occurs on the first of each month and there is no contamination on 1 January but there is contamination on the 1 February a Uniform distribution assumes that there is an equal probability that the contamination event happened on any of the intervening days.

In selecting a minimum and maximum value in DG>Plume for a Uniform or a Triangular PDF (see § 4.3.4) based on observed measurements, it is important to recognise that these are unlikely to describe the actual population range. For this reason, it may be appropriate to use expert opinion to define higher and lower values than those determined from observed measurements (although this would need to be justified). However, care needs to be exercised as the maximum and

minimum measurements may be anomalous (due to measurement error) or inappropriate to the problem (i.e. a very low value of hydraulic conductivity may relate to a clay lens within a sand and gravel deposit, and where contaminant movement is via the coarser sand and gravel fraction).

Uniform distributions typically are used to describe variation in porosity and measured lengths (e.g. source dimensions).

4.3.3 Log-Normal Distribution

A distribution is Log-normal if the logarithms of the values are distributed normally. A common example is hydraulic conductivity, which has been observed to vary in the field by several orders of magnitude. The true average of a Log-normal distribution is the geometric mean (which is the exponential of the arithmetic mean of the natural logarithms). A Log-normal distribution contains no negative values and is skewed.

A Log distribution is recommended for distributions that span more than one order of magnitude and which appear to be skewed. It is not appropriate where distributions appear to be linear, i.e. no bias to one end or the other, in which case a Uniform distribution should be used.

The Log-normal distribution is typically used to describe the variation in hydraulic conductivity values.

4.3.4 Triangular distribution

The Triangular distribution can be regarded as a simple approximation of the Normal distribution. It is called triangular because of the shape of the PDF. It has three parameters: a minimum value, a maximum value and a most likely value (mode). As for the Uniform distribution (see § 4.3.1) maximum and minimum values should be defined based on expert judgement rather than the observed range of measurements. By definition, values cannot be lower than the minimum or higher than the maximum. Most experts have a feeling for the range of a physical property in terms of a maximum credible value and minimum credible value rather than as a standard deviation or some other parameter of distribution. Understanding of these three parameters (maximum, minimum and mode) is fairly intuitive. Consequently for Uniform, Triangular and Log-triangular distributions the range of values are constrained compared to Normal and Log-normal distribution. For this reason, the Triangular distribution is useful for estimated and elicited distributions, where the variation (between lowest and highest values) is less than an order of magnitude. Triangular distributions are generally recommended if there are fewer than 10 readings since they are intuitive to estimate

4.4 Other distributions (from File)

There are a number of other less commonly used distributions including Exponential, Gamma, Binomial, Poisson, Log-Triangular and Log-uniform. These distributions are generally less appropriate for describing aquifer or contaminant properties. But one of those mentioned distributions or another distribution may be appropiate for certain case. Therefore a file with a user-defined PDF can be imported. This function is not implemeted yet in DG>Plume version 1.7.

4.5 Entering stochastic data

In most modelling and risk assessment scenarios the possible range of values for some parameters will not be known. There may be very limited or, in some cases, no site-specific data with which to define some parameter ranges and a method of selecting appropriate values and PDFs must be found. If there is no site-specific information on any of the parameters then modelling is inappropriate.

Certain parameters can readily be measured in the field (e.g. hydraulic conductivity, hydraulic gradient), but others are generally not measured (e.g. dispersivity) and values must be obtained from other sources. Where site-specific data are available they may be limited and consideration must be given to the way in which they are used to generate PDFs.

4.5.1 With sufficient data

The estimation of the PDF parameters should be made using site-specific data wherever possible. For example, the parameter μ in a Normal distribution is estimated by the sample mean and the parameter σ^2 is estimated by the sample variance. Similarly, for the Log-normal distribution, the parameter μ is estimated by the geometric sample mean (i.e. loge(μ) is estimated by the mean of the logarithms) and the parameter loge(σ^2) is estimated by the variance of the logarithms of the sample data.

The estimation of the PDF parameters should be made using site-specific data wherever possible. For example, the parameter μ in a Normal distribution is estimated by the sample mean and the parameter σ^2 is estimated by the sample variance. Similarly, for the Log-normal distribution, the parameter μ is estimated by the geometric sample mean (i.e. $\log_e(\mu)$ is estimated by the mean of the logarithms) and the parameter $\log_e(\sigma^2)$ is estimated by the variance of the logarithms of the sample data.

1. Check the characteristics of the data for patterns and trends. This will usually involve constructing a graph against time, or plotting maps and sections. Incorporate the understanding first in the deterministic model with aveage values. Only proceed when the data-points come from a single population.
2. Plot the data as a histogram, frequency plot, or cumulative frequency plot (e.g. use the Histogram function in Excel). If the curve has more than one mode, this is an indicator that the samples may be from more than one population and (1)

above should be revisited. Note that in DG>Plume only one PDF function per parameter can be entered.

3. The preparation of probability plots (involving plotting the data in order according to its percentile) is a useful graphical method of identifying the PDF. If the data form a straight line on normal graph paper, then this is a reasonable justification for assuming normality without formal proof.
4. If there are fewer than 30 data points, it will probably be necessary to assume the type of PDF as it may not be possible to prove the distribution with a high degree of statistical certainty. This will be the typical case for most site investigations such that the choice of a PDF will involve some expert judgement (see § 4.5.2).
5. Choose the distribution type most likely to fit the data from the shape of the histogram and knowledge of the property. Probability plots are also useful if the distribution is uncertain.
6. If the curve is skewed and if the data range over more than one order of magnitude then a Log distribution may be most appropriate.
7. Estimate the parameters (average, standard deviation) of the PDF from the data (see Figure 36). Some commercial packages have the option to fit PDFs to data; alternatively, most spreadsheets include statistical analysis packages. The estimation of the PDF parameters should be made using the data.
8. Use a statistical test procedure to determine if the selected distribution fits the data, i.e. is it statistically valid? For example, if a Normal distribution is proposed then a statistical test for normality should be undertaken. Such procedures include Chi-squared, Kolmogorov-Smimov, Shapiro-Wilks and D'Agostino. The Chi-squared test can be used to test the fit of any selected distribution. The Shapiro-Wilks and D'Agostine tests are better tests but are specific for Normal distributions (less effort and more reliable). If the test (e.g. Chi-squared) fails, then try other possible distributions until it succeeds.
9. Run the model.
10. Reality Check. The results of the modelling must be examined critically against any field data that exist (see Figure 36).

4.5.2 Limited or insuficient data

When there are only few site-specific data some assumptions must be made about the likely distribution of the parameter values whilst still taking into account the measured values. Experience suggests that certain parameters commonly exhibit certain types of distributions and that there are other preferred distributions based on the number of data points available.

Some recommendations are listed below:

- The recommended default distribution for hydraulic conductivity is Log-normal . In all cases where data spans an order of magnitude a log-based distribution should be used. If sufficient data are available to define that distribution, a PDF other than Log-normal may be more applicable.
- Normal distributions are recommended for other parameters (e.g. porosity), if there are more than 10 readings where the histogram suggests normality. The distribution should be checked to ensure that negative values are not assigned to a parameter which cannot be negative e.g. porosity. Also the mean value should be at least three standard deviations from zero. DG>Plume will automatically set the minimum value as 0,0001 for the porosity or zero for

other parameters, if the specified distribution results in negative values. It should be noted that this will skew the distribution slightly.

- Triangular distributions are generally recommended if there are fewer than 10 readings since they are intuitive to estimate. The paragraphs 3.4 and 3.5 give suggested distributions for different parameters. However, they can be over constrained it is unlikely that a set of 10 measurements will include either the lowest or highest real measurement. After defining the parameters and running the model the results of the modelling must be examined critically. The model runs can be improverd by using an uncertainity analysis (see § 4.8).

