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**LGMCAD, a Solute Transport Module of
the Groundwater Model for the Netherlands.
User's Manual**

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ABSTRACT

This report describes the input files for the program LGMCAD, which is the solute transport module of the National Groundwater Model for the Netherlands (LGM). Additionally, several accompanying programs are described. SHOWCLOUD is a program to display the location of the cloud of particles on the screen. Also described is a tool CLDGRID that converts the particle oriented output into solute concentrations on a 2-dimensional grid. The resulting grid files may be visualized with a commercial or public domain contour line program. In several appendices the formats are described of all the files that are involved in a complete solute transport simulation with LGMCAD.

SAMENVATTING

Dit rapport geeft een beschrijving van de invoerbestanden voor het programma LGMCAD. Dit is een module voor het transport van opgeloste stoffen, behorend bij het Landelijk Grondwater Model (LGM). Daarnaast zijn enkele hulpprogramma's beschreven. SHOWCLOUD is een programma om de locatie van een deeltjes wolk op het scherm zichtbaar te maken. Tevens is een hulpprogramma CLDGRID beschreven, dat de deeltjes georiënteerde uitvoer omwerkt tot concentraties opgeloste stof in een twee-dimensionaal grid. De grid-bestanden die hiervan het resultaat zijn, kunnen zichtbaar worden gemaakt met een commercieel of 'public domain' programma voor het maken van contourlijnen. In enkele appendices worden de formaten beschreven van alle bestanden die aan de orde komen bij een stof transport simulatie met het programma LGMCAD.

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1 INTRODUCTION

This manual describes the use of LGMCAD and several accompanying programs. LGMCAD is a solute-transport module which was developed for the National Groundwater Model of the Netherlands (LGM). LGM is one of the key models at RIVM for support of environmental policy analyses. The abbreviation CAD stands for 'Concentration of solutes based on Advective-Dispersive transport'. In addition to advective-dispersive transport, the module considers first order (exponential) decay and linear equilibrium adsorption.

LGMCAD is based on a Lagrangian concept, which means that point masses (or particles) are introduced that carry a certain, possibly varying, amount of solute mass. Accordingly, the displacement of the particles is calculated by solving the motion equations. This technique is known as *particle tracking*. The Lagrangian approach is consistent with Eulerian approaches such as Finite Elements Method. Its main advantage is that complications as numerical dispersion are more easily controlled. Several numerical tests have been carried to compare LGMCAD with known analytical solutions with satisfying results (Uffink, 1996).

The particle nature of the model has some consequences for the user, in particular for the preparation of input data and the visualization of output data. Most visualization techniques (contours plots) are based on Eulerian data, such as contaminant concentrations on a set of grid points. Therefore, frequently transformation of particle oriented output data to concentrations on a grid is necessary. For this purpose an auxiliary program, CLDGRID, has been developed and is described in this manual as well.

The results produced by LGMCAD cannot be displayed directly in graphical form. An additional program SHOWCLOUD displays the raw output data graphically. SHOWCLOUD is a simple and rudimentary tool, since development of a sophisticated graphical postprocessor was not considered a purpose of the project. For display of grid oriented output (LGMCAD+CLDGRID) several good packages exist, both in the commercial field and in the public domain.

The LGMCAD-code is written in Fortran (F77) and has been developed on an HP-Apollo workstation (series 9000). The additional programs CLDGRID and SHOWCLOUD are written partly in Fortran and partly in C. Their codes depend on the *X Toolkit* library of the X Windows System Series and the *curses* library for control of the HP terminal. Therefore, these programs are machine and terminal dependent. LGMCAD itself does not depend on terminal properties and, therefore, may run on a variety of machines. Calculation program and postprocessing tools have been disconnected deliberately in order to be able to use fast (super)

computers for the calculation of large and complex problems, while postprocessing is more conveniently carried out interactively at a desk-top machine.

The organization of the manual is as follows. Chapter 2 starts with a general description of LGMCAD and an overview of all types of input and output files. Chapter 3 is devoted entirely to the so-called *cad file*, which is the main input file. In the chapters, 4 and 5 the additional programs SHOWCLOUD and CLDGRID are discussed. Finally, in the appendix precise descriptions of several file formats are given.

The manual does not provide the theoretical background of the model. For more information on theoretical aspects, the reader is referred to Uffink (1990, 1996).

2 LGMCAD

2.1 General

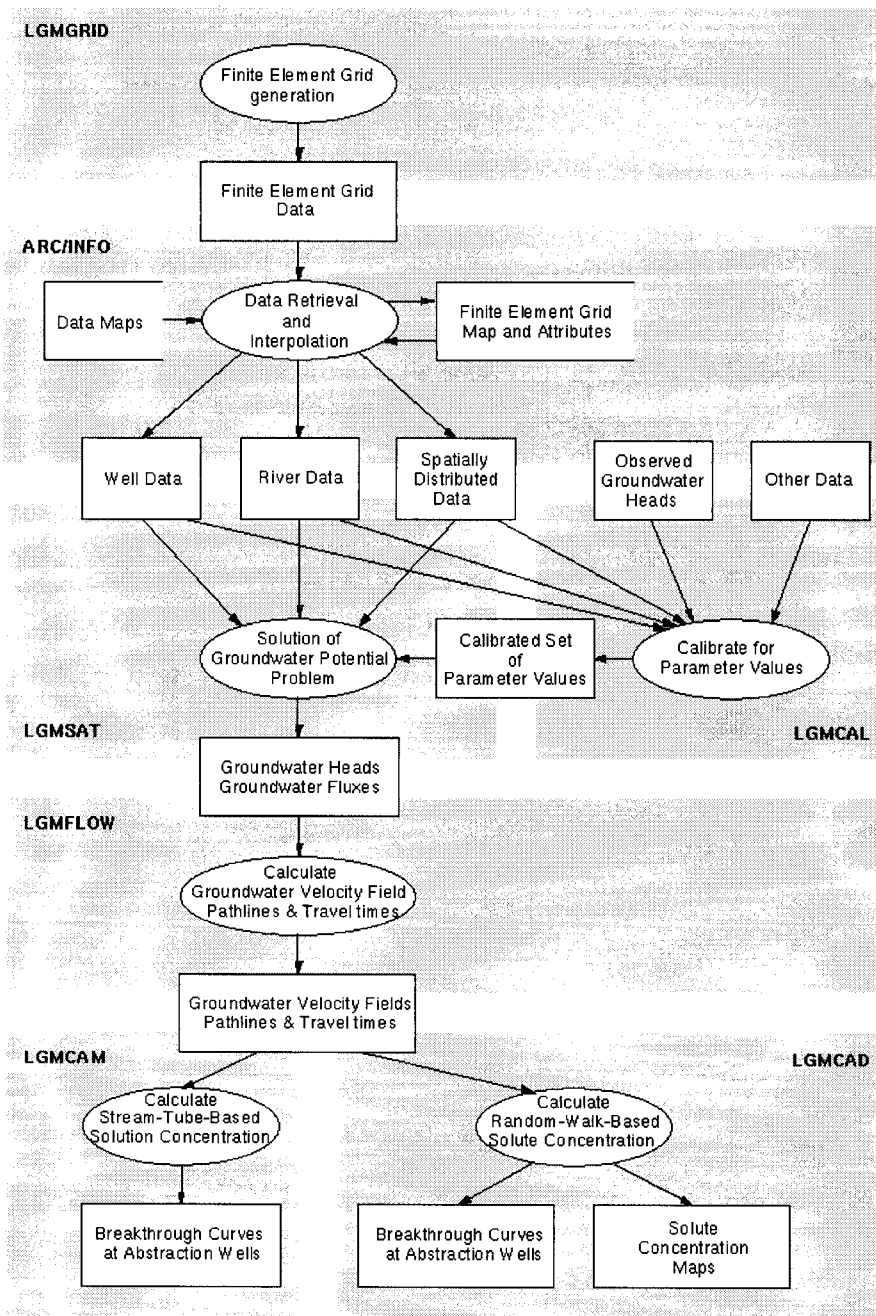


Figure 1 Relation between the various modules of the LGM software package

A complete simulation of a groundwater contaminant problem typically consists of several consecutive steps:

- i) modeling the groundwater flow and solving the groundwater heads (potentials).
- ii) calculate the groundwater velocity based on the distribution of the groundwater heads from step i).
- iii) modeling the solute transport and determination of the spatial/temporal distribution of the solute concentration, based on the velocity distribution obtained from step ii).

For the first and second step the LGM-modules LGMSAT and LGMFLOW are available.

LGMCAD provides the third step. An overview of all modules in the LGM software package and their relations is given in figure 1. As the figure indicates, LGMFLOW produces a file with the velocity field. This file also contains all relevant information on the geohydrological structure, the location of wells, rivers etc. Its is referred to as the *Efgofile*. The *Efgofile* is the link between the flow module and the solute transport module. For further details on the LGM program package see Pastoors (1992a, 1992b) and Kovar et al. (1992).

2.2 Command

The program is invoked by typing LGMCAD at the command-prompt, followed by one or more command-line arguments and concluded by pressing the ENTER key. The command-line arguments refer to the names of two basic input-files, the *Efgofile* and *Cadfile*. If these arguments are omitted, the program will prompt for them.

The general structure of the command is:

LGMCAD [-e EfgoFile] [-c CadFile] [-h]

- e** option: give name of *EfgoFile*
- c** option: give name of *CadFile*
- h** option: produces this information.

The *Efgofile* and *Cadfile* are essential files, which means that without these files LGMCAD does not run. Several additional input files may be involved, e.g. files to specify initial conditions or the spatial variation of contaminant input to the groundwater system (leaching rates). These non-essential or optional files are provided separately, while their names and locations are specified in the *Cadfile*.

2.3 Files

A calculation with LGMCAD involves several files. This paragraph gives an overview and a short description of their function and their contents. In the appendix the file formats are described in more detail.

Optional files are indicated by square brackets [] around the file-type name. All filenames may be chosen freely. An exception holds for the *lgm*cad.ini file, which is used to overwrite some default settings. All other file names are free, as well as the file name extensions. It is recommended, though, to use the extensions proposed in this manual, since this greatly helps to identify files during the various stages of the modeling process and postprocessing.

input files:

- EFGOFILE
- CADFILE
- [CLOUDFILE] initial concentration
- [GRIDFILE] rates of contaminant release into aquifer system
- [LGMCAD.INI]

output files:

- [CLOUDFILE's] if requested
- [KILLFILE] if contaminants leave the groundwater systems
- [BREAKTHROUGHFILE's] if requested

The output files contain only simulation results. Information about the course of the calculation process itself is sent by default to screen. Of course, screen output may be redirected to a file. The contents of this 'screen output file', are not discussed here.

EFGOFILE.

The *Efgofile* is the main output file of the groundwater flow module, LGMFLOW (formerly known as EFGO). Besides the velocity field, it contains information on the geohydrological structure, on the location of rivers and wells and on the spatial distribution of the groundwater recharge.

LGMCAD has been developed primarily to be used within the context of LGM, hence, in combination with LGMFLOW. However, an option exists to combine LGMCAD with an arbitrary groundwater flow model. This option is not described in this manual.

CADFILE

The *Cadfile* contains all the parameters concerning transport-processes (dispersion, decay-rates etc.), data on the initial contaminant concentration, rates of contaminant release into the aquifer system, etc. A detailed description of the *Cadfile* is given in Chapter 3.

CLOUDFILE

Cloud files contain data of a group of particles present in the system at a specific moment in time. Such a collection of particles is called a cloud. The cloud-data consist of the coordinates, the mass and some other, optional, attributes of the particles. The full format of a cloudfile is given in the appendix.

Cloud files can occur both as *input file* or as *output file*. As *input file*, it typically contains data on the particles in the system at the start of the simulation. These particles represents the initial contaminant distribution, if it exists. Such a cloudfile may be the output of a previous LGMCAD simulation. If the initial conditions of a groundwater contaminant problem are given in terms of concentrations, these data have to be converted first to a particle representation. The name of the cloudfile describing the initial conditions must be given in the *Cadfile*. If the name is omitted, the initial concentrations are assumed to be zero.

As *output file*, a cloud-file contains the data of all the particles in the system, i.e. their positions, their masses and an additional attribute for the sorption state of the particle (sorbed or free). During a simulation several cloud files can be produced, representing the state of the system at several moments in time. Cloud files may be visualized directly by the program SHOWCLOUD (chapter 5) or they may be converted first to concentration data on a grid by CLDGRID (chapter 5) and then visualized by a contour-lining program.

GRIDFILE

A gridfile is the Eulerian counterpart of the cloudfile. It contains solute concentrations on a regular spatial grid. Another important distinction exists between cloud files and grid files. Grid files contain concentrations in a *2-dimensional plane*, while a cloudfile contains *3-dimensional* information of all particles present in the system at a certain time. Out of one specific cloudfile several grid files can be derived, e.g. concentrations at several depths or the concentration distribution in a vertical cross-section. A grid file is obtained from a cloudfile by running CLDGRID. More details are given in Chapter 5.

Grid files may also appear as *input* for LGMCAD. In this case they contain information on the release rates of contaminants to the groundwater at the top of the aquifer system (leaching rates). The data may be expressed in terms of contaminant concentrations or directly as solute mass fluxes. More details are given in Chapter 3.

KILLFILE

One of the output files is the so-called *killfile*. This file contains information on the particles that leave the groundwater system during the simulation. In the terminology of LGMCAD these particles are 'killed' and no longer exist. The *killfile* is an ASCII file with exit times, masses and coordinates of the particles that leave the system, plus a code that identifies the well, river or boundary where the particle leaves. The *killfile* may be used during the postprocessing, e.g. to determine breakthrough curves in groundwater abstraction wells.

BREAKTHROUGHFILE

While a cloudfile or gridfile describes the spatial contaminant distribution at a fixed time, a breakthrough file contains the temporal contaminant distribution at a fixed point in space. The breakthrough file simply consists of a list of concentrations and times. Note that the data are already expressed in terms of concentrations. The data may be visualized by the RIVM-developed graphical program XY (Van Heerden and Tiktak, 1994) or any similar program.

LGMCAD.INI

The default settings may be overwritten by specifying new values in the *LGMCAD.INI* file. For instance, by default cloud files are written in ASCII format, but may also be written as unformatted (or binary) files by setting a switch in the *LGMCAD.INI* file. The advantage of unformatted files is that they are processed faster by CLDGRID, they occupy less disk space and the data do not suffer from a loss of significant figures. However, they cannot be read by a standard text editor.

The options that can be set in the *LGMCAD.INI* file are described in the appendix.

