User Manual

Visual MOCDENS3D

visualisation and processing software for MOCDENS3D, a 3D density dependent groundwater flow and solute transport model

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“All models are wrong, but some are useful”

George E.P. Box

“Models are to be used, but not to be believed”

Henri Theil

Visual MOCDENS3D

Visualisation and processing software for MOCDENS3D, a 3D density dependent groundwater flow and solute transport model.

ABSTRACT – MOCDENS3D is a density dependent groundwater flow and solute transport model (Oude Essink, 1998). It is based on the three-dimensional solute transport code MOC3D (Konikow et al., 1996), but adapted for density differences. Visual MOCDENS3D is a program package to process input and output for MOCDENS3D and to run the model. It is developed as a MATLAB toolbox but can also be used as a stand-alone application. Visual MOCDENS3D consist of different modules. *File Manager* loads and saves MOCDENS3D projects. The *Grid Builder* module assists in the preparation of the necessary MOCDENS3D input files and visualises the model input. The *MOCDENS3D* module assists in running the model and visualises the output. This is done using cross-sections, graphs, 3D plots and movie options. Also, MOCDENS3D output is used to calculate compaction of layers and surface subsidence. A comparison between observations and calculations and an analysis of residuals can be made. The *ParTrack* module uses a particle tracking algorithm to calculate flow paths, capture zones and travel times. The MOCDENS3D model can be run as a constant boundary type model (CBTM) whereby the boundary conditions such as status of cells (constant head, inactive or variable head), value of a constant head cell, or hydraulic parameters of cells are not variable. The model can also be run as a variable boundary type model (VBTM) whereby these boundary conditions can alter between different stress periods. Input of complex data is done using spreadsheets.

ACKNOWLEDGEMENT - Andy Louwyck of Ghent University, Research Unit Groundwater Modelling is acknowledged for assistance with his extensive MATLAB knowledge and Gualbert Oude Essink of TNO Geological Survey (Netherlands) is acknowledged for assistance with some MOCDENS3D issues.

Introduction – Installing Visual MOCDENS3D

Visual MOCDENS3D is developed to visualise and further handle MOCDENS3D output. The basic package consists of different modules:

- **File Manager**: regulates file flow of Visual MOCDENS3D

- **Grid Builder**: assist to make the necessary input files

- **MOCDENS3D**: runs MOCDENS3D and visualises the output. This requires that input files are already made. Also, observations and calculations can be compared and an analysis of the residuals can be made.

- **ParTrack**: uses particle tracking to calculate capture zones or flow paths

Visual MOCDENS3D is programmed as a toolbox within MATLAB but can also be used as a stand alone application. The advantage of using Visual MOCDENS3D as a MATLAB toolbox is that full use of the functionalities of MATLAB can be made. The latter program must thus be installed on your computer before Visual MOCDENS3D can be run in this way. The advantage of using Visual MOCDENS3D as a stand-alone application is that you don't need MATLAB.

Installing Visual MOCDENS3D as a MATLAB toolbox

Installing Visual MOCDENS3D is fairly simple. On the computer, a map 'c:\visualMOCDENS3D' must be made. In this map, all submaps must be copied. These are

vm program files
projects
basic mocdens files
manual

Visual MOCDENS3D must now be introduced in MATLAB so that you can use it as a toolbox. The procedure is simple and must be done only once.

From the Start button, select Shortcuts > New Shortcut. The Shortcut Editor dialog box appears. Create the shortcut by completing the dialog box, as shown in the figure 0.1.

The label, which will be shown as the name of the shortcut, is VM3D. In the callback, 'c:\visualMOCDENS3D' is set as the current directory if Visual MOCDENS is started and the command to start Visual MOCDENS3D is given. In category, it is indicated that a toolbar shortcut will be created and the path to the icon of the shortcut is given. After selecting save, all information is saved and a shortcut in the MATLAB toolbar is created.

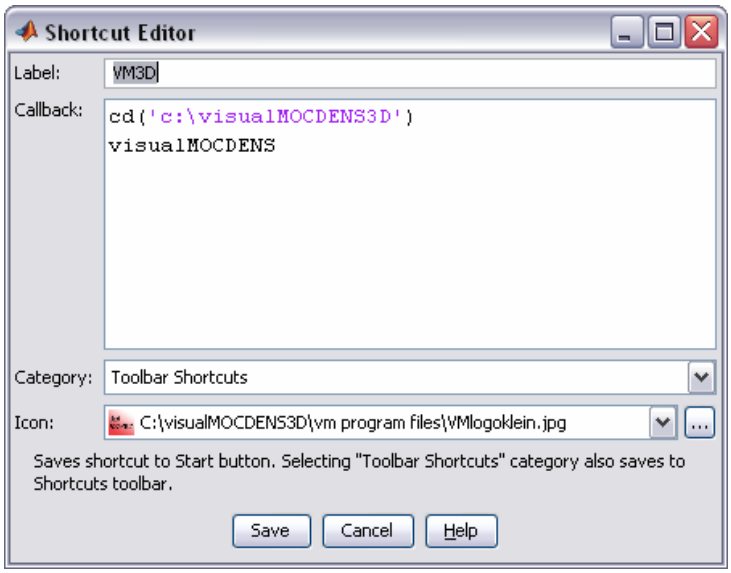


Figure 0.1 Example of the MATLAB shortcut editor to create a shortcut to Visual MOCDENS3D.

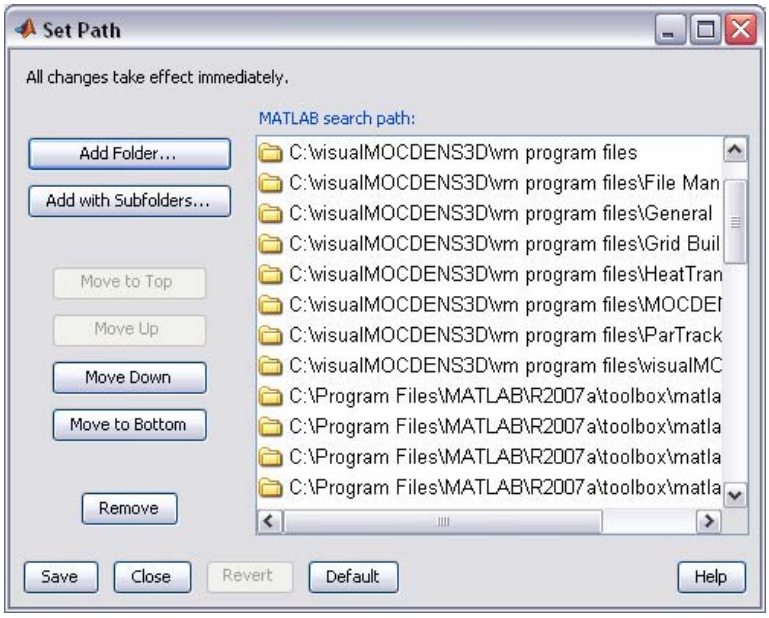


Figure 0.2 Window 'Set Path' which makes that Visual MOCDENS3D functions are readily recognised within MATLAB.

Then from File < set path … in MATLAB, the directory 'c:\visualMOCDENSD3D\vm program files' must be added ('add with subfolders' and push 'save'). All Visual MOCDENS3D functions can now be used without setting 'c:\visualMOCDENS3D\vm program files' as the current directory.

By selecting the VM3D icon on the MATLAB toolbar, Visual MOCDENS3D starts and is ready to be used.

Installing Visual MOCDENS3D as a stand-alone application

This makes it possible to use Visual MOCDENS3D without MATLAB on your computer. The folders 'projects', 'basic mocdens files' and 'manual' must be copied in the folder 'c:\visualMOCDENS3D'.

Also the files 'MCRInstaller.exe', 'VisualMOCDENS3D.exe', 'VisualMOCDENS3D.ctf', VMlogo.jpg and VMlogoklein.ico must be copied in the folder 'c:\visualMOCDENS3D'.

The first time you want to use a stand-alone application created with MATLAB, you have to install the MATLAB Component Runtime (MCR) on your computer. MCR is stand-alone set of shared libraries that enable the execution of MATLAB m-files. This is done by clicking on MCRInstaller.exe.

Thereafter, you can use Visual MOCDENS3D, simple by clicking on VisualMOCDENS3D.exe.

A short-cut with Visual MOCDENS3D logo can be made by right-clicking on the file VisualMOCDENS3D.exe. Then choose "Create Shortcut" and a shortcut will be made. To replace the shortcut icon with the Visual MOCDENS3D logo, right-click on the shortcut and select "properties". Go to the "shortcut" menu and click on "Change Icon" to select a new shortcut icon. The Visual MOCDENS3D logo can be found in the folder 'c:\visualMOCDENS3D'.

Installing Visual MOCDENS3D as a MATLAB toolbox and as a stand-alone application

Visual MOCDENS3D can be installed both as a toolbox and as a stand-alone application on one computer. In this case, the installation of Visual MOCDENS3D as MATLAB toolbox is done as already described. The installation of Visual MOCDENS3D as an stand-alone application is also done as described but all files are copied in a folder 'c:\visualMOCDENS3D_SA' and NOT in the folder 'c:\visualMOCDENS3D'.

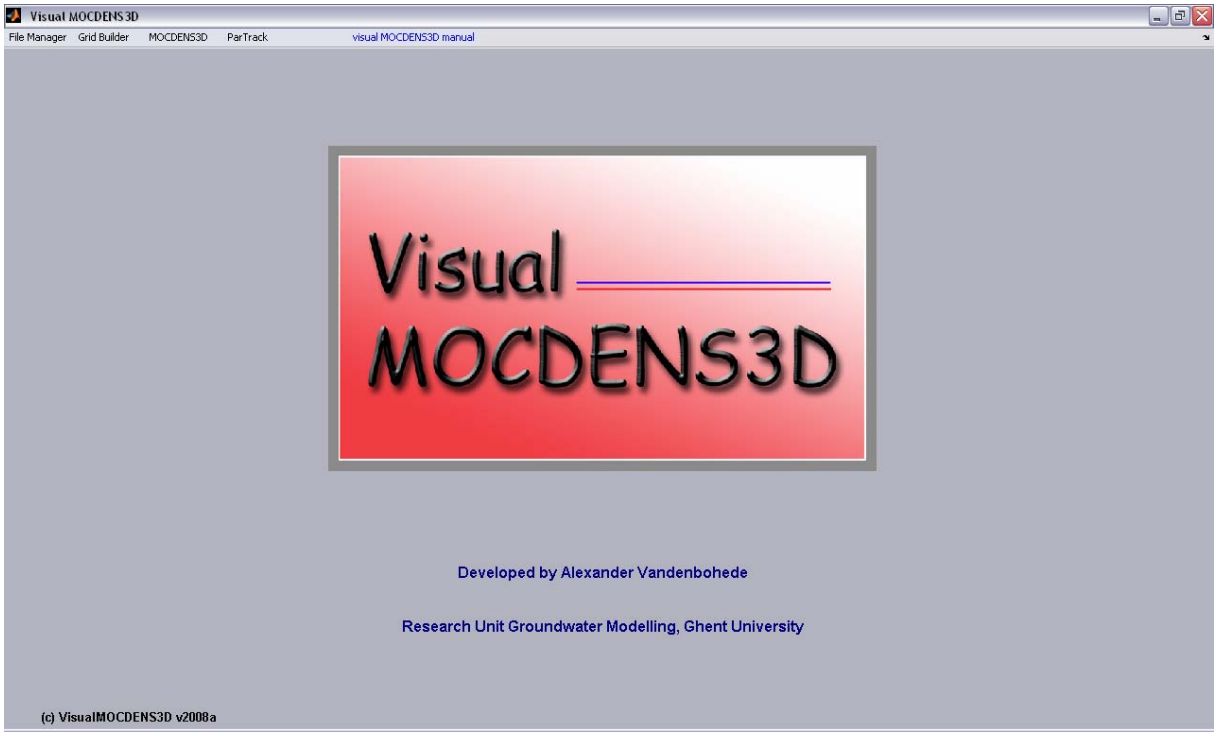


figure 0.3 *Visual MOCDENS3D window after starting up the program.*

Compatibility

Visual MOCDENS3D is made with MATLAB 7.5.0 (R2007b). Visual MOCDENS3D used as a MATLAB toolbox consist of p-files which are made with MATLAB 7.0.1. Consequently it runs on this and later MATLAB versions but not on earlier versions. The stand-alone application is compiled with MATLAB 7.5.0 (R2007b).

1 MOCDENS and Visual MOCDENS3D

1.1 Introduction

MOCDENS3D (Oude Essink, 1998) is a density dependent finite difference 3D groundwater flow model. It is an adaptation of the 3D solute transport model MOC3D (Konikow et al., 1996) to take into account density differences. The groundwater flow equation is solved by a module, which is in fact the MODFLOW computer code (McDonald and Harbaugh, 1988). Density differences are taken into account by adding buoyancy terms to the right-hand-side term of the basic equation of MODFLOW. The advection-dispersion equation is solved by the MOC module, using the method of characteristics (Konikow and Bredehoeft, 1978). An advantage of applying the method of characteristics is that the condition of spatial discretisation, characterised by the so-called grid Peclet number, is not strict. As a consequence, the displacement of fresh, brackish and saline groundwater in large-scale 3D aquifer systems can easily be simulated without severe numerical implications such as non-convergence as well as heavy over- and undershooting. Furthermore, retardation and a first-order reaction rate coefficient can be taken into account.

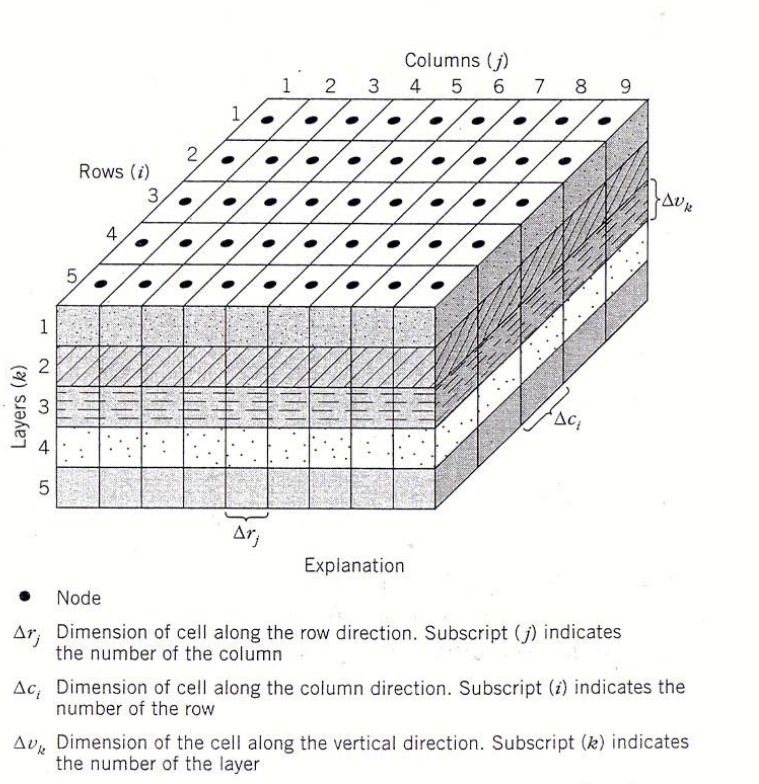


figure 1.1 *Discretisation of a three-dimensional groundwater reservoir (after McDonald and Harbaugh, 1988).*

The model area is subdivided in a number of layers, rows and columns (figure 1.1) and the groundwater flow and solute transport equations are solved for this finite difference grid. It is important to note that the grid used by MOCDENS3D must be a regular grid. This means that the width of a column or row remains constant throughout the model. Also all layers must have the same thickness.
MOCDENS3D consists of 2 modules which are fully integrated with each other:

- a solute-transport module, the MOC module,
- a groundwater-flow module, the MODFLOW module.

The MODFLOW module is adapted for density differences and this module computes transient density-dependent groundwater flow. This is possible by inserting a so-called buoyancy term in the basic equation of the MODFLOW module. The velocity filed distribution is derived from the computed fresh water head distribution. Subsequently, the velocity field distribution is derived from the computed fresh water head distribution. As such, the two modules are coupled with each other.

1.2 Governing equations

1.2.1 Flow equation

Three-dimensional flow for the finite difference grid in MODFLOW is given by the equation:

$$\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} - W = S_s \frac{\partial h}{\partial t} \qquad (1)$$

where x, y and z are coordinate directions; q_x, q_y and q_z are Darcian flow velocities (m/d) in x, y and z direction; W (d^{-1}) is a flux term accounting for pumping, recharge, or other sources and sinks; h is the hydraulic head (m); S_s is the specific elastic storage (m^{-1}) and t is time (d).

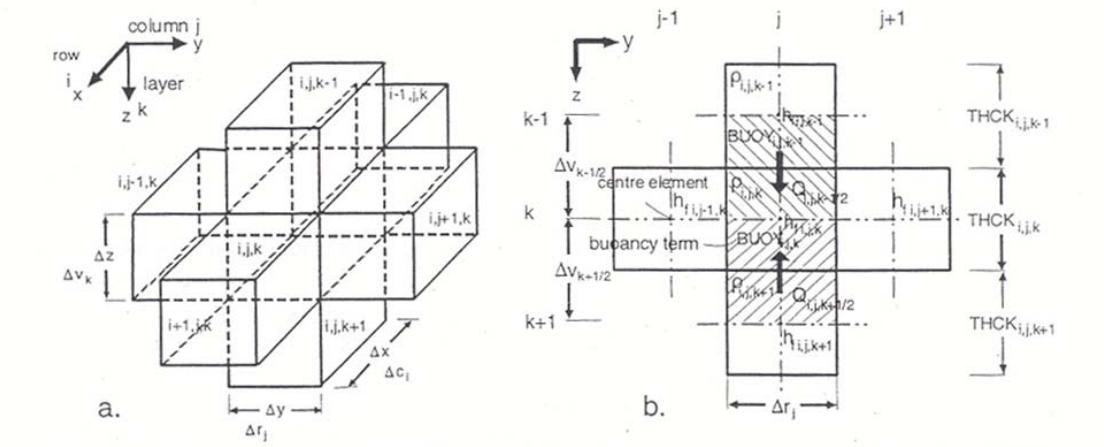


figure 1.2 *MODFLOW/MOCDENS3D grid cells more in detail (Oude Essink, 1998).*

The Darcy velocity components are given by:

$$q_x = -K_x \frac{\partial h}{\partial x}$$
$$q_y = -K_y \frac{\partial h}{\partial y} \qquad (2)$$
$$q_z = -K_z \frac{\partial h}{\partial z}$$

where K_x and K_y are horizontal hydraulic conductivities (m/d) and K_z is the vertical hydraulic conductivity (m/d).

Equation one states that outflow minus the inflow of water in every finite difference cell (these are thus six discharge rates, each for each side of a finite difference cell) equals the storage change of this cell.

The width of every column and every row is assumed to be equal, only density difference in the vertical direction must be taken into account to simulate density depended flow. The Darcy velocity components taken into account densities are given by

$$\begin{aligned} q_x &= -\kappa_{fx} \frac{\rho_f g}{\mu} \frac{\partial h_f}{\partial x} \\ q_y &= -\kappa_{fy} \frac{\rho_f g}{\mu} \frac{\partial h_f}{\partial y} \\ q_z &= -\kappa_{fz} \frac{\rho_f g}{\mu} \left(\frac{\partial h_f}{\partial z} + \frac{\rho - \rho_f}{\rho_f} \right) \end{aligned} \tag{3}$$

where μ is the dynamic viscosity (kg/md); ρ_f and ρ are the densities (kg/m³) respectively of fresh water and water; κ_{fx}, κ_{fy} and κ_{fz} are intrinsic permeability in the x, y and z direction and g the acceleration due to gravity (m²/d). Instead of a hydraulic head h, a fresh water head h_f is used:

$$h_f = \frac{p}{\rho_f g} - z \tag{4}$$

where p is the water pressure (kg/md²).

Small viscosity differences can however be neglected if density differences are taken into account (Verruijt, 1980; Bear and Verruijt, 1987). Then:

$$\begin{aligned} q_x &= -K_{fx} \frac{\partial h_f}{\partial x} \\ q_y &= -K_{fy} \frac{\partial h_f}{\partial y} \\ q_z &= -K_{fz} \left(\frac{\partial h_f}{\partial z} + \frac{\rho - \rho_f}{\rho_f} \right) \end{aligned} \tag{5}$$

The term $(\rho-\rho_f)/\rho_f$ is called the buoyancy term. This buoyancy is related to concentrations according through:

$$\frac{\rho - \rho_f}{\rho_f} = \frac{\rho_s - \rho_f}{\rho_f} \frac{C}{C_s} \tag{6}$$

where C is the concentration (mg/l), C_s is the concentration (mg/l) of salt water and ρ_s is the density of salt water (kg/m³).

Three-dimensional flow in MOCDENS3D is thus finally described by the following equation:

$$\frac{\partial q_x}{\partial x}+\frac{\partial q_y}{\partial y}+\frac{\partial q_z}{\partial z}-W=S_s\frac{\partial h_f}{\partial t} \tag{7}$$

1.2.2 Advection-dispersion equation

The advection-dispersion equation, describing the change of solute concentration in function of location and time is given in vector form by:

$$\frac{\partial(n_e C)}{\partial t}=\nabla.(n_e D.\nabla C)-\nabla.(qC)+q_s C_s \tag{8}$$

where C is the concentration (mg/l), t is time (d), n_e is the effective porosity (-), D the dispersivity tensor (m²/d), q, the Darcian velocity (m/d), q_s is the volumetric flow rate of sinks/sources (m/d) and C_s the concentration of sinks and sources (mg/l). It describes the total difference between inflow and outflow of solute mass for a volume aquifer obtained by summing the advective (second term RHS) and dispersive (first term RHS) terms in the coordinate directions.

With q_x, q_y and q_z the components of the Darcy velocity, D_{xx}, D_{yy}, D_{zz}, the diagonal terms of the dispersivity tensor and D_{xy}, D_{xz}, D_{yx}, D_{yz}, D_{zx} and D_{zy} the non-diagonal terms of the dispersivity tensor, this gives:

$$\begin{aligned}\frac{\partial(n_e C)}{\partial t}&=\frac{\partial}{\partial x}\left(n_e D_{xx}\frac{\partial C}{\partial x}+n_e D_{xy}\frac{\partial C}{\partial y}+n_e D_{xz}\frac{\partial C}{\partial z}\right)-\frac{\partial}{\partial x}(q_x C)\\&+\frac{\partial}{\partial y}\left(n_e D_{yx}\frac{\partial C}{\partial x}+n_e D_{yy}\frac{\partial C}{\partial y}+n_e D_{yz}\frac{\partial C}{\partial z}\right)-\frac{\partial}{\partial y}(q_y C)\\&+\frac{\partial}{\partial z}\left(n_e D_{zx}\frac{\partial C}{\partial x}+n_e D_{zy}\frac{\partial C}{\partial y}+n_e D_{zz}\frac{\partial C}{\partial z}\right)-\frac{\partial}{\partial z}(q_z C)+q_s C_s\end{aligned} \tag{9}$$

Equation 8 or 9 describes advective-dispersive solute transport in three dimensions with internal sources or sinks present.

Taking also into account retardation and first-order decay, equation 9 becomes:

$$\begin{aligned}\frac{\partial(n_e C)}{\partial t}&=\frac{1}{R_f}\frac{\partial}{\partial x}\left(n_e D_{xx}\frac{\partial C}{\partial x}+n_e D_{xy}\frac{\partial C}{\partial y}+n_e D_{xz}\frac{\partial C}{\partial z}\right)-\frac{1}{R_f}\frac{\partial}{\partial x}(q_x C)\\&+\frac{1}{R_f}\frac{\partial}{\partial y}\left(n_e D_{yx}\frac{\partial C}{\partial x}+n_e D_{yy}\frac{\partial C}{\partial y}+n_e D_{yz}\frac{\partial C}{\partial z}\right)-\frac{1}{R_f}\frac{\partial}{\partial y}(q_y C)\\&+\frac{1}{R_f}\frac{\partial}{\partial z}\left(n_e D_{zx}\frac{\partial C}{\partial x}+n_e D_{zy}\frac{\partial C}{\partial y}+n_e D_{zz}\frac{\partial C}{\partial z}\right)-\frac{1}{R_f}\frac{\partial}{\partial z}(q_z C)+\frac{q_s C_s}{R_f}-\lambda C n_e\end{aligned} \tag{10}$$

where R_f is the retardation factor (-) and λ is the first-order decay coefficient (d-1).

The dispersivity tensor D_{ij}, including diffusion can be written as:

$$
\begin{aligned}
D_{xx} &= \alpha_L \frac{V_x^2}{|V|} + \alpha_{Th} \frac{V_y^2}{|V|} + \alpha_{Tv} \frac{V_z^2}{|V|} + D_m \\
D_{yy} &= \alpha_L \frac{V_y^2}{|V|} + \alpha_{Th} \frac{V_x^2}{|V|} + \alpha_{Tv} \frac{V_z^2}{|V|} + D_m \\
D_{zz} &= \alpha_L \frac{V_z^2}{|V|} + \alpha_{Th} \frac{V_y^2}{|V|} + \alpha_{Tv} \frac{V_x^2}{|V|} + D_m \\
D_{xy} &= D_{yx} = (\alpha_L - \alpha_{Th}) \frac{V_x V_y}{|V|} \\
D_{xz} &= D_{zx} = (\alpha_L - \alpha_{Tv}) \frac{V_x V_z}{|V|} \\
D_{yz} &= D_{zy} = (\alpha_L - \alpha_{Tv}) \frac{V_y V_y}{|V|} \\
\text{with} \quad |V| &= \sqrt{V_x^2 + V_y^2 + V_z^2}
\end{aligned}
\tag{11}
$$

where V_x, V_y and V_z are the effective flow velocities (m/d) in the x-, y- and z-direction, α_L, α_{Th} and αTv are the longitudinal and transverse (in the horizontal and vertical direction) dispersivities (m) and D_m is the diffusion coefficient (m²/d). Instead of using longitudinal and transverse dispersivity, the latter is further subdivided. It was found by for instance Robson (1974), Robson (1978), Garabedian et al. (1991) and Gelhar et al. (1992) that the transverse dispersivity in the vertical direction is mush smaller than in the horizontal direction.

1.2.3 Numerical Methods

For an extensive treatment of the numerical methods, the reader is referred to the MODFLOW (McDonald and Harbaugh, 1988) and MOC3D manual (Konikow et al., 1996). Here a brief introduction is given.

MODFLOW offers several options to solve the implicit finite-difference equations, including the Strongly Implicit Procedure (SIP), Slice-Successive Overrelaxation (SSOR) methods, or Preconditioned Conjugate-Gradient matrix solvers (for instance Hill, 1990). The SIP method is used in MOCDENS3D.

After the head distribution has been calculated for a given time step or steady-state flow condition, the specific discharge across every face of each finite-difference cell within the transport subgrid is calculated next. These are further recalculated in effective velocities in the x-, y- and z-directions which form the basis for further calculations of solute transport.

The solute transport equation is, in general, more difficult to solve accurately using numerical methods than is the ground water flow equation, largely because the mathematical properties of the transport equation vary depending upon which terms in the equation are dominant in a particular system. When the solute transport is dominated by advective transport, as is common in many field problems, then the transport equation approximates a hyperbolic type of equation. In contrast, where a system is dominated by dispersive fluxes, such as might occur where fluid velocities are relatively low and aquifer dispersivities are relatively high, then the transport equation becomes more parabolic in nature. To further complicate matters, because system properties and fluid velocity may vary significantly, the dominant process may vary from point to point and over time within the same domain.

The method of characteristics (MOC) (Konikow & Bredehoeft, 1978) was developed to solve hyperbolic differential equations. A major advantage is that the method minimises numerical dispersion (or even eliminates it in limited cases). The approach taken by MOC is not to solve equation 10 directly, but rather to solve an equivalent system of ordinary differential equations. Advection is simulated with a particle tracking procedure whereas dispersion is calculated with a finite difference scheme. Equation 10 describes the change in concentration over time at fixed reference points within a stationary coordinate system, which is referred to an Eulerian framework. An alternative perspective is to consider changes in concentration over time in representative fluid parcels as they move with the flow of the fluid past fixed points in space. This, in effect, is a moving coordinate system, which is referred to as a Langrangian framework. Equation 10 is therefore converted from an Eulerian framework to a Langrangian framework. The material derivative of concentration with respect to time (dC/dt), or the change in concentration of a moving particle, describes the change in concentration in a parcel of water moving at the average effective velocity of water:

$$\frac{dC}{dT} = \frac{\partial C}{\partial t} + \frac{\partial C}{\partial x}\frac{dx}{dt} + \frac{\partial C}{\partial y}\frac{dy}{dt} + \frac{\partial C}{\partial z}\frac{dz}{dt} \tag{12}$$

The last three terms on the right side include the material derivatives of position, which are defined by the velocity in the x-, y- and z-direction:

$$\frac{dx}{dt} = \frac{V_x}{R_f} \qquad \frac{dy}{dt} = \frac{V_y}{R_f} \qquad \frac{dz}{dt} = \frac{V_z}{R_f} \tag{13}$$

A simpler form of the governing equation for the concentration of a reference point moving with the retarded velocity V/Rf is then obtained by substituting the right sides of equations 10 and 13 for the corresponding terms in equation 12:

$$\begin{aligned}\frac{d(n_e C)}{dt} &= \frac{1}{R_f}\frac{\partial}{\partial x}\left(n_e D_{xx}\frac{\partial C}{\partial x} + n_e D_{xy}\frac{\partial C}{\partial y} + n_e D_{xz}\frac{\partial C}{\partial z}\right) \\ &+ \frac{1}{R_f}\frac{\partial}{\partial y}\left(n_e D_{yx}\frac{\partial C}{\partial x} + n_e D_{yy}\frac{\partial C}{\partial y} + n_e D_{yz}\frac{\partial C}{\partial z}\right) \\ &+ \frac{1}{R_f}\frac{\partial}{\partial z}\left(n_e D_{zx}\frac{\partial C}{\partial x} + n_e D_{zy}\frac{\partial C}{\partial y} + n_e D_{zz}\frac{\partial C}{\partial z}\right) + \frac{q_s C_s}{R_f} - \lambda C n_e\end{aligned} \tag{14}$$

Although this concentration is now that of a moving point in space, the same symbol C is retained as a matter of convenience.