4.6 heterogeneity and uncertainty (upscaling)

For some contaminant problems, the ‘average’ parameter value may best describe the system behavior. In this case, measurements of a parameter at one scale (e.g. laboratory measurements) can be used to define the parameter at a larger scale. This approach of using sample measurements to define the `average' system behavior is described as upscaling. Where the system is believed to be heterogeneous, then upscaling should be used with care. In DG>Plume a heterogeneous system can be simulated by defining one average deterministic value. However it is advised to simulate a heterogenous system with a probabilistic approach.

It is emphasised that upscaling by averaging should be used only where it can be shown that the average value of a parameter is the controlling factor in contaminant transport. If the system behaviour is controlled by a small heterogeneous part of the system, it should not be used as the upscaling is only describing the uncertainty in the mean, not the heterogeneity of the system.

A pragmatic approach given below is based on simple analytic considerations of combining two blocks of different properties together and take no account of dispersion.

- For variation parallel to the direction of flow, hydraulic conductivity is upscaled using the harmonic mean of the data and porosity with the arithmetic mean (to get travel time).
- For variation perpendicular to the direction of flow, then hydraulic conductivity is upscaled using the arithmetic mean. Porosity is upscaled differently according to whether it is the first arrival that counts or the mode of arrival time. For first arrival, the minimum porosity counts and for the mode of arrival time it is the arithmetic mean.
- For variation in both directions in two dimensions (a quasi-random variability - the usual situation) it is generally considered that the hydraulic conductivity can be upscaled using the geometric mean of the data set and the porosity using the arithmetic mean.
- For variation in three dimensions [Gelhar 1993] has shown that the effective hydraulic conductivity is the geometric mean multiplied by the term $\exp(\sigma^2/6)$, where σ^2 is the variance of the distribution of the logarithm of the values of hydraulic conductivity.

4.7 Latin Hypercube sampling

The text of this paragraph is derived from A Users Guide to LHS: Sandia's Latin Hypercube Sampling Software [Wyss, G.D. and K.H. Jorgensen, 1998].

For stoachastic calculations DG>Plume is using the Latin Hypercube sampling method. Latin hypercube sampling was developed to address the need for uncertainty assessment for a particular class of problems.

A conventional approach to these questions is to apply Monte Carlo sampling. By sampling repeatedly from the assumed joint probability density function of the input parameters (i.e porosity, hydralic conductivity and dispersivity) and evaluating the calculated concentration for each sample, the distribution of the concentration, along with its mean and other characteristics, can be estimated. An alternative approach, which can yield more precise estimates, is to use a constrained Monte Carlo sampling scheme. One such scheme, developed by McKay, Conover, and Beckman is Latin hypercube sampling.

Latin hypercube sampling selects n different values from each of k variables X_1, ... X_k in the following manner. The range of each variable is divided into n nonoverlapping intervals on the basis of equal probability. One value from each interval is selected at random with respect to the probability density in the interval. The n values thus obtained for X_l are paired in a random manner (equally likely combinations) with the n values of XZ. These n pairs are combined in a random manner with the n values of X_3 to form n triplets, and so on, until n k-tuplets are formed. These n k-tuplets are the same as the n k-dimensional input vectors described in the previous paragraph. This is the Latin hypercube sample. It is convenient to think of this sample (or any random sample of size n) as forming an (n x k) matrix of input where the ith row contains specific values of each of the k input variables to be used on the ith run of the computer model.
For more information about the Latin Hypercube Sampling see § 6.2.

4.8 Uncertainty analysis

When several different distributions are combined in a calculation, the resulting distribution has its own characteristics and may not even be of the same type as any of the constituent distributions. To find the probability of the output parameter exceeding a certain value, it is necessary to search throughout the parameter space (all the possible parameter values) for the sub-space where the combination takes this value or larger and then find the probabilities of each of the parameters falling in this sub-space. Unfortunately the mathematics of determining such distributions are extremely complex and even the multiplication of two Normal distributions becomes very complicated.
Routinely when we attempt to calculate an impact we use scoping values in our equations. Sometimes they may be best-case estimates and sometimes they may be worst-case estimates, both of which are examples of combinations of extreme values of parameters. One problem with combinations of extreme estimates is that these may be far more unlikely than we appreciate. This is because the chance of all the parameters taking their extreme values simultaneously is far more remote than the chance of any one of them taking its extreme value individually.

The realisation of this fact is one of the reasons for using uncertainty analysis and trying to establish exactly how much of a worst case we are talking about. Is it 1 in a million chance, 1 in a billion, 1 in 10? These are all unlikely but there is significant difference between them. Whilst a worst-case analysis may be justified under the precautionary approach, decisions based solely on such results may have financial implications disproportionate to the actual level of risk.

4.9 Dependent parameters

One limitation of DG>Plume is that the sampling generally assumes all the parameters are independent of one another. Unfortunately this is not always true. For example, the hydraulic gradient is not independent of the hydraulic conductivity of an aquifer since there is a negative correlation between the two. For example, shallow hydraulic gradients are typically associated with higher values of hydraulic conductivity and steeper gradients by lower values of hydraulic conductivity.

DG>Plume does not allow dependency to be taken into account; the expectation is that expert users will input reasonable values given their knowledge of the hydrogeology. However, it should be recognised that the Monte Carlo method can and will pick extreme values from dependent ranges that would not be expected to occur in nature e.g. high hydraulic conductivity with low hydraulic gradient.

5 Examples and tutorial

The following lessons are discussed below:

- Lesson 1: Deterministic Plume Contour [see § 5.1]
- Lesson 2: Making and reviewing a calculation [see § 5.2]
- Lesson 3: Making a stochastic calculation [see § 5.3]
- Lesson 4: Plume Width [see § 5.4]
- Lesson 5: Stable Plume Length see § 5.5]
- Lesson 6: Test Monitoring Network [see § 5.6]

The input files belonging to these examples are located in the DG>Plume installation directory.

5.1 Lesson 1: Deterministic Plume Contour

Always start with a deterministic calculation. This is the most easy approach for setting up a problem definition. When the calculation results are satisfactory later a stochastic calculation can be made.

To make a deterministic plume contour:

- Start DG>Plume with *Start* > *Programs* > *DG>Plume*
- With *Tools* > *Options* > *Directories* a working directory can be set

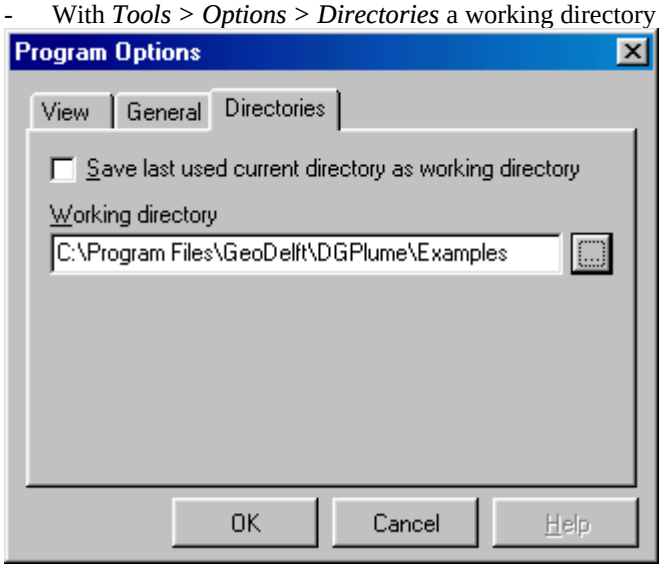


Figure 37 Lesson 1: Program Options

- Choose with the ... icon the working directory with the DG>Plume sample files. Default directory is: c:\Program Files\GeoDelft\DGPlume\Examples
- Open with icon the file: *Plume_Deterministic*
- Now you will see the Input View:

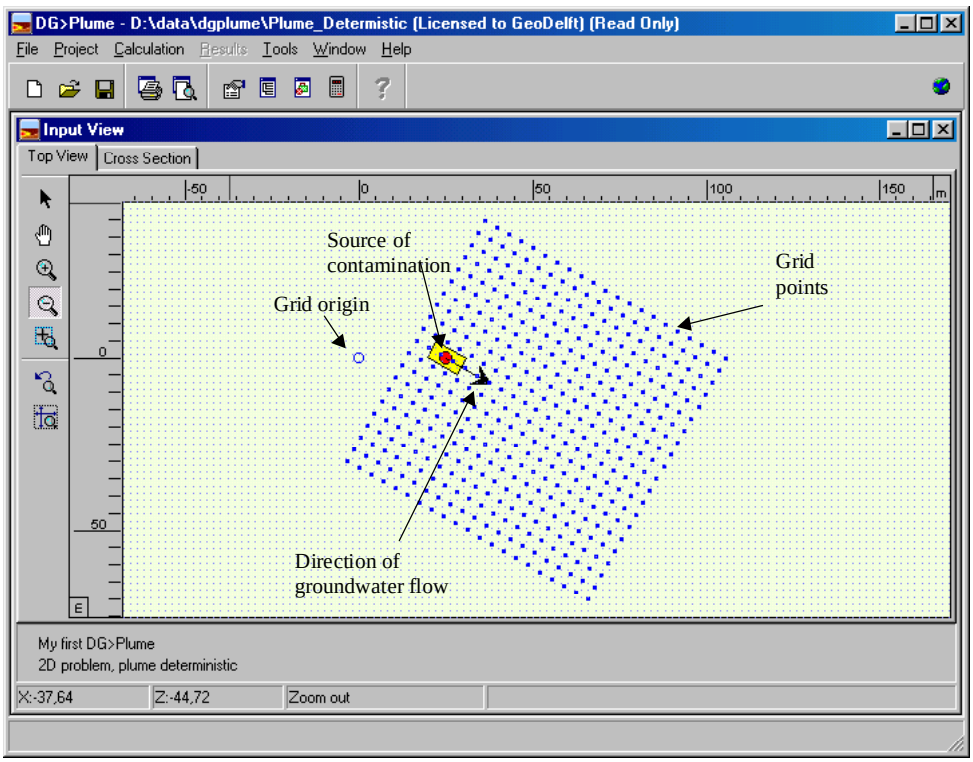


Figure 38 Lesson 1; explanation of the Input View

- Click on the tabpage *Cross Section* to see the cross section
- Click on the tabpage Top View to see the top view again
- Click on the icon:  to see the Input View.
- All the input parameters can be entered in this tree view
- Click on *Model > Type*
- The modeltype is set to Plume Contour
- Click on *Aquifer > Flow > Conductivity*
- Choose a Deterministic Conductivity value of *2 m/d*
- Click on *Contamination > Source Dimensions*
- Choose the tabpage *Width (Z)*
- Change the value from 5 in *10 meters*
- The source of contamination is now increased in size
- Click on *Calculation > Grid Mesh*
- Choose the tabpage *X'' locations*
- Change the End Location from 70 into 100 meters
- Click on the icon:  to see the Input View
- The Grid Mesh and Source of Contamination are changed now
- Click on *Project > Input* to see the Input View again
- Click on *File > Close*
- Choose *No* for not saving the file

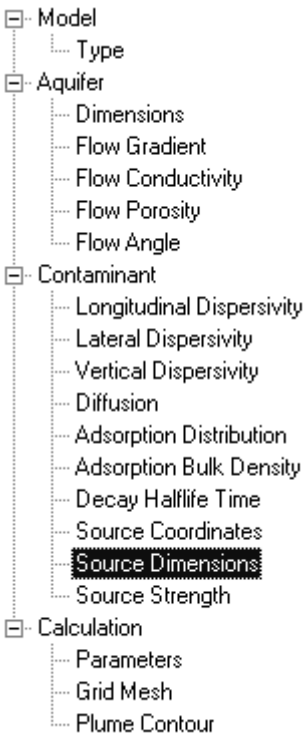


Figure 39 Lesson 1; Tree Input View

5.2 Lesson 2: Making and reviewing a calculation

- Open with  icon the file: *Plume_Deterministic*
- Choose *Tools* > *Options* > *General*
- Click on *Always Save As.* With this option the user will always be asked to specify the filename
- Click on the icon*:*  . Start and save the calculation as *Lesson 2*
- A DG>Plume calculation is started now.
- Click on *Results* > *Plume Contour* to see the contour plot

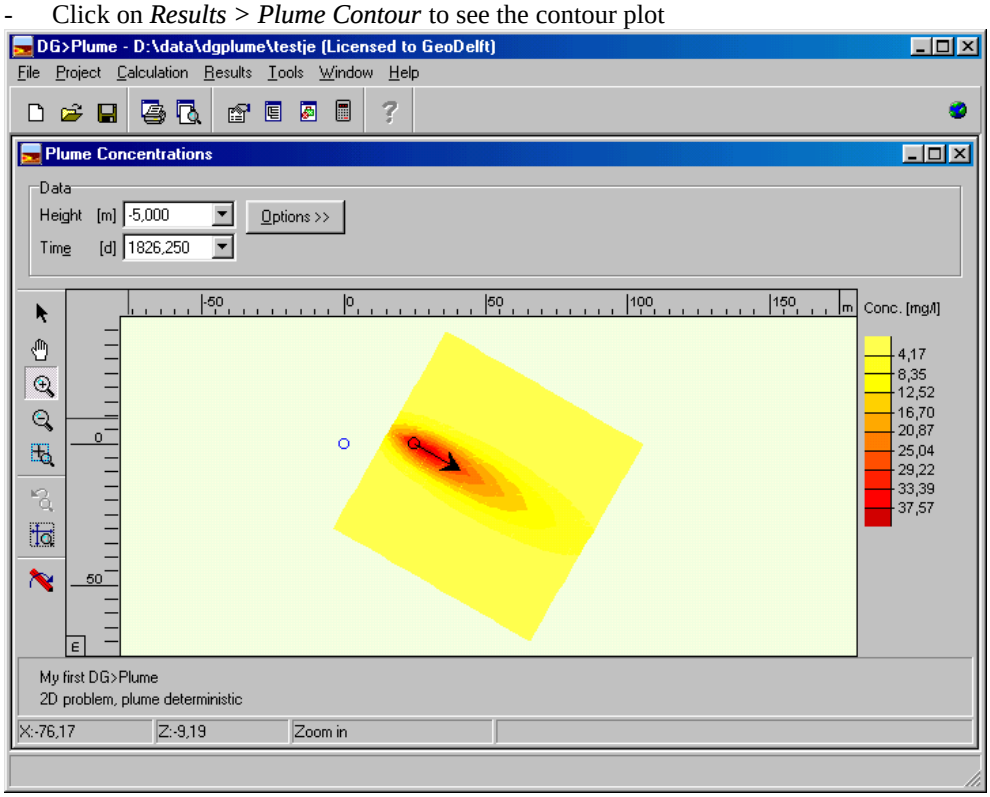


Figure 40 Lesson 2; Results of the Deterministic Plume calculation

- Click on *Options*>> to see the extra options for contouring
- Click *on Manual Range* and *Fit* to change the contouring range
- Click on *Time* to choose another time step
- Click on *Height* to choose another height
- Click on the icon:  and the plot window to zoom
- Click on the icon:  to undo the zoom action
- Click on *File* > *Page Setup*. Choose *Orientation Portrait*
- Click on *File* > *Copy Active Window to Clipboard*
- Start WORD program
- Click on Paste in WORD. The plot is now pasted in WORD and can be included in a report describing the project
- Return to DG>Plume
- Click on *Results* > *Report.* A report with all the input parameters is now generated
- Click on *File* > *Save as*.
- Type: *Test* to generate a report in Acrobat Reader format (PDF)
- Click *File* > *Exit* to leave the report generator

- Click on *Results* > *View* D*umpfile* to see the generated dumpfile. This ASCII file contains all the entered data and calculated values

5.3 Lesson 3: Making a stochastic calculation

- Open with  icon the file: *Plume_Deterministic*
- This file was used before in Lesson 2 for making a deterministic calculation
- Click *on Project* > *Input* to see the Tree Input View
- Click on *Type* > *Stochastic* to change the type of calculation
- *Click on Aquifer* > *Flow Conductivity* and choose a log-normal distribution
- Click on *Calculation* > *Parameters*
- Set the *Number of Realisations* to 10. Now 10 calculations will be made
- Click on *Calculation* > *Start* to start the calculation
- Note that it takes more time now to make a calculation. The highest calculated concentration is presented during the calculation process
- Click on *Results* > *Stochastic Plume Contour*
- Now the results can be reviewed on three tabpages: Average, Variation and Chance
- Choose the tabpage Average:

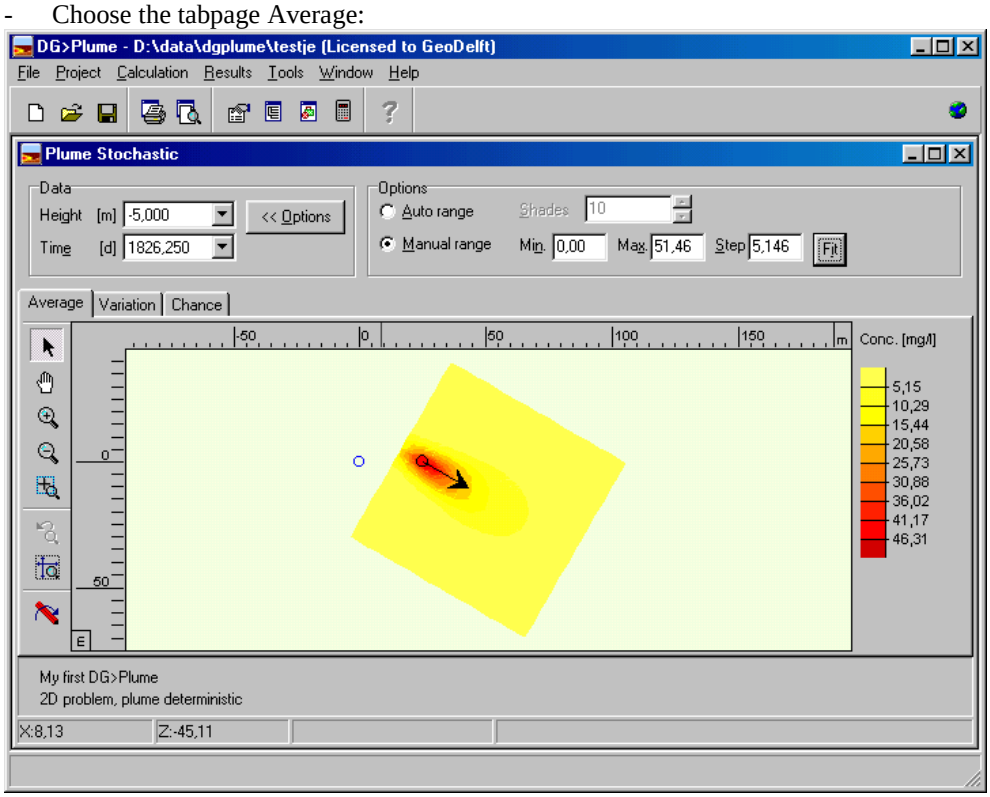


Figure 41 Lesson 3; Results of the Stochastic Plume calculation

- Choose *Options* >> *Manual Range* to change the contouring range
- Choose the  icon to zoom into the contouring plot
- Note that the calculated concentrations contours are more fanciful. This is caused by the different input parameters in the stochastic calculation
- Note that in the window the flow angle of the determinitic flow angle is presented (because it is not possible to show a range of flow angles). The same approach is chosen for the source of concentration
- Choose the tabpage *Variation*:
- Choose *Options* > *Manual Range* to change the contouring range

- Note that the variation is largest on the edges of the model area. The variation is defined as the standard deviation divided by the mean concentration.
- Choose the tabpage *Chance*:
- Choose *Options* > *Manual Range* to change the contouring range
- The chance is defined as the chance that the defined trigger concentration will be exceeded. This chance is decreasing towards the edges of the model area

5.4 Lesson 4: Plume Width

- Open with  icon the file: *PlumeWidth_Stochastic*
- Click on the icon*:* 
- A DG>Plume calculation is started now.
- Click on *Results* > *Stochastic Plume Width* to see the results

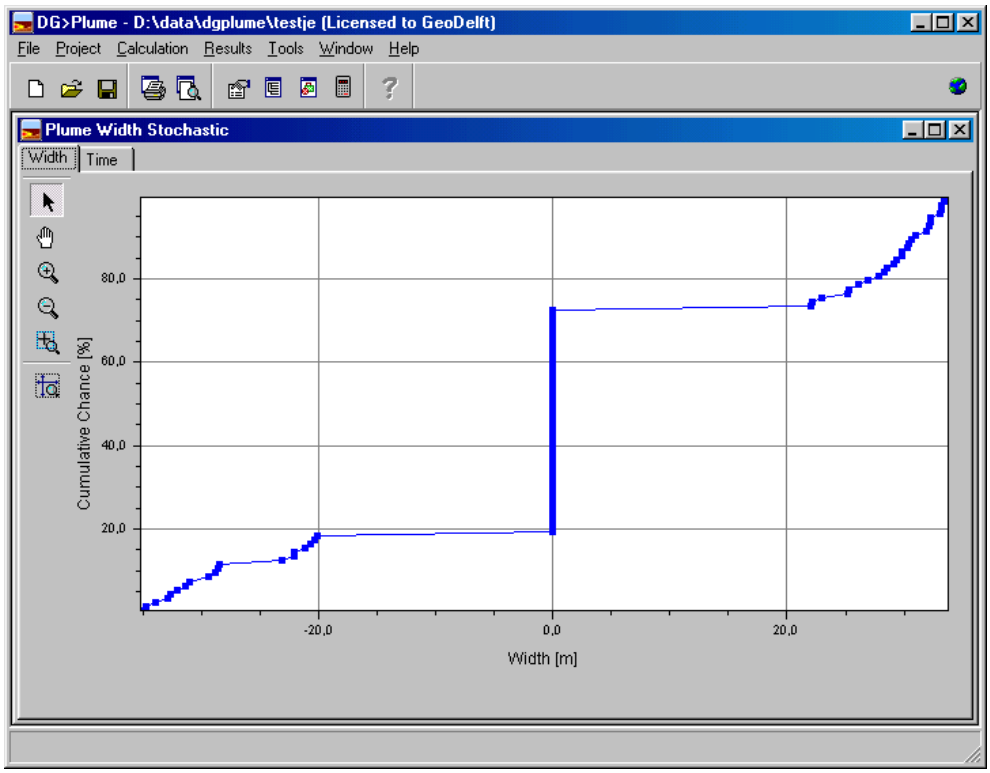


Figure 42 Lesson 4; Results of the Stochastic Plume Width calculation

- In Figure 42 can be seen that:
  - There is 0 – 20 % cumulative chance that the trigger concentration will not be exceeded in the obeservation points. The width of the plume is limited to a maximum of 20 meters
  - There is 20 – 75 % cumulative chance that the trigger concentration will be exceeded in the obeservation points, but not in the intervention point
  - There is 75 % -100 % cumulative chance that the trigger concentration will be exceeded in the intervention point. The plume width will be between 20 and 30 meters
- The results can be used for the design of the monitoring network

5.5 Lesson 5: Stable Plume Length

- Open with  icon the file: *PlumeLength_Stochastic*

- Click on the icon:  to see the Tree Input View.
- Click on *Calculation* > *Stable Plume Length*