3 CADFILE

3.1 General

The *Cadfile* contains all the specific data to characterize the transport-process, plus some data to control the calculation process. The data are divided into several sections:

- TIMES
- INITIAL CONCENTRATION
- RELEASE RATES
- PROCESS PARAMETERS
- OUTPUT CONTROL
- MISCELLANEOUS

There is no prescribed order for these sections in the *Cadfile*. However, within each individual section, the order of the data records is prescribed. A new section is opened by a record with the name of the section in capitals enclosed by square brackets. Only the first two characters of that name are significant. For instance, the section OUTPUT CONTROL may be opened by a record :

[OUTPUT]

or

[OUT]

Notice, that the closing bracket ']' is required. Comments may be inserted at any position by starting the record with the character '*' or by a semi-colon ';'. For numerical data free formats are applied, unless a format is mentioned explicitly. The field-separation symbol is a coma, a blank or both. Comments may also be included at the end of the record e.g.:

[TIMES]

; the following record contains the total simulation period and the initial time step.

200000, 15 Total simulation time = 200000 days, time step = 15 days

In the rest of this chapter the records of each section are described. The records are numbered by the first two letters of the section followed by a dot and a number. For example, the third

record in the section on release-rates is indicated as *(re.3)*. This identification is only for reference in the manual and does not have to be used in the file.

The very first line in the *cadfile* does not belong to any of the sections mentioned above and contains a text-string that identifies the problem that the cadfile belongs to. E.g., the first line may read:

Cadfile for Pesticide Transport Simulation; scenario 2a.

3.2 *TIMES*

[TIMES] (ti.1)

After the opening record (above) a single data record follows. The times-section contains only two parameters:

Tend, Tstep (ti.2)

where:

Tend indicates the time at which the calculation must be stopped.

Tstep denotes the time-step.

As unit of time 'days' are used

3.3 INITIAL CONCENTRATION

In this section information is given on particles initially present in the system. These particles represent the initial solute concentration. The information itself (location and masses of the particles) is expected to be described in a cloudfile (see appendix). The *Cadfile* simply contains the number of particles and the name of the cloudfile. The opening record of the section reads:

[INITIAL CONCENTRATION] (in.1)

The second record contains:

NPART (in.2)

NPART is the number of particles. If *NPART* = 0, the rest of the section is ignored.

P_ININAME (in.3)

P_ININAME is the name of a cloudfile representing the initial condition. In principle it contains *NPART* particles. If the number of particles in the file is higher than *NPART*, the program only reads the first *NPART* records. If the file contains less than *NPART* particles a warning is sent to screen and *NPART* is replaced by the actual number of records found in the file.

3.4 RELEASE-RATES

In this section data are entered on the amount of contaminants released to the groundwater system during the simulation period.

Two release options are distinguished: *individual cell-release* and *grid-distributed release*. The *cell-release* option considers an individual 3-dimensional (cubic) cell from where the contaminant release takes place. This cell may be located anywhere in the groundwater system (see figure 2). The user specifies the location and dimensions of this cell and the release rate at several consecutive moments in time. In case of *grid-release* the contaminants are released at the top of the groundwater system. This is the top of the upper aquifer in case of confined flow or the phreatic surface in case of unconfined flow. The rate may vary in space and in time. The spatial variation for a certain moment in time is specified by using a *gridfile* with the release-rates. This file is provided separately, while the *cadfile* holds the name of the *gridfile(s)*. Several grid files may be presented to specify the rate at different moments in time. The rate at an arbitrary point in time is obtained by linear interpolation between the two nearest point in time.

The release options differ with respect to the vertical position, where the release is taking place. Individual cells may be located at any depth in the aquifer, as desired by the user. Grid-release, however, always occurs at the top of the aquifer system. The vertical position is generated automatically by the program.

[RELEASE-RATES] (re.1)

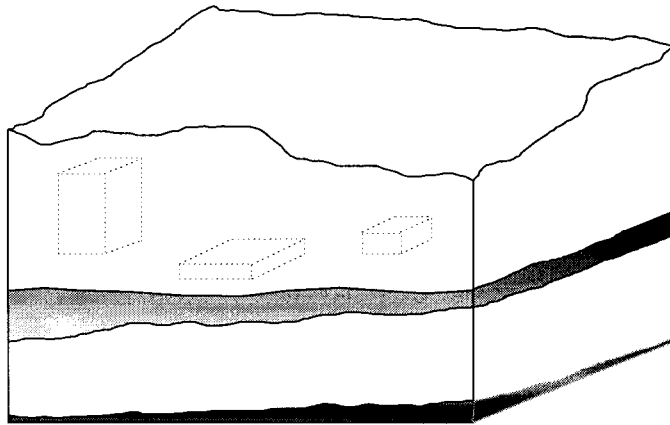
The first records following the opening line concern cell-release data:

NCELLS (re.2)

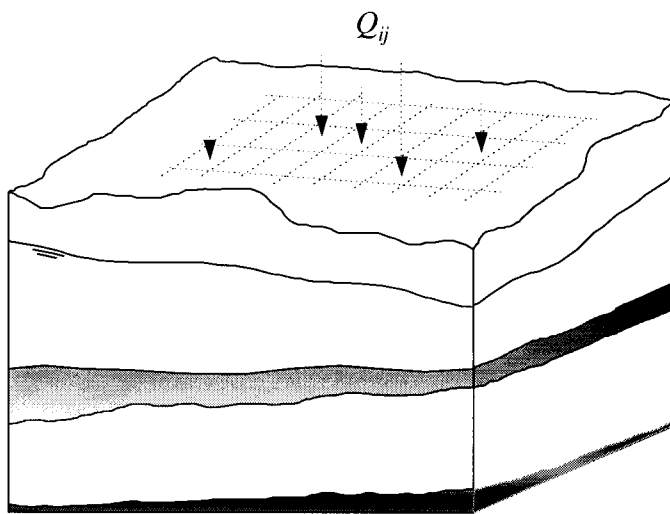
NCELLS defines the number of individual cells. If *NCELLS* > 1, the records below, (re.3), (re.4), (re.5) and (re.6), must be repeated *NCELLS*-times. For *NCELLS* = 0, these lines can be omitted.

CELLNAME (re.3)

CELLNAME is the name of a cell. This name is introduced merely to enhance the readability of the *CADFILE* and is relevant only for the user.



(a)



(b)

Figure 2. Two release options: (a) cell release and (b) grid-release

$X_CORNER, Y_CORNER, Z_CORNER, \Delta X, \Delta Y, \Delta Z$ (re.4)

On this record the location and dimensions of a cubic cell are specified. The coordinates of one of the corners are followed by the cell dimensions in x , y , and z direction. One may use the coordinates of any of the corners combined with positive dimensions or negative values for $\Delta X, \Delta Y, \Delta Z$. The results is that particles are generated with x, y, z coordinates in the intervals $[X_CORNER, X_CORNER+\Delta X]$, $[Y_CORNER, Y_CORNER+\Delta Y]$ and $[Z_CORNER, Z_CORNER+\Delta Z]$. The cubic cells may degenerate into plane cells, lines or point-sources by taking one or more of the cell dimensions equal to zero (figure 3)

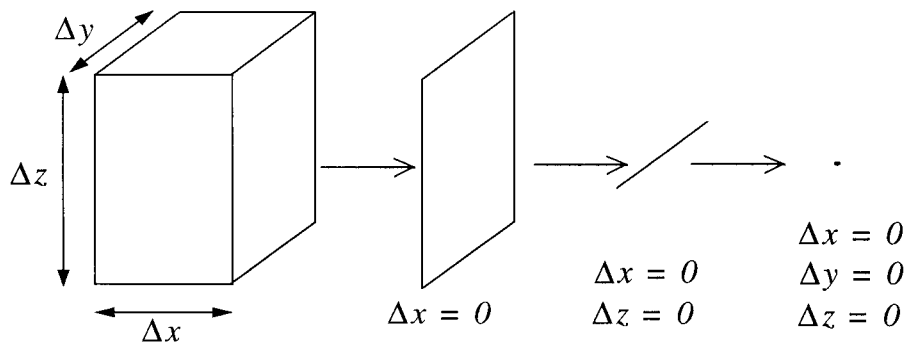


Figure 3. Degeneration of release cells into plane-, line-, or point-source

Temporally varying release rates will be approximated by a series of instantaneous mass pulses with a certain strength. The pulses act at a regular time interval ΔT , while the strength of each pulse is calculated by the program, based on the pulse interval and the release rate $Q(t)$. On the following three records data are given concerning the release period and the release rates.

$T_0, N_INTERVAL, \Delta T, NPART$ (re.5)

T_0 is the time of the start of the release period. The total period is divided into a number of intervals, $N_INTERVAL$, each with a length ΔT (figure 4). The number of pulses is $N_INTERVAL+1$. A pulse with index number j acts at time t_j given by:

$$t_j = T_0 + j \Delta T, \quad (3.1)$$

where j varies from 0 to $N_INTERVAL$.

On the next record the release rate $Q(t)$ is specified for each of the 'pulse' moments t_j :

$$Q_0, Q_1, Q_2, Q_3, \dots, Q_{N_INTERVAL} \tag{re.6}$$

where $Q_0, Q_1 \dots$ is shorthand for $Q(t_0), Q(t_1)$ etc. Figure 4 shows an example
 Each individual pulse consists of a number of particles, $NPART$, as given on the next record.

$$NPART \tag{re.7}$$

This means that the total amount of particles released into the aquifer is $NPART * (N_INTERVAL+1)$.

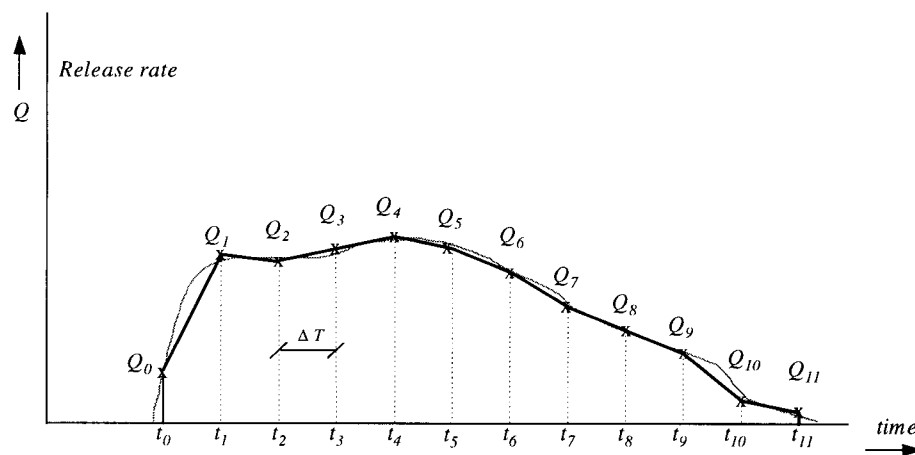


Figure 4 Approximation of release rate function $Q(t)$ by 11 intervals with piece-wise linear rate distribution

The strength of the pulses and the mass of each single particle is determined by the program according to the following scheme. First, it is assumed that between the pulse moments t_j and t_{j+1} the rate function $Q(t)$ varies linearly from Q_j to Q_{j+1} . Accordingly, the contribution of mass dM , released during a short period $d\tau$ on the pulse interval (see figure 5) is decomposed into two parts. One component is allocated to the pulse at t_j , the other to the pulse at t_{j+1} . For the decomposition linear weight factors are used. The total contribution is obtained by integration over the pulse interval with τ as

integration variable. The result of this procedure is that $Q(t)$ is approximated by a series of instantaneous mass releases (pulses) with strength P_j :

$$Q(t) \approx \sum_{j=0}^k P_j \delta(t - t_j) \quad (3.2)$$

where the pulse strength P_j are given by:

$$P_0 = [2Q(t_0) + Q(t_1)] \frac{\Delta T}{6} \quad (3.3)$$

$$P_j = [Q(t_{j-1}) + 4Q(t_j) + Q(t_{j+1})] \frac{\Delta T}{6} \quad (3.4)$$

$$P_{N_INTERVAL} = [Q(t_{N_INTERVAL-1}) + 2Q(t_{N_INTERVAL})] \frac{\Delta T}{6} \quad (3.5)$$

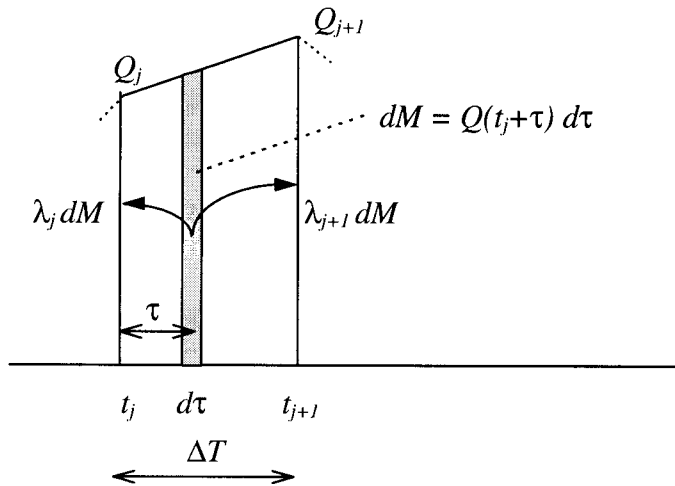


Figure 5. Decomposition of mass dM into $\lambda_j dM$ and $\lambda_{j+1} dM$,
where $\lambda_j = (\tau - 1) / \Delta T$ and $\lambda_{j+1} = \tau / \Delta T$

At each pulse $NPART$ particles are released. Thus, the mass of an individual particle released at t_j equals $P_j / NPART$.

NGRIDFILES, IFLAG

(re.8)

Apart from individual cell-release, it is possible to work with a spatially distributed release rate that also varies in time (*Grid-release*). The data (mass-rates) are now organized in a regular two-dimensional array or grid. In the following discussion the rate at a specific location and time, written as $Q(x_i, y_j, t_k)$, will be denoted shortly as $Q_{ij}(t_k)$. Note that the z -coordinate is not included in this notation, which is because in this option the release always takes place at the top of the aquifer system. For each t_k the rates $Q_{ij}(t_k)$ are given in an external file. The values t_k do not necessarily follow an equidistant pattern. The parameter *NGRIDFILES* on (re 8) defines the number of grid files. The second parameter, *IFLAG*, refers to how these data are interpreted. If *IFLAG* = 1, the data represent mass-fluxes per year per grid cell. If *IFLAG* = 2, the data represent concentrations of the natural recharge. In the latter case the mass-fluxes are determined by the program itself, using the values of the natural recharge from the *efgofile*. With the natural recharge, denoted by q_{ij} , one obtains $Q_{ij}(t_k)$ from:

$$Q_{ij}(t_k) = c_{ij} q_{ij} A, \quad (3.6)$$

where A is the area of a grid cell. For the option *IFLAG* = 1 the data $Q_{ij}(t_k)$, given in the gridfile can be converted to a convenient unit by specifying a conversion factor on the next record. This record is not included if *IFLAG* = 2.