The solutions of a system of equations 13 and 14 may be given as x = x(t), y = y(t), z = (t) and C = C(t) and these are called the characteristic curves of equation 10. A solution to the original partial differential equation may be obtained by following the characteristic curves. This may be accomplished by introducing a set of moving points (or reference particles) that can be traced within the stationary coordinates of a finite-difference grid. This is called particle tracking. Each particle corresponds to one characteristic curve, and values of x, y, z and c are obtained as functions of t for each characteristic curve (Garder et al., 1964). Each point has a concentration and position associated with it and is moved through the flow field in proportion to the flow velocity at its location (figure 1.3).

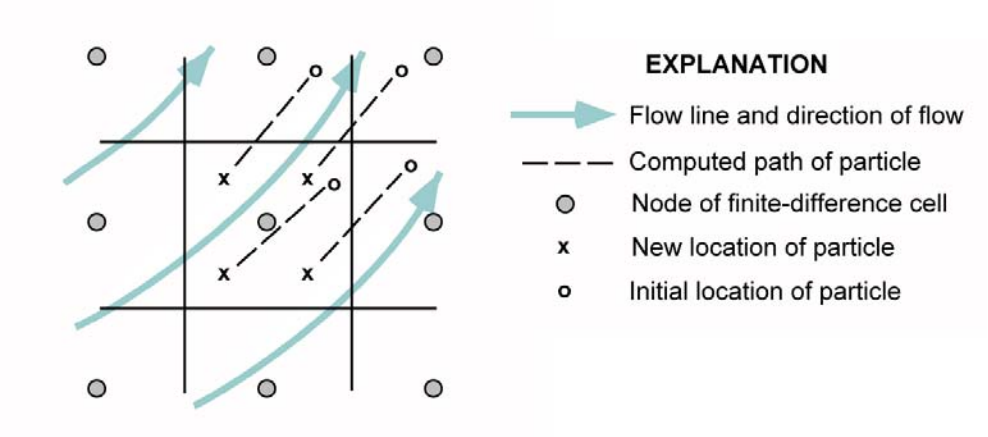


figure 1.3 *Path of hypothetical finite-difference grid showing relation of flow field to movements of points (or particles) in a MOC model for simulating solute transport (modified from Konikow and Bredehoeft, 1978).*

The change of concentration in a cell is calculated as the sum of the change due to advection and the change due to dispersion. For detailed treatment of the numerical solution the reader is referred to the MOC3D manual (Konikow et al., 1996). Advective transport is simulated by particle tracking where after the concentrations of every cell are calculated as the mean concentration of all particles in each cell. Then based on the dispersivity tensor, groundwater flow velocities and grid dimensions, dispersive transport is calculated. Advective and dispersive transport is thus solved sequentially. In real however, this happens simultaneously. To correct for this, the concentrations of the cells C(l,r,c) used to calculated dispersive transport are:

$$C_{(l,r,c)} = wC^{n*}_{(l,r,c)} + (1-w)C^{n-1}_{(l,r,c)} \tag{15}$$

whereby Cn*(l,r,c) is the concentration of cell in layer l, row r and column c, after the advective movement in time step n, and Cn-1(l,r,c) is the concentration in the same cell at the end of time step n-1. W is a weighting factor which is in most cases set at 0.5.

1.2.4 Stability Criteria

The above explained approach requires the considerations of a number of stability criteria. (Konikow and Bredehoeft, 1978). These may require that the time step used to solve the flow equation be subdivided into a number of smaller time increments to accurately solve the solute-transport equation.

First, consider the explicit finite-difference solution to calculate changes in concentration due to dispersion. It is found that:

$$\Delta t \le \min_{overgrid}\left[\frac{0.5}{\frac{D_{xx}}{R_f(\Delta x)^2}+\frac{D_{yy}}{R_f(\Delta y)^2}\frac{D_{zz}}{R_f(\Delta z)^2}}\right] \tag{16}$$

Next, by considering the effects of mixing ground water of one concentration with injected or recharged water of a different concentration. The change in concentration in a source node can not exceed the difference between the source concentration and the concentration in the aquifer and the

maximum possible change occurs when a source completely flushes out the volume of water in a cell at the start of a time increment. Therefore:

$$\Delta t \leq \min_{overgrid}\left[\frac{n_e R_f}{W_{i,j,k}}\right] \tag{17}$$

A third type of criterion involves the movement of point to simulate advective transport. The distance a particle moves during a time increment is equal to (or approximately so in case where particles cross a cell face and the adjacent cells have different properties) the velocity at the location of the particle times the length of the time increment. In effect, this constitutes a linear spatial extrapolation of the position of a particle from one time increment to the next. Konikow and Bredehoeft (1978) note that where streamlines are curvilinear, the extrapolated position of a particle will deviate from the streamline on which it was previously located. This deviation introduces an error into the numerical solution that is proportional to the time increment. Thus for a given velocity field and grid (the latter also determines the streamlines), some restrictions must be placed on the size of the time increment to assure that the distance a particle moves in the x-, y- and z-direction does not exceed some critical distances. These critical distances can be related to the grid dimensions by

$$\Delta t V_{x(p)} \leq \gamma \Delta x \qquad \Delta t V_{y(p)} \leq \gamma \Delta y \qquad \Delta t V_{z(p)} \leq \gamma \Delta z \tag{18}$$

where γ (or CELDIS in the input files) is the fraction of the grid dimensions that particles will be allowed to move (normally, $0 < \gamma < 1$). From equation 17 the smallest time increment can again be determined.

1.3 Overview MOCDENS3D model input

The model needs a relatively large amount of input data. The input for the groundwater flow model is equal to the input for MODFLOW and this is subdivided in a number of input packages (basic, block centred flow, river, dranaige, wells, obs). Adaptation for density differences is taken into account in an additional package (densin.dat) and small extras in other packages. One package (moc) regulates the solute transport.

Here, the input is summarised. Overview of the different input files is given elsewhere in this manual (chapter on the Grid Module). Details can be found in McDonald and Harbaugh (1988). Summary of the different input is given below.

Required basic input to solve the groundwater flow equation is:

- Schematisation of the groundwater reservoir in layers, rows and columns.
- Horizontal hydraulic conductivity of every layer, or more detailed of every cell.
- Vertical conductivity of every layer, or more detailed of every cell. This value is recalculated as a hydraulic conductance between the cells.
- Specific elastic storage and storage coefficient (or specific yield) for every layer or every cell if transient state flow is considered
- Model parameters

Boundary conditions are also required:

- Constant head boundaries
- Impermeable boundaries
- Constant inflow boundaries

Optional input is:

- Infiltration options
- Drainage options
- Well options
- River options

Solute transport simulations requires following input:

- Dispersivities
- Layer thickness
- Effective porosity
- Stability criteria
- Retardation and/or first order decay if required

Initial values for heads and concentrations are needed before starting the calculations.

1.4 Visual MOCDENS3D: an overview

Visual MOCDENS3D is designed to run MOCDENS3D, visualise the model output, use the model output to calculated capture zones and flow paths and provides tools for model calibration. It has also a grid builder for the design of the MOCDENS3D input files. This is done via graphical user interfaces (GUIs) programmed using the MATLAB software package. Visual MOCDENS3D contains the following modules:

File Manager: regulates file flow of Visual MOCDENS3D

Grid Builder: assist to make the necessary input files

- Basic grid: this assists in making the input files (bas, bcf, moc, wel, oba, obs, densin.dat, sip and name files) of a simple model. This is a model with all cells designated as active cells and with regular boundary conditions along the four sides of every layer.
- Advanced grid: this assists in making input files (bas, bcf, moc, wel, drn, ghb, riv, obs) based on irregular patterns using input via excel files.
- Grid visualiser: this option visualises model input
- Permanent to transient model: this options assist in making input files for a transient model from a permanent model

MOCDENS3D: runs MOCDENS3D and visualises the output. This requires that input files are already made.

- Running mocdens3D
- Horizontal cross-sections (heads, concentrations, effective velocities)
- Vertical cross-sections (heads, concentrations, effective velocities)
- Vertical effective flow velocities
- Differences between heads or concentrations between different layer/rows/columns or stress periods
- Head or concentration versus time or distance graphs
- In- or outflow of water or concentrations for cell(s)
- Calculation of solute mass and its evolution in the model
- 3D visualisation of heads, concentrations or velocities
- movies
- Comparison of calculations and observations
- Extra: visualisation of certain input files

ParTrack: uses particle tracking to calculate capture zones or stream lines

- 3D calculation and visualisation of stream lines
- Calculation and visualisation of capture zones

1.5 MOCDENS3D applications

MOCDENS3D can thus simulate 3D density depended solute transport. This has a large number of applications in coastal hydrogeology such as simulation of the distribution and evolution of fresh-salt water, human impact on this (for instance due to water catchments, drainage level changes, etc.) or influence of sea level and or recharge changes due to global change.

Second application is in contamination hydrogeology since the distribution and its evolution of contaminants can be calculated. Here also, density effects can be taken into account. This has for instance its applications in simulating the distribution of contaminants, design of remediation strategies etc.

At last, 'ordinary' groundwater flow simulations can also be performed. Disadvantage is here that a moc-file and other references to solute transport in the input files must be filled in. Concentrations can for instance be set at 0 and only the options for the processing of head calculations in Visal MOCDENS3D are used.

A number of applications which can be found in literature are hereafter given.

Oude Essink, G. H. P. (2001). Salt Water Intrusion in a Three-dimensional Groundwater System in The Netherlands : a Numerical Study. Transport in Porous Media 43(1): 137-158.

> Abstract - Salt water intrusion is investigated in a coastal groundwater system in the northern part of the province Noord-Holland, The Netherlands. Density dependent groundwater flow is modeled in three-dimensions with MOCDENS3D. This computer code is a version of MOC3D (Konikow et al., 1996) that has been adapted to simulate transient density-driven groundwater flow. Results from the model suggest that in this Dutch hydrogeologic system a severe and irreversible salinisation is already occurring. Within a few tens to hundreds of years, the salinity of the shallow aquifer is estimated to increase substantially. This salinisation process is a result of human activities such as the reclamation of the low-lying areas during the past centuries. Without changing the present boundary conditions, seepage into the low-lying areas will decrease slightly because of predicted increases in groundwater salinity. However, the rate in salt load through the Holocene aquitard into the low-lying areas will increase significantly due to an increase in salinity in the shallow aquifer. In addition, a relative sea level rise of 0.5m per century will intensify the salinisation process, causing an enormous increase in salt load in all low-lying areas in this part of The Netherlands.

Oude Essink, G. H. P. (2001). Density dependent groundwater flow at the island of Texel , The Netherlands. Proc. 16th Salt Water Intrusion Meeting, Miedzyzdroje-Wolin Island , Poland : 47-54.

> Salt water intrusion is investigated at Texel, which is a Wadden island in the northern part of The Netherlands with a surface area of approximately 130 km2. In this coastal groundwater system of Quatenary deposits, salinisation of the upper layers is taking place. At present, brackish water already occurs close to the surface of the low-lying polder areas at the eastern part of the island. Freshwater occurs up to –50 m M.S.L. in the sand-dune area at the western part. Density dependent groundwater flow in this system is modelled in three-dimensions by MOCDENS3D. The model is dimensioned 20 km by 29 km by 302 m depth, whereas about 125,000 active elements and one million particles simulate groundwater flow and salt transport

during 500 years. The salinity in the top layer as well as the salt load at the surface of the polders will increase substantially during the next centuries. In addition, a relative sea level rise of 0.75 meter per century definitely intensifies the salinisation process, causing a further increase in salt load in the polders. As such, the increased salinisation of the top layer will affect the surface water system from an ecological as well as a socio-economical point of view.

Vandenbohede, A. & Lebbe, L. (2002). Numerical modelling and hydrochemical characterisation of a fresh water lens in the Belgian coastal plain. Hydrogeology Journal, 10(5), 576-586.

Abstract - The distribution of fresh and salt water in coastal aquifers is influenced by many processes. The influence of aquifer heterogeneity and human interference such as land reclamation is illustrated in the Belgian coastal plain where, around 1200 AD, the reclamation of a tidally influenced environment was completed. The aquifer, which was filled with salt water, is thereafter freshened. The areal distribution of peat, clay, silt and sand influences the general flow and distribution of fresh and salt water along with the drainage pattern and results in the development of fresh water lenses. The water quality in and around the fresh water lenses below an inverted tidal channel ridge is surveyed. The hydrochemical evolution of the fresh water lens is reconstructed, pointing to cation exchange, solution of calcite and the oxidation and organic material as the major chemical reactions. The formation and evolution of the fresh water lens is modelled using a two-dimensional density depended solute transport model and the sensitivity of drainage and conductivities are studied. Drainage level influences mainly the depth of the fresh water lens where the time of formation is mainly influenced by conductivity.

Bouw, L. & Oude Essink, G.H.P. (2003). Development of a freshwater lens in the inverted Broad Fourteens Basin, Netherlands offshore, Journal of Geochemical Exploration (78-79), 321-325.

Abstract - The Mesozoic Broad Fourteens Basin is a northwest-southeast trending structural element, situated in the southern North Sea , Netherlands offshore. Biodegraded and water-washed oils in the southern Broad Fourteens Basin indicate topography-driven meteoric water flow during Late Cretaceous inversion. Density-driven groundwater flow models support the development of a freshwater lens in the northern Broad Fourteens Basin during Late Cretaceous inversion. Three model scenarios with basin-scale permeabilities and water table heads within the range of most likely values show the possible development of a freshwater lens in the northern Broad Fourteens Basin . The freshwater-saltwater interface is located at a depth of 200- 1200 m below mean sea level. Near steady-state flow conditions are reached within 1.5-4 Myr.

Oude Essink, G. H. P. (2003). Salinization of the Wieringermeerpolder, The Netherlands . Proc. 17th Salt Water Intrusion Meeting, Delft , The Netherlands : 399-411.

Bakker, M., G.H.P. Oude Essink, C.D. Langevin, (2004). The rotating movement of three immiscible fluids, Journal of Hydrology, 287: 270-278.

Abstract – A benchmark problem involving the rotating movement of three immiscible fluids is proposed for verifying the density dependent flow component of groundwater flow codes. The problem consists of a two-dimensional strip in the vertical plane filled with three fluids of different densities separated by interfaces. Initially, the interfaces between the fluids make a 45° angle with the horizontal. Over time, the fluids rotate to the stable position whereby the interfaces are horizontal; all flow is caused by density differences. Two cases of the problem are presented, one resulting in a symmetric flow field and one resulting in an asymmetric flow field. An exact analytical solution for the initial flow field is presented by application of the vortex theory and complex variables. Numerical results are obtained using three variable-density groundwater flow codes (SWI, MOCDENS3D, and SEAWAT). Initial horizontal velocities of the interfaces, as simulated by the three codes, compare well with the exact

solution. The three codes are used to simulate the positions of the interfaces at two times; the three codes produce nearly identical results. The agreement between the results is evidence that the specific rotational behaviour predicted by the models is correct. It also shows that the proposed problem may be used to benchmark variable density codes. It is concluded that the three models can be used to model accurately the movement of interfaces between immiscible fluids, and have little or no numerical dispersion.

Vandenbohede, A. & Lebbe, L. (2005). Density dependent groundwater flow model of the shore and dune area of the Westhoek nature reserve (Belgium). In: Araguas, L., Custodio, E. & Manzano, M., Groundwater and saline intrusion, selected papers from the 18th Salt Water Intrusion Meeting, Cartagena 2004, Spain, 197-205.

Abstract - The Westhoek nature reserve is a dune area situated along the French-Belgian border. Below the dunes a fresh water lens is found. A particular distribution of salt water occurring above fresh water is found under the adjacent shore. This less known water quality distribution is in dynamic equilibrium. A 2D density dependent groundwater flow model was made using the MOCDENS3D code. First, the groundwater flow and water quality evolution under the shore and in the dunes are modelled. Then the possible impact of sea level rise is simulated for a number of different scenarios. These scenarios reflect different reactions of coastal morphology and human intervention on the sea level rise. Depending on the scenario, the extent of the shore's salt water lens can increase, decrease of even completely disappear. Simultaneously, the extent of the dune's fresh water lens can alter significantly. The simulations illustrates also, besides the effects of sea level rise, that changes in boundary conditions (drainage levels, shore morphology, sea water level), natural or human induced, can alter importantly the water quality distribution. Because of the high ecological value of the area and the dune's importance for drinking water production, these changes should be well studied beforehand.

Vandenbohede, A. Linster, T. & Lebbe, L. (2005). Modelling of density dependent groundwater flow in the south-western Belgian coastal plain. In: Araguas, L., Custodio, E. & Manzano, M., Groundwater and saline intrusion, selected papers from the 18th Salt Water Intrusion Meeting, Cartagena 2004, Spain, 207-214.

Abstract - The Belgian coastal plain provides an excellent opportunity to study the development of fresh water lenses. Aquifer heterogeneity and human interference such as land reclamation determine the distribution of fresh and salt water. Before the land reclamation the Belgian coastal plain was a tidal flat and the groundwater reservoir was mainly filled with salt water. From around 1100 AD, with the completion of land reclamation, this salt water was replaced by fresh water leading to the now observed ground water quality distribution. The heterogeneous distribution of peat, clay, silt and sand influences the general flow and distribution of fresh and salt water along with the drainage pattern and results in the development of fresh water lenses. These fresh water lenses were surveyed in the polder 'Noordwatering Veurne' situated on the west bank of the IJzer river in the western Belgian coastal plain. Data of a preliminary field survey and literature data were combined to make a 3D groundwater flow model of the area using the MOCDENS3D code. This model shows the 3D development of fresh water lenses in a heterogeneous aquifer.

Vandenbohede, A., Luyten, K., & Lebbe, L. (2005). Impact of water catchment in the dune area along the French-Belgian border. In: Sadurski, A. and Balabanis, P. (ed.), Proceedings of the International conference on hydrogeological transboundary problems, West and East European Bridge, 22-26 November 2004, Warsaw, Poland, Polish Geological Institute Special Papers 18, p 93-97.

Abstract - The western Belgian coastal plain, along the French-Belgian border, consists of a shore, dunes and polders. A valuable nature reserve is present in the dunes as is a water catchment. In recent years, the water catchment has problems with salt water intrusion from

the polder. The aim of this study is to model the influence of the water catchment. Special attention goes to the evolution of the intrusion of salt water from the polder and from the sea in the dunes along the French-Belgian border. Therefore, a 3D density dependent groundwater flow model was made of the shore, dunes and part of the polder along the border using the MOCDENS3D code. The heterogeneous groundwater reservoir was schematised in the model based on numerous drilling descriptions and geophysical measurements and the simulations were calibrated using hydraulic heads and water quality observations. With the model it was shown that the salt water intrusion is restricted to the immediate surroundings of the water catchment, does not cross the border and does not influence the nature reserve.

Smith, K. A., Vandenbodehede, A., Maes, A., Verstraete, W. & Lebbe, L. (2005). Hydrogeological investigations in preparation of an in situ bioremediation strategy based on a novel bacterial Desulfitobacterium Dichloroeliminans strain DCA1, In Kalmar Eco-Tech '05 and The Second Baltic Symposium on Environmental Chemistry, Kalmar, Sweden, november 28-30, 2005, 413-424.

Abstract - Understanding the wide variety of aquifer physical, chemical and microbiological processes is necessary for the effective implementation of in situ bioaugmentation strategies. Therefore, a numerical density dependent 3D solute transport model MOCDENS3D was developed in combination with field experiments to characterise the subsurface control parameters. This also allowed for the study of the effect of aquifer heterogeneity upon the fate and transport of the reactive solutes and the injected bacterial strain.
These investigations were conducted during the evaluation of an in situ bioremediation strategy intended for the cleanup of a test site. The site lies within a historically 1,2-dichloroethane (1,2-DCA) contaminated sandy phreatic aquifer in Tessenderlo (Belgium). The halogenated compound has a putative carcinogenic effect and a high recalcitrance towards reductive dechlorination. The isolation of the novel anaerobic Desulfitobacterium dichloroeliminans strain DCA1 from the soil matrix of the Tessenderlo site at LabMET (Ghent University, Belgium) offered perspectives for the execution of a bioaugmentation strategy at this site, since this strain selectively degrades 1,2-DCA to ethene under anaerobic conditions without the production of toxic vinyl chloride. First, a step-drawdown pumping test followed by a forced gradient multiple-well tracer test was conducted to obtain values for the hydrogeological parameters such as hydraulic conductivity, longitudinal and transverse dispersivity and effective porosity. The solute transport model was used as a predictive field-scale modelling tool in aid of designing the preliminary field tests as well as the bacterial injection. The aim of the latter was the assessment of the transport of the augmented strain DCA1. Prior modelling of these experiments provides an insight in the possible design strategies and hence, it can be concluded that profound preliminary field investigation aided by a solute transport model such as MOCDENS3D, results in a more time- and cost-effective execution of large scale cleanup processes of contaminated sites.

Vandenbohede, A. & Lebbe, L. (2006). Occurrence of salt water above fresh water in dynamic equilibrium in coastal groundwater flow systems. Hydrogeology Journal, 14(4), 462-472.

Abstract - A salt water lens is found above fresh water under the shore between Dunkerque (France) and Nieuwpoort (Belgium). This inverse density distribution is in a dynamic equilibrium. It develops due to the infiltration of salt water on the back shore during high tide. Under this salt water lens, water infiltrated in the adjacent dune area flows towards the sea and discharges at the seabed. This water quality distribution differs from the classic salt water wedge under fresh water described in the literature. Here, the evolution to this water quality distribution is simulated with a density dependent numerical model. A large tidal range, shore morphology and a permeable groundwater reservoir are the main conditions for the observed water quality distribution. By altering these conditions, intermediate water quality distributions between the classic salt water wedge and the one discussed here develop. Based on these simulations, it is expected that similar kinds of inverse density distribution could be

present in a number of coastal areas, which have tides, a gently sloping shore and a permeable substratum.

Vandenbohede, A. en Lebbe, L. (2006). Groundwater discharge along the western Belgian coast. In: Proceedings HydroEco 2006, International Multidisciplinary Conference on Hydrology and Ecology, the Groundwater/Ecology connection, Karlsbad, Czech Reblic, 11-14 september 2006. (Edited by K. Kovar, Zbynek Hrkal and Jiri Bruthans), 37-42.

Abstract - The interaction of fresh water flowing from the main land towards the sea and the saline sea water is complex but very important since this occurs in valuable ecological areas. This interaction is studied here in the nature reserve "De Westhoek" situated in the western Belgian coastal plain. A peculiar water quality distribution is found under the shore, with dens saline water above less dens fresh water, in a dynamical equilibrium. Fresh water discharges around the low water line, seaward from a shallow salt water lens under the shore. The dynamics of this fresh water zone are here studied in detail. Influences of tides and monthly recharge variations are modeled using MOCDENS3D, a density dependent finite-difference numerical model. These show that the influence of tides on the discharge is important, influence of monthly recharge variations is small.

Giambastiani, B.M.S., M. Antonellini, G.H.P. Oude Essink & R.J. Stuurman (2007). Saltwater intrusion and water management in the unconfined coastal aquifer of Ravenna (Italy): a numerical model. Journal of Hydrology, 340, 91-104.

Abstract - The Ravenna pinewoods represent an historical landmark in the Po Plain and they have a great environmental, historical – tourist values. The San Vitale pinewood forest is located approximately 8- 10 km from north of Ravenna and it is surrounded by the complex urban system of Ravenna , by the city industrial infrastructure and by the waterworks of the agricultural drainage system. Most of this study area is below sea level, such as the water table depth, and there is no natural freshwater hydraulic gradient to contrast the density gradient of saltwater. In the last century, many events (land subsidence; land reclamation and drainage; urban and industrial development and gas and deep groundwater extractions; coastal dunes destruction) have resulted in the occurrence of large volumes of brackish and saline groundwater. Nowadays the freshwater in this coastal aquifer consists of low salinity water lenses floating on top of the saltwater wedge and the present system is not yet in a steady state situation. This study is aimed to understand how the past and present human activities have been affecting the saltwater intrusion process in this phreatic aquifer and how the future sea level rise gets the salinisation process faster. For these reasons a model has been developed to quantify these effects on the density dependent groundwater flow, head and salinity distribution, and seepage and salt load fluxes to the surface water system. The code MOCDENS3D (Oude Essink, 1999) is used to assess above mentioned aspects.

Vandenbohede, A., Luyten, K. & Lebbe, L. (2007). Impacts of global change on heterogeneous coastal aquifers: case study in Belgium. Journal of Coastal Research, 24(2B), 160-170.

Abstract - Coastal plains are in the frontline of climate change. Predicted increase in recharge and sea level rise will alter groundwater flow, water quality distribution, recharge and discharge considerably. This is simulated here in the Belgian western coastal plain. It consists of a shore, dunes and polder (low-lying area) with a heterogeneous groundwater reservoir of quaternary age. A 3D density dependent groundwater flow model based on numerous (hydro)geologic observations was made. First the current groundwater flow and distribution between fresh and salt water was simulated. Then the effects of a 15 % recharge increase and 0.4 m of sea level rise in the next 100 years were modelled. Sea level rise results in an increased flow of fresh water towards the polder and a decreased flow towards the sea. An increase in recharge results in more water flowing towards both the polder and the sea. Brackish water present in the polder will be pushed back as is a current salt water intrusion

from the polder in the dunes. The simulations also show that groundwater levels will rise. This will put strain on the ecological valuable dunes and the drainage system in the polders.

Vandenbohede, A. en Lebbe, L. (2007). Effects of tides on a sloping shore: groundwater dynamics and propagation of the tidal wave. Hydrogeology Journal, 15, 645-658.

Abstract - The influences of tides on a coastal environment with a sloping shore are investigated by means of field observations and groundwater flow modelling. The Belgian western coastal plain consists of a wide shore, dunes and polders where diurnal tides with large amplitude occur. The effects of tides on the groundwater flow are studied using the MOCDENS3D code. First, MOCDENS3D is validated to simulate accurately the propagation, attenuation and lag of a tidal wave in an aquifer. Then groundwater flow and influences of tides are modelled for a cross-section along the French-Belgian border. This gives an exhaustive insight in the spatial and temporal varying groundwater flow and propagation of the tidal wave in the aquifer. Simulation shows that there are two interfering flow cycles. The first is a shallow tidally fluctuating flow cycle on the shore due to the interaction of the gently sloping shore and the tidally oscillating sea level. The second is a deeper flow cycle from the dunes towards the sea. Further, it is indicated that the propagation and attenuation of the tidal wave follows a complex pattern with lateral as well as vertical components. The interaction between tides and shore topography influences also the salinity distribution.

Additionally, more information of MOCDENS3D can be found in the following publications:

Oude Essink, G.H.P. (1993). A sensitivity analysis of the adapted groundwater model MOC. Proceedings 12th Salt Water Intrusion Meeting, Barcelona, Nov. 1992, 371-389.
Oude Essink, G.P. (1998). MOC3D adapted to simulate 3D density-dependent groundwater flow. In: Proc. of MODFLOW '98 Conference, October, 4-8, 1998, Golden, Colorado, USA, Volume I, 291-303.
Oude, Essink, G.H.P. (1999). Simulating 3D density-dependent groundwater flow: the adapted MOC3D. Proceedings 15th Salt Water Intrusion Meeting, 1998, 69-79.

2 Visual MOCDENS3D workflow and File Manager Module

2.1 Introduction

Visual MOCDENS3D is developed to visualise and further handle MOCDENS3D output. It also assists in putting together the MOCDENS3D input files and in running the MOCDENS3D model. Visual MOCDENS3D is designed as a MATLAB toolbox but can also be used as a stand-alone application. In the first case, MATLAB must be installed on the computer.

Figure 2.1 gives an overview of the Visual MOCDENS3D workflow. The first step is the compilation of the required input files which are used by the MOCDENS3D code to run the model. Running the model results in an output file (grafile.out) which is then translated by a program (matvis.m) in two data structures (grif.mat and data.mat) which can be imported in MATLAB by Visual MOCDENS3D or in the stand-alone application. These mat-files are further used in the Visual MOCDENS3D modules.