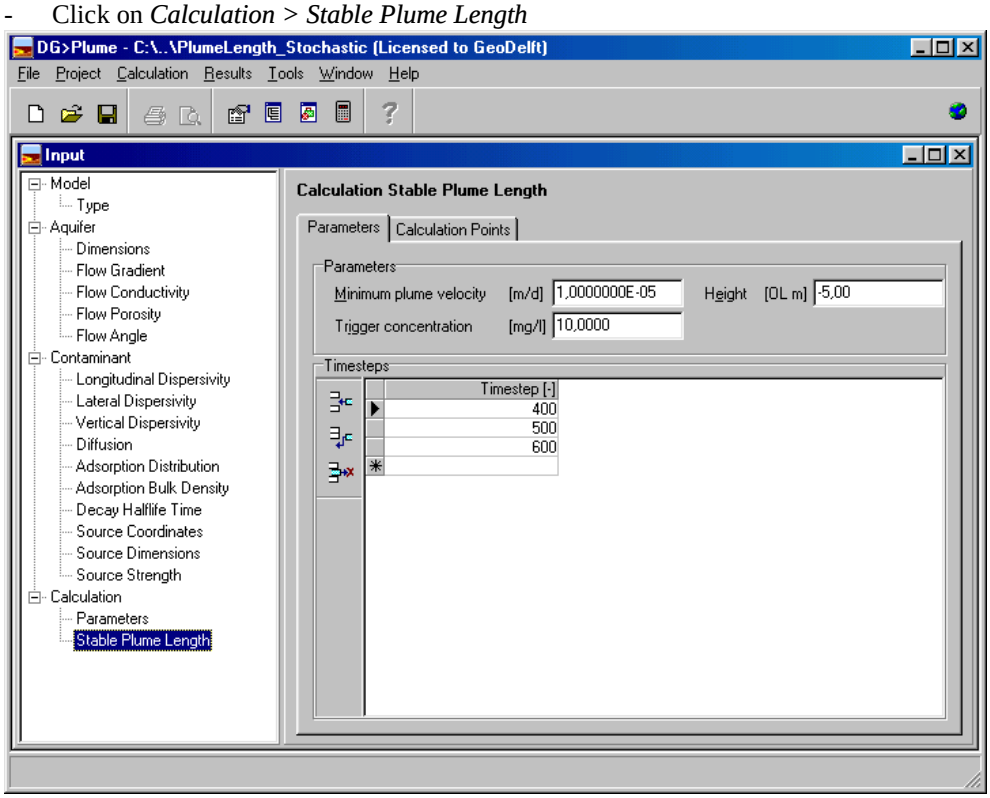


Figure 43 Lesson 5; Tree Input View for Stable Plume Length

- Note that a stable plume is defined as a situation where areas with a concentration of 10 mg/l are moving less than 0,00001 m/d

- Click on the icon: 
- A DG>Plume calculation is started now.
- Click on *Results* > *Stochastic Stable Plume Length*

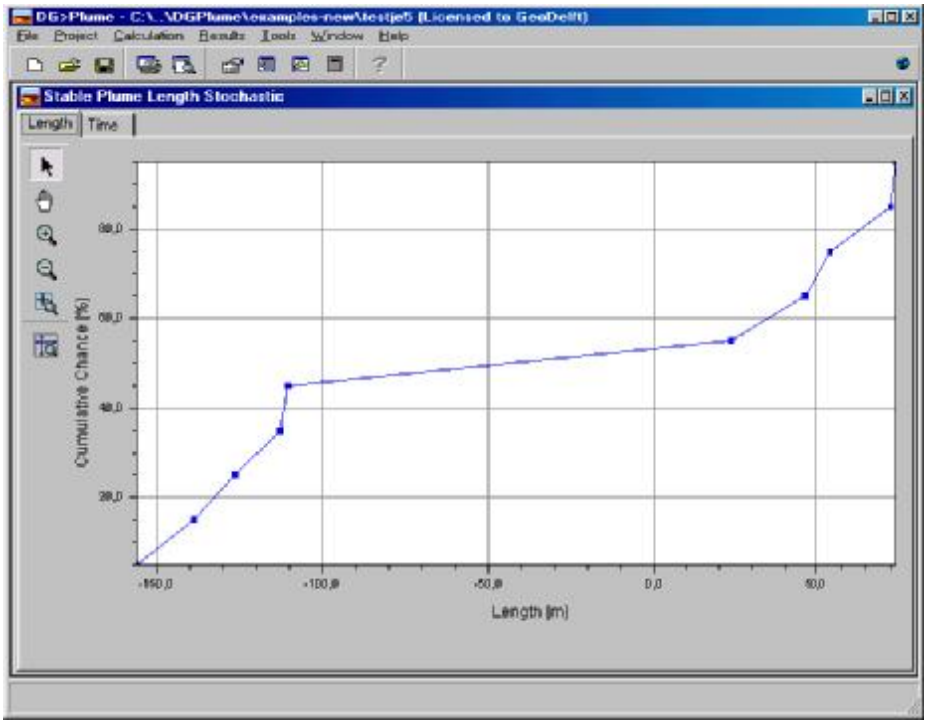


Figure 44 **Results of the stochastic Plume Length calculation**

In

- **Figure 44** can be seen that:
  - There is 0 – 50 % cumulative chance that no stable plume will be reached (negative plume length). In this case the plume length will be between 100 and 150 meters
  - For the remaining 50 % of the cases a stable plume will be reached. The stable plume length will differ between 25 and 75 meters

5.6 Lesson 6: Test Monitoring network

- Open with  icon the file: *Monitoring_Stochastic*

- Click on the icon:  to see the Input View.
- Click on *Calculation >Test Monitoring*

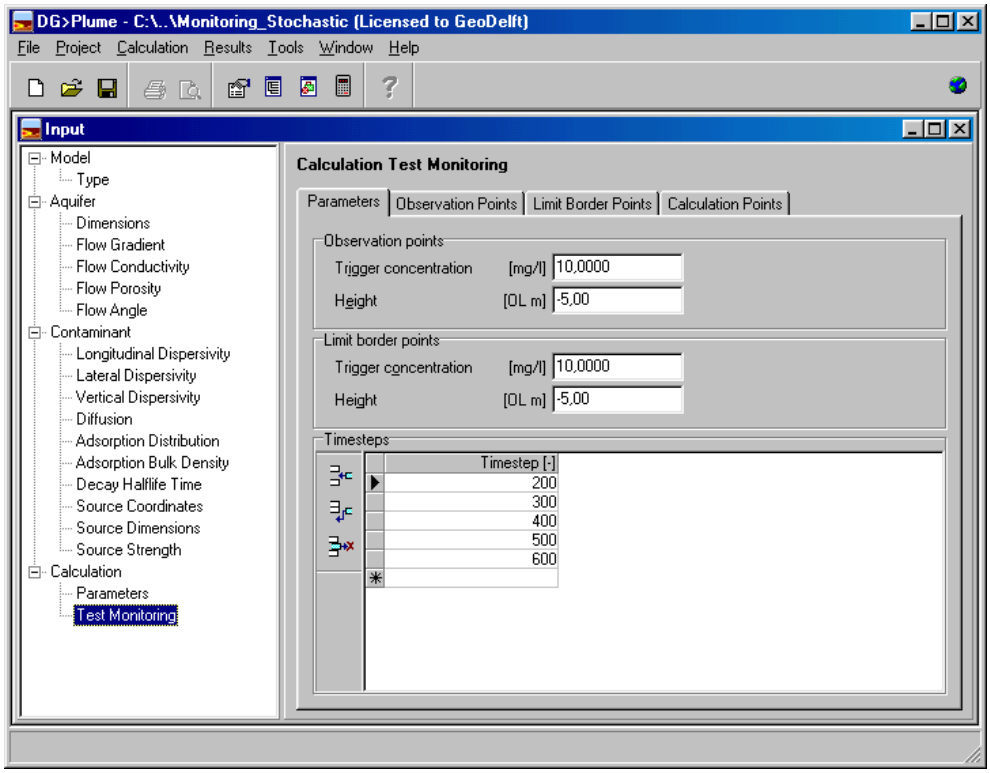


Figure 45 Tree Input View: Test Monitoring: Parameters

- A trigger concentration of 10 mg/l is set for both the observation points and the limit border points. It will be checked whether this trigger concentration will be exceeded in the observation and limit border points

- Click on the icon*:* 
- A DG>Plume calculation is started now.
- This calculation takes more time, because 100 realisations will be calculated
- Click on *Results > Stochastic Test Monitoring*
- Click on the tab page *Surface*