CONVERS

(re.9)

The next record is repeated *NGRIDFILES* times and reads:

'FILENAME', t_k , $N_SUBINTVAL$, $NPART$

(re.10)

This record contains the name of the gridfile between quotes. This file is expected to be in ARC-INFO format (see appendix). The record is repeated *NGRIDFILES* times. For every k between 1 and *NGRIDFILES* a file name is entered that contains the data $Q_{ij}(t_k)$ or $c_{ij}(t_k)$ (depending on the value of *IFLAG*). The release rate during an interval between t_k and t_{k+1} is considered to vary linearly between $Q_{ij}(t_k)$ and $Q_{ij}(t_{k+1})$. This continuously varying rate is approximated by a number of instantaneous pulses. Therefore, the interval is divided into a number of subintervals, which is determined by the parameter *N_SUBINTVAL*. Every pulse is modeled by *NPART* particles. The release period starts at t_1 , and ends at $t_{NGRIDFILES}$. By specifying several intermediate times t_k the release period can be divided into *NGRIDFILES* - 1 intervals. During such an interval the release rate is considered to be continuous and varying linearly between $Q_{ij}(t_k)$ and $Q_{ij}(t_{k+1})$. An interval between t_k and t_{k+1} is divided into *N_SUBINTVAL* subintervals. The

continuous release rate during this is approximated by $N_SUBINTVAL$ pulses at each grid cell, which are modeled each by $NPART$ particles. The mass of an individual particle released at a certain time is now:

$NSUBWINDOW$ (re.11)

The grid files mentioned above (grid-release) may cover a large part of the model area, leading to a large amount of generated particles. Sometimes, only part of that area is of interest. The option to choose a selected part of the grid area, without preparing a new series of grid files, is provided using *subwindows*. Figure 6 illustrates a hierarchy of windows. On record (re.11) the number of subwindows is given. If $NSUBWINDOW$ is greater than zero, data on the location of these windows must be entered on the next record.

$SUBXMIN, SUBYMIN, SUBXMAX, SUBYMAX$ (re.12)

This line contains the coordinates of the lower left corner of the subwindow, the point ($SUBXMIN, SUBYMIN$) and the coordinates of the upper right corner, the point ($SUBXMAX, SUBYMAX$). If $NSUBWINDOW > 1$, this line has to be repeated $NSUBWINDOW$ -times.

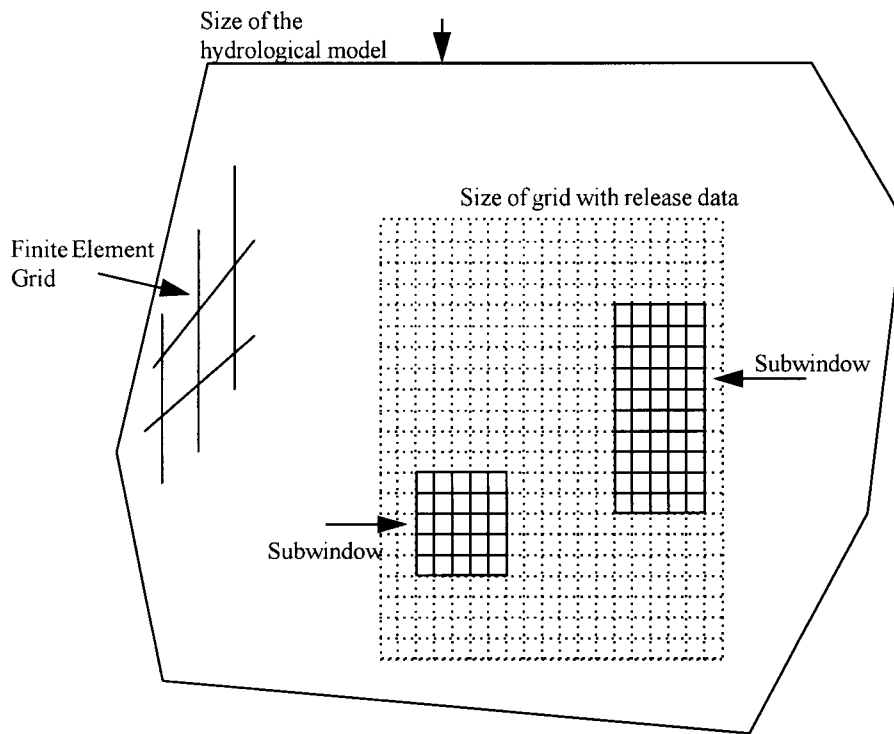


Figure 6. Hierarchy of windows.

3.5 OUTPUT

The OUTPUT-section contains information on the type of requested output. Output data become available in two types of files (see also Chapter 2).

- *.cld* files, or cloudfiles
- *.brk* files, or breakthrough files

The opening record of this section reads:

[OUTPUT] (ou.1)

On the next line a name is given that is used to generate new filenames for the output of particle data:

Cld_Filename (ou.2)

This is the part of the name shared by all generated *.cld* files. The final filename consists of this name, plus a three number code and the standard extension *.cld*. For example, if *CldFilename* = 'PLUME', the first file becomes *PLUME000.cld*. When the second cloudfile is generated, the three figure code is increased by one, unless that file already exists. Hence, subsequent cloud files are *PLUME001.cld*, *PLUME002.cld*, etc. The files contain the coordinates, mass and other attributes of the particles present at a given time. If instead of *CldFilename* the record is left blank, 'cloud' is assumed as default name and output is stored on *cloud000.cld*, *cloud001.cld*, etc.

N_CldFiles, I_Offset (ou.3)

N_CldFiles is the number of requested cloud files. *I_Offset* is a parameter that indicates how values for times are interpreted. If *I_Offset* = 0, the time is taken as an absolute value. For *I_Offset* = 1 the time indicates the time since the start of the simulation.

CldTime1, CldTime2 (ou.4)

(This record is omitted for *N_CldFiles* = 0.)

CldTime1, *CldTime2*, etc. are the times for which a cloud-file is created. Normally, the number of data on this record is equal to *N_CldFiles*. If the number of data is less than *N_CldFiles* (e.g. *Ndata*), *N_CldFiles* is modified to *Ndata*. If *Ndata* is larger, only the first *N_CldFiles* data are read and the rest is ignored.

NMON (ou.5)

NMON is the number of monitoring wells. Each of these wells is specified on a record.

MONNAME, XMIN, YMIN, ZMIN, ΔX, ΔY, ΔZ

(ou.6)

This record must be omitted if $NMON = 0$. If $NMON > 0$ the record is repeated $NMON$ -times. The record contains 6 parameters for the position and dimensions of the monitoring cell, preceded by a text string holding a name to identify the spot under consideration. After each time step the program checks if mass is present in the specified cell and it calculates the concentration. The values of time and concentrations are written to a file (ASCII-format), with the name *MONNAME.brk*.

3.6 PROCESS-PARAMETERS

[PROCESS-PARMS] (pr.1)

This section contains parameters that describe the transport processes: dispersion, adsorption and degradation. The parameter that controls the dispersion is the *dispersivity*. On the next record the dispersivity values are given for a constant background value that holds throughout the system. In certain specified regions the background value may be overwritten.

ALFA_L, ALFA_T_h, ALFA_T_v (pr.2)

ALFA_L : longitudinal dispersivity (m)
ALFA_T_h : transverse dispersivity in the horizontal plane (m)
ALFA_T_v : transverse dispersivity in the vertical plane (m)

The second record contains the number of regions where the background value must be overwritten:

NCH_ALFA (pr.3)

where *NCH_ALFA* is the number of cell-blocks with a dispersivity that differs from the background value.

XMIN, YMIN, ZMIN, ΔX, ΔY, ΔZ, ALFA_L, ALFA_T_h, ALFA_T_v (pr.4)

This line specifies the location and dimension of an areas where dispersivity values differ from the background values. This line has to be repeated *NCH_ALFA* times.

ISORPTION (pr.5)

The program has a number of options to simulate the sorption process. The parameter *ISORPTION* indicates one of the following options:

ISORPTION = 0 : no adsorption;

In this case the transport is pure advection-dispersion and no further data are required

ISORPTION = 1 : linear equilibrium adsorption.

Linear equilibrium adsorption is assumed and the program expects the retardation coefficient on the next record.

RETARD (pr.6)

RETARD is the retardation factor, which may be calculated by the formula:

$$R = 1 + \frac{(1-\varepsilon)\rho_g K_d}{\varepsilon} \quad (3.7)$$

where:

- R = retardation factor (dimensionless)
- ε = porosity (dimensionless)
- ρ_g = mass density of grain skeleton (kg/m³)
- K_d = partitioning coefficient (m³/kg) solutes to grain

IDECAY (pr.7)

The parameter *IDECAY* indicates whether decay (degradation) occurs and whether the decay parameter is a spatial variable or a constant. It also indicates if the decay parameter is given in terms of decay rates [T⁻¹] or as a half lifetime [T]. Table 3.1 shows the meaning of the values for *IDECAY*.

Table 3.1 Codes for *IDECAY*

<u><i>IDECAY</i></u>	<u>property</u>	<u>decay parameter</u>
0	no decay	--
1	constant	λ
2	constant	$T_{1/2}$
3	variable in space (cells)	λ
4	variable in space (cells)	$T_{1/2}$
5	variable in space (grids)	λ
6	variable in space (grids)	$T_{1/2}$

The lines following record (pr.7) depends on the value of *IDECAY*. In case *IDECAY* = 0, there is no decay and there are no additional record required. The cases *IDECAY* = 1 and *IDECAY* = 2 correspond to a spatial constant decay rate. Now, a record follows with the value of the decay parameter (pr.8). The parameter expected on (pr.8) is the

decay rate λ in days⁻¹, when *IDEDECAY* = 1. If *IDEDECAY* = 2, the record contains the half-life time T_{50} .

DECAY_PARM (pr.8)

The value of *IDEDECAY* determines whether *DECAY_PARM* is interpreted as a decay rate λ or as a half-life time T . In the program days are used as unit of time. Thus, if the decay parameter represents the decay rate it must be expressed in day⁻¹. If it represents the half-life time, it is given in days. T and λ are interrelated by:

For *IDEDECAY* = 3 or 4, the line (pr.8) must be included as well, but now the parameter is interpreted as a background (default) value that may be overwritten in several specific regions. Information on these specific values are added on (pr.9) and (pr.10) *IDEDECAY* = 3 expects the parameters as decay rates, while *IDEDECAY* = 4 expects half-life times. Secondly, a number of 3D cells is specified, where the background value can be overwritten.

NCH_DECAY (pr.9)

Here *NCH_DECAY* is the number of cell-blocks with a decay parameter that differs from the background value given on (pr.8).

XMIN, YMIN, ZMIN, ΔX, ΔY, ΔZ, C_DECAY (pr.10)

This line specifies the location and dimension of an area where the decay parameter differs from the background values. The line above has to be repeated *NCH_DECAY* times.

In case *IDEDECAY* is 5, or 6 the variation in the decay-parameter is expected to be available as a 2-dimensional grid. Several layers in vertical direction may be used. Apart from the decay parameter itself, also the z -elevation of top and bottom of the grid cells must be provided. The records (pr.11) . and (pr.12).follow now directly after (pr.8).

N_LAYERS (pr.11)

For the first layer 3 separate grid files are necessary. The first contains the z -level of the top of the layer, the second file contains the decay parameter, while the third file contains the z -level of the bottom of the layer. If a second layer is defined, the bottom of the first layer is taken as the top of the second layer. Thus, for each additional layer two additional grid files are required, one for the decay-parameters and one for the

bottom of that layer. The maximum number of layers at present is 3, which requires the following order of grid files (from top to bottom):

- file-1* (top level of the 1st layer)
- file-2* (decay parameter for 1st layer)
- file-3* (bottom of 1st layer)
- file-4* (decay parameter for 2nd layer)
- file-5* (bottom of 2nd layer)
- file-6* (decay parameter for 3rd layer)
- file-7* (bottom of 3rd layer)

Consequently, line (*pr.12*) must be repeated $(2 N_LAYERS + 1)$ times.

filename

(*pr.12*)

3.7 MISCELLANEOUS

[MISCELLANEOUS] (mi.1)

This category contains various parameters not covered by any of the previous sections.

IRAN (mi.2)

The parameter, *IRAN*, is the seed for the random generator. Using the same seed for two different runs of the same problem, means that the same series of random number is generated and, consequently, the same output will be produced. This may be necessary e.g. to locate a problem during the calculation. A reason to **change** the seed may be when various runs for the same problem are executed and the cloudfiles are added afterwards. The effect of the addition is that the number of particles is increased, which means a better accuracy.

ICLIP (mi.3)

ICLIP is a switch, set to either 1 or 0. It indicates whether the CLIP-option is used or not. With the CLIP option execution of the simulation may be accelerated considerably. It is useful, if the study area only covers part of the total hydrological model area. If the solute transport is relevant in a part of the total model area, a clip-window may be specified on the next record. This means that transport is only simulated as long as the solute particles are inside this window. If the CLIP option is set (*ICLIP* = 1) the following record contains the dimensions of the clip window.

C_XMIN, C_XMAX, C_YMIN, C_YMAX (mi.4)

[END]

This last line indicates that no more data follow. Text that is written beyond this record is ignored. Any comments can be included after this line.


```

[RELEASE-RATES]
0                number of locations for cell release
7, 10           number of files for grid release
0.00273973      Conversion (=1/365); original data given in kg/year
; Grid-release
; -----
; the following files contain the data of nitrate release at the years
; 1950, 1960, 1970, 1980, 1990, 1995, 2005
; (the situation at 2005 is a copy of that at 1995)
; Files are located in the directory /home/lbg6/lbguffi/lgm/nitraat/gasfiles

'/home/lbg6/lbguffi/lgm/nitraat/gasfiles/a0n1950.g2a', 0, 20 , 5000
'/home/lbg6/lbguffi/lgm/nitraat/gasfiles/a0n1960.g2a', 3650, 20 ,5000
'/home/lbg6/lbguffi/lgm/nitraat/gasfiles/a0n1970.g2a', 7300, 20, 5000
'/home/lbg6/lbguffi/lgm/nitraat/gasfiles/a0n1980.g2a', 10950, 20 , 10000
'/home/lbg6/lbguffi/lgm/nitraat/gasfiles/a0n1990.g2a', 14600, 10 , 5000
'/home/lbg6/lbguffi/lgm/nitraat/gasfiles/a0n1995.g2a', 16425, 20 , 10000
'/home/lbg6/lbguffi/lgm/nitraat/gasfiles/cop1995.g2a', 20000, 1 , 0
; data on subwindows
0                no subwindows selected; next record will be ignored
200000, 435000, 240000, 465000 (subwindow data)

[MISCELLANEOUS]
2                seed for random generator
1                switch indicating clip-option is ON
200000, 240000, 435000, 465000 xmin, xmax, ymin, ymax for clip-window
[END]

```

Any additional text may be included here.