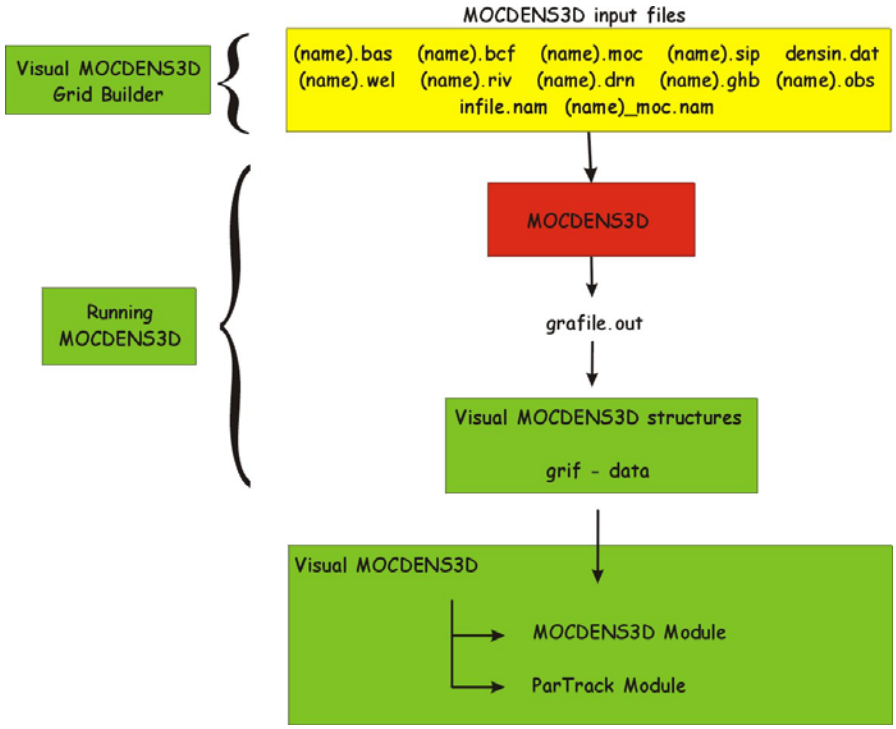


figure 2.1 *Workflow of Visual MOCDENS3D. Input files are indicated in yellow, Fortran codes are given in red, and Visual MOCDENS options are given in green.*

2.2 Scalars, arrays and structures

For users not familiar with MATLAB, a short introduction to the most common MATLAB data types is given. For more explanation, the reader is referred to the excellent MATLAB help.

A single number is called a *scalar*, e.g. A = 5. An *array* is a list of different scalars. This can be one-dimensional or two-dimensional as in the next examples:

one-dimensional: *B = [1 2 3 4]*
two-dimensional: *B = [1 2 3 4; 5 6 7 8]*

This is here given in MATLAB notation. The two-dimensional array (called a matrix) consists of two rows of four elements (or columns).

The structure data type offers users a most convenient way to handle data describing different aspects. Structures are MATLAB arrays with named "data containers" called fields. The fields of a structure can contain any kind of data. For example, one field might contain a text string representing a name, another might contain a scalar representing a billing amount, a third might hold a matrix of medical test results, and so on. An example is the structure observations:

observations =
x: [1 2]
y: [5 3]
h: [9.6000 3.7000]

This structure contains three fields each holding two scalars.

2.3 MOCDENS3D input and running the model

2.3.1 Input files

After installing Visual MOCDENS3D on the computer (see introduction), a MOCDENS3D model can be made. MOCDENS3D needs a number of input files and the first step is the construction of these files. Different possible input files of which a number are required (indicated with an *) are:

- (name).bas-file *: basic input such as number of layers, rows and columns, grid with indication of boundary conditions, initial heads and length of stress periods
- (name).bcf-file *: dimensions of rows and columns and the hydraulic parameters
- (name).sip-file *: model parameters such as maximum number of iterations and closure criterion for the strongly implicit procedure solver package
- (name).moc-file *: input for the solute transport such as initial concentrations, dispersivities, diffusivity, retardation, decay, layer thickness and effective porosity
- densin.dat-file *: input to calculate buoyancy
- (name).wel-file: input for wells in the model
- (name).riv-file: input for rivers in the model
- (name).drn-file: input for drainage in the model
- (name).ghb-file: input for general head boundaries in the model
- infile.nam-file *: list of file-names which are used in the model
- (name)_moc.nam-file *: idem, specifically for the solute transport

These input files are text files and can be made in a basic text processor (such as notepad), editor of a FORTRAN compiler or the MATLAB editor. Alternatively, they can be constructed using the Grid Builder Module of Visual MOCDENS3D (see chapter 3).

In the directory where the model is made (called in MATLAB “working directory”), following files must be present:

moc3d.exe
tnt.ext

These can for instance be found in 'c:\VisualMOCDENS3D\basic mocdens files' after installing Visual MOCDENS3D on the computer. By running MOCDENS3D using the running options in the MOCDENS3D module, these files are automatically copied in the working directory. Otherwise, this must be done by the user.

2.3.2 Running the model

Running of the model consists of a number of commandos which must be given. These are

*!del *.out*
!moc3D
[grif data] = matvis(pathname)

These can be given in the MATLAB Command Window. The first two commando's are dos commando's, hence the preceding '!' which evaluates a dos commando in MATLAB. Of importance is that the first commando (!del *.out) deletes the output of any previous model made in the directory. The second commando runs the MOCDENS3D model. The third uses a MATLAB function *matvis.m* to translate the MOCDENS3D output (*grafile.out*) in the grif and data structures which are used in Visual MOCDENS3D.

Because of the commando (!del *.out) any previous model output is deleted. Thus be sure that this is saved under another name (without the extension out) if you want to keep the grafile.out file or that the grif and data structures are saves (see further) before closing Visual MOCDENS3D.

Running of the model can also be performed via Visual MOCDENS3D (see chapter 4) whereby the output visible during the run is given in the MATLAB Command Window.

As explained before, the *grafile.out* file is translated by the *matvis* function in two structures data and grif. The grif structure contains as fields the maximum and minimum head in the model (hmax, hmin), maximum and minimum concentration in the model (cmax, cmin), thickness of each layer (thick), number of layers, (nslay), number of columns (nscol), number of rows (nsrow), width of each column (cdel), width of each row (rdel), constant layer thickness of the simulation (zdel), porosity (poros), number of stress periods (nper) and length of the stress periods (periods). For instance:

grif =
nscol: 65
nsrow: 55
nslay: 5
cdel: 20
rdel: 20
zdel: 4
thick: [4 4 4 4 4]
nper: 21
poros: 0.3000
periods: [1x21 double]
hmin: 3.2000
hmax: 11.5569
cmin: 499.4200

cmax: 1.9710e+004

The *data* structure contains the fresh water heads (head), concentrations (conc), velocities along the columns (vc), velocities along the rows (vr) and velocities along the layers (vl). For instance:

data =
21x5 struct array with fields:
head
conc
vc
vr
vl

This includes data of a model of 21 time steps and 5 layers.

2.4 File Manager

2.4.1 Set directory

In different options in Visual MOCDENS3D a file name or path to a directory must be given. To facilitate this, the current or working directory can be given by selecting the options 'set directory' in the File Manager module.

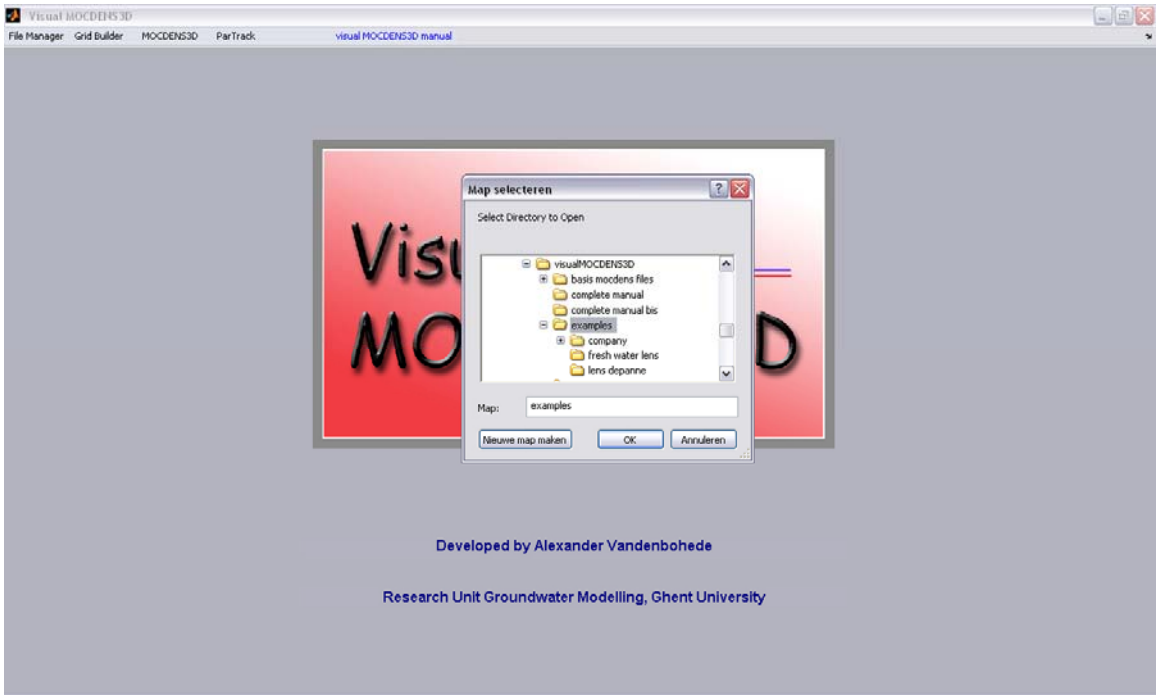


figure 2.2 *Set current directory gui.*

2.4.2 Load/save projects

By running MOCDENS3D with the Visual MOCDENS3D interface or by converting the *grafile.out* file using the *matvis* function, *grif* and *data* structures are in the workspace. The two structures data

and grif are called a project in Visual MOCDENS3D since they contain all information of a model or model run. These two structures are all what is needed to continue working with Visual MOCDENS3D.

The structures can be saved as a project in Visual MOCDENS3D. This is done with the load/save projects GUI (figure 2.3). By saving a project, structures are saved as mat files:

(name)_grif.mat
(name)_data.mat

(name) is the name of the project. It is perhaps advisable to indicate a project with a distinct part in the name for easy recognition, e.g. proj_company, which is than saved as proj_company_grif.mat and proj_company_data.mat.

Loading of a project is done by selecting one of the two project structures (e.g. proj_company_grif.mat or proj_company_data.mat in the previous example). If successfully, an echo of the basic model dimensions are given.

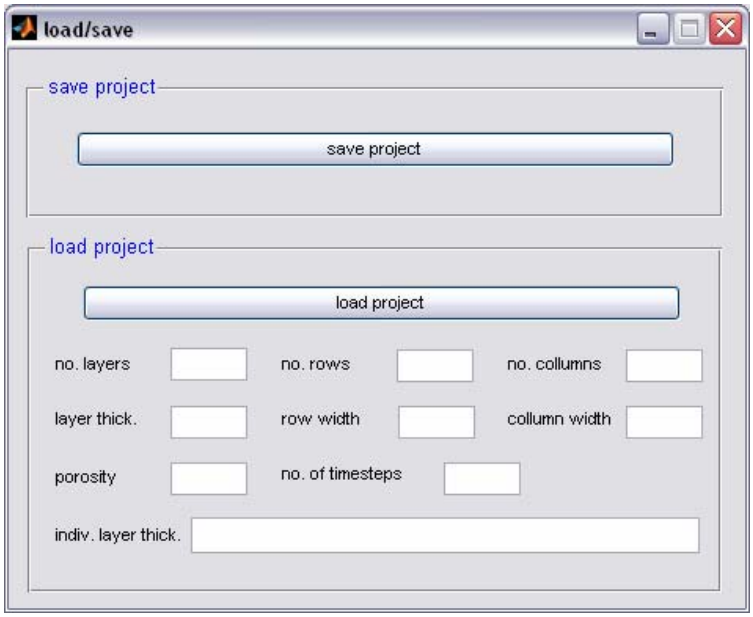


figure 2.3 *Load/save gui.*

2.4.3 Load MOCDENS3D output

MOCDENS3D output (grafile.out or a renamed grafile.out file) can be imported using the "Load MOCDENS3D output" option. This basically runs the *matvis* function through a GUI.

2.4.4 Clear options

This option makes it possible to clear the workspace whereby all variables are cleared or clear only the grif and data structures. It is advisable to do this before loading a new project.

2.4.5 Layer thicknesses

The thicknesses of all layers are the same in a MOCDENS3D model. In some particular instances it can be convenient to changes these layer thicknesses. This can be done using this option (figure 2.4).

One instance where this can be useful is when simulating only groundwater flow and no solute transport. In this case only transmissivities are of importance, not the absolute layer thicknesses. Taking into account that layer thicknesses must be equal in MOCDENS, transmissivities (conductivity times thickness) in such model includes thickness. A small example consisting of three layers is given below:

Field situation	thickness (m)	conductivity (m/d)
Layer 1	5	1
Layer2	10	0.1
Layer3	1	5

Model	thickness (m)	conductivity (m/d)
Layer 1	1	5
Layer2	1	1
Layer3	1	5

These two models are equal from a point of view of groundwater flow. Taking into account only layers of 1 m and not recalculating conductivity, 16 layers would be needed.

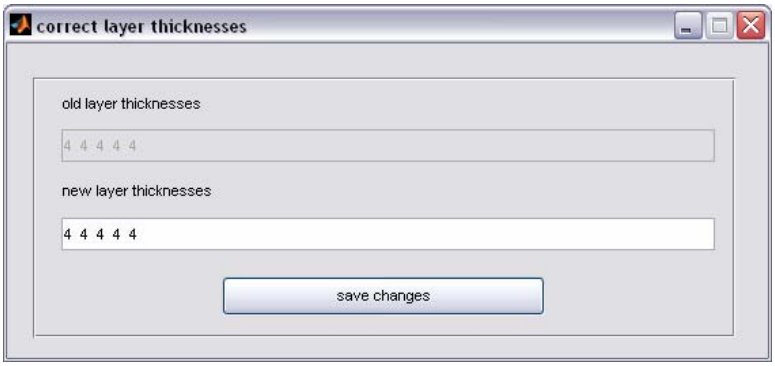


figure 2.4 *GUI for changing the layer thicknesses.*

3 Grid Builder

3.1 Constant versus varying boundary type models

3.1.1 Input files

Visual MOCDENS3D Grid Module assists in the preparation of the necessary MOCDENS3D input files. These are related to package in MODFLOW and MOCDENS. The input files are

- (name).bas-file *: basic input such as number of layers, rows and columns, grid with indication of boundary conditions, initial heads and length of stress periods
- (name).bcf-file *: dimensions of rows and columns and the hydraulic parameters
- (name).sip-file *: model parameters such as maximum number of iterations and closure criterion for running the "strongly implicit procedure" solver
- (name).moc-file *: input for the solute transport such as initial concentrations, dispersivities, diffusivity, retardation, decay, layer thickness and effective porosity
- densin.dat-file *: input to calculate buoyancy
- (name).wel-file: input for wells in the model
- (name).riv-file: input for rivers in the model
- (name).drn-file: input for drainage in the model
- (name).ghb-file: input for general head boundaries in the model
- infile.nam-file *: list of the above file-names which are used in the model
- (name)_moc.nam-file *: idem

Files marked with an * are files which are required, the other files are optional. A short description of the format of these files is given in appendix 1. A more detailed description is given in McDonald, M.G. & Harbaugh, A.W. (1988).

It is important to note that the grid used by MOCDENS3D must be a regular grid. This means that the width of a column or row remains constant throughout the model. Also all layers must have the same thickness.

3.1.2 CBTM versus VBTM

From the above list of files, it is obvious that a model needs a lot of information. Basically, this information can be divided in three main categories:

- boundary conditions: Cells of the finite difference grid can be assigned a constant head, no flow boundary or constant flux boundary.
- hydraulic parameters: hydraulic parameters of the model layers, transmissivity, hydraulic conductance and optionally storativity.
- model stresses: recharge, drainage, influence of rivers and general head boundaries.

In most models, boundary conditions and hydraulic parameters of model layers do not change. Such models are referred to in Visual MOCDENS3D as *constant boundary type models (CBTM)*. Boundary conditions are determined by hydrological/geographical boundaries and these do not change during the time which is modelled. The same holds for the hydraulic parameters, the geology of the aquifer which is modelled does not change. Stresses can, however, change. For instance, recharge can change due to surfacing, wells can be added during the time which is simulated or contact factors of rivers or drainage systems can alter.

A model where boundary types and hydraulic parameters can also vary is called a *varying boundary type model (VBTM)* in Visual MOCDENS3D. This is for instance the case when dynamic landscape evolutions are to be modelled, e.g. shifting position of sea, dunes and hinterland.

3.1.3 Grid Builder workflow

All the MOCDENS3D input files can be constructed via Visual MOCDENS3D GUI's. For a CBTM they can also be made using a text editor but then a number of possibilities to view or corrected the input, specific to Visual MOCDENS3D, is lost.

CBTM

All input GUI's have common features. Figure 3.1 gives an example of an input GUI for the bas file. A header, boundary condition and stress period box allow defining the specific input of for the bas file. Finally, there is a specific box regulating the work flow, here called bas structure. First, it allows saving the date for the bas file. In case a constant boundary type model is selected, the input is saved in two ways: a bas file and a structure. The bas file is in the correct format and can be immediately used by MOCDENS3D. The bas structure is a MATLAB structure (see 2.2) and contains all the information which is given in the GUI. By clicking on the import button, data of an earlier made bas file can be imported and changed. This is done by importing the structure which was saved. The clear button clears the GUI.

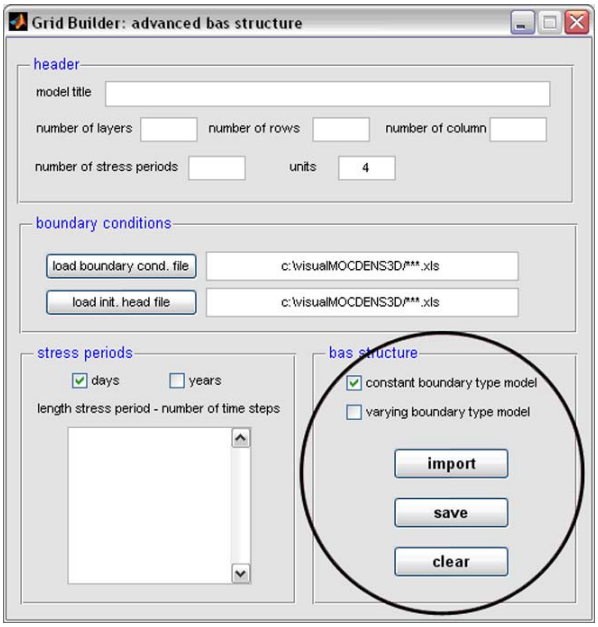


Figure 3.1 *General lay-out of a Grid Builder GUI. A common feature of all GUI's is encircled.*

By saving input, a name must be assigned. This is translated in specific names for the, in this example, bas file and bas structure. This is done for reasons of quick identification. If a (name) is ascribed, the bas file is saved as (name).bas and the bas structure is saved as (name)_bas.mat. Table 3.1 gives these identifiers for all input files.

Table 3.1 *Overview of file names constructed for a CBTM. Files indicated with a * are required, the others are optional.*

	file name	structure name
bas *	(name).bas	(name)_bas.mat
bcf *	(name).bcf	(name)_bcf.mat
moc *	(name).moc	(name)_moc.mat
sip *	(name).sip	(name)_sip.mat
densin.dat *	(name).dat	(name)_dat.mat
nam *	(name).nam	(name)_nam.mat
wel	(name).wel	(name)_wel.mat
riv	(name).riv	(name)_riv.mat
drn	(name).drn	(name)_drn.mat
ghb	(name).ghb	(name)_ghb.mat

So the work flow is fairly simple. With the GUI's the different input is given and this is saved as a file required by MOCDENS3D and a MATLAB structure. From 3.2 onwards the different input GUI's are described and an example of a CBTM is given in chapter 6.

A very important remark is that the names you ascribe to a file can only have 8 characters. This is because MOCDENS3D is a Fortran code and this can not handle name assignments larger than 8 characters.

VBTM

For a variable boundary type model, workflow is mainly the same. Using the input GUI's the different structures given in table 3.1 are made. In the different GUI's the VBTM option must be chosen. However, no MOCDENS3D files are made yet. This is because these file change over the time domain of the modelling due to changing boundary conditions. These files are made during the model run which will be discussed in chapter 4. An example is given in chapter 6.

3.2 Grid Builder lay-out

The grid module consists of four main parts:

- Basic grid: This option creates the input files for a simple model with a rectangular grid of active cells. Hydraulic parameters can only vary between layers.
- Advanced grid: This option makes it possible to construct input files of irregular grids
- Grid visualiser: Visualises model input.

CBTM and VBTM can be made from basic and advanced grid. Input of complex data is done via excel-files. 2D as well as 3D grids can be made using the grid module. However, 2D grids must be oriented according to the rows.

3.3 Basic grid

3.3.1 Basic (bas) package

Figure 3.2 gives the GUI for constructing a bas file. The *header box* gives general input such as the number of layers, number of rows, number of columns and number of stress periods. Optionally a model title can be given which will be put in the first line of the (name).bas-file. The units options makes it possible to chose between different time units in the model:

- 1: seconds
- 2: minutes
- 3: hours
- 4: days
- 5: years

Boundary conditions are given in the *boundary condition box*. Therefore the boundary type along the north, south, west and east boundary must be given. This must be done for every layer, under each other. The different options which can be chosen are:

- < 0: constant head boundary. A difference between different constant head boundaries (for instance with regard to the inflow of water with different concentration) can be made be using different numbers (-1, -2, etc) which are called zones (see also moc-file),
- 0: no flow boundary. A zero in the model grid actually designates a non-active cell of the grid,
- > 0: active cell.

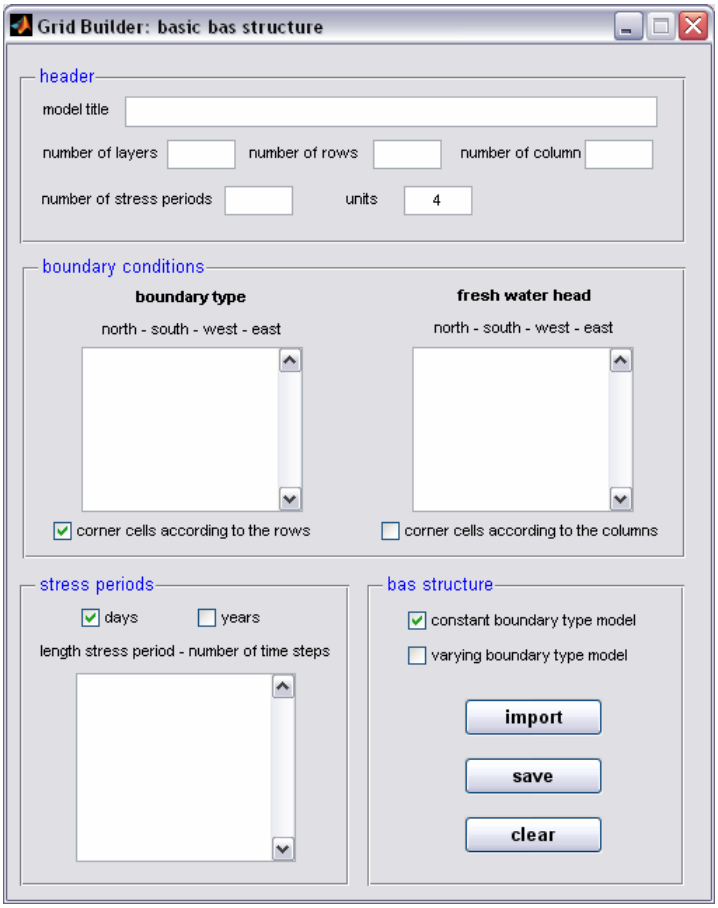


figure 3.2 *Basic grid: bas package input GUI.*

Next the fresh water head of the north, south, west and east border of the grid must be given for every layer. Only one value per north, south, west or east border and per layer can be given.

Last, it must be indicated if boundary type and head of the corner cells of the grid must be according to the north/south border (or according to the rows) or according to the west/east border (or according to the columns).
If the boundary type and heads are equal for every layer, this must be given only ones. If not, the input in the two boxes must exist of n-rows (n the number of layers) and 4 columns.
In the *stress periods box*, the length of every stress period and the number of time steps in which every stress period is subdivided is given. If these are the same for every stress period, this must be given only ones. Otherwise the input of the boxes consist of n rows (n the number of stress) periods and 2 columns. The length of the stress periods can be given in days or years. These will be recalculated with regard to the units chosen in the *header box*.

3.3.2 Block-centered flow (bcf) package

Figure 3.3 gives the GUI for constructing a (name).bcf file. The *header box* gives general input such as the number of layers, number of rows, number of columns, width of a row and width of a column.

Hydraulic parameters are given in the *hydraulic parameter box*. First it must be designated if one value per layer will be used or if a matrix of the parameter is chosen. In both cases, the parameters are constant for each layer, but by choosing for a matrix, small changes can be made directly in the bcf-file, for instance to add layer heterogeneity. Also, choice between steady state and transient state simulation must be made. In case of the latter, the storativity box will become active. Thereafter, the values for the hydraulic parameters must be assigned. A transmissivity value for every layer must be given. If these values are the same for every layer, only one value must be given. The same applies for the storativity. For the hydraulic conductance, the number of layers minus one values must be given since the lower boundary is impermeable. Again, only one value can be given if all values are the same. Finally, the anisotropy (ratio of transmissivity in the column direction to transmissivity in the row direction) is given.

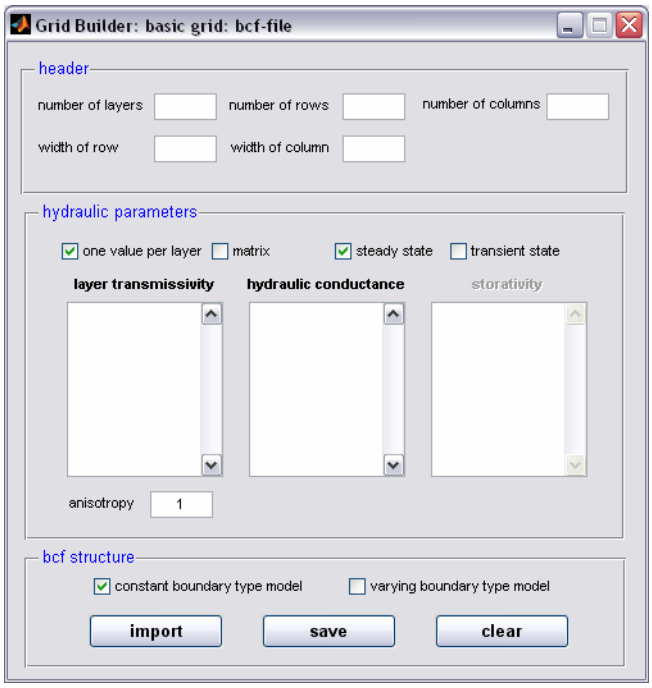


figure 3.3 *Basic grid: bcf-file input GUI.*

3.3.3 Method of characteristics (moc) package

Figure 3.4 gives the GUI for constructing a (name).moc file. The *header box* gives general input such as the layers, rows and columns involved in the solute transport grid. In the original MOC3D program, an area in the model grid for which solute transport is calculated could be chosen. Here the entire model area is involved in the solute transport calculations and the values which are given in the *header box* are thus equal to the number of layers, rows and columns of the model. Further, the number of particles per cell and the celdis parameter must be given. The number of parameters must be n^2 or n^3 with n an integer value, respectively for a two- and three-dimensional model. Celdis is the percentage of cell distance which a particle can travel during a time step. According to the celdis, the time steps are further subdivided by the model. Optionally, a model title can be added which will appear in the first line of the moc-file.

In the *solute transport parameter box*, initial concentrations for every layer are given. If this is the same for every layer, only one value must be given. Also, the thickness of each layer and its effective porosity must be given. Here also, if these are the same for every layer, this must be indicated only ones.

Also the number of constant head boundary zones must be indicated and for every of these zones, the used indication in the bas-file (-1, -2, etc) with the corresponding concentration must be indicated.

Solute transport parameters are given in the *solute transport parameter box*.

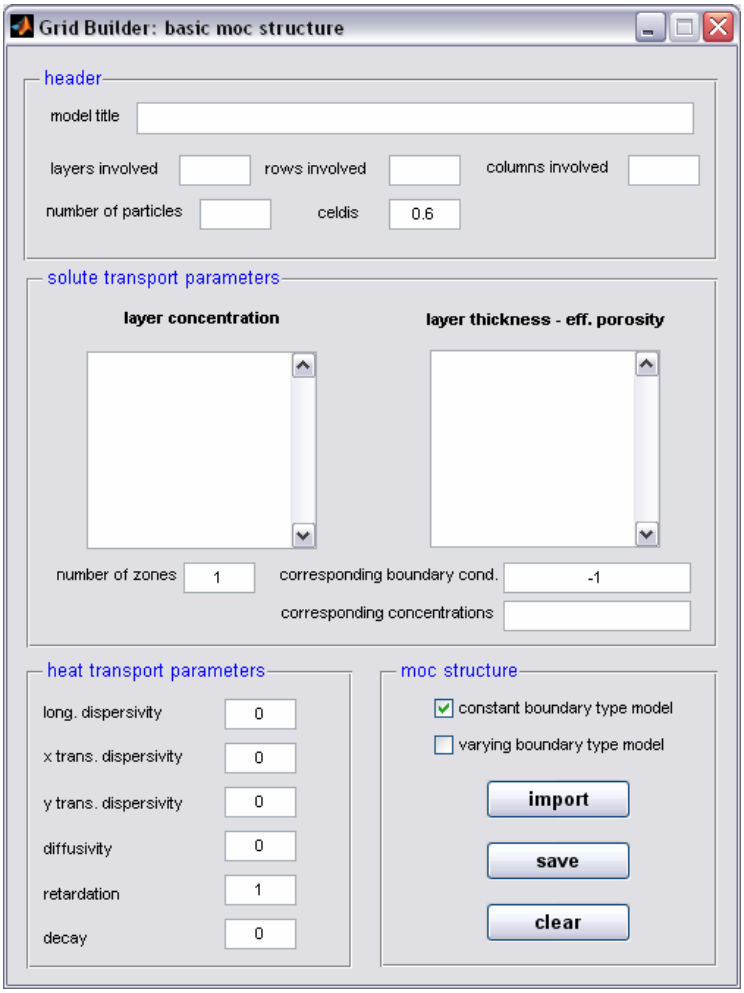


figure 3.4 *Basic grid: moc-file input GUI.*

3.3.4 Strongly implicit (sip) package

Figure 3.5 shows the input GUI for the sip-file. In the *input box*, the maximum number of iterations and the closure criterion must be given.