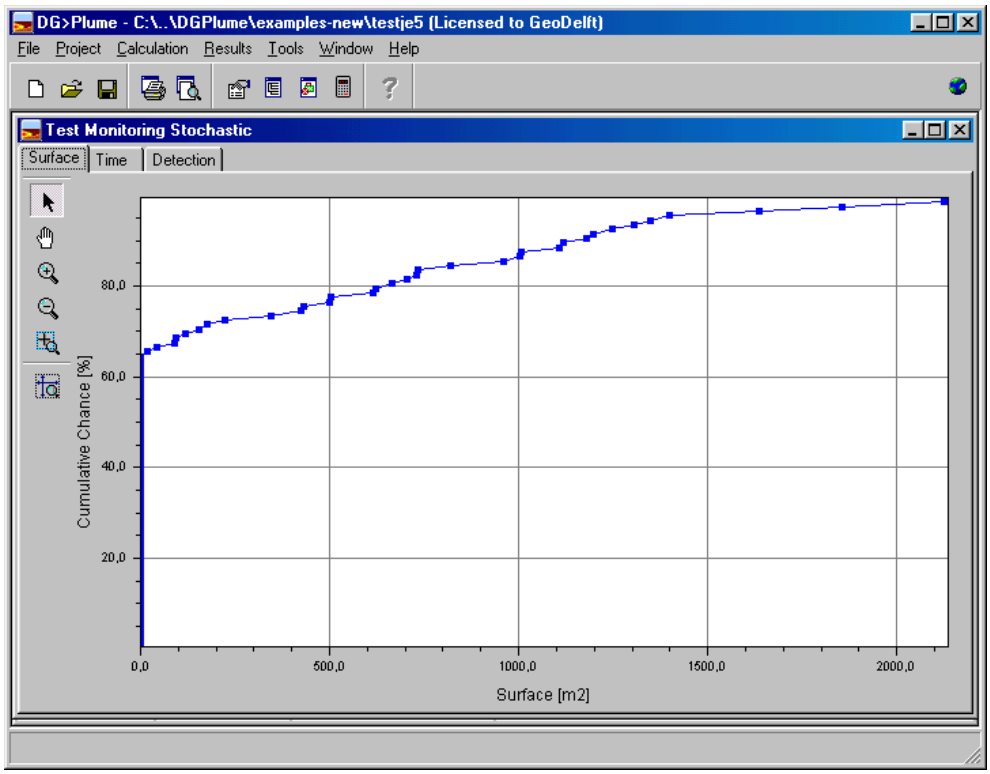


Figure 46 Results of the Stochastic Test Monitoring calculation: Surface

- The chance that the limit border will not be reached is 65 %
- For the remaining 25 % the limit border will be exceeded. In the graph it can be seen that the surface beyond the limit border will vary between 0 and 2100 m^2
- Click on the tab page *Detection*

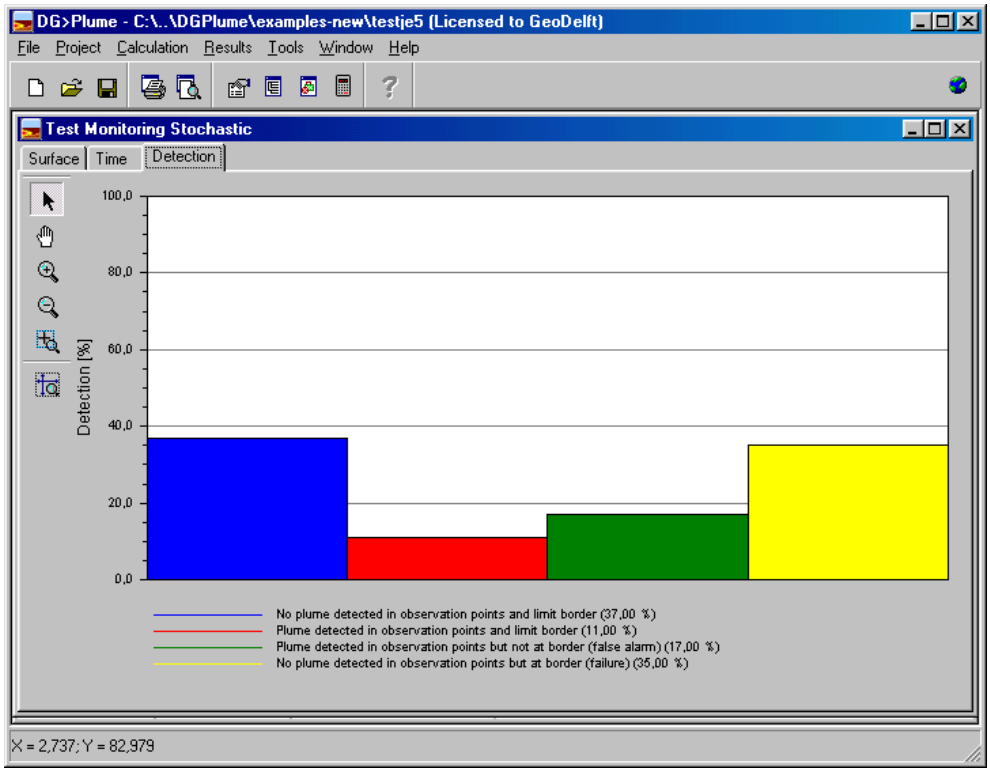


Figure 47 Results of the Stochastic Test Monitoring calculation: Detection

- In this tab page the detection chance of the monitoring network is presented
- The meaning of the four colors is explained before in this manual in Figure 34

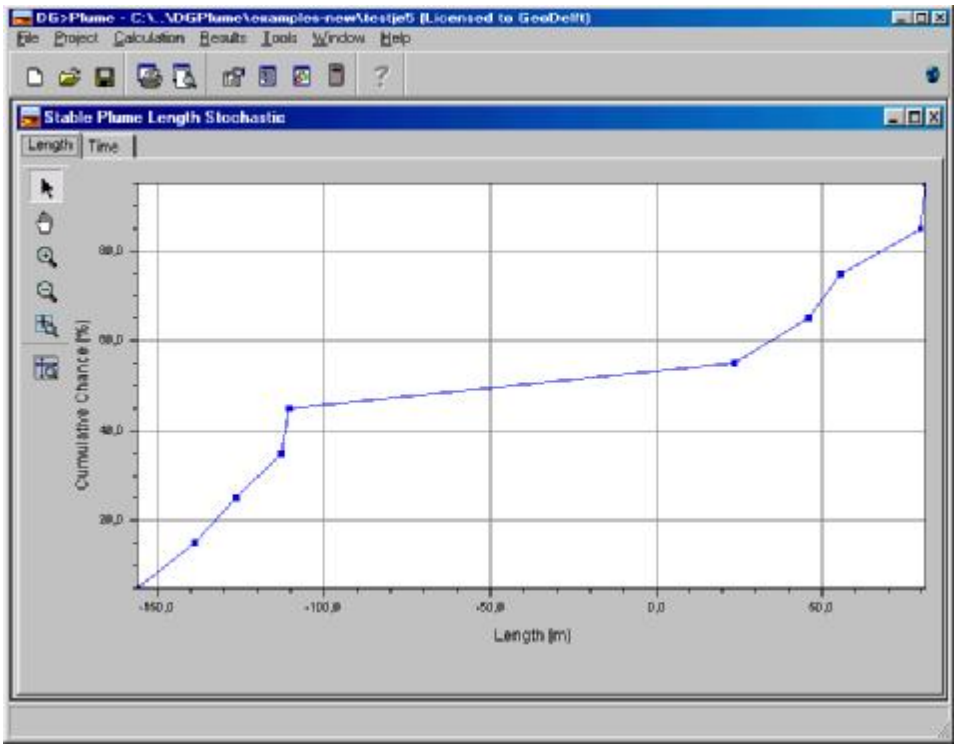


Figure 48 Results of the stochastic Plume Length calculation

- In Figure 48 can be seen that:
  - There is 0 – 50 % cumulative chance that no stable plume will be reached (negative plume length). In this case the plume length will be between 100 and 150 meters
  - For the remaining 50 % of the cases a stable plume will be reached. The stable plume length will differ between 25 and 75 meters

6 Background information

Below, you will find background information on the following topics:

- The concept of Flexible Emission Control (FEC) [§ 6.1]
- Latin Hypercube Method [§ 6.2]

6.1 Flexible Emission Control (FEC)

The text of this article is derived from the article Flexible Emission Control: a process-like approach [Van Meurs, et. al, 2000].