4 SHOWCLOUD

4.1 *General*

The graphical tool SHOWCLOUD can be used in batch mode or in interactive mode. In this chapter first we discuss SHOWCLOUD in interactive mode followed by a description of the batch-mode. SHOWCLOUD produces pictures on screen with the spatial distribution of the particles (the particle cloud). The program is meant as an aid to view the data and to get a general idea of the solute distribution, for instance to select areas for further investigation. Hard copies of the pictures can be obtained after using a screen-grabber and saving the pictures on a file. A suitable public domain screen grabber for an X-terminal is XV (Bradley, 1994). Note that SHOWCLOUD only shows the position of the particles. The pictures are not representative for the solute concentration, as the mass may vary from particle to particle.

4.2 *Interactive mode*

In interactive mode the program is invoked by typing:

SHOWCLOUD

No command-line arguments are given. After the program is invoked a prompt for the cloudfile name appears [figure 7]. The user now enters the name of the cloudfile. Accordingly, the program prompts for the coordinates and the dimensions of the window (figure 8). The window is the part of the model area that will be displayed. At the right-upper corner of the screen the maximal and minimal particle coordinates are given, which may be helpful in choosing appropriate window dimensions. The extreme particle coordinates are taken as default window coordinates. The defaults are accepted by pressing the ENTER key. Else, the requested dimensions are typed in. Next, a graphical screen is opened and the positions of the particles are plotted. Figure 9 gives an example.

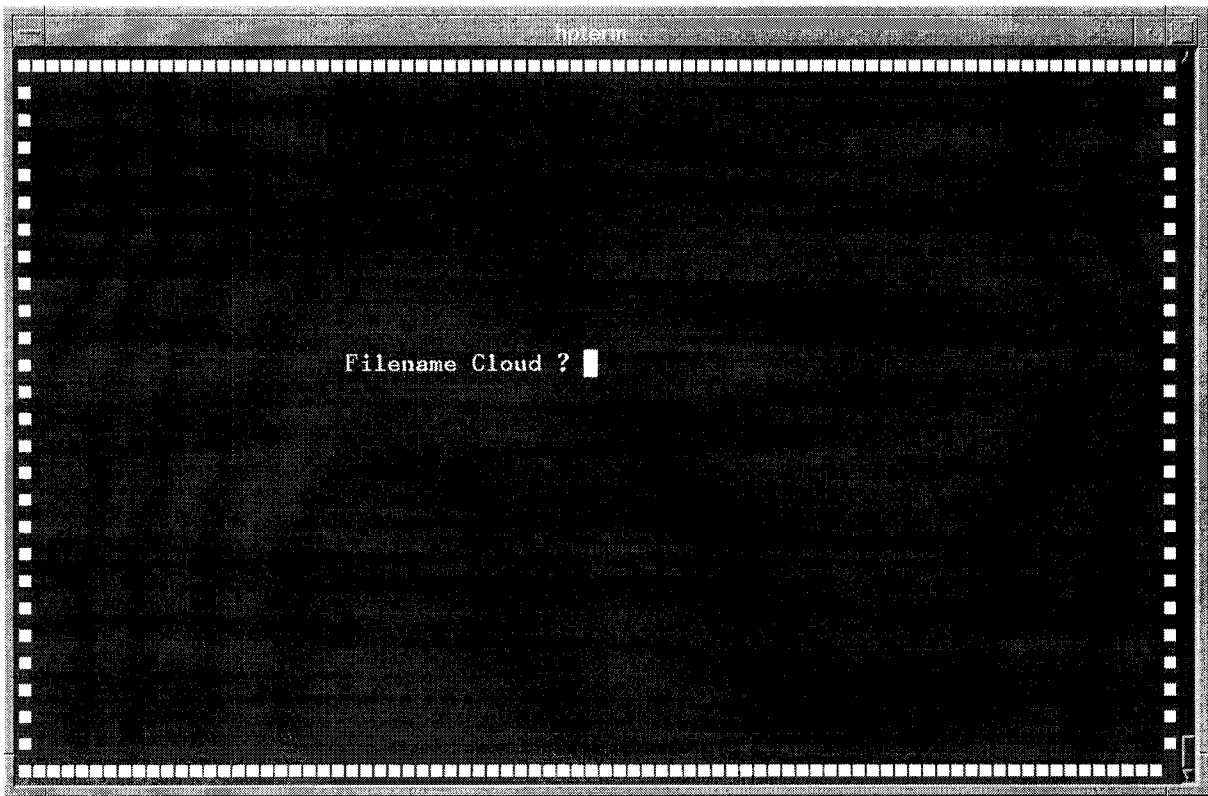


Figure 7 Prompt for name of Cloudfile

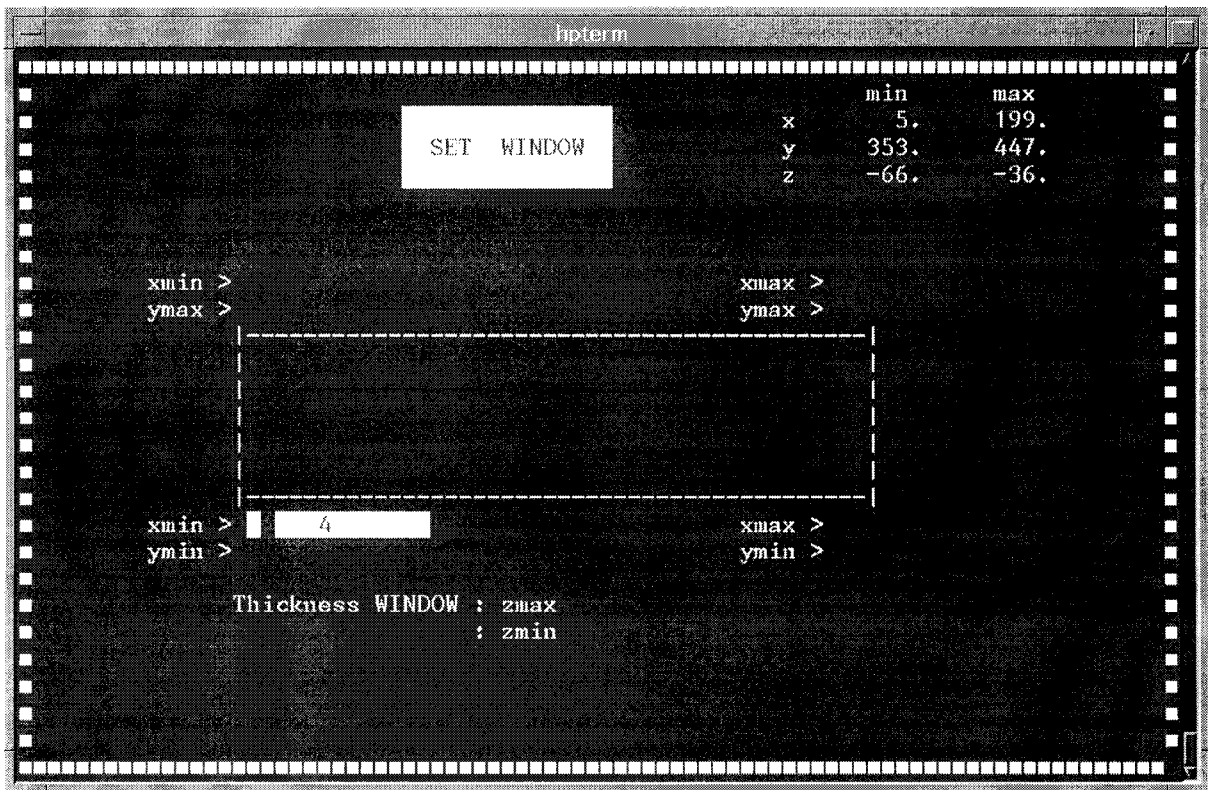


Figure 8 Prompt for dimensions of window

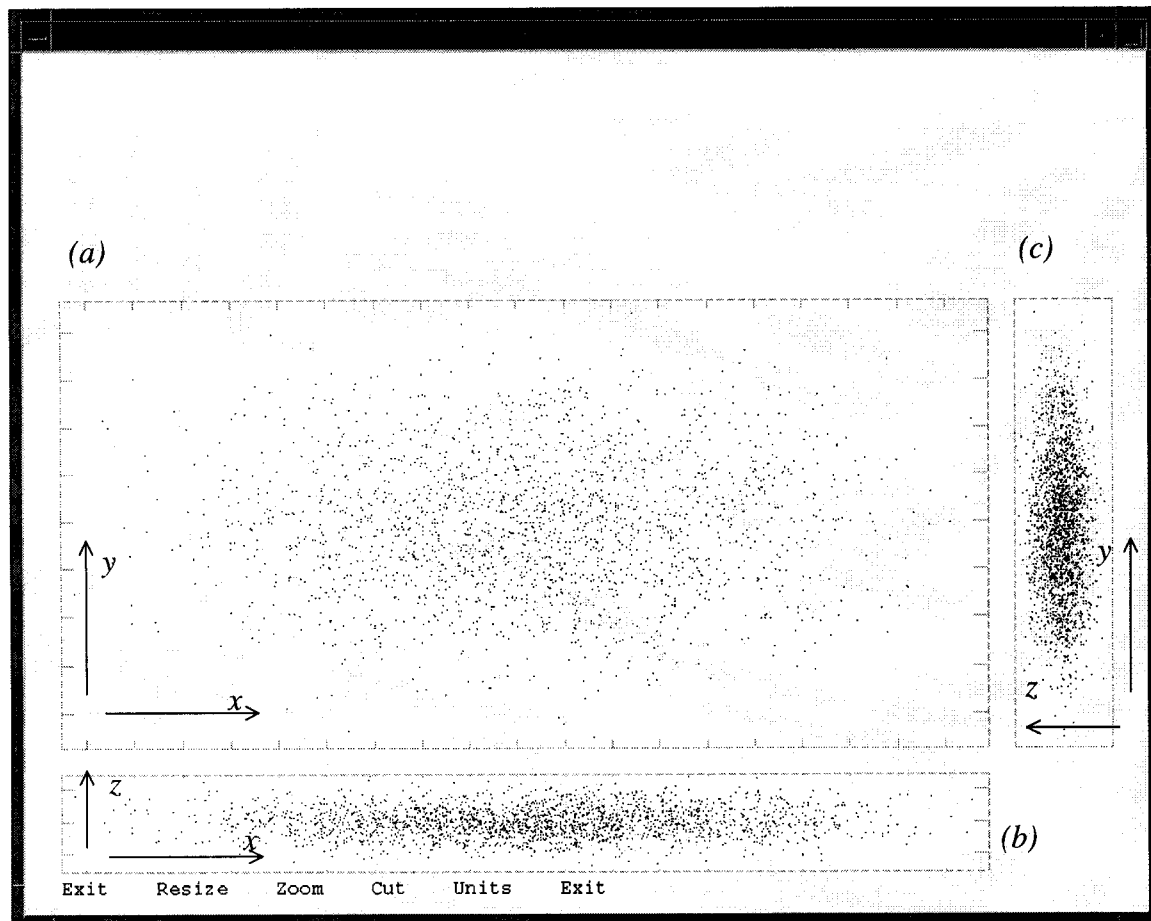


Figure 9. Particle positions (a) in x - y plane, (b) in x - z plane and (c) in y - z plane.

Figure 9 consists of three views, (a) a top view, with a horizontal x -axis from $XMIN$ to $XMAX$ and a vertical y -axis from $YMIN$ to $YMAX$; (b) a side view with the x -axis horizontally and the z -axis vertically from $ZMIN$ to $ZMAX$ and (c) a second side view with the z -axis horizontally and the y -axis vertically. In other words (a) shows the x,y coordinates, (b) shows the x,z coordinates and (c) the y,z coordinates. A menu at the lower end of the screen becomes visible by pressing the space bar. If the menu bar does not show, the reason may be that the program is still reading the cloudfile and the newly read particles fall outside the specified window. Another possibility is that the program has finished reading, but the mouse pointer is not inside the graphic screen.

The menu-bar shows a few options that can be selected by moving the highlight. Moving the highlight to the left is possible by pressing the key ' l '. The highlight moves to the right by pressing the key ' h '. These keys correspond with the cursor control keys in the *vi*-

editor. When the highlight is on the required option the ENTER key is pressed. Below the options are discussed.

RESIZE

With this option the screen given in figure 8 reappears and new window dimensions can be entered.

ZOOM

It is possible to zoom-in on the top view. The new values for $XMIN$, $YMIN$, $XMAX$, $YMAX$ are entered using the mouse. After choosing the ZOOM-option, the original mouse pointer disappears from the screen. As soon as the mouse is touched, a new pointer becomes visible. First, the lower left corner of the zoom-area is selected by bringing the pointer to the required position and clicking the left mouse button. The new coordinates $XMIN$ and $YMIN$ are now established. Accordingly, the upper-right corner is selected and the coordinates $XMAX$ and $YMAX$ are read. After pressing the ENTER key a new screen appears with the new window dimensions. (Figure 9a and 9b).