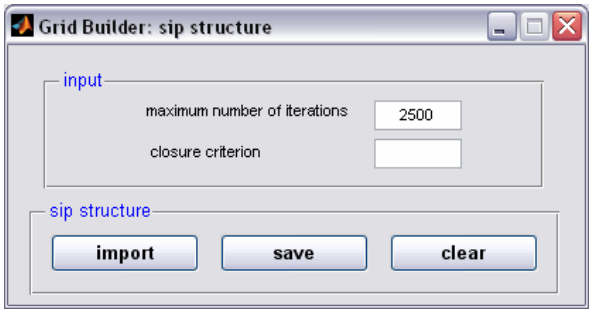


figure 3.5 *Basic grid: sip-file input GUI.*

3.3.5 densin.dat-file

Figure 3.6 shows the input GUI for the densin.dat file. In the *input box*, the maximum concentration and the corresponding density must be given. Take into account that the file which is used by MOCDENS3D must be called densin.dat. The name you ascribe during saving holds here only for the structure and not for the MOCDENS3D file.

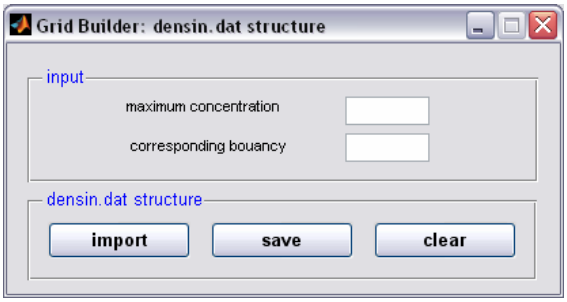


figure 3.6 *Basic grid: densin.dat input GUI.*

3.3.6 Well (wel) package

Figure 3.7 shows the input GUI for the wel-file. Via the wel- file, two different sinks/sources are given:

- pumping or injection in the aquifer via wells,
- recharge (or infiltration).

The first part of the *well input box* gives general input. This is the number of layers, rows and columns and number of stress periods.

If recharge will be included in the model, the recharge box must be indicated. Further the amount of recharge and the concentration of the recharge water can be given.

Sinks/sources in case of pumping or injection wells are directly given in the GUI or via external input. In the first case, the additional recharge option is chosen and the beginning and end stress period, layer, row, column, discharge rate and concentration of every sink/source is filled in. In the latter case this is

via an excel-file. This is done be indicating the additional recharge from file box and given the path to the file.

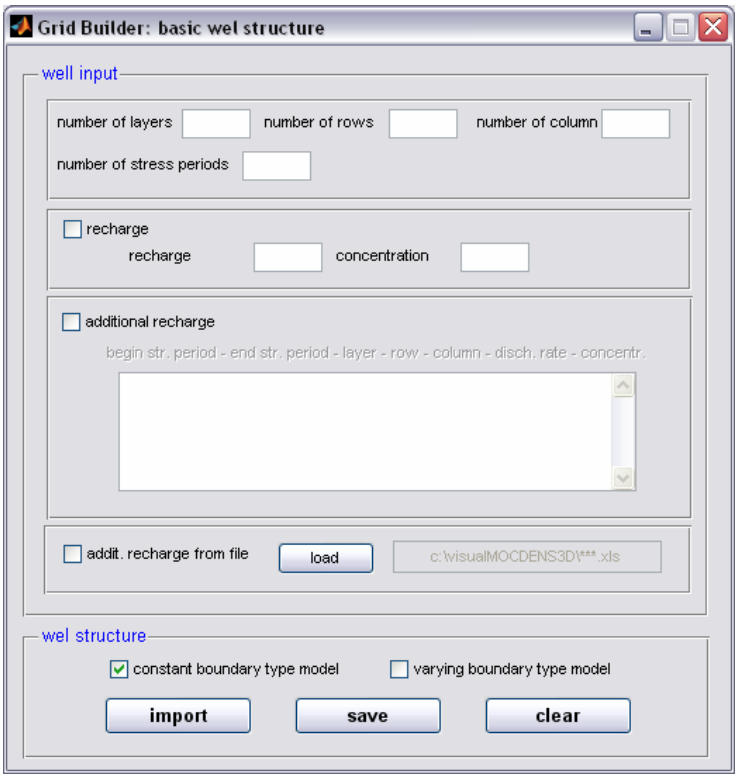
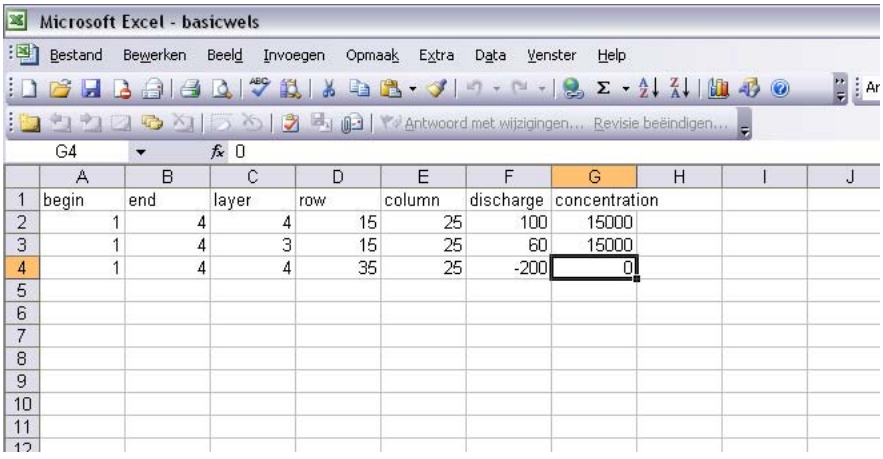


figure 3.7 *Basic grid: wel-file input GUI.*

The excel-file has the following format (example in figure 3.8):

- column 1: begin stress period of the pumping/recharge
- column 2: end stress period of the pumping/recharge
- column 3: layer of the pumping/recharge
- column 4: row of the pumping/recharge
- column 5: column of the pumping/recharge
- column 6: discharge of the pumping/recharge
- column 7: concentration of the pumping/recharge



	A	B	C	D	E	F	G	H	I	J
1	begin	end	layer	row	column	discharge	concentration			
2	1	4	4	15	25	100	15000			
3	1	4	3	15	25	60	15000			
4	1	4	4	35	25	-200	0			
5										
6										
7										
8										
9										
10										
11										
12										

figure 3.8. *Example of input of additional sinks/sources via excel.*

3.3.7 Name (nam) package

Figure 3.9 shows the input GUI for the creation of the name-files. The name-files are a list of files of the packages which are used in the model. Two such name-files must be made. The first is called infile.nam and list which (if used) bas, bcf, wel, drn, ghb, and sip file is used. Secondly, a (name).nam file must be made which gives which moc file is used. The name of the (name).nam file must also be included in infile.nam. The user must not be concerned about this all. The names of the files must be simply filled in.

First it must be indicated if a CBTM or a VBTM will be used. If you use a CBTM the left part of the GUI will be active, the right part inactive. The names of the different files must be filled in. These are the files which will be read by the MOCDENS3D model, e.g. company.bas, company.bcf, etc. The densin.dat file must always be called densin.dat and the moc name file is the name of the (name).nam file containing the name of the moc file. This file must have the extension nam.

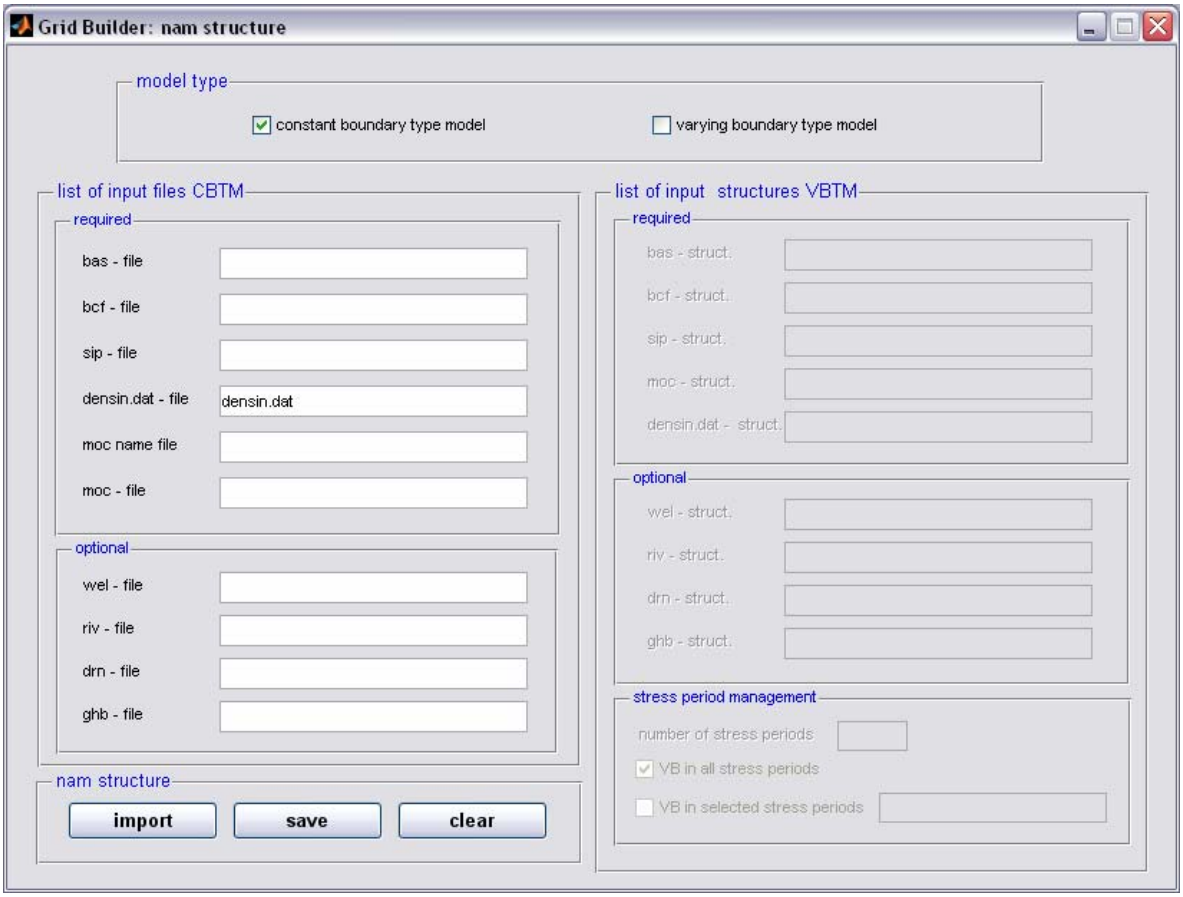


figure 3.9 *Basic grid: nam-file input GUI.*

In case you choose for a VBTM the right part of the GUI will be active, the left part inactive. Now, the names of the structures containing the data of the different packages (company_bas, etc.) must be given. The specific MOCDENS3D files will be constructed while running the model since these will change.

Additional here is the *stress period management box*. First, it is given how many stress periods the model contains. Secondly, it must be indicated if variable boundary conditions changes occur between all stress periods or between certain stress periods. Changes in all stress periods are irrelevant using VBTM as described here but is an option for additional packages (e.g. simulation of heat transport). This is clarified with an example. 20 stress periods are for instance considered whereby a first set of

boundary conditions are valid in stress periods 1 to 5, a second in stress periods 6 to 17 and a third in stress periods 18 to 20. Then 20 is filled in as the number of stress periods and 6 and 18 as variable boundary conditions in these stress periods since these change in stress period 6 and in stress period 18.

3.4 Advanced grid

3.4.1 Introduction

The advanced grid option assists in the construction of irregular grids. This means that inactive cells occur in the model grid or that properties (hydraulic parameters, boundary conditions, etc.) vary in model layers.

3.4.2 Basic (bas) and block centered flow (bcf) packages

Figure 3.10 shows the input GUI's for the bas- and bcf-file in the advanced grid option. These are more or less the same as the GUI's in the basic grid option instead that the boundary conditions and hydraulic heads (for the bas-file) and the transmissivities, hydraulic conductances and optionally the storativities (for the bcf-file) are now given via an excel file.

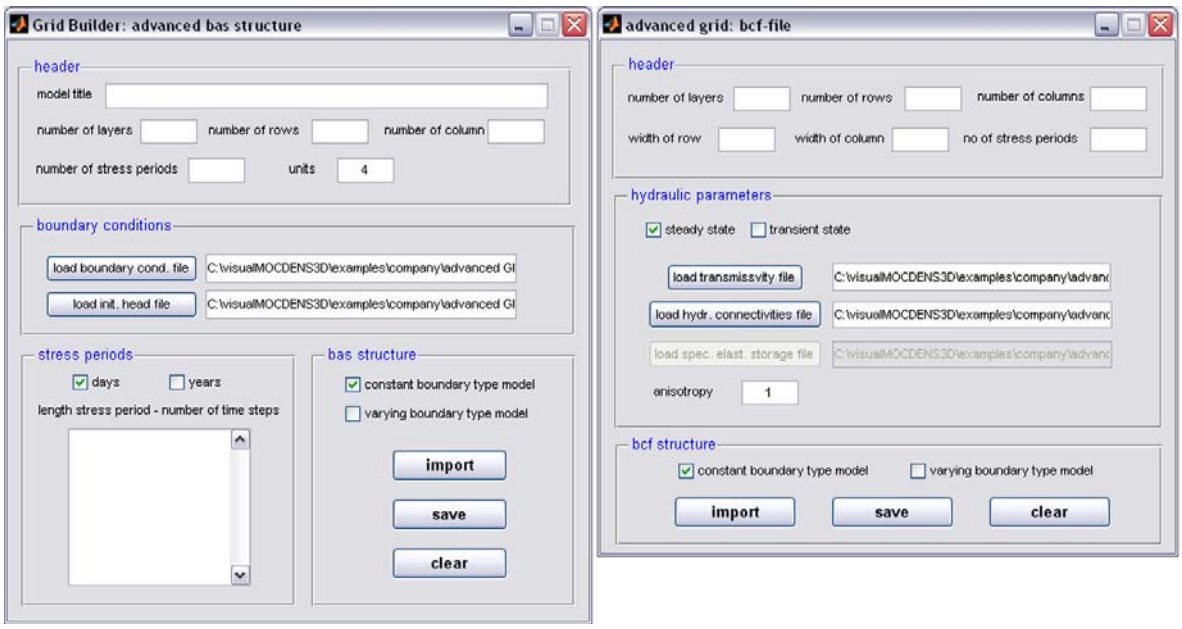


figure 3.10 *Advanced grid: bas- and bcf-file input GUI.*

Figure 3.11 shows an example of the grid input for bas- and bcf-file via excel. The input for the boundary conditions for a 5 stress period, 3 layer, 5 row and 5 column example is given. Also, figure 3.11 shows the input format for a CBTM. In the first line, the first and the last stress period are indicated followed by the boundary conditions for every layer. A blank line is present between the matrices of every layer. **Notice that only one excel sheet is present, blank sheets must be deleted.** Every excel sheet in a file stands for different boundary conditions (see input for VBTM). Input for initial fresh water heads, transmissivities, hydraulic conductances (minus one layer!) and storativities occurs identically.

Input for a VBTM occurs identical. Figure 3.12 gives an example for a 5 stress period, 3 layer, 5 row and 5 column model whereby the boundary conditions change from stress period 3. Two sheets are present in the excel file, one for every set of boundary conditions which are applied. Sheet 1 gives the boundary conditions for stress period 1 to 2 and sheet 2 gives the boundary conditions for stress period 3 to 5. The first stress period on sheet two must follow directly on the second stress period of sheet 2. The sheets must be ordered according to increasing stress period and no empty sheet can be present in the file. Input for initial fresh water heads, transmissivities, hydraulic conductances (minus one layer!) and storativities occurs identically.

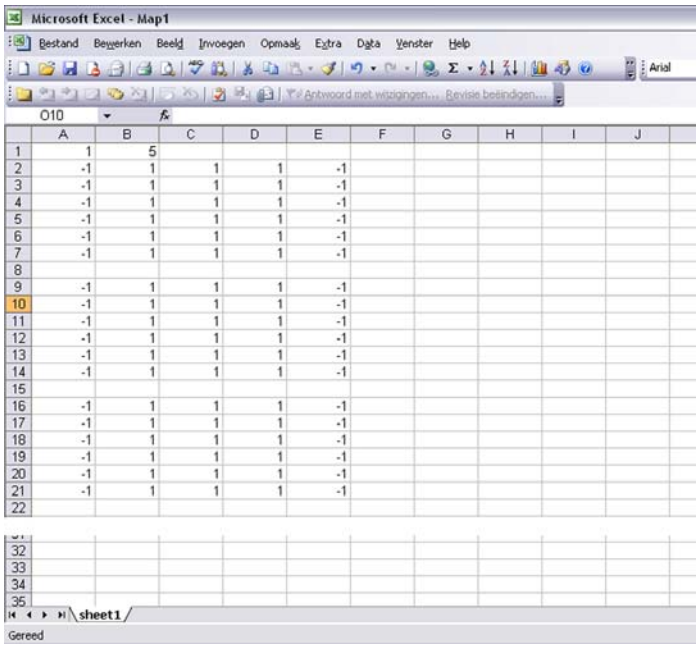


figure 3.11 *Example of input of boundary conditions for a CBTM via an excel file. Input for initial fresh water heads, transmissivities, hydraulic conductances (minus one layer!) and storativities occurs identically.*

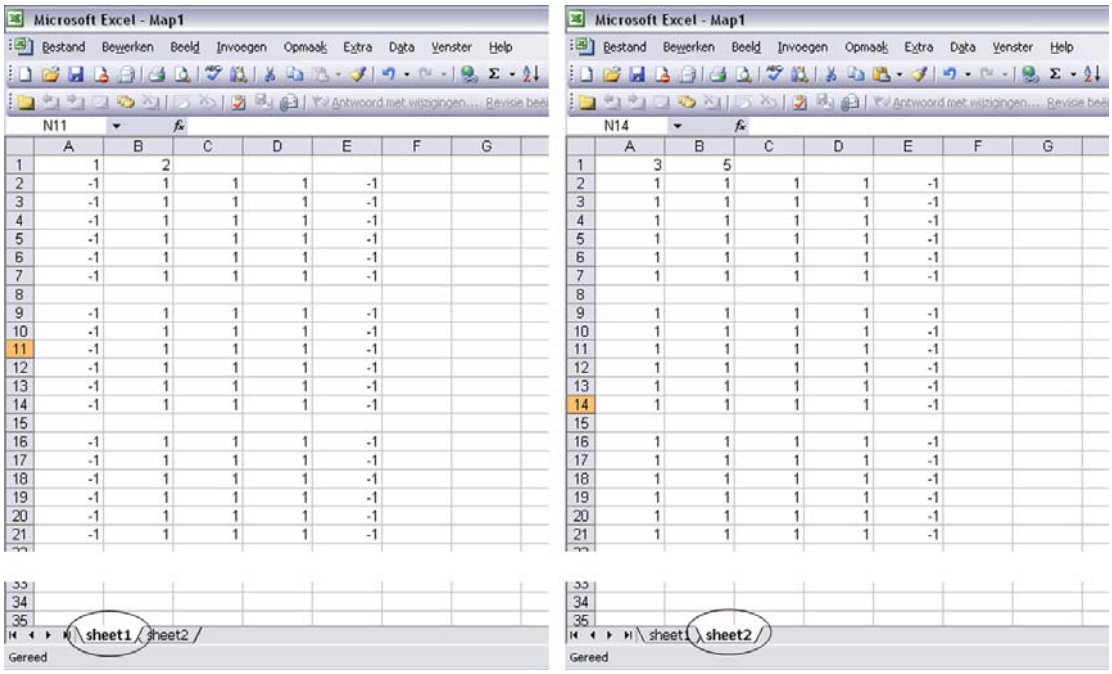


figure 3.12 *Example of input of boundary conditions for a VBTM via an excel file. Input for initial fresh water heads, transmissivities, hydraulic conductances (minus one layer!) and storativities occurs identically.*

3.4.3 Method of characteristics (moc) package

Figure 3.13 shows the input GUI for the moc-file. This is the same as in the basic grid option save for the input of layer concentrations. These are also given via an excel file which has almost the same format as the example in figure 3.11. The single exception is that the header with the stress periods is not needed since the concentrations are initial concentrations.

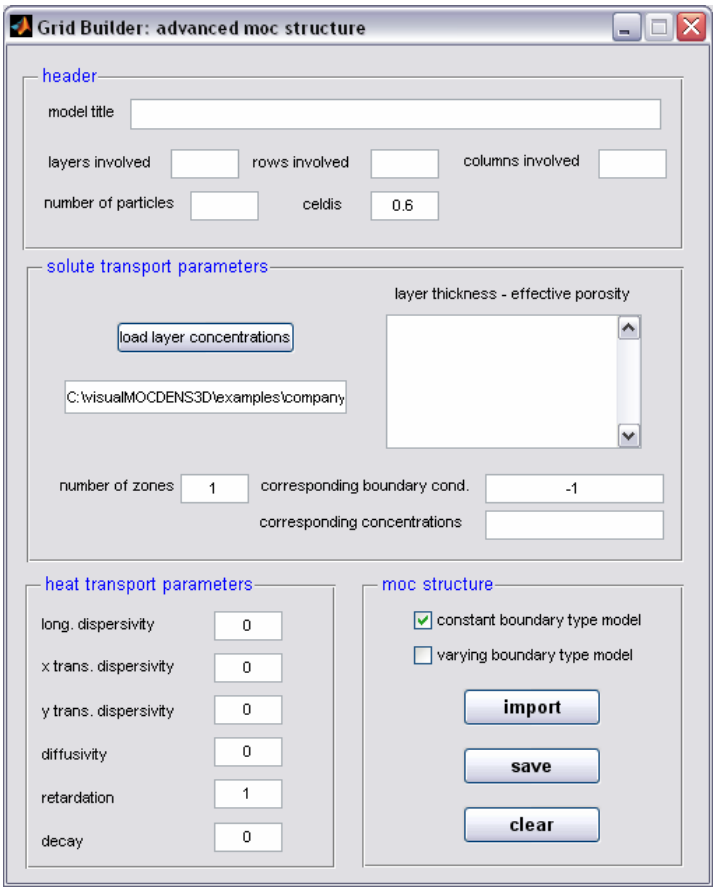


figure 3.13 *Advanced grid: moc-file input GUI.*

3.4.4 Strongly implicit (sip) package and densin.dat and name (nam) files

The input for these files is identical as in the basic grid option.

3.4.5 Well (wel) package

Figure 3.14 shows the input GUI for the wel-file. These GUI is more less the same as the input for a wel-file using the basic grid option. Additional recharge (for instance wells) is given via an excel file or directly in the GUI as is the case in the basic grid option. Main difference is the input for the recharge. Two options are here possible:

- Matrices of the recharge and the concentration are given. This is done by indicating the recharge matrix checkbox. Two excel files must be given. The first gives the amount of recharge whereas the second gives the concentration of the recharge for the model area. An example is given in figure 3.15. It gives the input of recharge for a 10 row and 10 column model. The same recharge for stress period 1 to 3 is considered. So the first and last stress

period for which a certain recharge is valid is given in the firs row of the excel file followed by a rows x columns matrix with the recharge values. A second period in which recharge changes is given on the next sheet in the same excel file and so on. The sheets must be ordered according to increasing stress period and no empty sheet can be present in the file. This is in the case were recharge is given in the first layer of the model. Otherwise the list options should be chosen or the boundary conditions can be used to specify in which cell the recharge takes place. In the latter case the bas structure ((name)_bas.mat) is imported by indicating the appropriate box and giving the name of the file. The recharge is now attributed to the uppermost active cell for each position instead of to the first layer.

- List of the recharge and the concentration is given. This is illustrated in figure 3.16. This is an excel file containing 7 columns with the beginning and end stress period, layer, row, column, recharge rate and concentration of all cells.

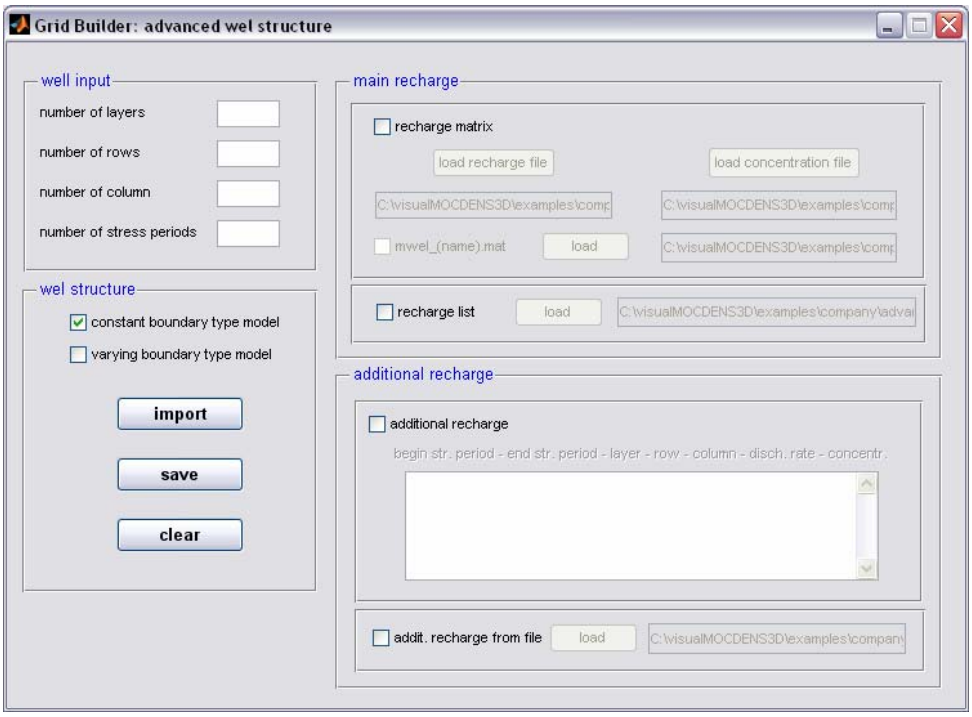


figure 3.14 *Advanced grid: wel-file input GUI.*

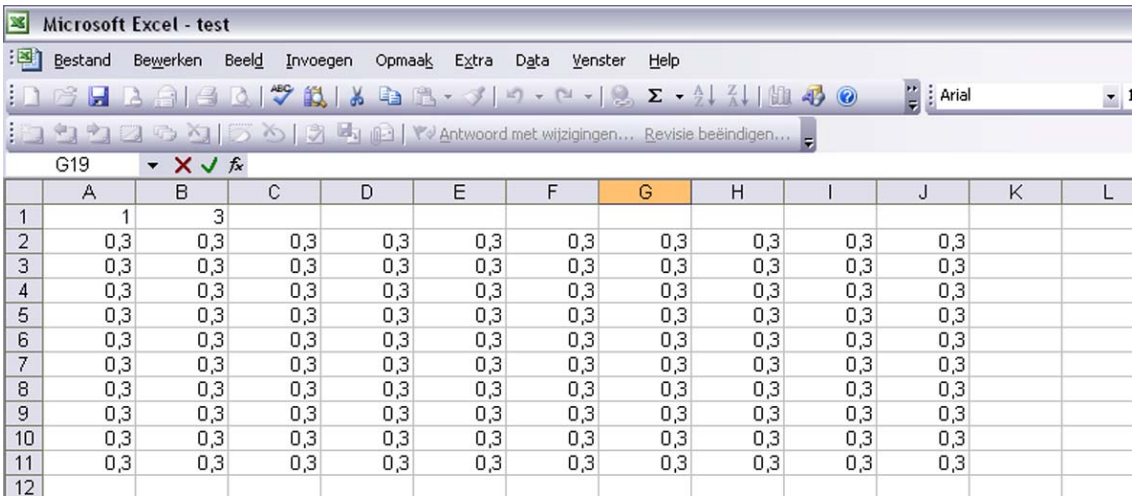
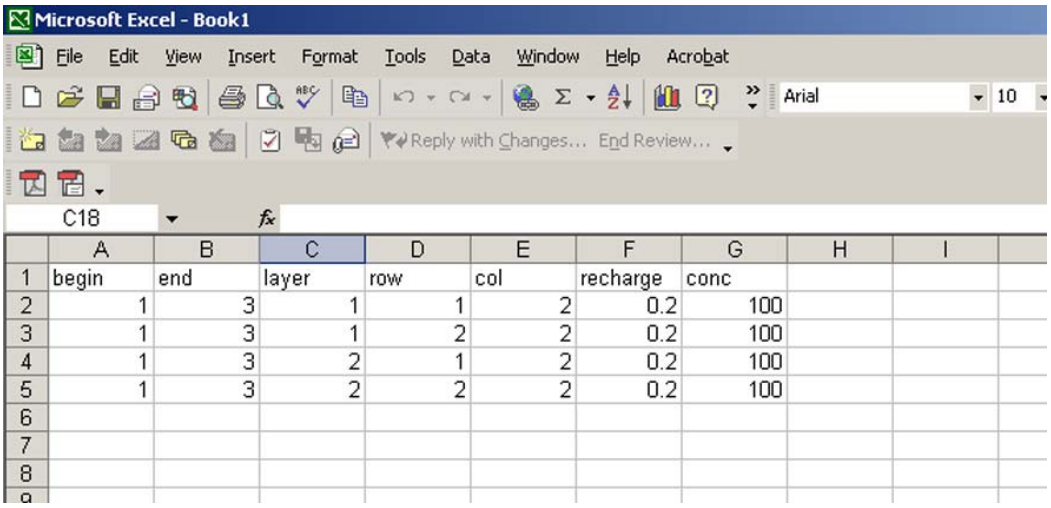


figure 3.15 *Example for the input of recharge in 2 layer, 10 rows and columns model. The concentration file has the same format.*



	A	B	C	D	E	F	G	H	I
1	begin	end	layer	row	col	recharge	conc		
2	1	3	1	1	2	0.2	100		
3	1	3	1	2	2	0.2	100		
4	1	3	2	1	2	0.2	100		
5	1	3	2	2	2	0.2	100		
6									
7									
8									

figure 3.16 *Example for the input of recharge with a list file.*

3.4.6 River (riv), drainage (drn) and general head boundary (ghb) package

Input for the construction of the river, drain and general head boundary file is almost identical. The input GUI's are given in figure 3.17. In each case, the positions of the cells (layers, rows, columns) were a river, ghb or drain is considered must be given plus some additional information.