6.1.1 Introduction

Flexible Emission Control (FEC) delivers a conceptual framework for the analyses of the risk of migration. This means that FEC is applicable for mobile dissolved contaminants. Within FEC, the risk analyses is based upon the local soil properties, the type and extension of the pollution, the presence distance of local vulnerable objects and the local dynamics of the fate and behaviour of the contaminants. FEC is developed in the Netherlands [CUR/NOBIS 2000]. It gives a framework in which on the one hand space and thus time is given to natural attenuation of the contaminants or to the application of extensive remedial techniques. The maximum space is depending upon the distance between the current contaminated area of a the plume, the location of a vulnerable object e.g. a groundwater extraction well for drinking purposes, and an area in which, whenever necessary, additional counter measures (fall-back scenario) must be carried out. On the other hand, restrictions to the migration are imposed in order to maintain a safe situation nearby locations with a vulnerable object.

6.1.2 Framework of FEC; phased approach

The concept of FEC is a phased approach and it consists of three steps. The first step is governed by site investigation, risk analyses and the feasibility of counter measures primarily within the contaminated area (current source and plume) whenever necessary. A hypothesis about the plume behaviour is formulated both with and without counter measures but the emphasis is addressed to control and to monitor the current situation. Therefore, the behaviour of the current pollution (fate and transport) is closely followed. So, field measurements partly take over the protection given by the costly containment measures. Based upon the gathered characteristics of the situation (fate and migration of the contaminants in relation with the soil properties), a decision can be made about the realisation of further actions whenever needed.

The second step is collecting data from the field by monitoring. Monitoring consists of a verifying part and a controlling part. Within the verifying part, the hypothesis is judged about the behaviour and dynamics of the fate of the contaminants. Within the controlling part of monitoring the rate of migration is followed to judge whether the pollution remains within certain limits. Based upon this judgement, it might necessary to carry out the third step. The third step contains additional remedial actions, continuation of the monitoring or the ending of any involvement when the remaining risk is acceptable.

6.1.3 Framework of FEC; division into sub-areas

The division of the subsoil into sub-areas is strongly based on the methodology of 'source-path-target' This methodology is a rational framework to approach a soil contamination problem. The problem now is broken down into three elements: the contaminated source, a target in the vicinity which might be threatened and a pathway which connect both of them [Holdgate, 1979].

In the concept of FEC, four areas are distinguished in the subsoil:

- *System area*: in which the contamination is located and remedial actions can be carried out;
- *Monitoring area*: where control and monitoring takes place to acquire information about the fate and migration (emission) of the contaminant;
- *Back-up control area*: where additional remedial actions can be carried out;
- Area bordered by a *'fail-safe' limit* where the flux/concentration of the contaminants has to be in agreement with standards for sustainable circumstances.

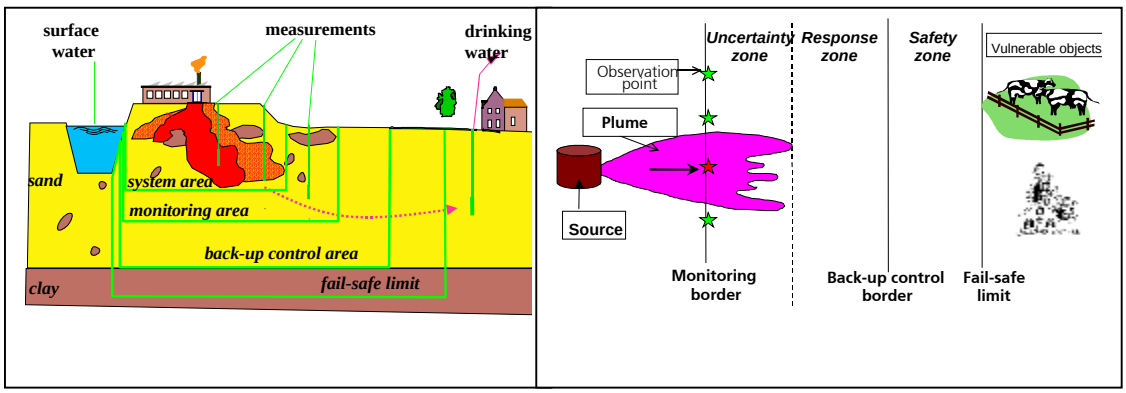


Figure 49 FEC concept

The area between the fail-safe limit and the border of the fall-back area can be seen as a safety zone for the vulnerable object like a groundwater extraction well. The area between the border of the monitoring area and border of the back-up control area is based on two aspects: uncertainty and delay. Uncertainty consists of two parts. On the one hand an observation point at the monitoring border may detect contamination which is at the edge of the plume, whereas the front of the plume has already passed this border. On the other hand the plume contains irregularities (fingering) e.g. due to soil heterogeneity (uncertainty zone). Delay is caused by the time necessary for sampling and evaluation, and the time necessary to carry out additional measures the so-called fall back scenario (response zone).

The design of the different areas within FEC and the design of the monitoring system, among others, are based on:

- The dynamics of the system (groundwater velocity, retardation, natural attenuation etc.);
- The trigger values applied within the monitoring system;
- The frequency of the sampling;

- The accuracy of the analytical measurements;
- The variation of the properties in the subsoil;
- The mutual distance between observation points;
- The acceptable standards nearby the vulnerable object;
- The optimisation of costs (monitoring costs vs. costs of realisation of fall-back scenario).

6.2 Latin Hypercube method

The text of this paragraph is derived from A Users Guide to LHS: Sandia's Latin Hypercube Sampling Software [Wyss, G.D. and K.H. Jorgensen, 1998].

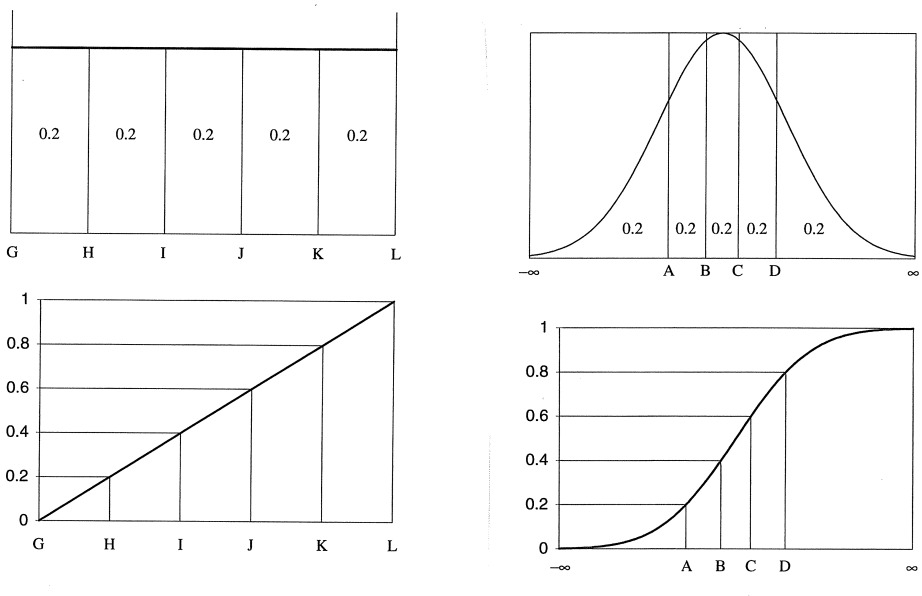


Figure 50 Intervals used with a Latin hypercube sample of Size n = 5 with a Normal distribution and an Uniform distribution

To help clarify how intervals are determined in the Latin hypercube sample, consider a simple example where it is desired to generate a Latin hypercube sample of size n = 5 with two input variables. Let us assume that the first random variable X_1 has a normal distribution with a mean value of μ and a variance of σ^2. The endpoints of the intervals are easily determined based on the parameters μ and σ^2. The intervals for n = 5 are illustrated in Figure 50 in terms of both the density function and the more easily used cumulative distribution function (CDF). Thus each of the five intervals corresponds to a 20% probability.