CUT

The CUT option operates like the ZOOM option. Only particles inside the selected area are displayed, but the scale of the picture remains unchanged. (Figure 10a and 10b)

UNITS

With the UNITS-option the values of the coordinates are written along the axes. [figure 11]

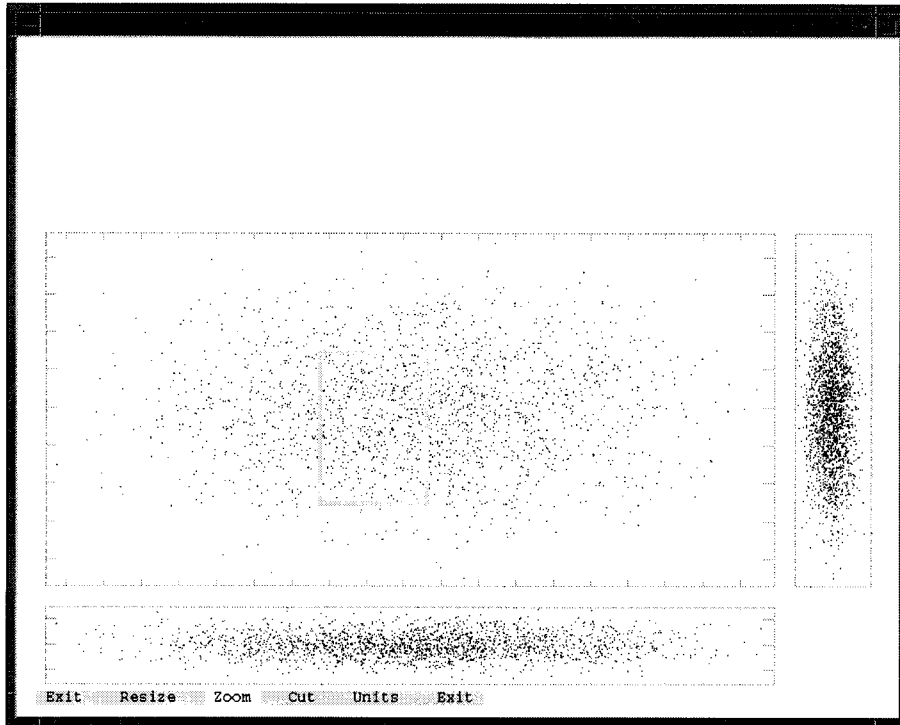


Figure 10a. Selecting an area with the ZOOM option

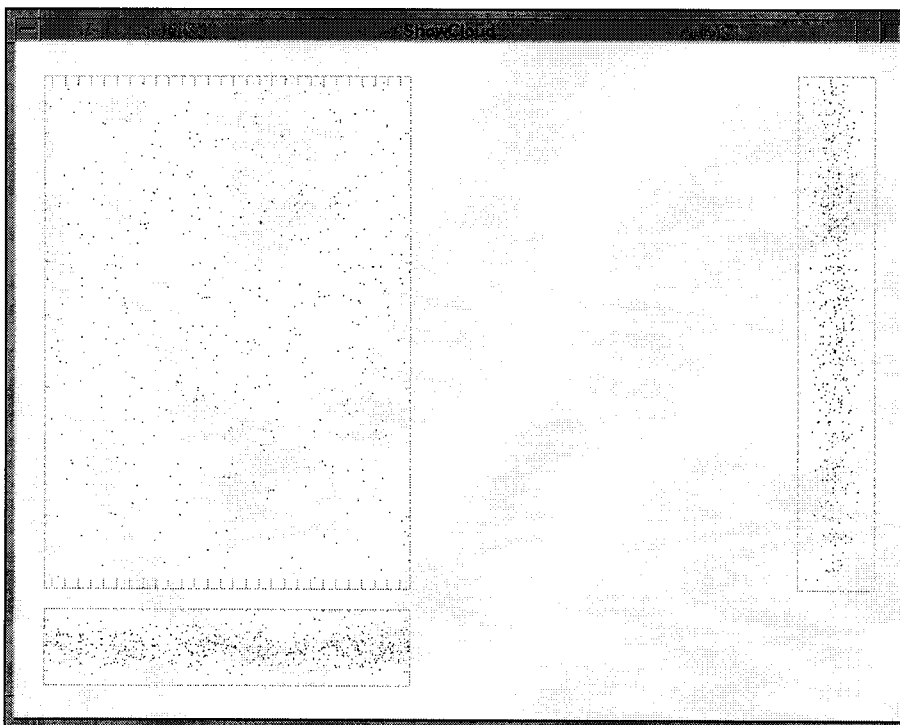


Figure 10b. Result of ZOOM option as shown in 10a

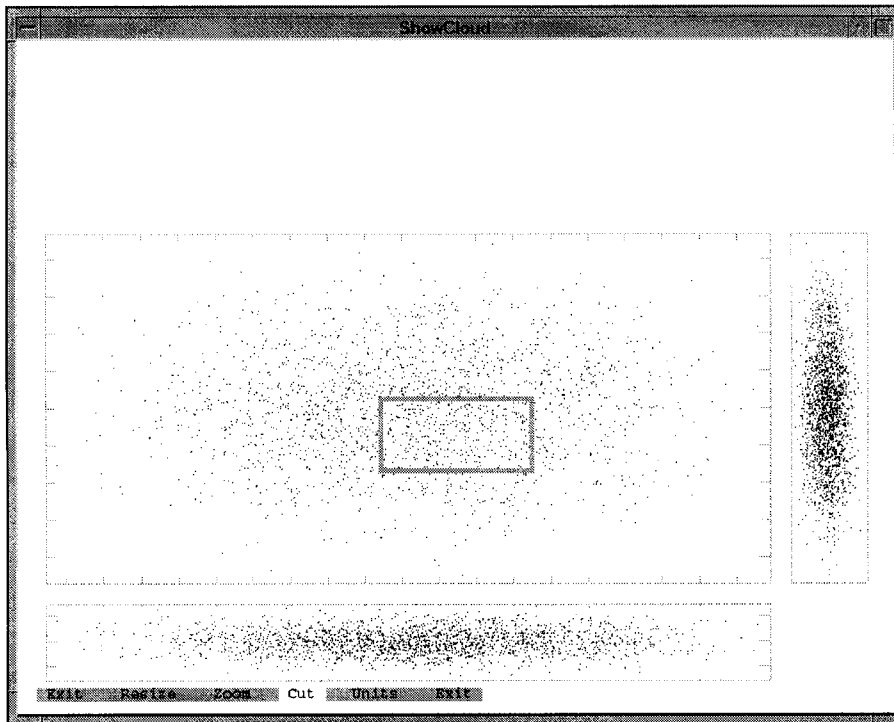


Figure 11a. Selecting an area with the CUT option

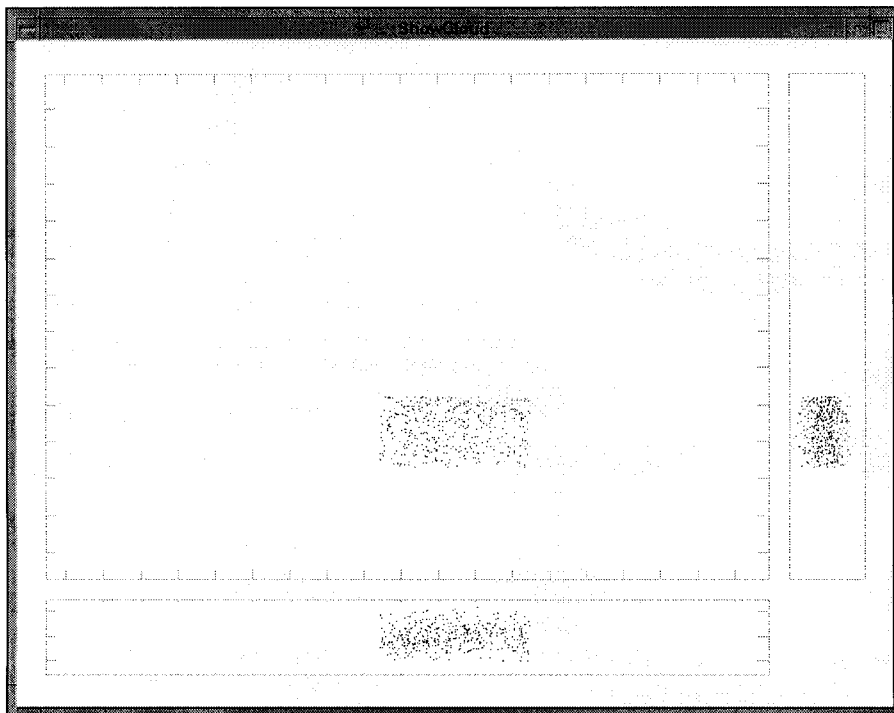


Figure 11b. Result of CUT option as given in 11a

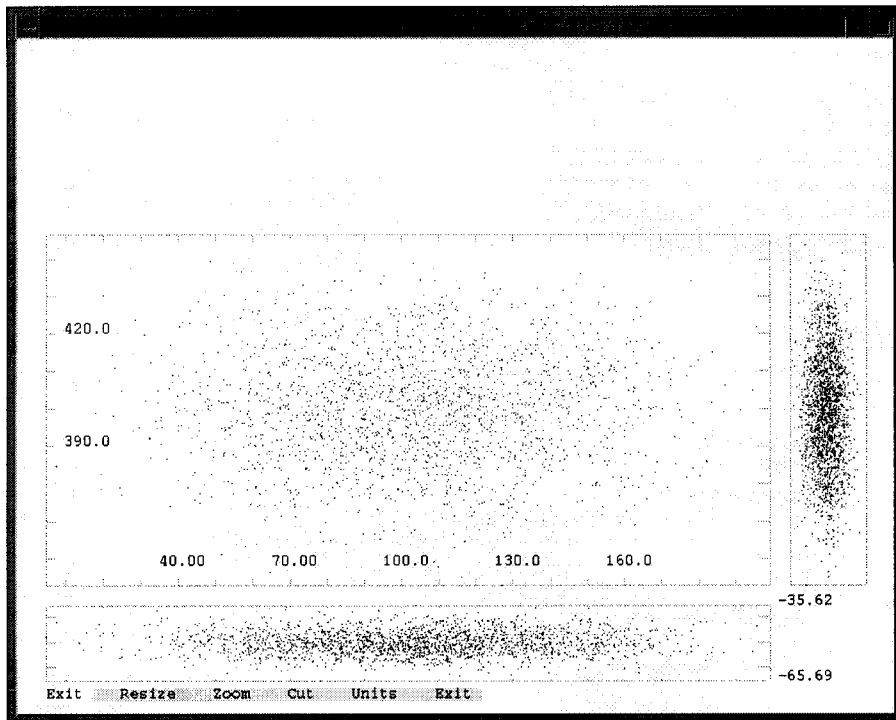


Figure 12 ShowCloud picture with units along the axes.

4.3 Batch-Mode

In batch mode the prompts are suppressed. Input is given in files that are specified on the command-line. The program is now invoked by:

SHOWCLOUD [-f LISTFILE] [-c CLDFILE] [-w WINFILE]

- f** option: name of a LISTFILE (File with list of names of *.cld files)
Shows the files successively by pressing the spacebar)
- c** option: name of CLDFILE; read particle positions directly from CLDFILE
- w** option: name of WINFILE; read window dimensions from a file
- h** option: produces this information.

The files involved with SHOWCLOUD in batch-mode are:

input files:

- CLOUDFILE
- [LISTFILE]
- [WINFILE]

output file:

(none)

CLOUDFILE

The name of the .cld file with the particle coordinates.

LISTFILE

Instead of visualizing a single Cloud File, the program can show a series of Cloud Files. When these file hold successive positions of a contaminant plume, it produces the impression of an animation (moving plume). The batch mode is now used with the **-f** option and a file is included (the List File) that contains the names of these Cloud Files. The files are displayed successively by pressing the space-bar. The **-f** option and **-c** option can not be used simultaneously.

Example of a List File

```
cloud01.cld  
cloud02.cld
```

```
.  
.
```

WINFILE

This file contains the dimensions of the window.

XMIN, YMIN, ZMIN

XMAX, YMAX, ZMAX

For instance:

220000., 455000., 10.

230000., 465000., 12.

5 CLDGRID

5.1 General

LGMCAD produces output in a particle oriented format. To visualize the results as concentration contourlines, the first thing to do is transform the raw (three-dimensional) data to concentrations on a two-dimensional grid. This is achieved by the program CLDGRID.

In CLDGRID a grid cuts a slice with a certain thickness out of the 3-dimensional modeling area which is occupied by the particles. The cells of the grid are arranged in a two-dimensional array. The grid also has a dimension in the third direction, which will be referred to as the 'thickness'. The standard arrangement of the grid cells is horizontal at a fixed elevation (see figure 12) and a constant thickness. The dimensions in the horizontal direction are denoted by L (length) and W (width), while the thickness is denoted by d .

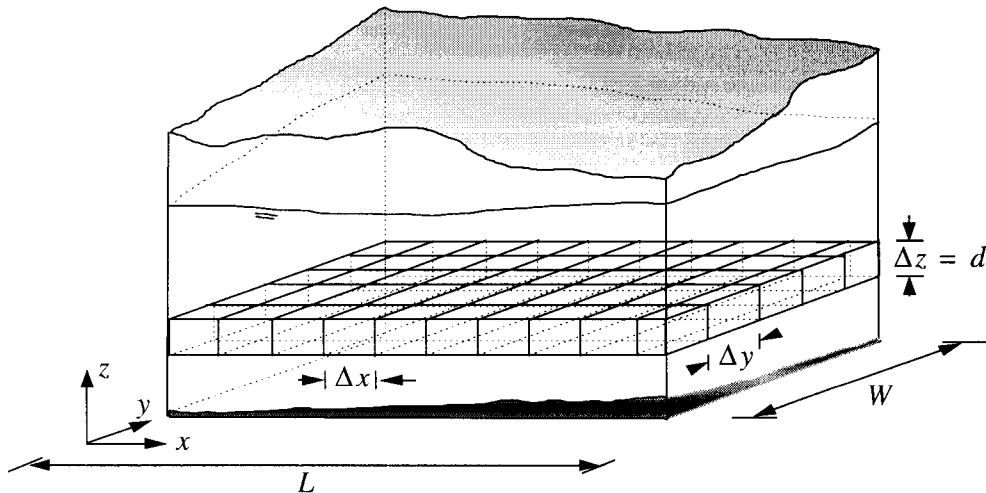


Figure 13. Horizontal Grid with constant elevation; constant Δx , Δy and Δz

In addition to the 'standard' arrangement, an option exists to create a 'more or less' horizontal grid that follows a plane with a varying elevation (figure 14). This can be used e.g. to obtain concentrations at a certain depth below a varying groundwater table, or half-way a certain aquifer whose elevation and thickness varies.