This additional information is for a river cell

- Head in river
- Riverbed hydraulic conductance
- Bottom elevation
- Concentration in river

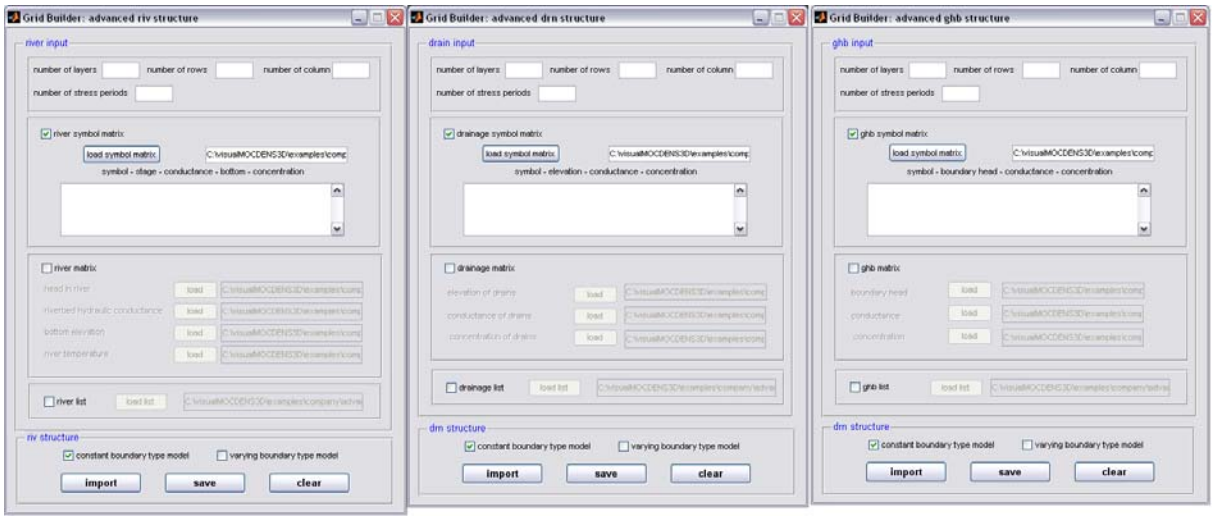


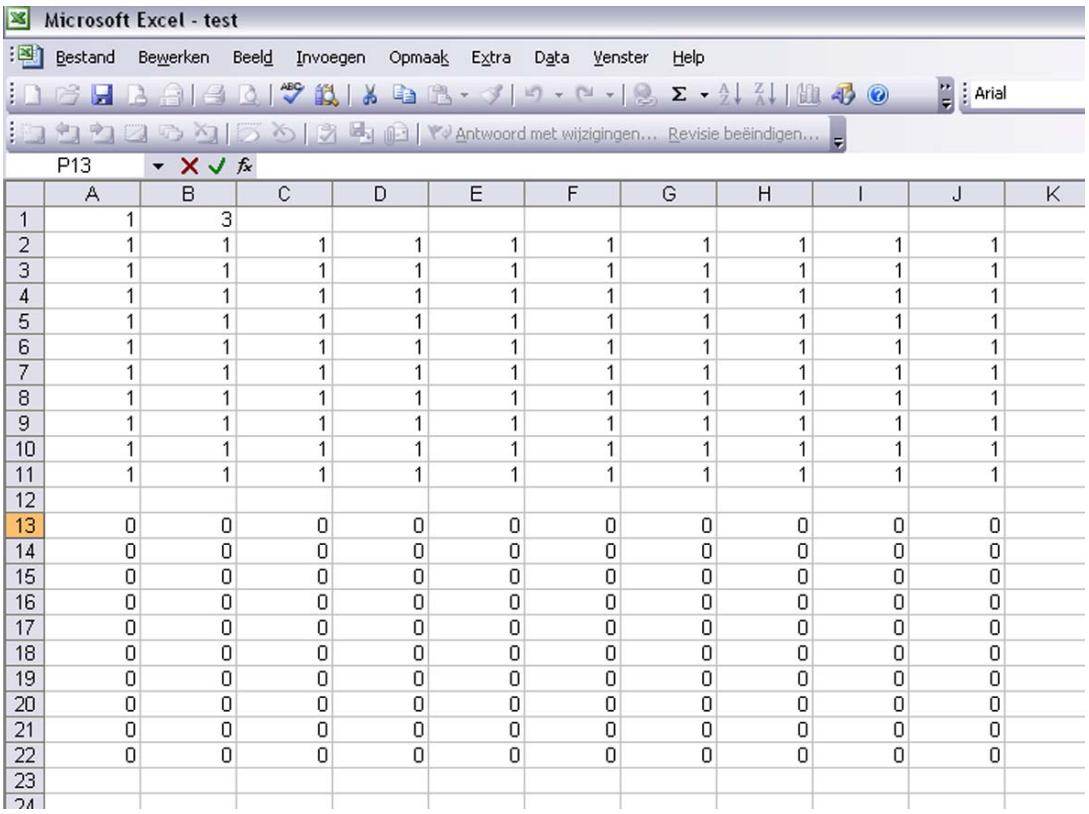
figure 3.17 *Advanced grid: river, drain and general head boundary input GUIs.*

This additional information is for a ghb cell:

- Boundary head
- Conductance
- Concentration

This additional information is for a drainage cell:

- Elevation of drains
- Conductance of drains
- Concentration of drains



	A	B	C	D	E	F	G	H	I	J	K
1	1	3									
2	1	1	1	1	1	1	1	1	1	1	
3	1	1	1	1	1	1	1	1	1	1	
4	1	1	1	1	1	1	1	1	1	1	
5	1	1	1	1	1	1	1	1	1	1	
6	1	1	1	1	1	1	1	1	1	1	
7	1	1	1	1	1	1	1	1	1	1	
8	1	1	1	1	1	1	1	1	1	1	
9	1	1	1	1	1	1	1	1	1	1	
10	1	1	1	1	1	1	1	1	1	1	
11	1	1	1	1	1	1	1	1	1	1	
12											
13	0	0	0	0	0	0	0	0	0	0	
14	0	0	0	0	0	0	0	0	0	0	
15	0	0	0	0	0	0	0	0	0	0	
16	0	0	0	0	0	0	0	0	0	0	
17	0	0	0	0	0	0	0	0	0	0	
18	0	0	0	0	0	0	0	0	0	0	
19	0	0	0	0	0	0	0	0	0	0	
20	0	0	0	0	0	0	0	0	0	0	
21	0	0	0	0	0	0	0	0	0	0	
22	0	0	0	0	0	0	0	0	0	0	
23											

figure 3.18 *Example for the input of drainage from using the symbolic matrix options. The values differing from 0 refer to a combination of elevation, conductance and concentration which are given in the symbol box. This system is identical for the input of river or general head boundary cells using the symbolic option. In the case the matrices with values (for instance of elevation, conductance and concentration for the drainage) are imported, the format is the same but the actual values are given.*

This can be done in three ways:

- Symbolic matrix: Figure 3.18 gives an example of this option. Cells which contain a river, ghb or drain are given a number differing from 0. Every value stands for a combination of the additional information as given above. Figure 3.18 shows an example for a 2 layer, 10 row and 10 column model. Symbols are valid for the stress periods 1 to 3. So the first and last stress period for the first input period is given in the firs row of the excel file followed by a rows x columns matrix for every layer with the value. The symbols for another range of stress periods are given on the next sheet of the same excel file. The sheets must be ordered according to increasing stress period and no empty sheet can be present in the file. The values are to be coupled on the additional information needed for the river, ghb or drainage cells. This is given in the symbol box were for every river, ghb or drainage cell respectively the symbol – river head – riverbed conductance – bottom - concentration, symbol – conductance – concentration or symbol – elevation – conductance – concentration must be given.
- Matrices of different properties: Matrices for the different properties are given via excel files. These have the same format as illustrated in figure 3.18 but the actual values are given. Four such file must be constructed for river input and three for the ghb and drainage input
- List file: This is an excel file given for every cell where a river, ghb or drain is present the properties. This is identical on the example given in figure 3.16 except for the number of columns. For river input 9 columns are needed (first and last stress period, layer, row, column,

river head, conductance, river bottom and concentration). 8 columns are needed for ghb input (first and last stress period, layer, row, column, boundary head, conductance and concentration). 8 columns are also needed for drainage input (first and last stress period, layer, row, column, elevation, conductance and concentration).

3.5 Model overview

The visual MOCDENS3D Grid Builder contains a GUI to provide you with an overview of the file names and types you have made. This is handy to see which files are already made, what there names are, if they are made with the basic or advanced option and if they are a CBTM or a VBTM. Figure 3.19 shows the GUI. The only thing you need to do is to load the appropriate nam-structure ((name)_nam.mat). Basic grid info is given and the information for every file. This is done in case you have given the input using the Visual MOCDENS3D Grid Builder input GUIs. If the different files (bas, bcf etc.) are made using a text editor, they will not show up here.

Any general errors (for instance incompatible grid definitions between files) are reported. The grid dimensions of the bas package serve hereby as reference.

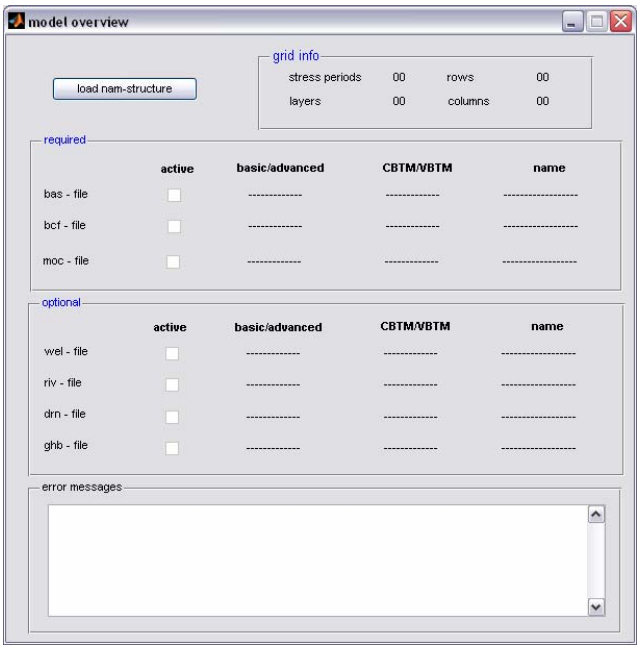


Figure 3.19 *GUI to give a general model overview based on the name files.*

3.6 Grid Visualiser

3.6.1 Introduction

With the Grid Visualiser of some of the most important input can be plotted. These are the bas, bcf and well files. The other files (drn, ghb and riv) must be visualized by the user in another way since these are (in most cases) no continuous matrices.

Input can be plotted from an excel file or from the input structure. The excel-files are files with matrices (e.g. 3.11 and 3.12) and no list files.

3.6.2 Basic (bas) package

Figure 3.20 shows the GUI for plotting the basic package input. First, the way the input is read must be chosen. This can be done from the excel input files (here the boundary condition or initial head file) or from the input structure ((name)_bas.mat).

Stress period and layer you want to plot is indicated next as are the number of rows, number of columns, number of layers and width of columns and rows. These latter values are filled in automatically if a grif structure is loaded in the workspace. Finally, it must be chosen if boundary conditions or initial heads will be plotted (if chosen for input via the structure) and if interpolation will be used. Labels and title can be assigned and data can be copied in the workspace.

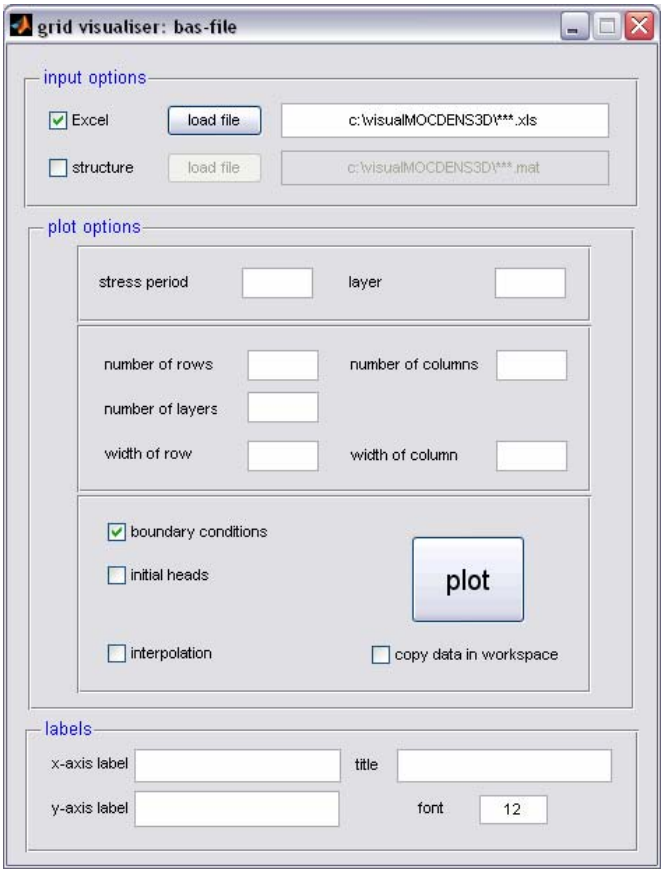


Figure 3.20 *GUI visualizing the basic package input.*

3.6.3 Block centered flow (bcf) package

Figures 3.21 and 3.2 show the GUIs for plotting the block centered flow package input, respectively for horizontal and vertical cross-sections. First, the way the input is read must be chosen. This can be done from the excel input files (here the boundary condition or initial head file) or from the input structure ((name)_bcf.mat).

Stress period and layer or column/row you want to plot is indicated next as are the number of rows, number of columns, number of layers and width of columns and rows. These latter values are filled in automatically if a grif structure is loaded in the workspace. Finally, it must be chosen if transmissivities, hydraulic conductances or specific elastic storages will be plotted (if chosen for input via the structure) and if interpolation will be used. Labels and title can be assigned and data can be copied in the workspace.

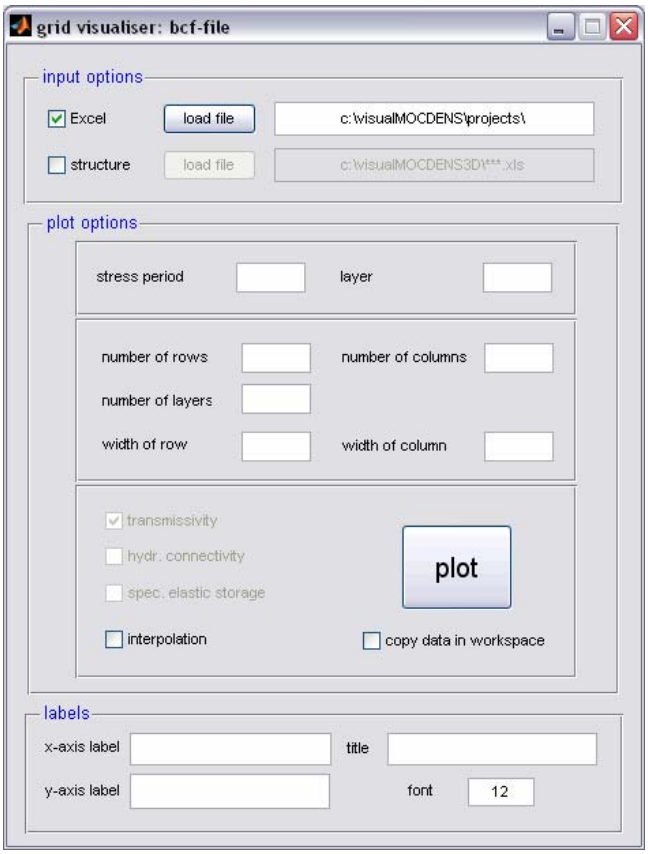


Figure 3.21 *GUI visualizing the block centered flow package input, horizontal cross-sections.*

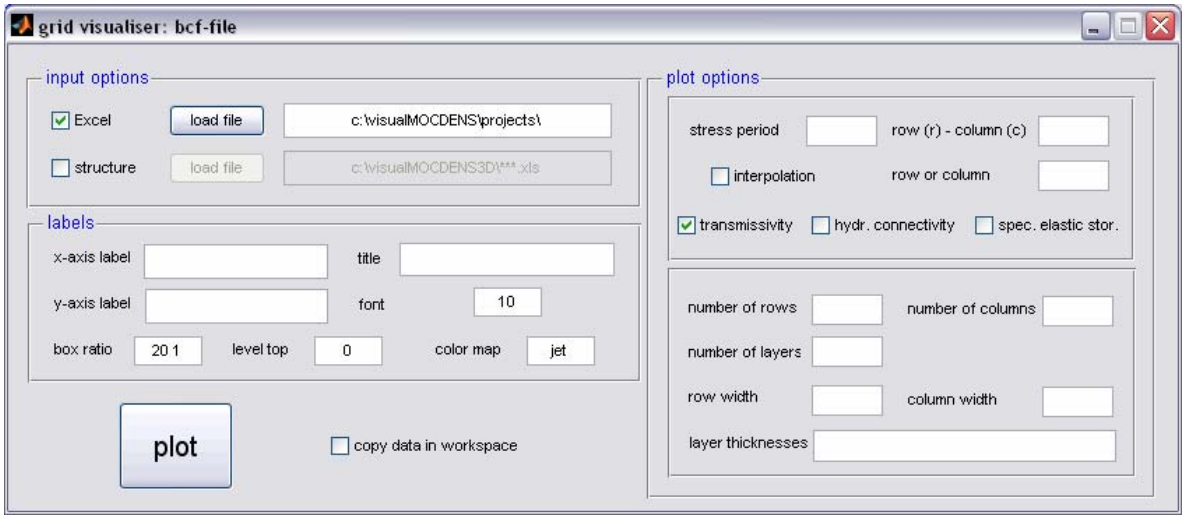


Figure 3.22 *GUI visualizing the block centered flow package input, vertical cross-sections.*

3.6.4 Well (wel) package

Figure 3.23 shows the GUI for plotting recharge given through the well package input. It thus plots the recharge or pumping in the uppermost cells of the model. First, the way the input is read must be chosen. This can be done from the excel input files (here the boundary condition or initial head file) or from the input structure ((name)_wel.mat).

Stress period and layer you want to plot is indicated next as are the width of columns and rows. These latter values are filled in automatically if a grif structure is loaded in the workspace. Finally, it must be chosen if recharge or concentrations will be plotted (if chosen for input via the structure), select units and if interpolation will be used. Labels and title can be assigned and data can be copied in the workspace.

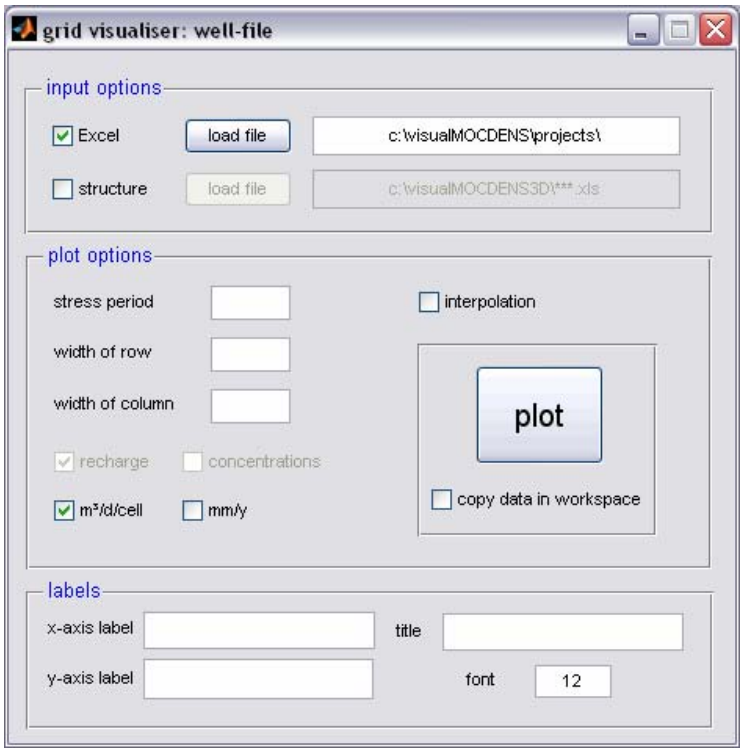


Figure 3.23 *GUI visualizing the well package input.*

3.7 Permanent to transient model

With this option a bas or a moc-file is constructed from an existing model. **This applies only to a CBTM.** The boundary conditions, initial heads and/or the initial concentrations from one model are then used to construct a new bas or moc-file. This is for instance useful for extracting the boundary conditions, heads and/or the concentrations from a permanent model for determining the initial conditions in a transient model.

Figure 3.24 shows the GUI. The *grid info box* first gives some details about the current model. The *bas file box* helps in constructing a new bas file. First the stress period of the current model which will be used to construct the new bas-file must be given. Then the mat file referring to the bas file of the current model can be given. In this way, the new initial heads will be written in a bas-file format, using the information (number of rows, layers, columns and boundary conditions) of the older model.

Additionally, thee number of stress periods, the length of these stress periods and the number of time steps of each stress period must be filled out.

Finally, the name of the output file must be given.

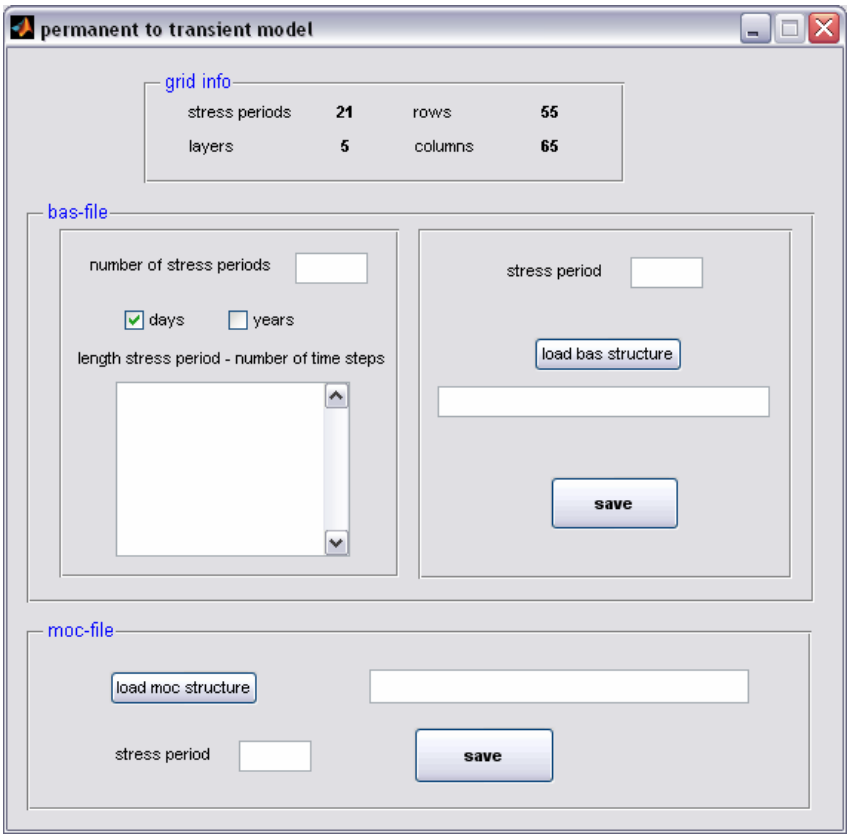


figure 3.24 *Permanent to transient model GUI.*

If no mat-file referring to a bas-file is present, or it is for some reason not required that all is written in the bas file format, the mbas_(name).mat-file checkbox must not be indicated. In this way, by pushing the build button, only the head matrices will be build. An example of the result is for instance:

```
        95         1(50F7.2)                        1   ; HEAD 1
4.50   4.50   4.50   4.50   … NCOL
.
.
.
NROW
Repeated for every layer
```

This can be pasted in an existing bas-file.

The same system applies for constructing a moc-file. In the *moc-file box*, first the stress period of the current model which will be used to construct a new moc-file must be indicated. If the mmoc_(name).mat checkbox is not indicated and reference to a mat file is not given, only the concentration matrices will be build. An example of the result is then:

```
     96       1.0(50F9.2)                        1    ; CONC  1
      0.00      0.00      0.00      0.00      0.00      0.00      0.00 … NCOL
.
.
.
NROW
Repeated for every layer
```

3.8 View structures

If you are not sure what kind of input structure a certain structure is of if it is compatible as a Visual MOCDENS3D input structure at all, this GUI can be handy.

It gives for a mat-file the type of input structure (bas, bcf, etc.), the model type (CBTM, VBTM) and the fields. If you want to look to it more in detail, the structure can be copied in the workspace.

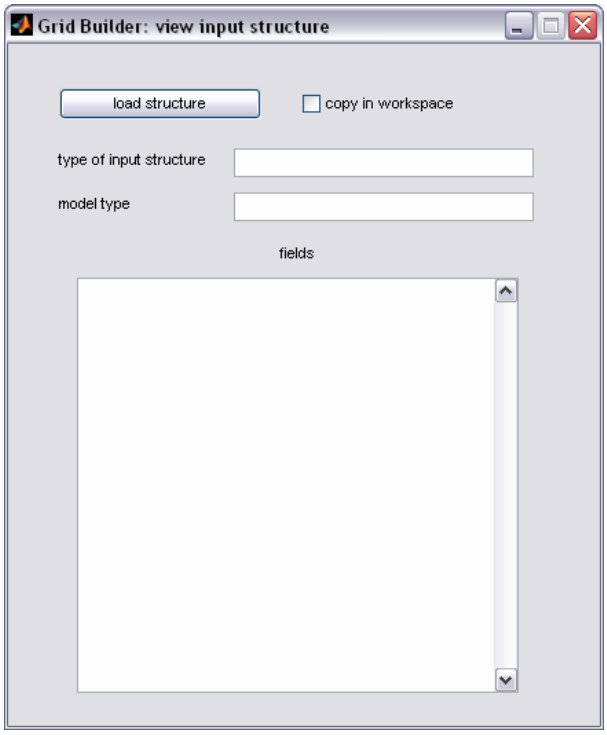


figure 3.25 *GUI gives a quick overview of the nature and content of an input structure.*

4 MOCDENS3D module

4.1 Introduction

The MOCDENS3D module of visual MOCDENS3D gives the commandos to run the model and to visualise its output with a number of cross-sections, graphs and 3D visualisation options.

4.2 Controlling input and running MOCDENS3D

4.2.1 Introduction

MOCDENS3D consist of a number of FORTRAN routines. After the input files are prepared a number of commands must be given to run the model and prepare the output of the model to be compatible with visual MOCDENS3D. These are two dos commands and a MATLAB function. These can be given in the MATLAB Command Window. In the MATLAB Command Window, dos commands can be given when proceeded by an "!".

The different dos commands are:

*!del *.out*
!moc3D
[grif data] = matvis(pathname)

The first two commando's are dos commando's, hence the preceding '!' which evaluates a dos commando in MATLAB. Of importance is that the first commando (!del *.out) deletes the output of any previous model made in the directory. The second commando runs the MOCDENS3D model. The third uses a MATLAB function *matvis.m* to translate the MOCDENS3D output (*grafile.out*) in the grif and data structures which are used in Visual MOCDENS3D.

Instead of given the above dos commands in the MATLAB Command Window. Running the model can also be done via Visual MOCDENS3D GUI's. There is a difference between a constant and a variable boundary type model.