We will assume in this example that the second random variable, X_2, has a uniform distribution on the interval from G to L. The corresponding intervals used in the Latin hypercube sample for X_2 are given in Figure 50 in terms of both the density function and the CDF.

The next step in obtaining the Latin hypercube sample is to pick specific values of X_1 and X_2 in each of their five respective intervals. This selection must be done in a random manner with respect to the density in each interval; that is, the selection

must reflect the height of the density across the interval. For example, in the (-∞, A) interval for X_1, values close to A will have a higher probability of selection than those values in the tail of the distribution that extends to -∞. Next, the selected values of X_1 and X_2 are randomly paired to form the five required two-dimensional input vectors. In the original concept of Latin hypercube sampling as outlined in McKay, Conover, and Beckman, the pairing was done by associating a random permutation of the first n integers with each input variable. For illustration, in the present example consider two random permutations of the integers (1, 2, 3, 4, 5) as follows:

Permutation Set No. 1: (3, 1, 5, 2, 4)
Permutation Set No. 2: (2, 4, 1, 3, 5)

By using the respective position within these permutation sets as interval numbers for X_1 (Set 1) and X_2 (Set 2), the following pairing of intervals would be formed:

Computer run	Interval no. Used for X_1	Interval no. Used for X_2
1	3	2
2	1	4
3	5	1
4	2	3
5	4	5

Thus, on computer run number 1, the input vector is formed by selecting the specific value of X_1 from the interval number 3 (B to C) and pairing this value with the specific value of X_2 selected from interval number 2 (H to 1). The vectors for the second and subsequent runs are constructed in a similar manner.

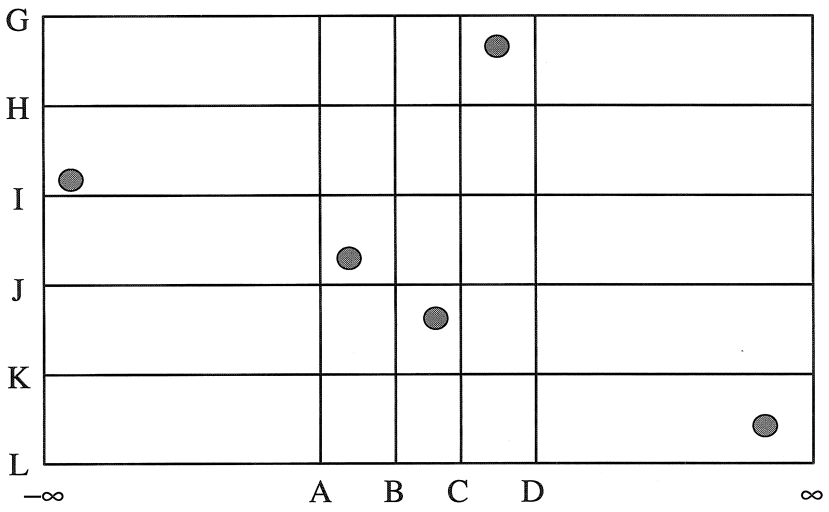


Figure 51 A Two-Dimensional Representation of One Possible Latin Hypercube Sample of Size 5 Utilizing X_1 and X_2

Once the specific values of each variable are obtained to form the five input vectors, a two-dimensional representation of the Latin hypercube sample such as that given in Figure 51 can be made. Note in Figure 51 that all of the intervals for X_1 have been sampled, and the same is true of X_2. In general, a set of n Latin hypercube sample points in k-dimensional Euclidean space contains one point in each of the intervals for each of the k variables.

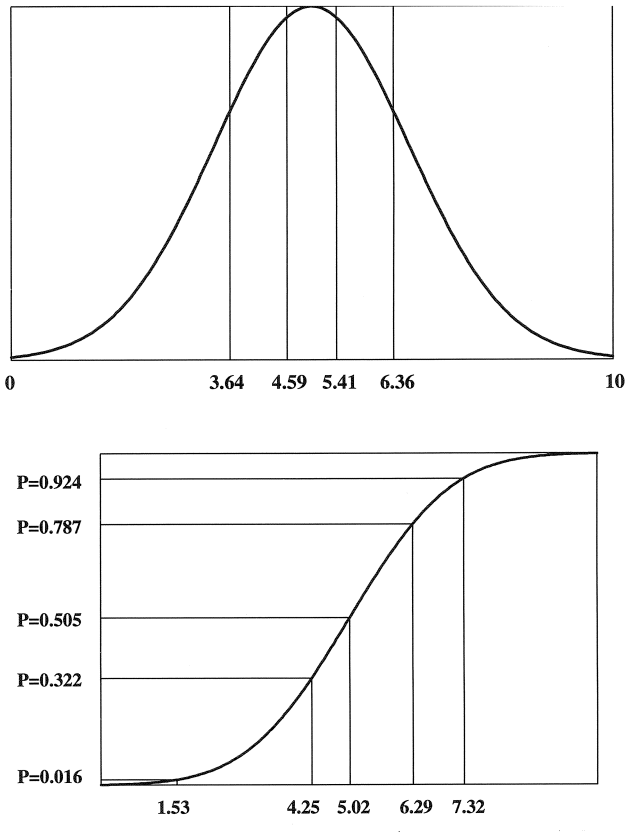


Figure 52 Interval Endpoints Used with a Latin hypercube sample of Size 5 (top) and Specific Values of X Selected Through the Inverse of the Distribution Function (bottom)

To illustrate how the specific values of a variable are obtained in a Latin hypercube sample, consider the following example. Suppose it is desired to obtain a Latin hypercube sample of size n = 5 from a normal distribution with a mean of 5.0 and a variance of 2.618 as indicated in Figure 50. The density characteristics of the normal distribution allow for the definition of the equal probability intervals. These intervals are shown in Figure 50 in terms of a density function. The next step is to randomly select an observation within each of the intervals. This selection is not done uniformly within the intervals shown in Figure 50, but rather it is done relative to the probability density function distribution being sampled (in this case, the normal distribution). This is equivalent to uniformly sampling from the quantiles of the distribution (equivalent to sampling the vertical axis of the CDF) and then "inverting" the CDF to obtain the actual distribution values that those quantiles represent. This process is illustrated in Figure 50.

Therefore to get the specific values, n = 5 numbers are randomly selected from the standard uniform distribution (uniformly distributed between 0 and 1). Let these be denoted as U_m, where m = 1, 2, 3, 4, 5. These values will be used to select distribution values randomly from within each of the n = 5 intervals. To accomplish this, each of the random numbers U_m, is scaled to obtain a corresponding cumulative probability, P, so that each P_m lies within the m^{th} interval. Thus, for this example with n = 5,

$$P_m = \left(\frac{1}{5}\right)U_m + \left(\frac{m-1}{5}\right)$$

This ensures that exactly one probability, P_m, will fall within each of the five intervals (0, 0.2), (0.2, 0.4), (0.4, 0.6), (0.6, 0.8) and (0.8, 1). The values P_m are used with the inverse normal distribution function to produce the specific values to be used in the final Latin hypercube sample. Note that exactly one observation is taken from each interval shown in Figure 50. Figure 50 makes it clear that when obtaining a Latin hypercube sample, it is easier to work with the CDF for each variable.

Figure 50 shows how one input variable having a normal distribution is sampled with Latin hypercube sampling. This procedure is repeated for each input variable, each time working with the corresponding cumulative distribution function. If a random sample is desired, then it is not necessary to divide the vertical axis into n intervals of equal width. Rather, n random numbers between 0 and 1 are obtained and each is directly (i.e., without scaling) mapped through the inverse distribution function to obtain the specific values. The final step in the sampling process involves pairing the selected values.

7 Literature

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