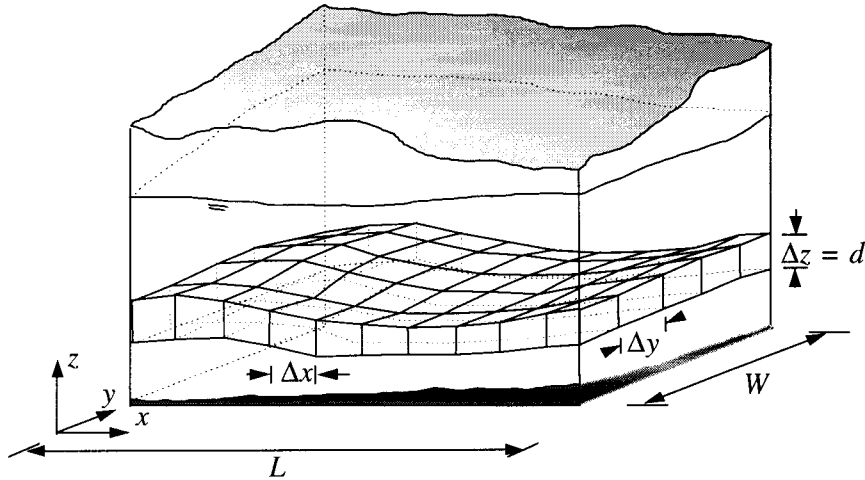


Figure 14. Horizontal Grid; constant Δx and Δy ; varying elevation and thickness d

Apart from ‘horizontal’ grids, vertical grids can be defined for concentrations in a vertical cross-section (figure 16). For convenience, a set of new horizontal coordinates (ξ, η) is now introduced. The new coordinates are obtained after a horizontal translation of the origin to point A, with coordinates (x_A, y_A) , and a rotation over α , being the angle of the cross-sectional plane the x, z plane. The new and original coordinates are related by (see figure 15):

$$\xi = (x - x_A) \cos(\alpha) + (y - y_A) \sin(\alpha) \tag{5.1}$$

$$\eta = -(x - x_A) \sin(\alpha) + (y - y_A) \cos(\alpha)$$

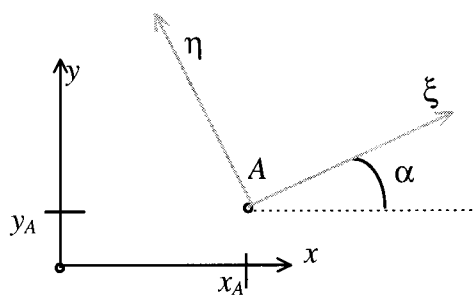


Figure 15. Relation between new coordinates (ξ, η) and original (x, y) coordinates

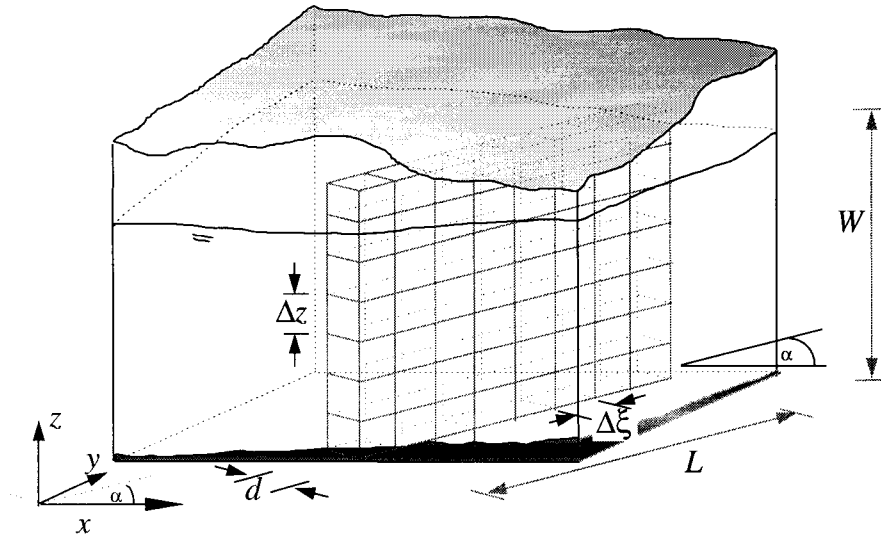


Figure 16. Vertical Grid with new horizontal coordinates ξ and η ;
Gridcell dimensions $\Delta\xi$, $\Delta\eta = d$ and Δz constant.

After definition of the position and structure of the grid, the program reads the Cloud File, counts the particles in each cell, sums the mass of the particles in the grid-cells and calculates the concentration. Accordingly, the calculated concentration is allocated to the center of the each grid-cell and these values are written on an output file (Grid File).

5.2 Interactive mode

First the interactive mode is discussed. The program is now invoked by typing:

CLDGRID

The program prompts for the type of grid (figure 17), as discussed in the previous paragraph (also see figures 13, 14, 16). The subsequent screens depend on the chosen type and will be discussed below one by one.

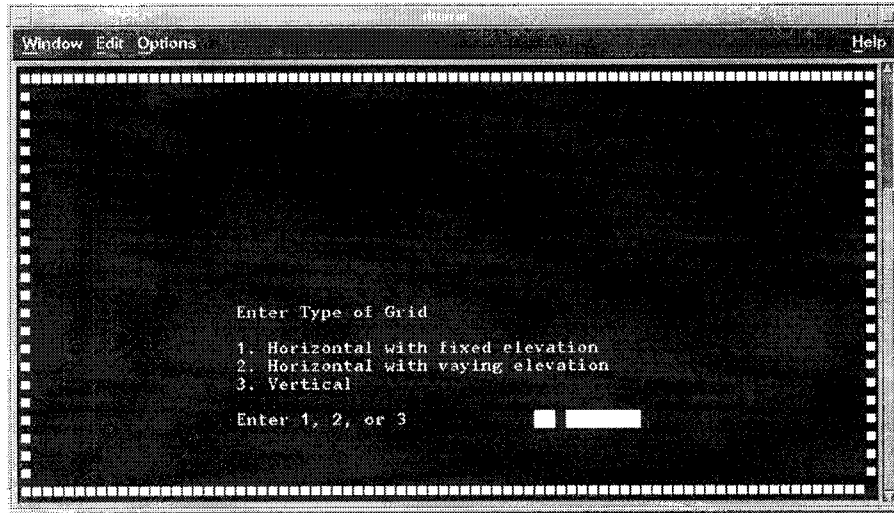


Figure 17. Prompt for type of grid

5.2.1 Horizontal Grid with Fixed Elevation

For a horizontal grid with fixed elevation, the program prompts for the dimensions and the position of the grid (see figure 18). The user enters the coordinates of the lower-left corner (x_{min}, y_{min}) , and the upper-right corner (x_{max}, y_{max}) of the grid on the x,y plane. The program comes with default values that can be accepted by pressing ENTER. Besides the horizontal position, the vertical position must be given. This is done by specifying z_{min} and z_{max} . In the present case the thickness of the grid d is equal to $\Delta z = z_{max} - z_{min}$. Note that in this grid type Δz is constant for all grid-cells.

The horizontal dimensions of the grid-cells are:

$$\Delta x = (x_{max} - x_{min}) / n_x \quad (5.2)$$

$$\Delta y = (y_{max} - y_{min}) / n_y$$

where n_x and n_y are the number of grid-cells in the x - and y -direction, which are also entered in the screen shown on figure 18. Here, we deal with a horizontal grid, so the number of cells in the z -direction is equal to 1.

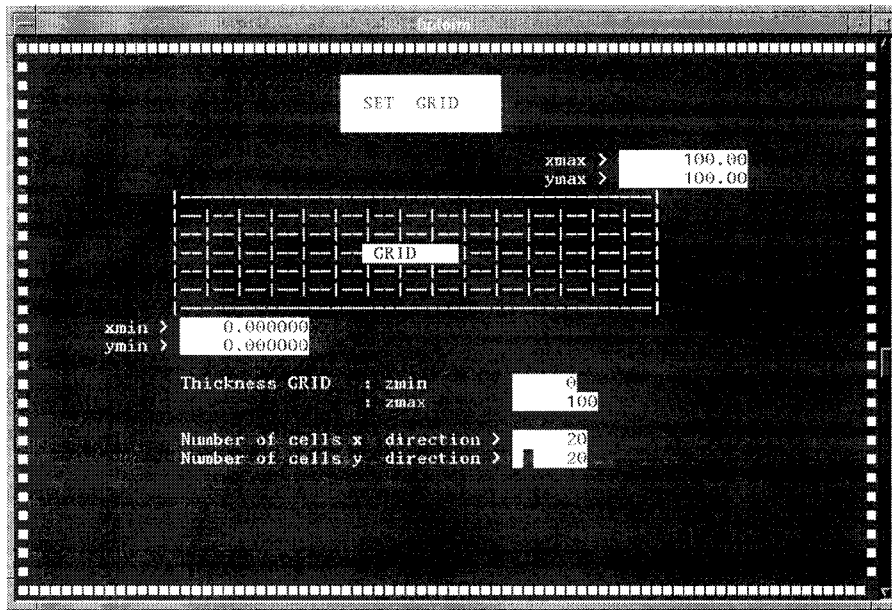


Figure 18. Prompt for dimensions of horizontal grid

5.2.2 Horizontal Grid with Varying Elevation

For the definition of a grid with a variable elevation and varying vertical thickness, two additional files must be provided. One holds the z-levels of the bottom of the grid at the center of the grid cells, while the second contains the upper levels at the center of the cells. These files must be in the gridfile format, which is described in the appendix. Since these files already contain the information on the horizontal structure of the grid, this information does not have to be entered again. The prompts for the filenames of lower and upper elevation of the grid-cells are shown in figure 19.

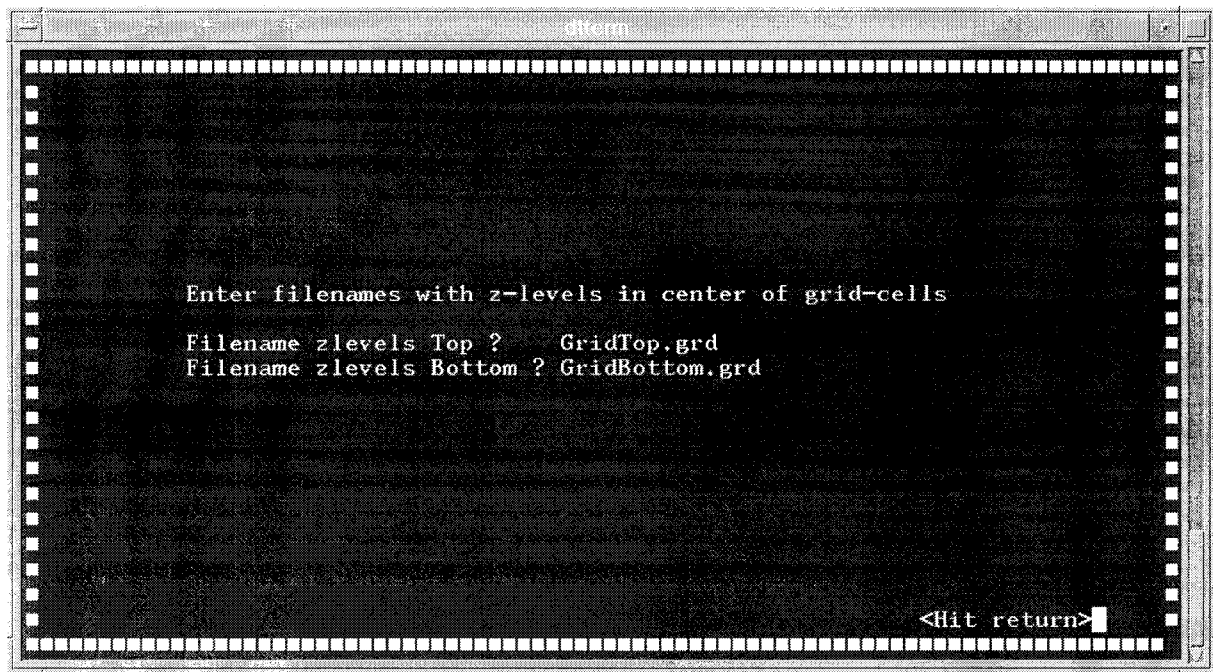


Figure 19. Prompt for Filenames

5.2.3 Vertical Grids

Verticals grids are used to obtain concentration distributions in a cross-section. The position of the cross-section and the dimensions of the grid are determined by several variables. Figure 20 illustrates the meaning of these variables. Let γ be the plane of the cross-section. This plane intersects the horizontal x - y plane along a line A - B . The direction of the cross-sectional plane is given via the coordinates of the points A and B , which are respectively (x_A, y_A) and (x_B, y_B) . In the new coordinate system (see figure 15) the line A - B corresponds with the ξ -axis. The dimension of the grid in ξ -direction, the length L , is equal to $\sqrt{[(x_B - x_A)^2 + (y_B - y_A)^2]}$, or the distance A - B . The grid height H follows from the z -values of the bottom and the top of the grid, respectively z_{min} and z_{max} . The dimension perpendicular to the cross-sectional plane, $\Delta\eta$, is also called the grid thickness d . The number of grid-cells in horizontal direction and vertical direction is denoted by n_ξ and n_z . The grid cell dimensions are:

$$\Delta\xi = \sqrt{(x_B - x_A)^2 + (y_B - y_A)^2} / n_\xi$$

$$\Delta z = (z_{max} - z_{min}) / n_z$$
(5.3)

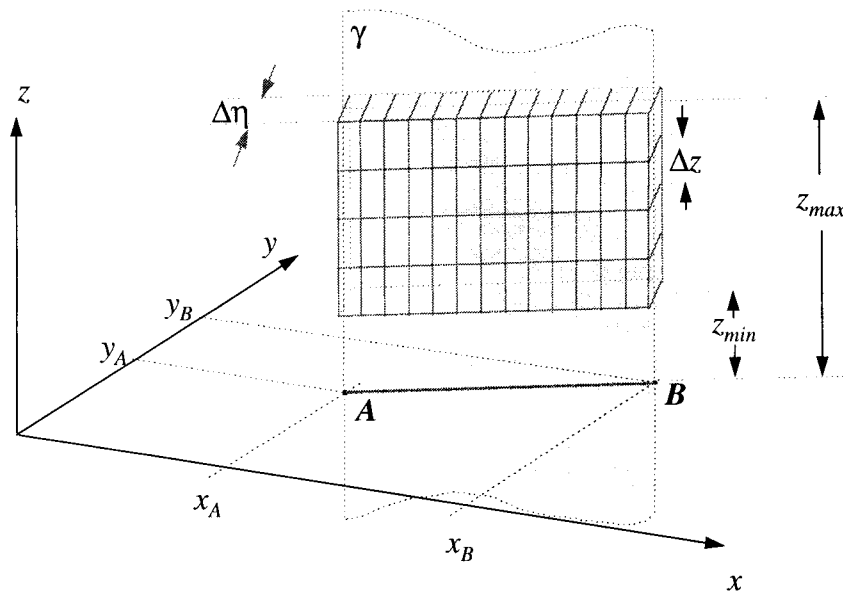


Figure 20. Position of vertical grid

5.2.4 Porosity and Filename

After data on the structure of the grid, the porosity of the aquifer are entered (figure 21) plus the name of the cloud file to be processed (figure 22). The results are finally stored on an output file with a name GRID000.GRD