4.2.2 CBTM

Two GUI's assist in running a MOCDENS3D model. A first GUI checks the model input (figure 4.1. Checking the model does not mean that all the input files are controlled. It means that the model structure is checked using the nam-files (infile.nam and moc-nam file). First of all, it is controlled if all necessary files (bas, bcf, sip, moc and densin.dat) are included in the model and if the reference to it (file number, file name etc) in the nam-files is correct. Further it checks if references to optional files are correct. It also checks if the necessary exe-files (moc3d.exe and tnt.exe) are present in the model's directory. If not, these files are copied automatically. The model check is initiated by giving the model

directory and pressing on the 'check model files' button. In the two windows an overview is given of all input files and of the errors which were found.

The Running MOCDENS3D GUI (figure 4.1) assists in running MOCDENS3D. First the directory of the MOCDENS3D model is given and a project name must be assigned. Then the "run MOCDENS3D" button is pushed. The model can be seen running in the MATLAB Command Window or in the dos window of the stand-alone application.

The results of a model run are two structures, grif and data, which are copied in the MATLAB workspace or which are available to the stand-alone application. The matvis.m function is thus executed automatically. The grif and data structures are also saved in the designated directory. If the name of the project is (name), the grif and data structures are saves as (name)_grif.mat and (name)_data.mat.

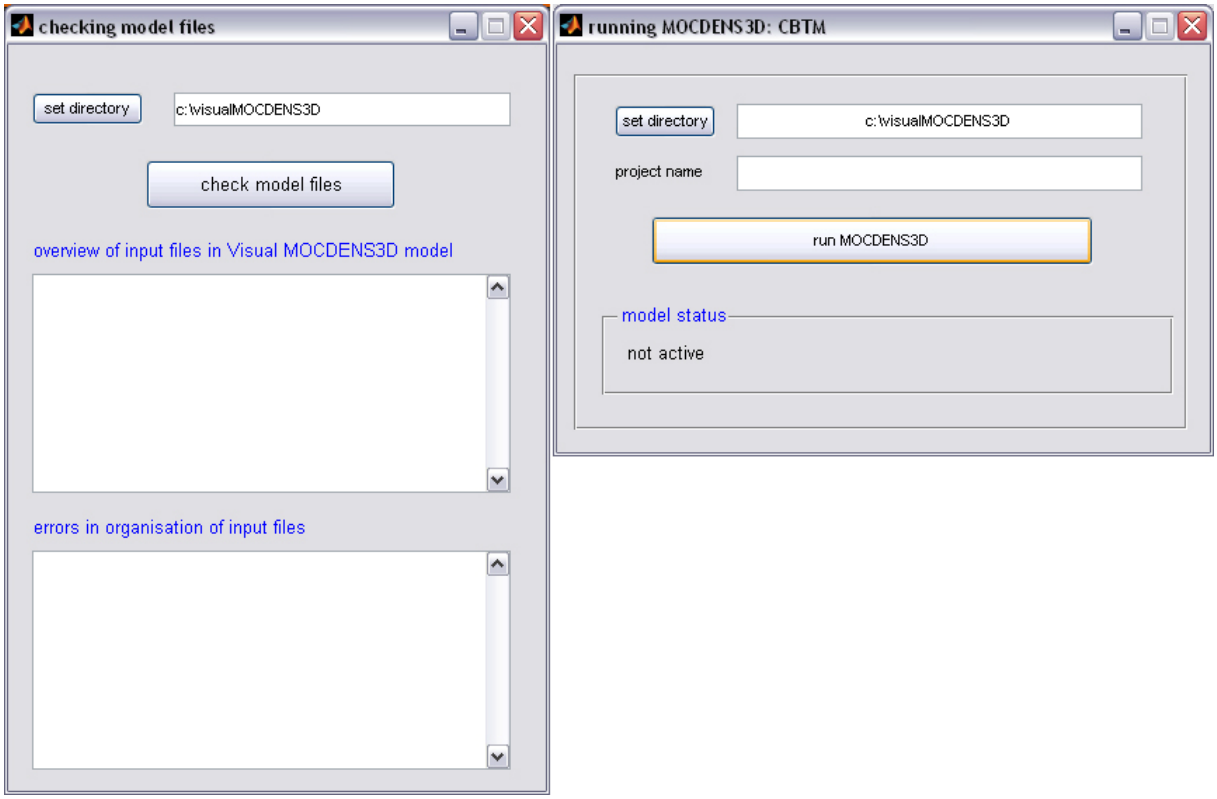


figure 4.1 *GUI assisting in controlling (left) and running (right) the MOCDENS3D CBTM models.*

4.2.3 VBTM

Figure 4.2 shows the GUI for running a VBTM. First the nam-structure is loaded. This nam-structure contains reference to all packages which are used by the model and contains thus all information to run the model.

The number of different boundary conditions should appear below the name of the nam structure. In the *model output box*, the directory and project name must be given.

Then the 'start calculations' button is pressed and the model run starts. The results of a model run are again two structures, grif and data, which are copied in the MATLAB workspace or which are available to the stand-alone application. The grif and data structures are also saved in the designated

directory. If the name of the project is (name), the grif and data structures are saves as (name)_grif.mat and (name)_data.mat.

It is possible to include a MATLAB function which can be called every time the boundary conditions changes. Such a function is of the general form:

[tempconc] = *functionname*(tempconc, grif, k)

tempconc is the concentration distribution of every layer, row and column (tempconc(1:number of layer, 1:number of rows,1:number of columns)) after the k^{th} change of boundary conditions. The function thus takes this concentration distribution as input, this distribution can be changed and the new one is used in the subsequent calculation. It can thus be used to make changes to this concentration distribution for instance in the simulation of a clean-up a contaminated site where the reactions one wishes to simulate are more complicated than a first-order decay. The MATLAB function must be present in the folder with model files.

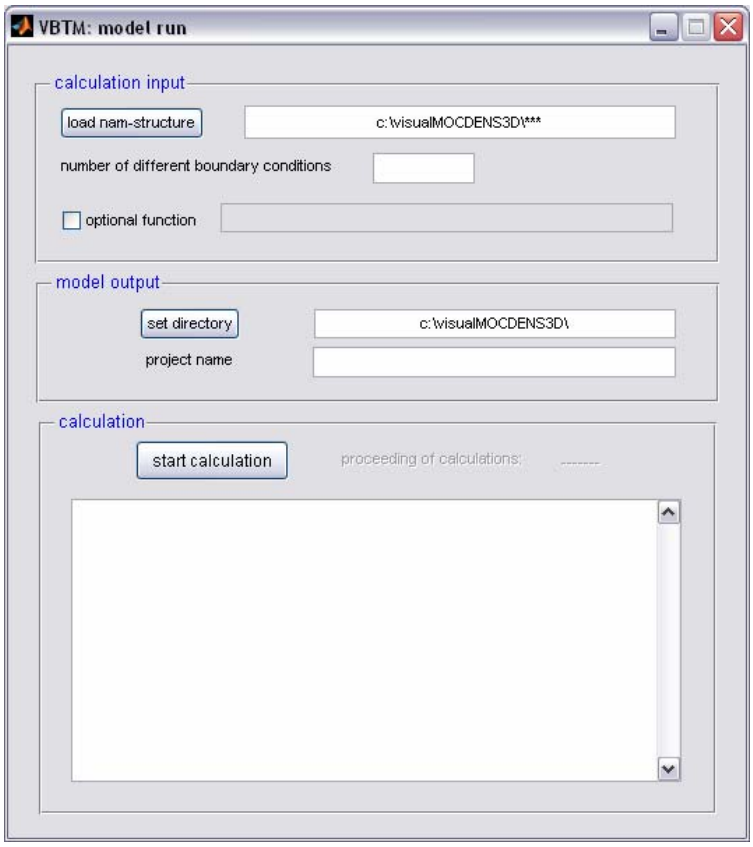


figure 4.2 *GUI assisting running the MOCDENS3D VBTM model.*

4.3 Cross-sections

4.3.1 Horizontal cross-sections

This GUI (figure 4.3) assists in the visualisation of head, concentration and/or effective velocities with horizontal cross-sections. Head and/or concentrations can be plotted with contours or with color maps. Effective velocities are visualised with arrows.

The *grid info box* summarises the grid sizes of the model and selects the number of layer and stress period for which data are plotted.

Layer: give layer number
Stress period: give stress period

In the *heads box*, options for plotting the heads are selected. Choose contour lines or color map by designating the appropriate box.

Plot interval: this gives by default the minimum and maximum hydraulic head occurring in the model. Alter this given the preferred plot interval, plot step and label step
Plot step: gives the step with which a contour is plotted
Label step: gives the step with which a label is plotted on the contours.
Line thickness: regulates line thickness
Font: regulates the font of the labels
Color: regulates color of labels and lines. Regular MATLAB colors are used.

Colormap: regulates color map. If an 'i' is given after the regular MATLAB color maps, the color map is inverted.
Close interval: if the close interval box is indicated, every head outside the interval is indicated in white, other less the cells are given the color of the minimum or maximum head.

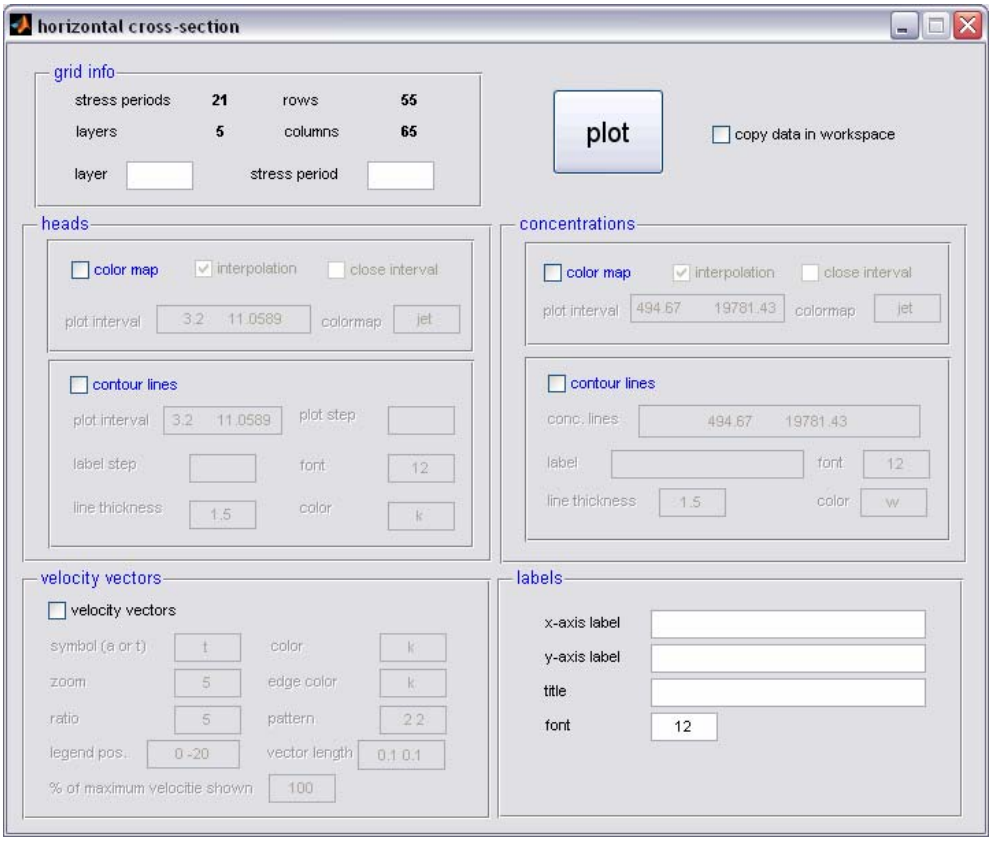


figure 4.3 *Horizontal cross-section GUI.*

In the *concentration box*, options for plotting the heads are selected. Choose contour lines or color map by designating the appropriate box.

Plot interval: this gives by default the minimum and maximum concentration occurring in the model. Alter this given the preferred plot interval, plot step and label step

Plot step: gives the step with which a contour is plotted
Label step: gives the step with which a label is plotted on the contours.
Line thickness: regulates line thickness
Font: regulates the font of the labels
Color: regulates color of labels and lines. Regular MATLAB colors are used.

Colormap: regulates color map. If an 'i' is given after the regular MATLAB color maps, the color map is inverted.
Close interval: if the close interval box is indicated, every concentration outside the interval is indicated in white, other less the cells are given the color of the minimum or maximum concentration.

In the *velocity vector box*, options for plotting the heads are selected.
Choose velocity vectors by designating the velocity vector box

Symbol (a or t): designate the symbol, arrow (a) or triangle (t)
Zoom: regulates the size of the velocity vector
Ratio: regulates the ratio of the length to the width of the velocity vector
Color: regulates the color of the velocity vector. Regular MATLAB colors are used.
Edge color: regulates the edge color of the velocity vector. Regular MATLAB colors are used.
Pattern: regulates the pattern with which velocity vectors are plotted, 2 by 2 means that in every two model cells a velocity vector is plotted.
Legend position: regulates the position of the legend. The legend is by default plotted above the figure but can be altered by changing the coordinates.
Vector: regulates the size of the velocity vectors used as reference in the legend

Options for labels are given in the labels box. Label on the x-axis, y-axis and title can be plotted. Font regulates the font of the axes, labels and title.

4.3.2 Vertical cross-sections

This GUI (figure 4.4) assists in the visualisation of head, concentration and/or effective velocities with vertical cross-sections. Head and/or concentrations can be plotted with contours or with color maps. Effective velocities are visualised with arrows.

The *grid info box* summarises the grid sizes of the model and selects the number of the row or column and stress period for which data are plotted.

Row (r) or column (c): cross-section according to a row or column
Stress period: give stress period
Row or column number: give row or column number

In the *heads box*, options for plotting the heads are selected. Choose contour lines or color map by designating the appropriate box.

Plot interval: this gives by default the minimum and maximum hydraulic head occurring in the model. Alter this given the preferred plot interval, plot step and label step
Plot step: gives the step with which a contour is plotted
Label step: gives the step with which a label is plotted on the contours.
Line thickness: regulates line thickness
Font: regulates the font of the labels
Color: regulates color of labels and lines. Regular MATLAB colors are used.

Colormap: regulates color map. If an 'i' is given after the regular MATLAB color maps, the color map is inverted.
Close interval: if the close interval box is indicated, every head outside the interval is indicated in white, other less the cells are given the color of the minimum or maximum head.

In the *concentration box*, options for plotting the heads are selected. Choose contour lines or color map by designating the appropriate box.

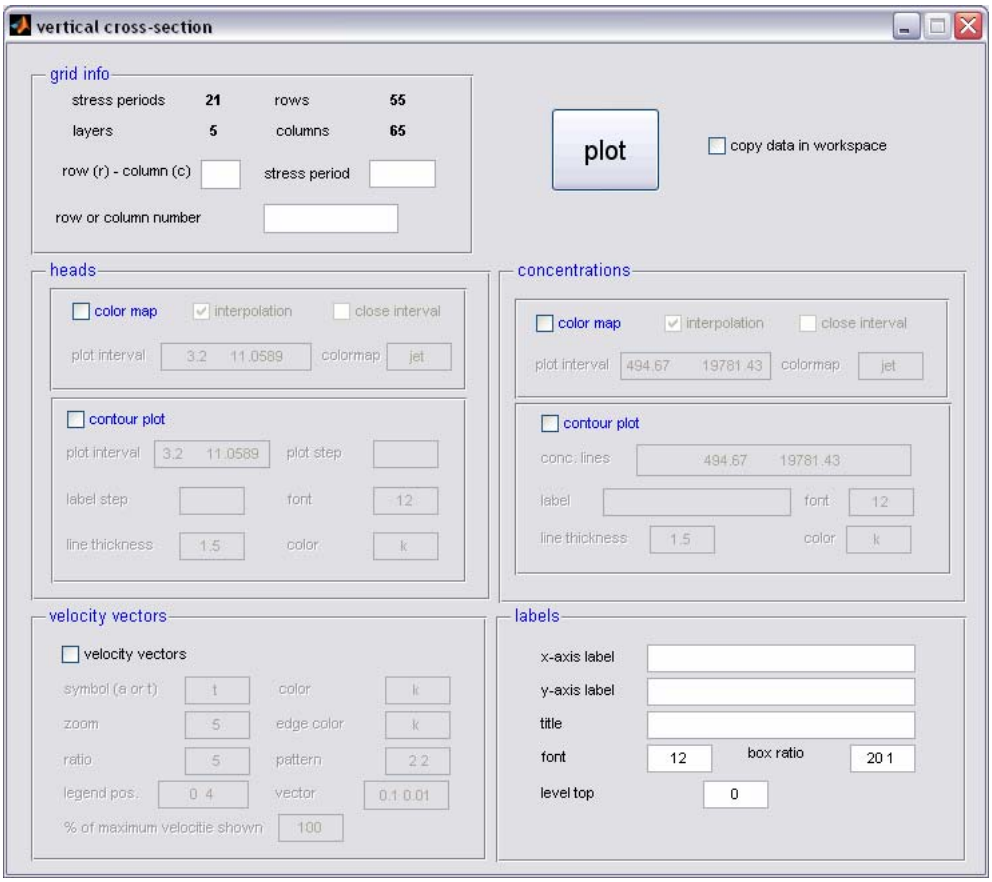


figure 4.4 *Vertical cross-section GUI.*

Plot interval: this gives by default the minimum and maximum concentration occurring in the model. Alter this given the preferred plot interval, plot step and label step
Plot step: gives the step with which a contour is plotted
Label step: gives the step with which a label is plotted on the contours.
Line thickness: regulates line thickness
Font: regulates the font of the labels
Color: regulates color of labels and lines. Regular MATLAB colors are used.

Colormap: regulates color map. If an 'i' is given after the regular MATLAB color maps, the color map is inverted.
Close interval: if the close interval box is indicated, every concentration outside the interval is indicated in white, other less the cells are given the color of the minimum or maximum concentration.

In the *velocity vector box*, options for plotting the heads are selected. Choose velocity vectors by designating the velocity vector box

Symbol (a or t): designate the symbol, arrow (a) or triangle (t)
Zoom: regulates the size of the velocity vector

Ratio: regulates the ratio of the length to the width of the velocity vector
Color: regulates the color of the velocity vector. Regular MATLAB colors are used.
Edge color: regulates the edge color of the velocity vector. Regular MATLAB colors are used.
Pattern: regulates the pattern with which velocity vectors are plotted, 2 by 2 means that in every two model cells a velocity vector is plotted.
Legend position: regulates the position of the legend. The legend is by default plotted above the figure but can be altered by changing the coordinates.
Vector: regulates the size of the velocity vectors used as reference in the legend

Options for labels are given in the *labels box*. Label on the x-axis, y-axis and legend can be plotted. Font regulates the font of the axes, labels and title.

4.3.3 Horizontal cross-sections of vertical velocities

This GUI (figure 4.5) assists in the visualisation of effective vertical velocities with horizontal cross-sections. Head and effective horizontal velocities can also be plotted to serve as a 'background' or framework. Heads and vertical velocities can be plotted with contours or with color maps. Effective horizontal velocities are visualised with arrows.

The *grid info box* summarises the grid sizes of the model and selects the number of layer and stress period for which data are plotted.

Layer: give layer number
Stress period: give stress period

If the proceed button is pushed, the minimum and maximum vertical velocity for the selected layer and stress period is shown in the *head box* of the *vertical velocity* box.

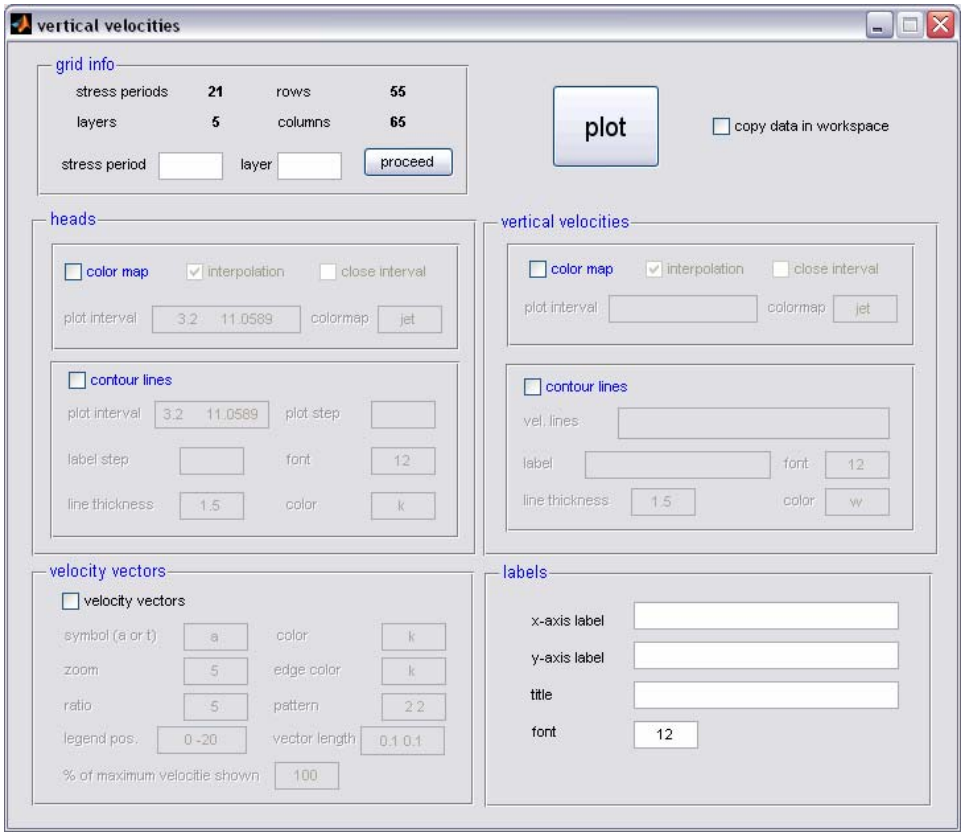


figure 4.5 *Vertical velocity GUI.*

In the *head box*, options for plotting the heads are selected. Choose contour lines or color map by designating the appropriate box.

Plot interval: this gives by default the minimum and maximum hydraulic head occurring in the model. Alter this given the preferred plot interval, plot step and label step
Plot step: gives the step with which a contour is plotted
Label step: gives the step with which a label is plotted on the contours.
Line thickness: regulates line thickness
Font: regulates the font of the labels
Color: regulates color of labels and lines. Regular MATLAB colors are used.

Colormap: regulates color map. If an 'i' is given after the regular MATLAB color maps, the color map is inverted.
Close interval: if the close interval box is indicated, every head outside the interval is indicated in white, otherless the cells are given the color of the minimum or maximum head.

In the *vertical velocity box*, options for plotting the heads are selected. Choose contour lines or color map by designating the appropriate box.

Plot interval: this gives by default the minimum and maximum concentration occurring in the model. Alter this given the preferred plot interval, plot step and label step
Plot step: gives the step with which a contour is plotted
Label step: gives the step with which a label is plotted on the contours.
Line thickness: regulates line thickness
Font: regulates the font of the labels
Color: regulates color of labels and lines. Regular MATLAB colors are used.

Colormap: regulates color map. If an 'i' is given after the regular MATLAB color maps, the color map is inverted.
Close interval: if the close interval box is indicated, every concentration outside the interval is indicated in white, other less the cells are given the color of the minimum or maximum concentration.

In the *velocity vector box*, options for plotting the heads are selected.
Choose velocity vectors by designating the velocity vector box

Symbol (a or t): designate the symbol, arrow (a) or triangle (t)
Zoom: regulates the size of the velocity vector
Ratio: regulates the ratio of the length to the width of the velocity vector
Color: regulates the color of the velocity vector. Regular MATLAB colors are used.
Edge color: regulates the edge color of the velocity vector. Regular MATLAB colors are used.
Pattern: regulates the pattern with which velocity vectors are plotted, 2 by 2 means that in every two model cells a velocity vector is plotted.
Legend position: regulates the position of the legend. The legend is by default plotted above the figure but can be altered by changing the coordinates.
Vector: regulates the size of the velocity vectors used as reference in the legend

Options for labels are given in the *labels box*. Label on the x-axis, y-axis and title can be plotted. Font regulates the font of the axes, labels and title.

4.4 Differences

4.4.1 Layers – different stress periods

This GUI (figure 4.6) makes it possible to visualise differences in head and/or concentrations in horizontal cross-sections between different stress periods. This is done with contour plots and/or color maps. This option makes it for instance possible to calculate drawdowns based on head data.

The *grid info box* summarises the grid sizes of the model and selects the layer and the two stress periods between which differences will be plot. Then the "proceed" button must be pushed and the head and concentration interval for the specific layer are given as aid to continue.

Layer: give layer number
Stress period 1 minus 2: this gives the two stress periods between which the differences are calculated. Data of stress period one minus stress period two is calculated.

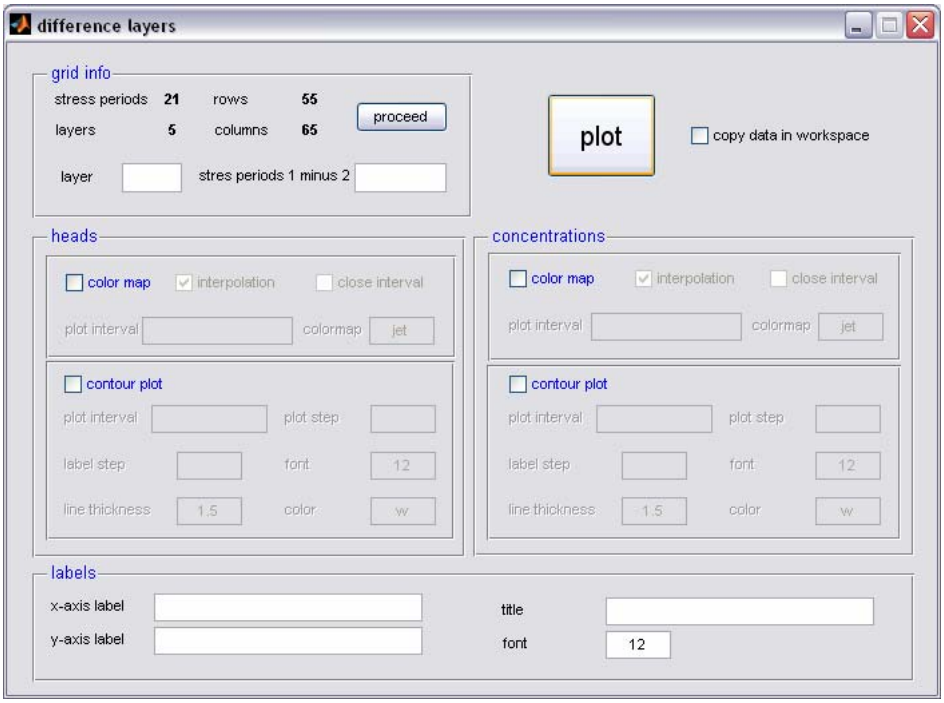


figure 4.6 *Differences between different stress periods (layers) GUI.*

In the *heads box*, options for plotting the heads are selected. Choose contour lines or color map by designating the appropriate box.

Plot interval: this gives by default the minimum and maximum hydraulic head occurring in the model. Alter this given the preferred plot interval, plot step and label step
Plot step: gives the step with which a contour is plotted
Label step: gives the step with which a label is plotted on the contours.
Line thickness: regulates line thickness
Font: regulates the font of the labels
Color: regulates color of labels and lines. Regular MATLAB colors are used.

Colormap: regulates color map. If an 'i' is given after the regular MATLAB color maps, the color map is inverted.

Close interval: if the close interval box is indicated, every head outside the interval is indicated in white, otherless the cells are given the color of the minimum or maximum head.

In the *concentration box*, options for plotting the heads are selected. Choose contour lines or color map by designating the appropriate box.

Plot interval: this gives by default the minimum and maximum concentration occurring in the model. Alter this given the preferred plot interval, plot step and label step
Plot step: gives the step with which a contour is plotted
Label step: gives the step with which a label is plotted on the contours.
Line thickness: regulates line thickness
Font: regulates the font of the labels
Color: regulates color of labels and lines. Regular MATLAB colors are used.

Colormap: regulates color map. If an 'i' is given after the regular MATLAB color maps, the color map is inverted.
Close interval: if the close interval box is indicated, every concentration outside the interval is indicated in white, otherless the cells are given the color of the minimum or maximum concentration.

Options for labels are given in the *labels box*. Labels on the x-axis and y-axis can be plotted. Font regulates the font of the axes, labels and title.

4.4.2 Row/column – different stress periods

This GUI (figure 4.7) makes it possible to visualise differences in head and/or concentrations in vertical cross-sections between different stress periods. This is done with contour plots and/or color maps. This option makes it for instance possible to calculate drawdowns based on head data.

The *grid info box* summarises the grid sizes of the model and selects the row/column and the two stress periods between which differences will be plot. Then the "proceed" button must be pushed and the head and concentration interval for the specific layers are given as aid to continue.

Row (r) or column (c): choose between cross-section according to a row (r) or column (c)
Stress period 1 minus 2: this gives the two stress periods between which the differences are calculated. Data of stress period one minus stress period two is calculated.
Row or column number: give row or column number

In the *heads box*, options for plotting the heads are selected. Choose contour lines or color map by designating the appropriate box.

Plot interval: this gives by default the minimum and maximum hydraulic head occurring in the model. Alter this given the preferred plot interval, plot step and label step
Plot step: gives the step with which a contour is plotted
Label step: gives the step with which a label is plotted on the contours.
Line thickness: regulates line thickness
Font: regulates the font of the labels
Color: regulates color of labels and lines. Regular MATLAB colors are used.