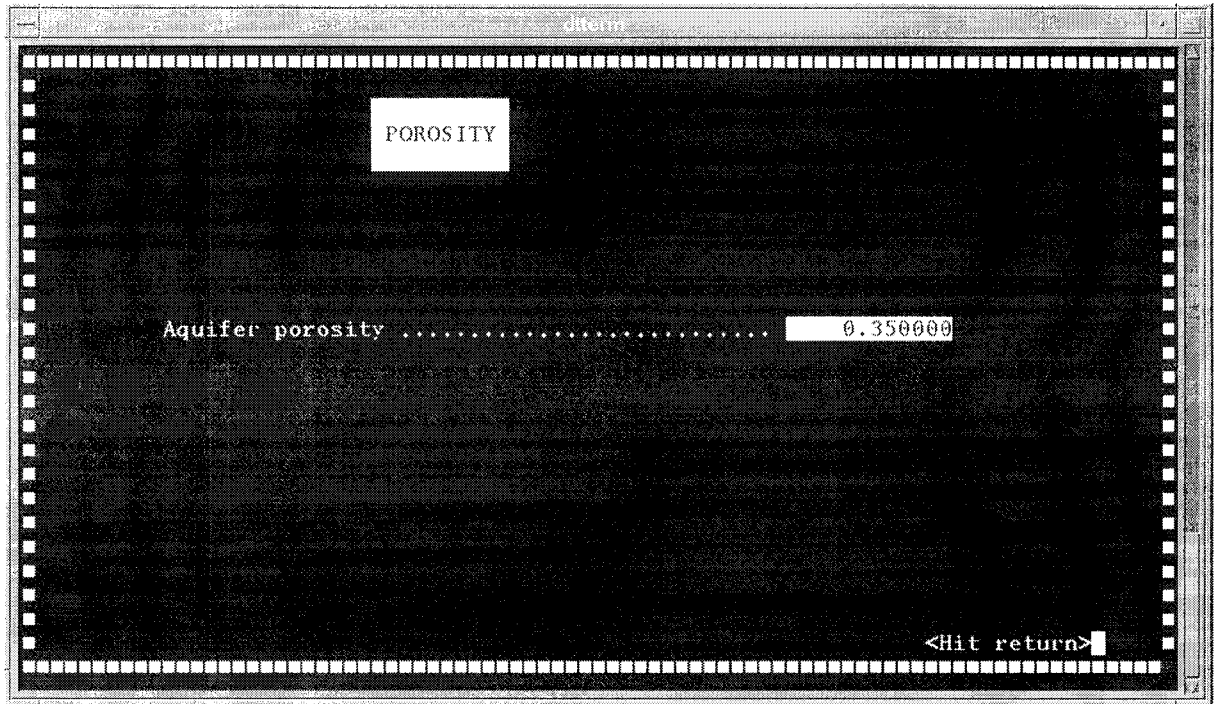


Figure 21. Prompt for aquifer porosity.

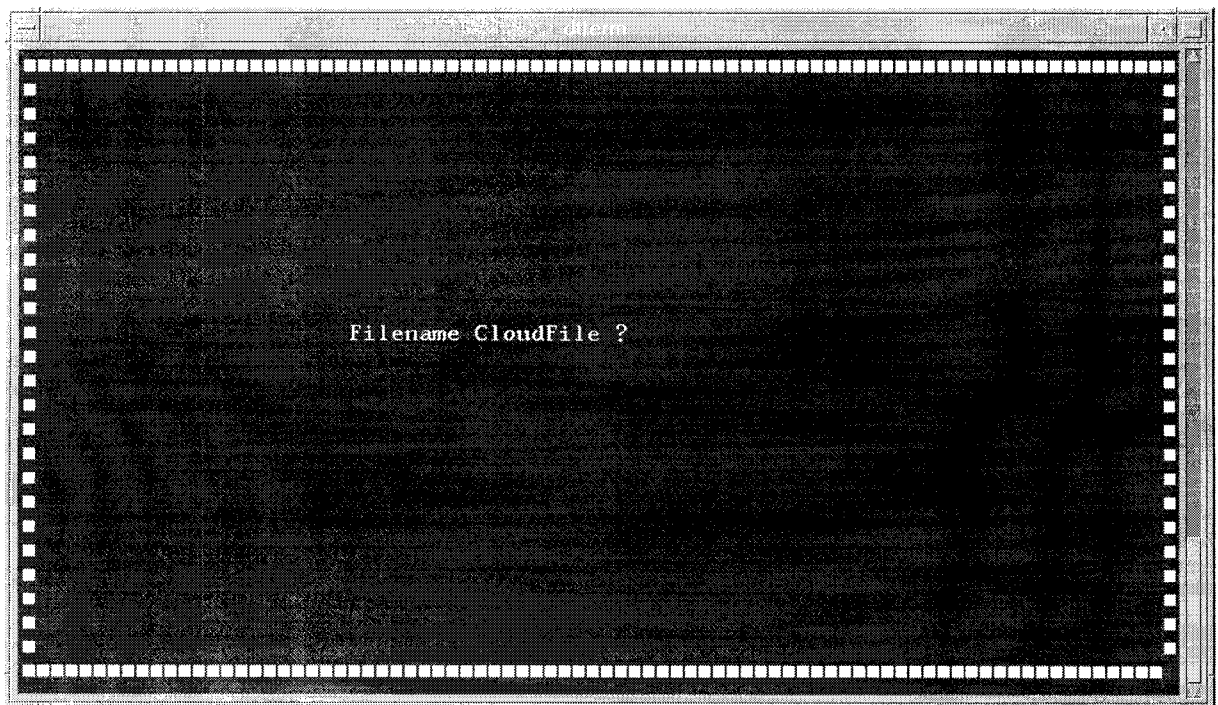


Figure 22. Prompt for name of Cloud file.

5.3 Batch-Mode

In batch mode the prompts are suppressed and input is given in files specified on the command-line. The program is invoked in by:

CLDGRID [-f INFILE] [-c CLOUDFILE] [-g GRIDFILE]

- f** option: give name of INFILE; This file contains information on the grid structure (shown as animation by pressing the spacebar)
- c** option: give name of CLOUDFILE (input file);
(if -c not used, program prompts for filename)
- g** option: give name of gridfile (output-file)
(if -g not used, filename GRIDnnn.GRD is used)
- h** option: produces this information.

The files involved with the batch mode of CLDGRID:

input files:

- INFILE
- CLOUDFILE

output file:

- GRIDFILE

INFILE

Definition of the grid structure is read from a file with the name given on the command line. The contents of this file are.

xmin, ymin, zmin
xmax, ymax, zmax
nx, ny
porosity

CLOUDFILE

The name of the cloud file that contains the particle coordinates and other attributes.

GRIDFILE

The name of the grid file with the concentrations (output file).

References

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Appendix A CLOUD FILES

Structure

Cloud files contain the data of all particles present in the system at a specific moment in time. The structure of the file is as follows. The first record is a one-line header that only contains the time. Each following record contains 6 particle attributes. For each new particle a new record is used:

T

$M_1, X_1, Y_1, Z_1, S_1, P_1$

$M_2, X_2, Y_2, Z_2, S_2, P_2$

..., ..., ..., ..., ..., ..

, X_i, Y_i, Z_i, S_i, P_i

..., ..., ..., ..., ..., ..

$M_n, X_n, Y_n, Z_n, S_n, P_n$

where:

- i the record number of the cloudfile (excluding the header)
- M_i mass of particle P_i
- X_i x -coordinate of particle P_i
- Y_i y -coordinate of particle P_i
- Z_i z -coordinate of particle P_i
- S_i code indicating the sorption status of particle P_i ($S = 0 \rightarrow$ free; $S = 1 \rightarrow$ sorbed)
- P_i particle identification number

The first 4 particle-attributes are real variables (single precision). The last 2 are integers. The particle identification number P is a unique number that a particle receives when it is generated. It identifies the particle and it is the only attributes that never changes. This number makes backtracking possible. Backtracking is a technique in which for a given particle (or group of particles) earlier locations are traced until the location is found where it entered the groundwater system. A typical example where backtracking is applied is the determination of capture zones for groundwater pumping stations. A 'backtracking' post-processor is under development. A prototype is available, but not included in this manual.

Format

A cloud file may be a formatted ASCII file (text-file) or an unformatted (binary) file. The advantage of unformatted files is the faster postprocessing (CLDGRID), no loss of significant figures in the data and less disk space. However, they cannot be read by a standard text editor or spreadsheet. The default is to write the clouds in unformatted files, but this may be changed by setting the appropriate switch in the *LGMCAD.ini* file (appendix D). The program CLDGRID recognizes both formatted and unformatted cloud files. In ASCII mode, the variables are read in a free format.

Appendix B GRID FILES

A grid is a rectangular region of evenly spaced rows and columns, defined by horizontal and vertical grid lines. The grid lines make up a wire mesh, while the intersection of the lines define the location of *grid nodes*. A rectangular block defined by four adjacent grid nodes is a *grid cell*, while the center of it is referred to as the *cell center* (see figure B-1).

Structure

Grid files generally consist of a series of header lines in which the structure (size/limits) of the grid is described, followed by a series of values (concentrations) that are assigned either to the grid nodes or to the cell centers, depending on grid convention. Several conventions are around. Some conventions focus on the grid-nodes, others on the cell centers. Another point that varies is the order in which the values are stored: row order or column order. Also the direction may vary: starting at the row with the minimum y-coordinate or the maximum y-coordinate. Three file conventions are described here.

CLDGRID
SURFER
ARC-INFO

CLDGRID Convention

This is the originally applied format in LGMCAD. The header, that consists of 3 records, contains data on the dimension and location of the grid. The rest of the data represent concentrations at the **cell centers**. The concentration values in the file are organized in **row order** starting with the minimum y-coordinate row. Thus, the first *C* value represents the concentration at the center of the cell in the lower left corner of the *x, y* plane. The general format is

<i>nx ny</i>	number of cells in <i>x</i> direction; number of cells in <i>y</i> direction
<i>dx dy</i>	dimension of grid cells in <i>x</i> , or <i>y</i> direction
<i>xmin ymin</i>	<i>x</i> and <i>y</i> coordinates of lower left corner of lower left grid cell
C_1, C_2, \dots, C_{nx}	grid row 1
$C_{nx+1}, \dots, \dots, C_{nx+nx}$	grid row 2
.	
$C_{nx(ny-1)+1}, C_{(ny-1)nx+2}, \dots, \dots, C_{nx \cdot ny}$	grid row <i>ny</i>

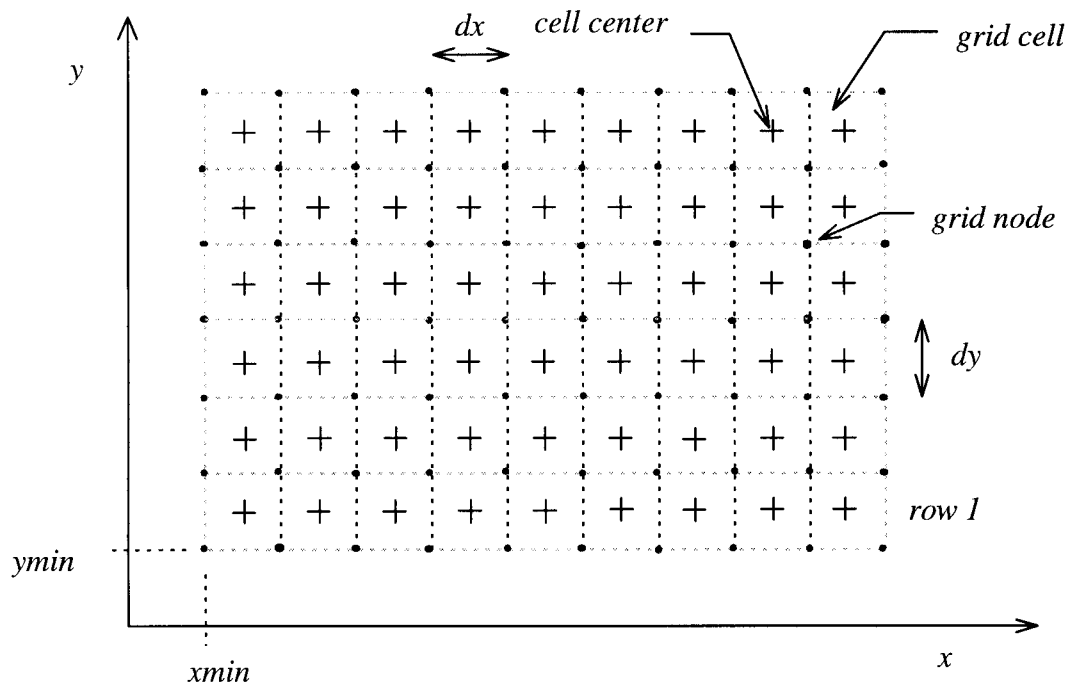


Figure B-1

The coordinates that belong to the first two C-values are:

$$\begin{aligned} &xmin + dx/2, \quad ymin + dy/2 \\ &(xmin + dx) + dx/2, \quad ymin + dy/2 \end{aligned}$$

where the grid cell dimensions dx and dy are given by:

$$dx = \frac{(xmax - xmin)}{nx}; \quad dy = \frac{(ymax - ymin)}{ny}$$

The following example is a part of a correctly formatted CLDGRID file. The grid consists of 80 X 60 grids. Only data for the first 3 rows are given.

```

80 60
500 500
200000 435000
19.12 18.98 18.96 18.91 18.84 18.85 18.86 18.77 18.68 18.65
18.53 18.25 17.94 17.58 17.05 16.53 15.94 15.44 14.99 14.5
14.07 13.79 13.64 13.64 13.82 14.24 14.99 15.56 15.2 15.21
15.46 15.87 16.25 16.5 16.67 16.78 16.91 16.99 17.02 16.99
16.95 16.92 16.94 17. 17.12 17.47 17.38 16.69 16.05 15.57
15.14 14.8 14.51 14.2 13.87 13.62 13.42 13.2 12.97 12.74
12.48 12.17 11.8 11.43 11.05 10.65 10.17 9.63 9.04 8.52
8.09 7.55 6.9 6.1 5.17 4.3 3.58 2.91 2.28 1.73
19.21 19.21 19.15 19.07 19.03 18.98 18.89 18.88 18.86 18.83
18.77 18.48 18.14 17.76 17.18 16.58 15.97 15.49 15.11 14.62
14.15 13.82 13.66 13.64 13.78 14.08 14.5 14.81 14.92 15.15
15.5 15.99 16.4 16.68 16.82 16.92 17.06 17.11 17.16 17.15
17.1 17.08 17.13 17.28 17.52 17.37 16.89 16.27 15.7 15.29
14.93 14.6 14.29 13.97 13.65 13.43 13.22 13.04 12.86 12.63
12.37 12.06 11.73 11.38 10.97 10.57 10.18 9.67 9.08 8.61
8.11 7.53 6.88 6.08 5.17 4.22 3.35 2.57 1.86 1.21
19.34 19.35 19.31 19.34 19.3 19.21 19.07 19.07 19.1 19.04
18.96 18.7 18.35 17.85 17.26 16.68 16.15 15.69 15.27 14.83
14.36 13.88 13.73 13.7 13.79 14.02 14.35 14.61 14.8 15.1
15.51 16.07 16.54 16.83 16.97 17.1 17.22 17.32 17.36 17.33
17.31 17.31 17.39 17.6 17.37 16.9 16.44 15.9 15.38 15.01
14.65 14.33 14.05 13.74 13.46 13.26 13.06 12.86 12.7 12.48
12.2 11.87 11.59 11.31 10.95 10.59 10.26 9.75 9.16 8.65
8.22 7.72 7.18 6.41 5.51 4.44 3.44 2.56 1.74 1.
    
```

80 values for first row of cells

80 values for second row of cells

80 values for third row of cells

Figure B-2 Example of a Grid File with CLDGRID convention

SURFER Convention

Surfer is a grid-based contouring and three dimensional surface plotting program for the PC developed by Golden Software (1996). It produces contour maps and surface plots for data that are organized on a regularly spaced grid. The structure of the grid files that Surfer uses differs slightly from the CLDGRID files. Surfer grids are oriented on the **grid nodes** instead of the cell centers. This means that the concentration values given in the file are associated to the nodes. Also, the structure of the grid is described by the number of grid lines, which is always one more than the number of grid cells. The order in which the concentration values are stored is the same as in the CLDGRID file: row order, starting with the minimum y coordinate row. Thus, the first function value in the grid file (after the header lines) corresponds to the grid node at lower left corner of the grid. Surfer knows two formats for the grid files: a text files (ASCII) file and a binary or unformatted file. Here we shall only deal with the text (formatted) file type. The general structure is:

id	The code letters DSAA, which identifies the file as an ASCII grid file for Surfer
$nx \ ny$	The number of grid lines along the x -axis and y -axis respectively
$xlo \ xhi$	The minimum and maximum x values of the grid lines
$ylo \ yhi$	The minimum and maximum y values of the grid lines
$Clo \ Chi$	The minimum and maximum C values of the grid
C_1, C_2, \dots, C_{nx}	grid row 1
$C_{nx+1}, \dots, C_{nx+nx}$	grid row 2
.	
$C_{nx(ny-1)+1}, C_{nx(ny-1)+2}, \dots, C_{nx \cdot ny}$	grid row ny

These are the rows of C values of the grid organized in row order. Each row has a constant y -coordinate. The grid row 1 corresponds to ylo and the last grid row to yhi . Within each row the C values are arranged from xlo to xhi

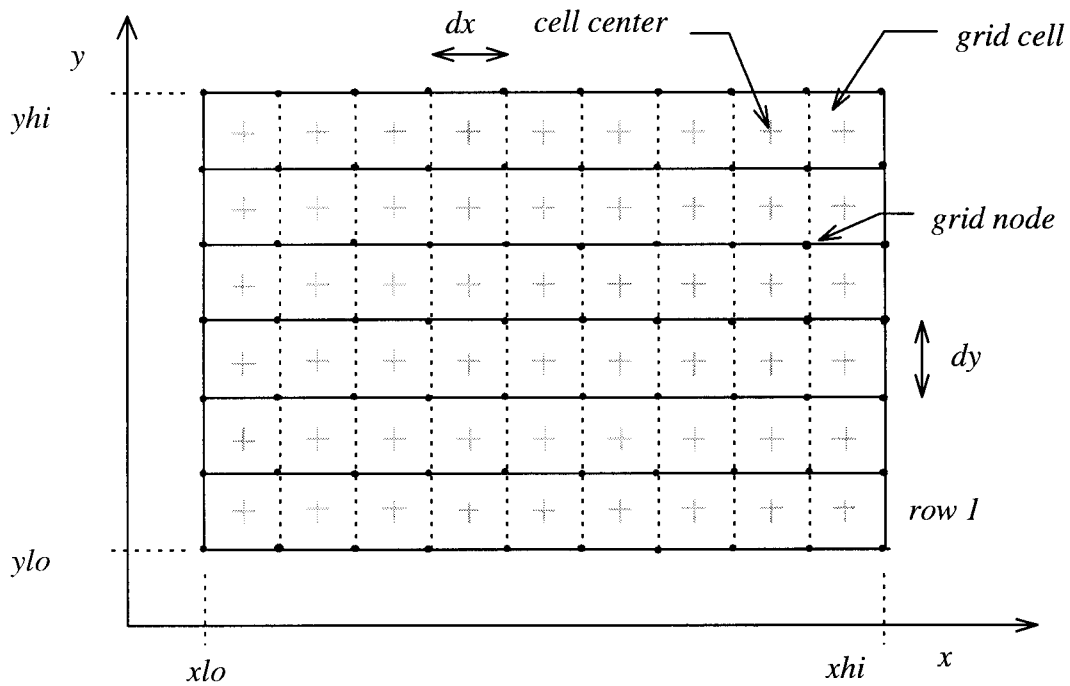


Figure B-3

Note in the SURFER header the parameters nx and ny stand for the number of grid lines, where in the CLDGRID header nx and ny denote the number of grid cells. In a Surfer grid file the coordinated for the first two C-value C_1, C_2 , are:

$$(x_1, y_1) = (xlo, ylo)$$

$$(x_2, y_2) = (xlo + dx, ylo)$$

where xlo and ylo are the coordinates of the lower dx and dy are the grid cell dimensions following from:

$$dx = \frac{(xhi - xlo)}{(nx - 1)}; \quad dy = \frac{(yhi - ylo)}{(ny - 1)}$$

Below an example is given of as Surfer Grid file. This file describes a 100 X 100 grid. Only data for the first two rows are given.

```
DSAA
100 100
200250.0 249750.0
425250.0 474750.0
.0 17821.08
2232.88 3047.61 .00 .00 .00 .00 .00 .00 .00 .00
3350.45 2631.28 2964.89 693.80 1178.94 3626.52 2924.95 .00 .00 .00
.00 .00 .00 .00 .00 .00 .00 .00 .00 .00
.00 .00 .00 .00 .00 .00 4009.65 .00 .00 .00
.00 .00 3768.75 3316.50 2529.34 3760.81 2496.96 1871.92 2210.25 3734.98
.00 .00 .00 .00 .00 .00 .00 .00 .00 .00
.00 .00 .00 .00 .00 .00 .00 .00 .00 .00
.00 .00 .00 .00 .00 .00 .00 .00 .00 .00
.00 .00 .00 .00 .00 .00 .00 .00 .00 .00
4565.79 3015.78 .00 .00 .00 .00 .00 2413.91 3043.27 3280.51
6211.60 2406.09 2836.55 2299.81 2917.92 4123.93 243.07 .00 .00 .00
.00 .00 .00 .00 .00 .00 .00 .00 .00 .00
.00 .00 .00 .00 .00 .00 2709.93 2589.78 2488.39 2145.04
3572.57 3478.31 4903.87 3020.14 3285.28 2829.77 2240.69 2350.22 2523.41 2036.62
4129.47 .00 .00 .00 .00 .00 .00 .00 .00 .00
.00 .00 .00 .00 .00 .00 .00 .00 .00 .00
.00 .00 .00 .00 .00 .00 .00 .00 .00 .00
.00 .00 .00 .00 .00 .00 .00 .00 .00 .00
.00 .00 .00 .00 .00 .00 .00 .00 .00 .00
```

Data first row

Data second row

Figure B-4 Example of a Grid File with CLDGRID convention

ARC-INFO Convention

Arc-info is a software package for file maintenance in a GIS environment. It is frequently used at RIVM to extract data from databases. These data become available in several formats. For grid oriented data one of the file format is called ASCIIGRID. This format is also recognized by LGMCAD.

The ARC-INFO ASCIIGRID format is based on cells, which means that the functions values (concentration) are allocated to the centers of the grid cells. Only square grid cells are possible, so here $dx = dy = h$. The organization of the grid values is again in row order, but starting with the **maximum** y-coordinate row. The values given per row start with the **minimum** x-coordinate cell.

The file begins with a 6 line header. Each record contains a keyword and a value. These keywords are given in bold font in the example below and must be included in the record:

NCOLS	<i>nx</i>	number of grid cells in x-direction
NROWS	<i>ny</i>	number of grid cells in y-direction
XLLCORNER	<i>xmin</i>	
YLLCORNER	<i>ymin</i>	
CELLSIZE	<i>h</i>	
NODATA_VALUE	<i>a</i>	
C_1, C_2, \dots, C_{nx}		grid row 1
$C_{nx+1}, \dots, \dots, C_{nx+nx}$		grid row 2
.		
$C_{nx(ny-1)+1}, C_{nx(ny-1)+2}, \dots, C_{nx \cdot ny}$		grid row <i>ny</i>

The first two C-values, C_1, C_2 , are the concentration that hold for the points with coordinates:

$$(x_1, y_1) = (xmin + h/2, ymax - h/2)$$

$$(x_2, y_2) = (xmin + dx + h/2, ymax - h/2)$$

where the grid cell dimension h is given in the header and $ymax$ follows from

$$ymax = ymin + ny \cdot h$$

The **nodata_value** a is a value assigned to those cells whose true value is unknown.

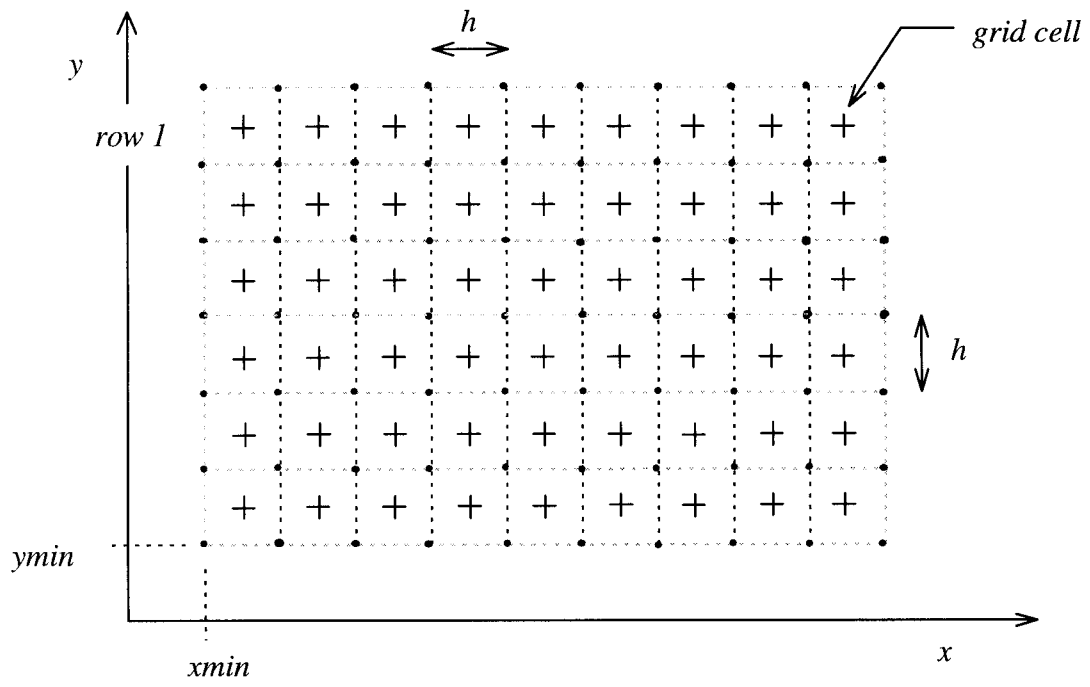


Figure B-5

Appendix C LGMCAD.INI

Normally, when LGMCAD runs and in the working directory there is no LGMCAD.INI file, several standard options are set. For more advanced use, these options can be modified, which is done by including an initialization file under the name LGMCAD.INI. At present there are 4 options that may be modified. The option is modified by including a line in the LGMCAD.INI file, that contains a keyword and a value. The explanation of the options is given below.

TOL *tl*

This keyword stands for tolerance and has to do with the catchment of particles by a pumping well. The standard procedure is that the program calculates a radius, and draws a circle with that radius around the well. All particles within this circle are considered to be caught by the well. R_{catch} is derived from the dimensions of the finite element grid. If the circumference of the element where the pumping well is located is denoted by O , then standard procedure is to define $R_{catch} = (O \cdot tl) / 8$, where the default value for tl is 1.0. With the keyword **TOL** it is possible to modify the value of tl and to increase or reduce R_{catch} .

IFF *iformat*

This keyword controls the format of the cloudfiles that are produced. The default value of *iformat* = 1, which means that cloudfiles are produced as text-files (formatted files). Any other integer value for *iformat* results in binary (unformatted) files.

BACK *iback*

This keyword is related to an option that is currently not yet fully operational. The default value for *iback* is 0. When the value is set to 1, all particles that occur in the system will obtain an identification code and at the start of the particles lifetime, its original position (coordinates) and the code will be written in a so-called *gen-file*. With the help of a post-processor program it is possible to relate particles that end in a certain well of surface water element, with their starting positions. This option can be used, for instance, to determine catchment areas of groundwater pumping stations and to define protection zones.

NMIN *nm*

The value *nm* gives the minimum amount of particles that is generated within each grid cell, when the grid release rate is used. Normally this value is 1, which means that for every pulse at

least one particle is generated, even if the amount of mass is very small. The value may be increased, which results in a larger amount of particles per cell per pulse.

Appendix D INSTALLATION

For the auxiliary programs CLDGRID and SHOWCLOUD are using graphical subroutines from the package XVIG (Demaree, 1993). It is necessary to set the following environment-variables in the .profile or .kshrc file of the user's home directory.

XVIGDIR

This is the pathname of the root directory of the XviG system installations. Usually it will be set as:

```
XVIGDIR=$HOME/xvig
```

XVIG

This is the pathname of the XviG child program. Usually one will set this as

```
XVIG= $HOME/xvig/bin/xvig or
```

```
XVIG=$XVIGDIR/bin/xvig
```

Finally, the following line must be included in the .profile or .kshrc file

```
EXPORT XVIG XVIGDIR
```