Colormap: regulates color map. If an 'i' is given after the regular MATLAB color maps, the color map is inverted.
Close interval: if the close interval box is indicated, every head outside the interval is indicated in white, otherless the cells are given the color of the minimum or maximum head.

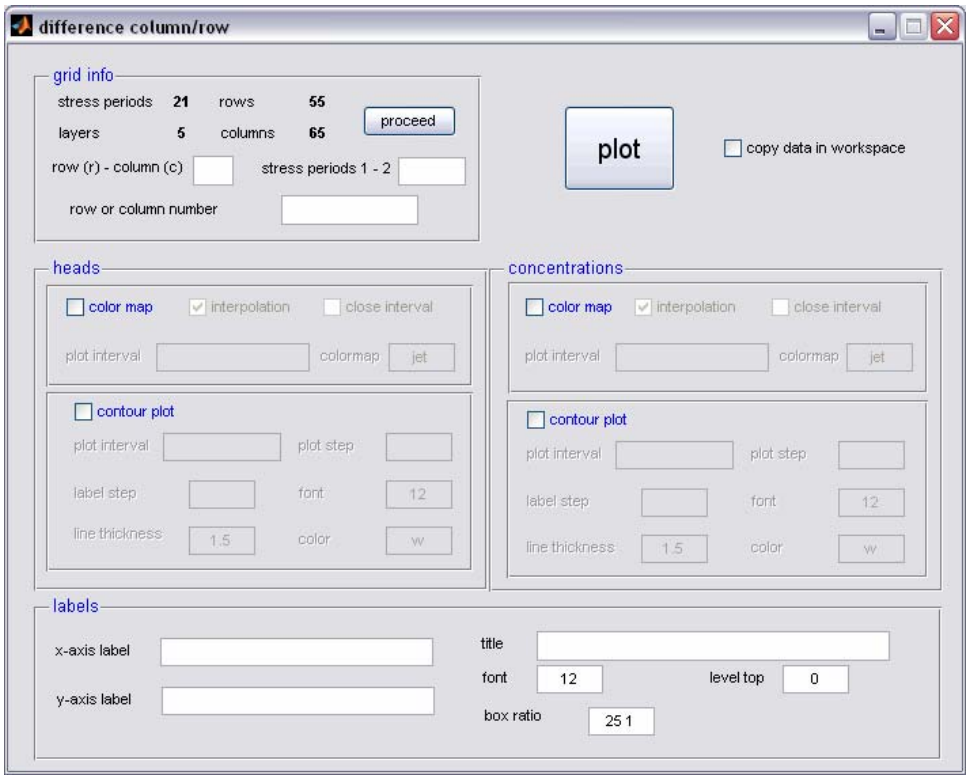


figure 4.7 *Differences between different stress periods (row/column) GUI.*

In the *concentration box*, options for plotting the heads are selected. Choose contour lines or color map by designating the appropriate box.

Plot interval: this gives by default the minimum and maximum concentration occurring in the model. Alter this given the preferred plot interval, plot step and label step
Plot step: gives the step with which a contour is plotted
Label step: gives the step with which a label is plotted on the contours.
Line thickness: regulates line thickness
Font: regulates the font of the labels
Color: regulates color of labels and lines. Regular MATLAB colors are used.

Colormap: regulates color map. If an 'i' is given after the regular MATLAB color maps, the color map is inverted.
Close interval: if the close interval box is indicated, every concentration outside the interval is indicated in white, otherless the cells are given the color of the minimum or maximum concentration.

Options for labels are given in the *labels box*. Labels on the x-axis and y-axis can be plotted. Font regulates the font of the axes, labels and title.

4.4.3 Layers – same stress period

This GUI (figure 4.8) makes it possible to visualise differences in head and/or concentrations in horizontal cross-sections in a same stress period. This is done with contour plots and/or color maps.

The *grid info box* summarises the grid sizes of the model and selects the two layers and the stress period between which differences will be plot. Then the "proceed" button must be pushed and the head and concentration interval for the specific layer are given as aid to continue.

Layer 1 minus 2: gives the layer numbers between which differences are calculated. Data of layer one minus layer two is calculated.
Stress period: gives the stress period

In the *heads box*, options for plotting the heads are selected. Choose contour lines or color map by designating the appropriate box.

Plot interval: this gives by default the minimum and maximum hydraulic head occurring in the model. Alter this given the preferred plot interval, plot step and label step
Plot step: gives the step with which a contour is plotted
Label step: gives the step with which a label is plotted on the contours.
Line thickness: regulates line thickness
Font: regulates the font of the labels
Color: regulates color of labels and lines. Regular MATLAB colors are used.

Colormap: regulates color map. If an 'i' is given after the regular MATLAB color maps, the color map is inverted.
Close interval: if the close interval box is indicated, every head outside the interval is indicated in white, otherless the cells are given the color of the minimum or maximum head.

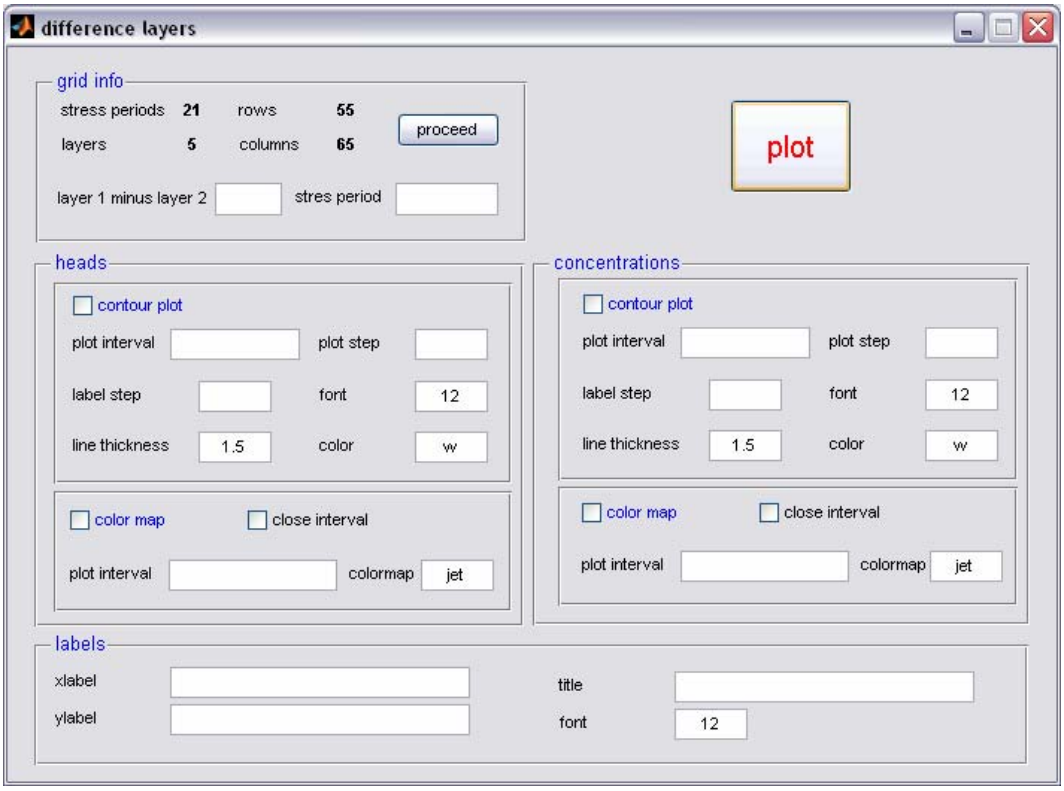


figure 4.8 *Differences between different stress periods (layers) GUI..*

In the *concentration box*, options for plotting the heads are selected. Choose contour lines or color map by designating the appropriate box.

Plot interval: this gives by default the minimum and maximum concentration occurring in the model. Alter this given the preferred plot interval, plot step and label step
Plot step: gives the step with which a contour is plotted
Label step: gives the step with which a label is plotted on the contours.
Line thickness: regulates line thickness

Font: regulates the font of the labels
Color: regulates color of labels and lines. Regular MATLAB colors are used.

Colormap: regulates color map. If an 'i' is given after the regular MATLAB color maps, the color map is inverted.
Close interval: if the close interval box is indicated, every concentration outside the interval is indicated in white, otherless the cells are given the color of the minimum or maximum concentration.

Options for labels are given in the *labels box*. Labels on the x-axis and y-axis can be plotted. Font regulates the font of the axes, labels and title.

4.5 Graphs

4.5.1 Head/concentration vs time

This option makes it possible to plot head or concentration data for given grid cells versus time. The *grid info box* summarises the grid sizes of the model.

In the *head and concentration info box*, the checkboxes make it possible to choose between different options:

- head vs time: head for given layer(s) along row(s) or column(s) in function of distance
- concentration vs time: concentration for given layer(s) along row(s) or column(s) in function of distance
- time in years: time on the x-axis is given in years
- time in days: time on the x-axis is given in days

Time interval: time interval plotted on the x-axis
Layer: layer number of cells
Row: row number of cells
Columns: column number of cells

More than one cell can be given. If in this case the value for each choice is the same, only one value must be given.

Labels for x-axis, y-axis can be indicated in the *labels box*.
Font: regulates the font of the axes, labels and legend
Line width: width of the graph line
Start time: start of the time on the x-axis. This must be given in accordance with the time option (years or days)

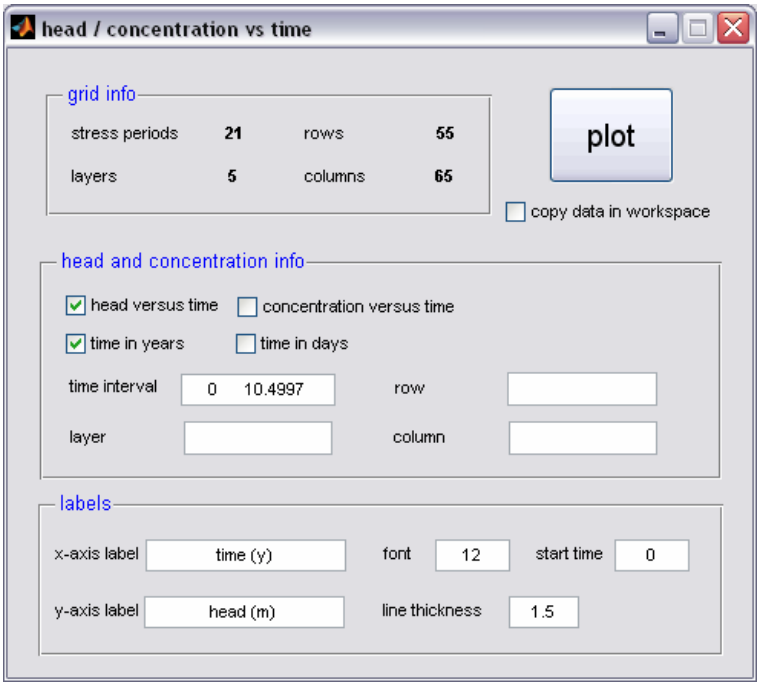


figure 4.9 *Head/concentrations vs time GUI.*

4.5.2 Head/concentration vs distance

This option makes it possible to plot head or concentration data for given layer(s) along row(s) or column(s) in function of distance.

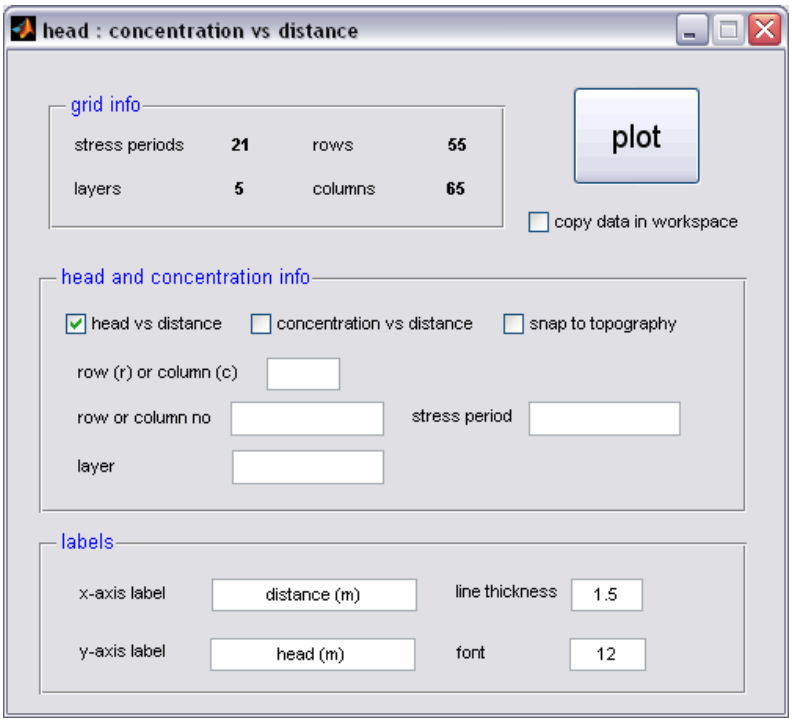


figure 4.10 *Head/concentrations vs distance GUI.*

The *grid info box* summarises the grid sizes of the model.

In the *head and concentration info box*, the checkboxes make it possible to choose between different options:

- head vs distance: head for given layer(s) along row(s) or column(s) in function of distance
- concentration vs distance: concentration for given layer(s) along row(s) or column(s) in function of distance
- snap to topography: head or concentration (as indicated by the other boxes) is given row(s) or column(s) for each first active cell. It thus gives the head or the concentration for the water table, independent of model layers.

Row or column (r or c): choose for cross-section via a column (c) or row (r)
Row or column number: give number of row(s) or column(s)
Stress period: give stress period(s)
Layer: give layer(s)

More than one row or column, stress period or layer can be given. If in this case the value for each choice is the same, only one value can be given.

Labels for x-axis, y-axis can be indicated in the *labels box*.
Font: regulates the font of the axes, labels and legend
Line width: width of the graph line

4.5.3 Head/concentration vs depth

This option makes it possible to plot head or concentration data for given layer(s) along row(s) or column(s) in function of depth.

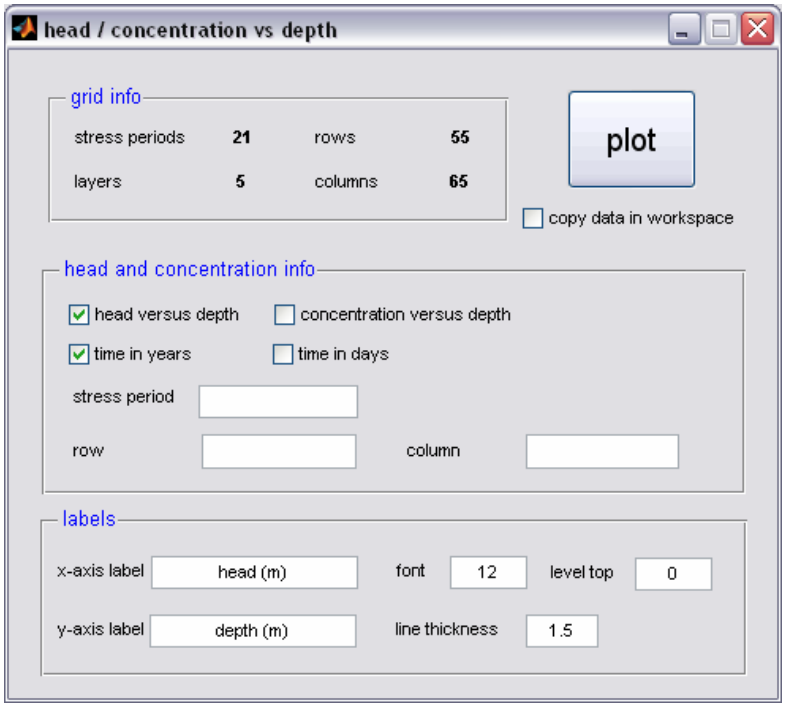


figure 4.11 *Head/concentrations vs distance GUI.*

The *grid info box* summarises the grid sizes of the model.

In the *head and concentration info box*, the checkboxes make it possible to choose between different options:

- head vs depth: head for given layer(s) along row(s) or column(s) in function of depth
- concentration vs depth: concentration for given row(s) or column(s) in function of depth

Rows: row number of cells
Columns: column number of cells
Stress period: give stress period(s)

More than one row, column or stress period can be given. If in this case the value for each choice is the same, only one value must be given.

Labels for x-axis, y-axis can be indicated in the *labels box*.
Font: regulates the font of the axes, labels and legend
Line width: width of the graph line

4.6 Inflow/outflow

4.6.1 For stress period

This option makes it possible to calculate in- or outflow for given grid cells for a given stress period.

The *grid info box* summarises the grid sizes of the model. Then three different options are possible.

First, in the *point selection box*, cells are given by their layer(s), row(s) and column(s) and in or outflow is calculated for these cells.

Stress period: stress period
Layer: layer number of cells
Row: row number of cells
Columns: column number of cells

More than one cell can be given. If in this case the value for each choice is the same, only one value must be given. The checkboxes make it possible to chose the unit, either m/y or m^3/d. By pressing the calculate button, the calculated outflow/inflow is printed in the outflow/inflow box.

Secondly, a graph can be made of the inflow/outflow of the cells according to a row or column of a certain layer. The checkboxes make it possible to chose the unit, either m/y or m^3/d. By checking the snap to grid checkbox, the in or outflow is calculated for the first active layer of the selected column or row, or by other words the in or outflow near the water table is calculated.

Layer: number of the layer(s)
Stress period: number of the stress period(s)
Row (r) or column (c): chose between row or column
Row/column: number of the row(s) or column(s)
Font: regulates the font of the axes, labels and legend
Line width: width of the graph line

Labels for x-axis, y-axis can also be indicated. If different graphs are to be plotted but they are for instance of the same layer, only one value for the layer must be filled out.

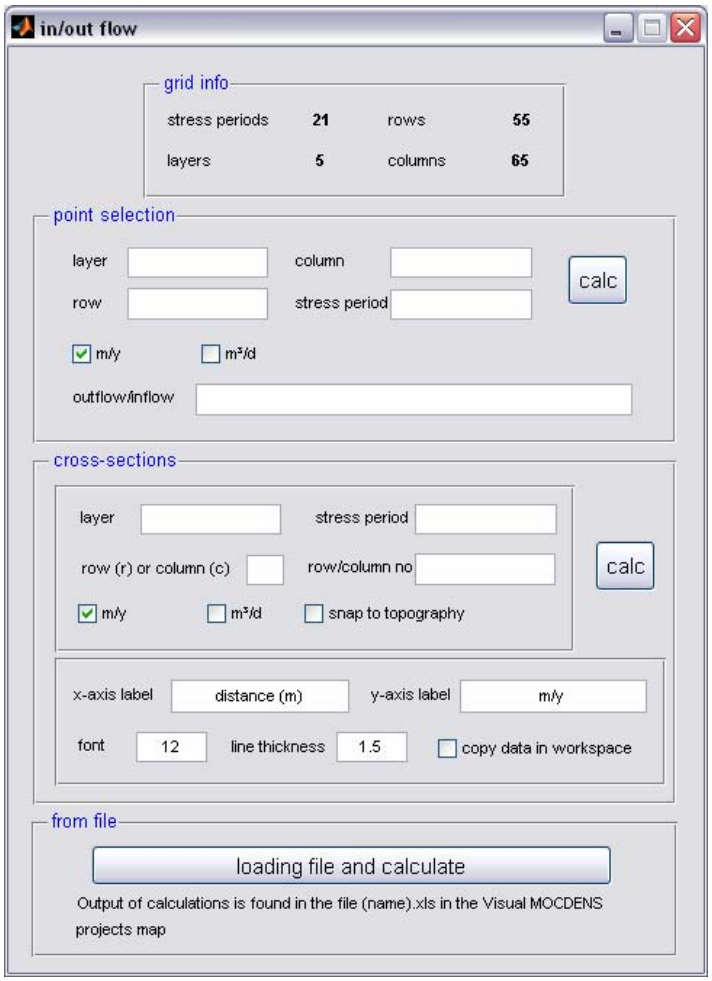
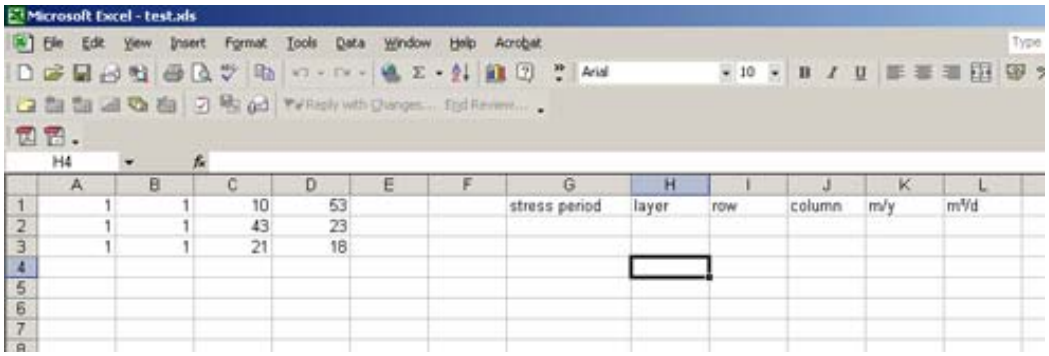
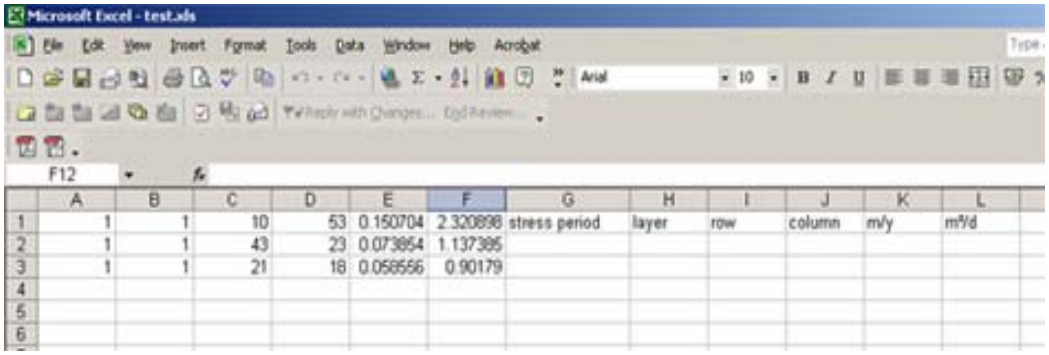


figure 4.12 *Inflow/outflow for a stress period GUI.*

Finally, stress period, layer, row and column can also be given *from file*. This must be an excel file using the following format:



After pressing the 'calc' button, in or outflow is calculated and added in the fifth (in m³/m/d) and sixth (m³/d) (E and F) column of the same excel sheet:



4.6.2 In time

This option makes it possible to plot in or outflow for given grid cells in function of time. The *grid info box* summarises the grid sizes of the model.

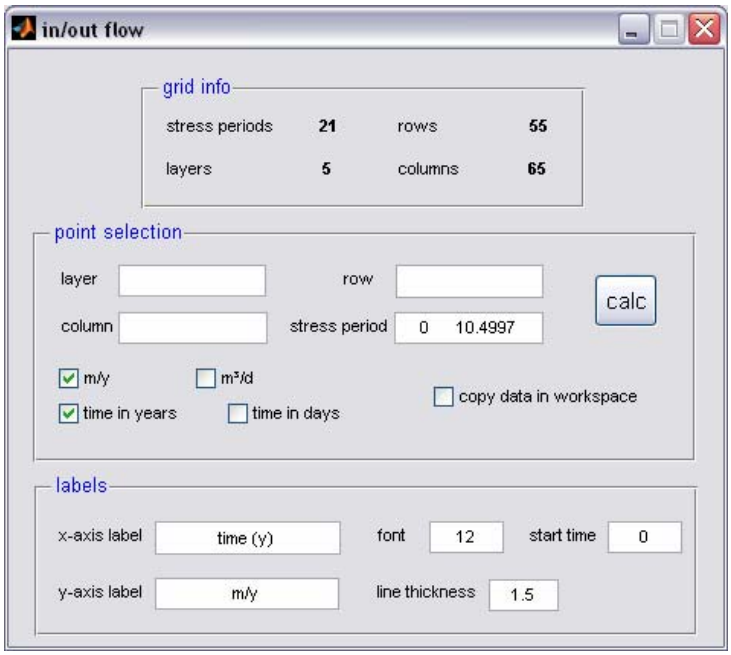


figure 4.13 *Inflow/outflow (in time) GUI.*

In the *point selection box*, cells are given by their layer(s), row(s) and column(s) and in or outflow is calculated.

Layer: layer number of cells
Row: row number of cells
Columns: column number of cells
Time period: time period which should be considered

More than one cell can be given. If in this case the value for each choice is the same, only one value can be given. The checkboxes make it possible to choose the unit, either m/y or m³/d and the time units (days or years).

Labels for x-axis, y-axis can be indicated in the *labels box*.

Font: regulates the font of the axes, labels and legend

Line width: width of the graph line
Start time: start of the time on the x-axis. This must be given in accordance with the time option (years or days)

4.6.3 Cross-sections

This option visualises inflow and outflow through horizontal cross sections. The inflow and outflow is given for the first model layer or for the first active cell going from the first to the last layer if all cells in the upper layer(s) are not active.

The *grid info box* summarises the grid sizes of the model and selects the stress period for which data are plotted. The unit in which the in and outflow will be plotted (m/y or m^3/d) must be indicated

Stress period: give stress period

If the proceed button is pushed, the minimum and maximum inflow and outflow for the selected stress period is shown in the options box.

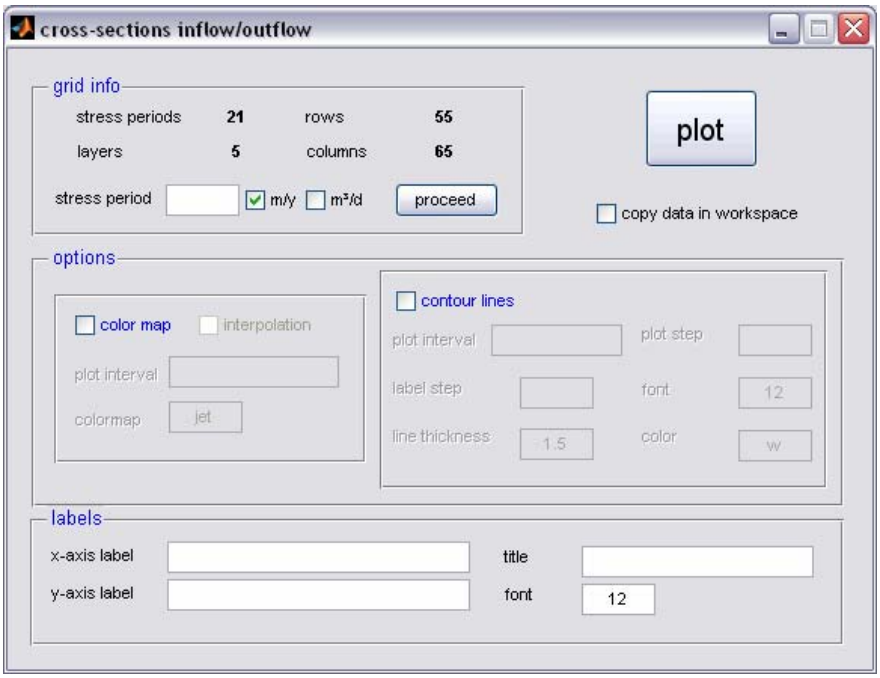


figure 4.14 *Inflow/outflow cross-sections GUI.*

In the *options box*, options for plotting the in and outflow are selected. Choose contour lines or color map by designating the appropriate box.

Plot interval: this gives by default the minimum and maximum hydraulic head occurring in the model. Alter this given the preferred plot interval, plot step and label step
Plot step: gives the step with which a contour is plotted
Label step: gives the step with which a label is plotted on the contours.
Line thickness: regulates line thickness
Font: regulates the font of the labels
Color: regulates color of labels and lines. Regular MATLAB colors are used.

Colormap: regulates color map. If an 'i' is given after the regular MATLAB color maps, the color map is inverted.

Options for labels are given in the *labels box*. Label on the x-axis, y-axis and title can be plotted. Font regulates the font of the axes, labels and title.

4.7 Solute mass

4.7.1 Solute mass versus time in an aquifer volume

This option visualises the solute mass present in a certain volume of aquifer. The *grid info box* summarises the grid sizes of the model and the maximum simulation time. Solute mass can be expressed in different units:

- kg of the solute present in the designated volume of aquifer,
- kg/m³of the designated volume of aquifer which is water saturated thus per m³ of pore volume,
- mean concentration in mg/l in the designated volume of aquifer,
- volume, which is the water saturated volume (or m³ of pore volume) of the designated volume of aquifer in which the solute is present.

This must first be indicated in the *options box*.

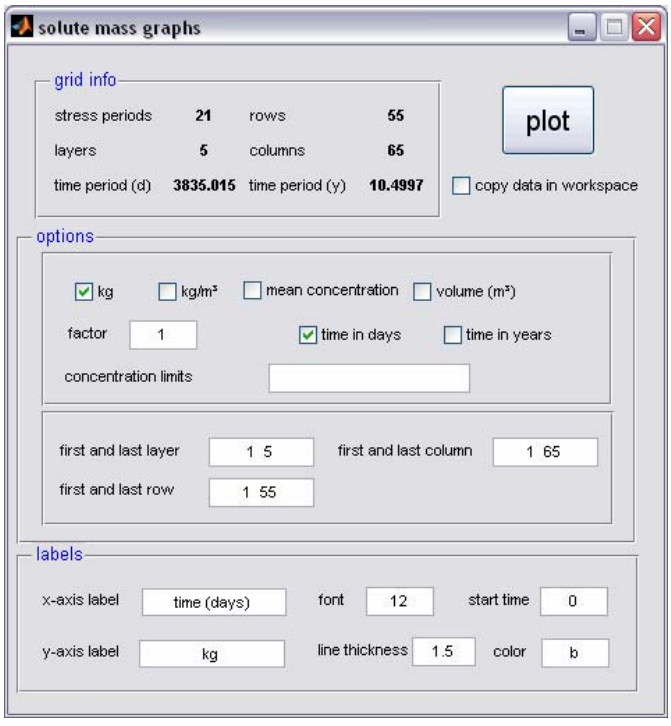


figure 4.15 *GUI to calculate solute mass in a designated part of the aquifer.*

The units of the solute mass in this option are kg, kg/m³, m³ or mg/l. If solute concentrations in the input file are not given in mg/l, a correction factor must be given or the labels of the graphs must be adjusted. If for instance concentration is given in µm/l , this factor must be 0.1.

The solute mass is calculated taken into account concentrations larger than the background concentration. If this is set at '0', the total solute mass is calculated. Using another value makes it possible to calculate surplus mass for instance due to a contamination source. Time can be indicated in days or years.

The part of the aquifer for which the solute mass will be calculated must be given next. This comprises the first and last layer, first and last row and the first and last column.

Options for labels are given in the *labels box*. Label on the x-axis and y-axis can be plotted.

Font: regulates the font of the axes, labels and legend
Line width: width of the graph line
Start time: start of the time on the x-axis. This must be given in accordance with the time option (years or days)

4.7.2 Solute mass versus time in wells

This option visualises the solute mass pumped by wells. It calculates the mean concentration (in the unit which is used in the model, in most cases mg/l) or in kg/d which would be pumped up by a number of pumping wells. This option can for instance be used to evaluate salt load in pumping wells of a water catchment or solute mass which will be pumped up by a number of wells used for aquifer clean-up. The *grid info box* summarises the grid sizes of the model and the maximum simulation time.

Then choice must be made between graphs of mean concentration or in kg/d. The units of the solute mass in this option are kg/d or mg/l. If solute concentrations in the input file are not given in mg/l, a correction factor must be given or the labels of the graphs must be adjusted. If for instance concentration is given in µm/l , this factor must be 0.1. Time can be given in days or in years.

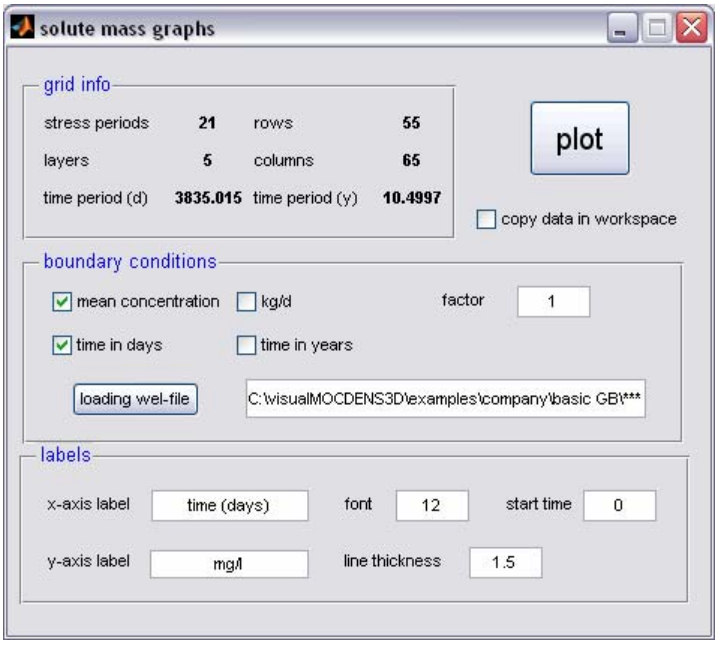
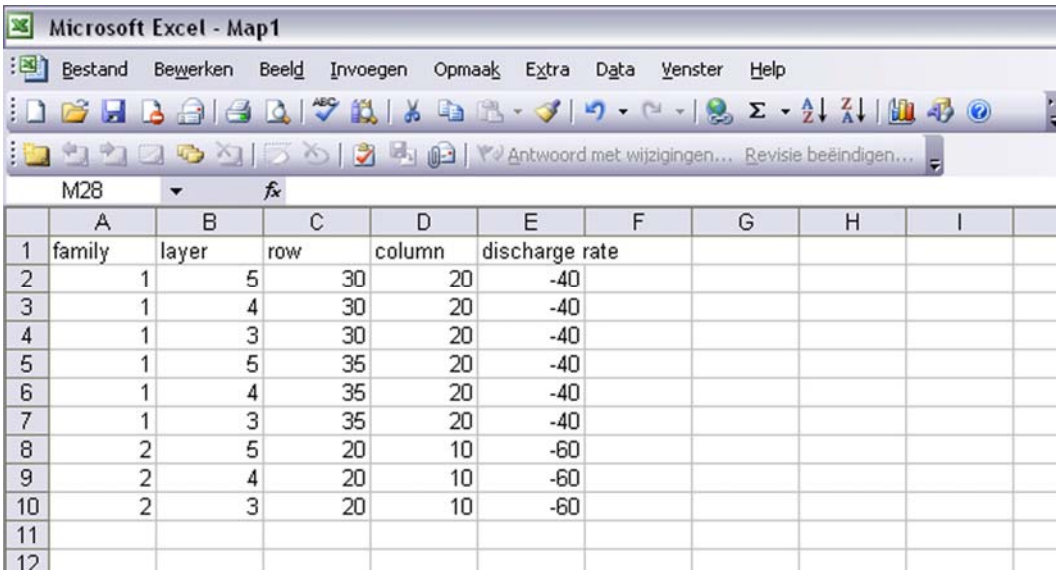


figure 4.16 *GUI to calculate solute mass in pumping wells.*



	A	B	C	D	E	F	G	H	I
1	family	layer	row	column	discharge rate				
2	1	5	30	20	-40				
3	1	4	30	20	-40				
4	1	3	30	20	-40				
5	1	5	35	20	-40				
6	1	4	35	20	-40				
7	1	3	35	20	-40				
8	2	5	20	10	-60				
9	2	4	20	10	-60				
10	2	3	20	10	-60				
11									
12									

figure 4.17 *Example of the well input file.*

The position of the wells must be given via an excel file. To calculate solute mass in kg/d, the discharge rate of each well must also be given. Figure 4.17 gives an example of an input file. Wells are subdivided in a number of families. The mean concentration or accumulated mass of all wells of a family is calculated and this is plotted in function of time. For every well, the family number, layer, row, column and discharge rate must be given.

Options for labels are given in the *labels box*. Label on the x-axis and y-axis can be plotted.

Font: regulates the font of the axes, labels and legend
Line width: width of the graph line
Start time: start of the time on the x-axis. This must be given in accordance with the time option (years or days)

4.7.3 Horizontal and vertical cross-sections of solute mass

Horizontal and vertical cross-sections of solute mass can be plotted using these options. The unit of the solute mass is kg per m³ of water saturated aquifer material (or per m³ of pore volume). If solute concentrations in the input file are not given in mg/l, a correction factor must be given or the labels of the graphs must be adjusted. If for instance concentration is given in µm/l, this factor must be 0.1.

The other options in the GUI are the same as for horizontal and vertical cross-sections of head and concentration (4.4.2 and 4.4.3). Besides the solute mass, hydraulic heads and effective velocities can be plotted.

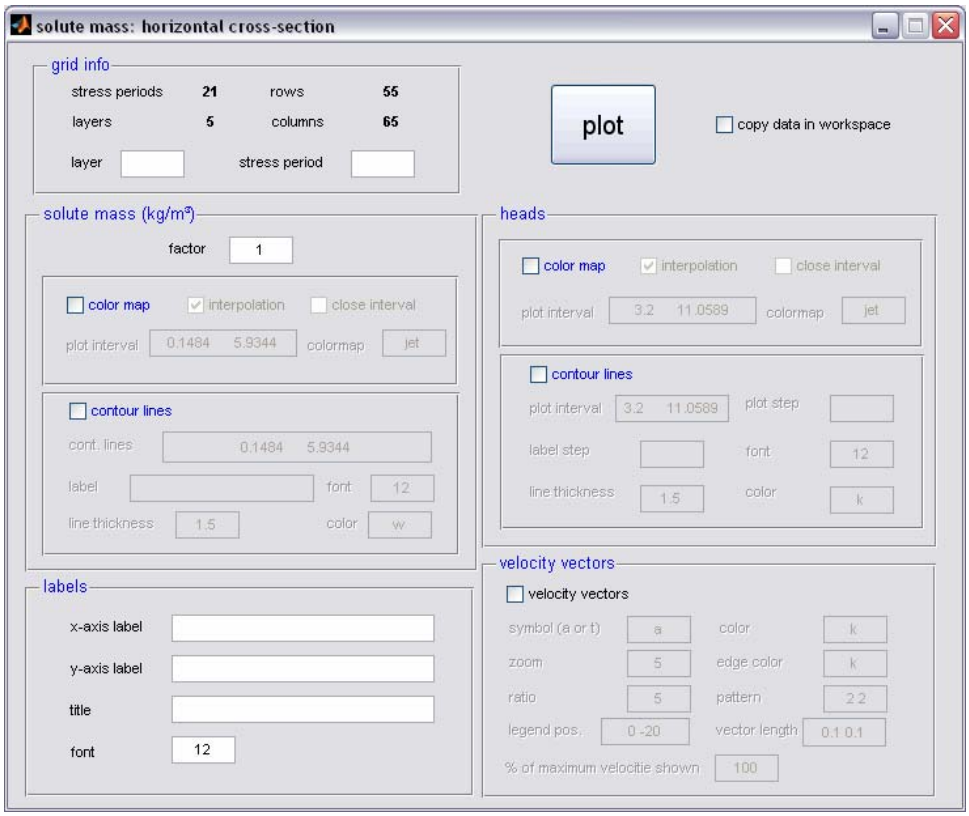


figure 4.18 *Input GUI for horizontal cross-sections of solute mass.*

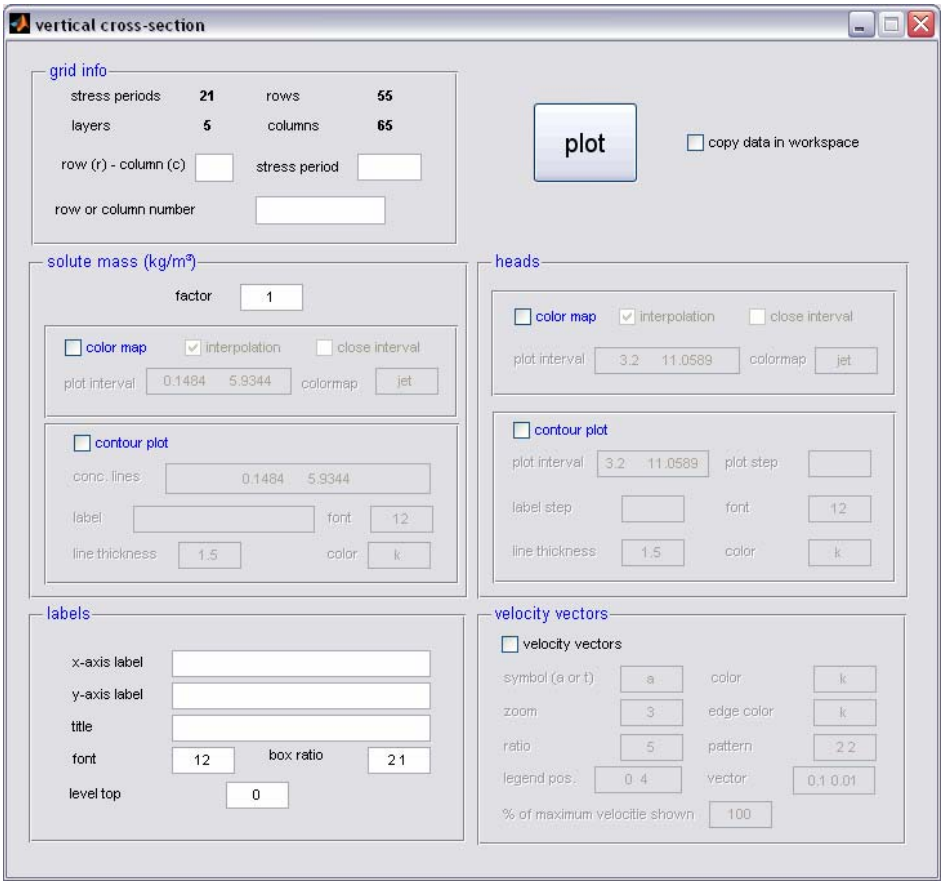


figure 4.19 *Input GUI for vertical cross-sections of solute mass.*

4.8 Subsidence and compaction

4.8.1 Introduction

Proper use and understanding of the applications and limitations of this option is needed. It is also important that subsidence can be calculated using a variable boundary type model but that the specific elastic storage is constant throughout the model time domain.

In Visual MOCDENS3D compaction of a layer with thickness Δb (m) is calculated using a one-dimensional formula:

$$\Delta b = \left(S_S - \rho_w g n_e \beta_w\right) b \Delta s$$

where S_S is the specific elastic storage (m^{-1}), ρ_w is the density of the pore water (kg/m^3), g acceleration due to gravity (m/s^2), n_e the effective porosity (-), b the initial thickness of the layer (m) and β_w the compressibility of water (ms^2/kg). Subsidence at a level is then the sum of the compactions of all layers below that level.

This means that a value for the specific elastic storage must be known. The other parameters are grid dimensions or physical constants. When a transient model is used, values for specific elastic storage are readily available. This is not the case for a permanent flow model. Then there are two options. Specific elastic storages are given as new input or they are be calculated according to the relation developed by Van der Gun (1979):

$$S_S = 1.8\ 10^{-6} + 2.59\ 10^{-4} d^{-0.7}$$

Where d is the depth below surface (m).

By calculating the compaction in this way, you must be aware of some points:

- Compaction is calculated using a one-dimensional formula using stress-independent parameters. No distinction is for instance made between elastic and inelastic compaction. In this way compaction of a layer is slightly overestimated and must be regarded as a worst case estimation.
- Compaction is a transient phenomenon: it evolves in function of head evolution. Therefore, there are inherent drawbacks of computing compaction with a permanent model. Between different stress periods drawdowns evolve immediately to a new permanent situation without calculating the transient behaviour. The same holds for compaction.
- De “Van der Gun” relation is an approximation how specific elastic storage changes in function of depth. This was determined in the Dutch dune area in sandy sediments. Consequently, it forms only a first approximation.

4.8.2 Specific elastic storage input

First step in the calculation is loading the specific elastic storage in the workspace. This is done by the specific elastic storage input GUI (figure 4.20). Two options are possible: defining values which are constant for one layer using the GUI or loading the specific elastic storage from an excel file.

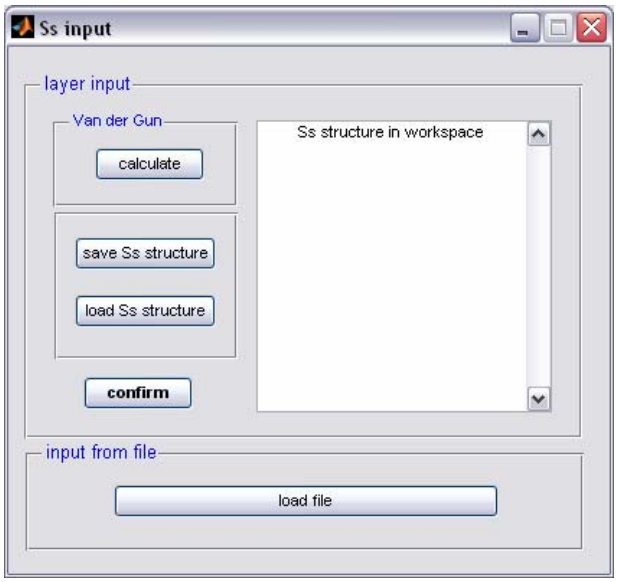


figure 4.20 *GUI regulating the input for the specific elastic storage coefficient..*

For the first option, the values can be typed in the GUI window. The same number of values as layers must be given. By pushing the "confirm" button, these values are loaded in the workspace and ready to be used. The specific elastic storage values can also be calculated according to the Van der Gun relation. This is done simply by pushing the "calculate" button and the values appear in the GUI window. Again, the values must be confirmed to load them in the workspace. The values can be saved for later use by pressing the "save S_S structure" button and can be loaded by pressing the "load S_S structure" button.

Using specific elastic storages from an excel file is done by loading the file. The values are set automatically in the workspace.

4.8.3 Horizontal and vertical cross-sections

Horizontal and vertical cross-sections of compaction and subsidence can be plotted using these options. Compaction and subsidence is calculated in mm.

First the layer and stress period for which compaction or subsidence is calculated must be given as is the reference stress period. This reference stress period is the stress period where compaction and subsidence is zero. The hydraulic head differences needed to calculate compaction of layers is the differences of heads between the stress period you want to plot and this reference stress period.

The other options in the GUI are the same as for horizontal and vertical cross-sections of head and concentration (4.4.2 and 4.4.3) with the exception that no velocity vectors can be plotted.

If subsidence is chosen for a layer different from layer 1, then this is the sum of compaction of all layers below and including the selected layer.

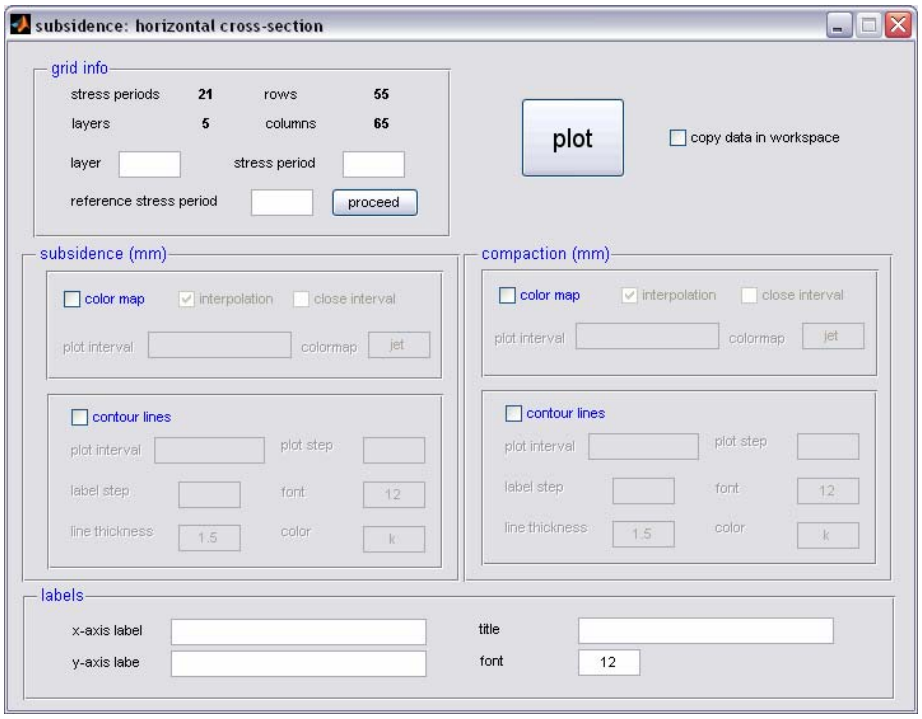


figure 4.21 *Input GUI for horizontal cross-sections of compaction and subsidence.*

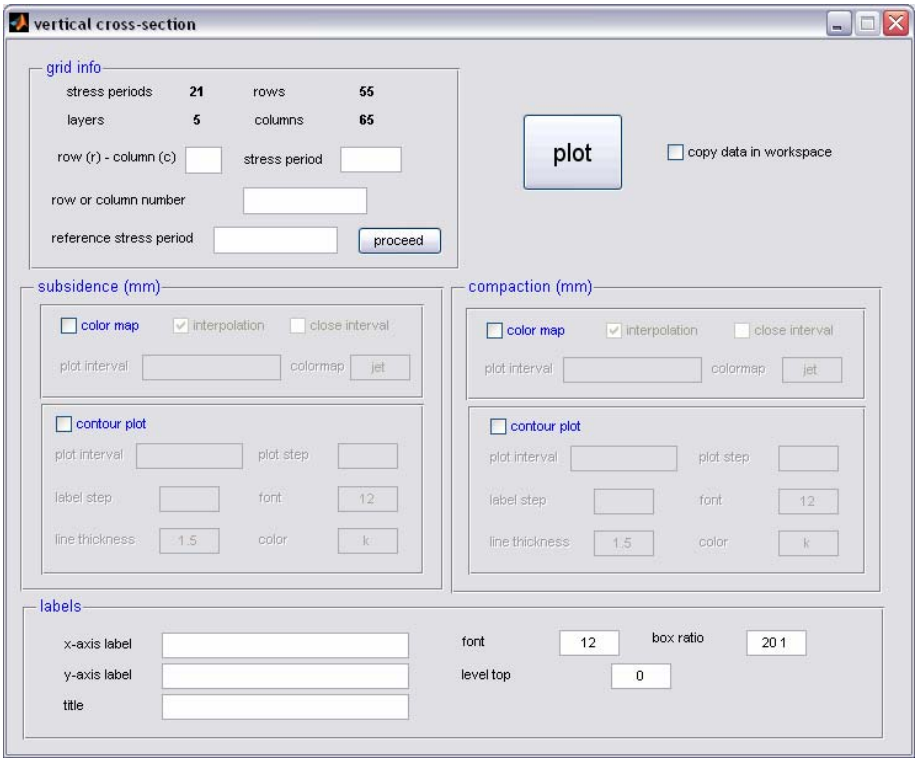


figure 4.22 *Input GUI for vertical cross-sections of compaction and subsidence.*

4.8.4 Graphs

figure 4.23 *Input GUI for f compaction and subsidence graphs.*

This option plots compaction of a layer or subsidence up to a level in function of time (figure 4.23). First it subsidence versus time or compaction versus time is chosen as are the time units (days or years). Secondly the reference stress period is given as is the time interval you want to plot. By default the time intervals spans the whole time domain of the model. Then layers, rows and columns of which you want to plot compaction or subsidence are given. More than one cell can be given. If in this case the value for each choice is the same, only one value must be given.

Finally, labels for x and y axis, font size and line width size can be given as is the start time of the graph.

4.9 3D plots

4.9.1 3D cross-sections

This option makes it possible to visualise head, concentration or effective velocities with different cross-sections through the model domain. Effective velocities are calculated as the sum of the effective velocities in the x-, y- and z-directions.

The *grid info box* summarises the grid sizes of the model.

The *3D cross-sections box* regulates the input for the cross-sections. These cross-sections can be drawn with slices through the aquifer for which heads, concentrations or effective velocities can be plotted with color maps or superposed contour lines.

First, indicate by using the check boxes if heads, concentrations or velocities are plotted. Velocities are calculated as the absolute velocity. Choose then the cross-sections by indicating the levels (z-

coordinates, in m), the x-coordinates (in m) and the y-coordinates (in m). by default, cross-sections according to the last column and first row are given.

Stress period: give time step
z-coord.: give the levels for horizontal cross-sections, in m
y-coord.: give the y-coordinate of the vertical cross-section, in m
x-coord.: give the x-coordinate of the vertical cross-section, in m
Plot interval: this gives by default the minimum and maximum hydraulic head occurring in the model. Alter this given the preferred plot interval, plot step and label step
Close interval: if the close interval box is indicated, every head outside the interval is indicated in white, otherless the cells are given the color of the minimum or maximum head.
Map: give the color map, standard MATLAB color maps are used. If an 'i' is given after the regular MATLAB color maps, the color map is inverted.
Ramp down/up: choose between the rampdown or rampup MATLAB option
Trans. Factor: factor determines the translucency of the cross-sections
Ratio: give ratio of between the x-, y- and z-directions
Level top (mTAW): indicates the level of the top of the model in mTAW
Font: font of the labels
Contour lines: if filled in, the given contourlines are drawn on the different cross-sections
Color: color of the isolines, default MATLAB colors are to be used
Line width: width of the contour lines

Labels on the x-axis, y-axis and legend can be plotted via the *labels box*. Font regulates the font of the axes, labels and title.

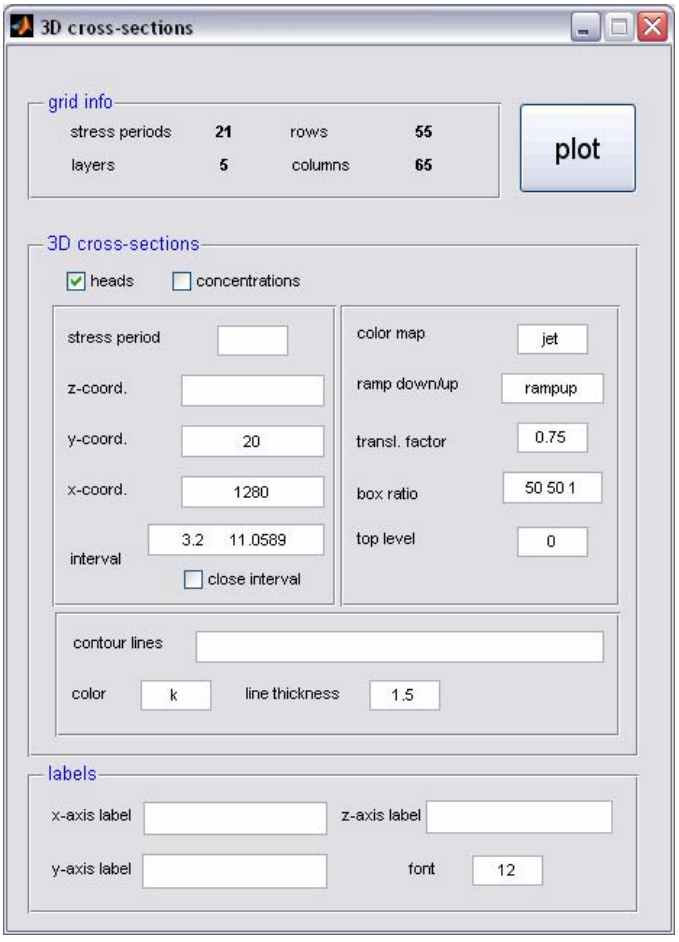


figure 4.24 *3D cross-sections GUI.*

4.9.2 Isosurfaces

This option plots 3D surfaces of head or concentration using the isosurface or isocaps function in MATLAB. More than one isosurface can be plot but only one isosurface can be plotted if isocaps are chosen.

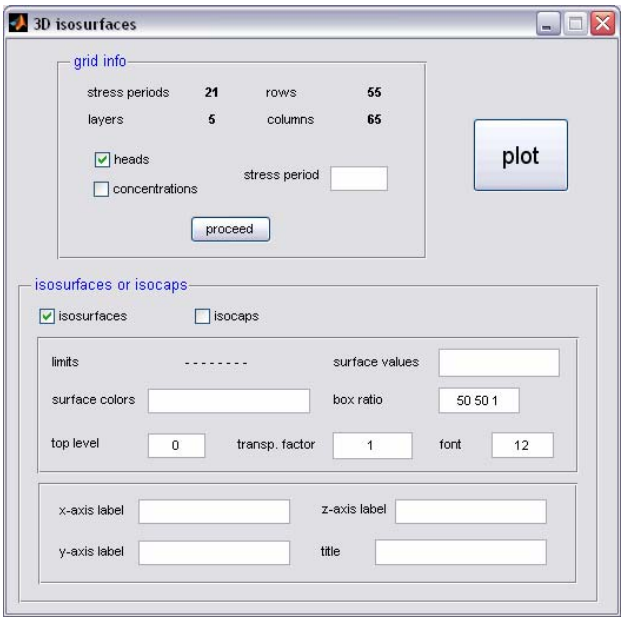


figure 4.25 *3D isocaps GUI.*

The *grid info box* summarises basic grid input. Also a choice must be made of heads, or concentrations isosurfaces will be plotted for a given time step.

Stress period: give stress period

By pushing the 'proceed' button, minimum and maximum values are given in the limits section of the *isosurfaces or isocaps box*.

The *isosurfaces or isocaps box* gives the options for plotting the surfaces. Indicate by clicking on the appropriate box if isosurface or isocaps are to be used.

Surface value: give the value of the surfaces. By using isosurfaces, more than one value can be chosen. By using isocaps, only one value can be chosen.
Colors: give the colors of the surfaces. By using isosurfaces, more than one value can be chosen. By using isocaps, only one value can be chosen.
Limits: repetition of the limits which can be chosen.
Ratio: give ratio of between the x-, y- and z-directions
Level top (mTAW): indicates the level of the top of the model in mTAW
Trans. Factor: factor determines the translucency of the cross-sections
Font: font of the labels

Labels on the x-axis, y-axis and legend can be plotted via the *labels box*. Font regulates the font of the axes, labels and title.

4.10 Movie options

4.10.1 Horizontal and vertical cross-sections

With these options, a movie is made showing the evolution of the fresh water heads, concentrations and/or the effective velocities in function of time. This movie is in an avi-format. Horizontal as well as vertical cross-sections can be made.

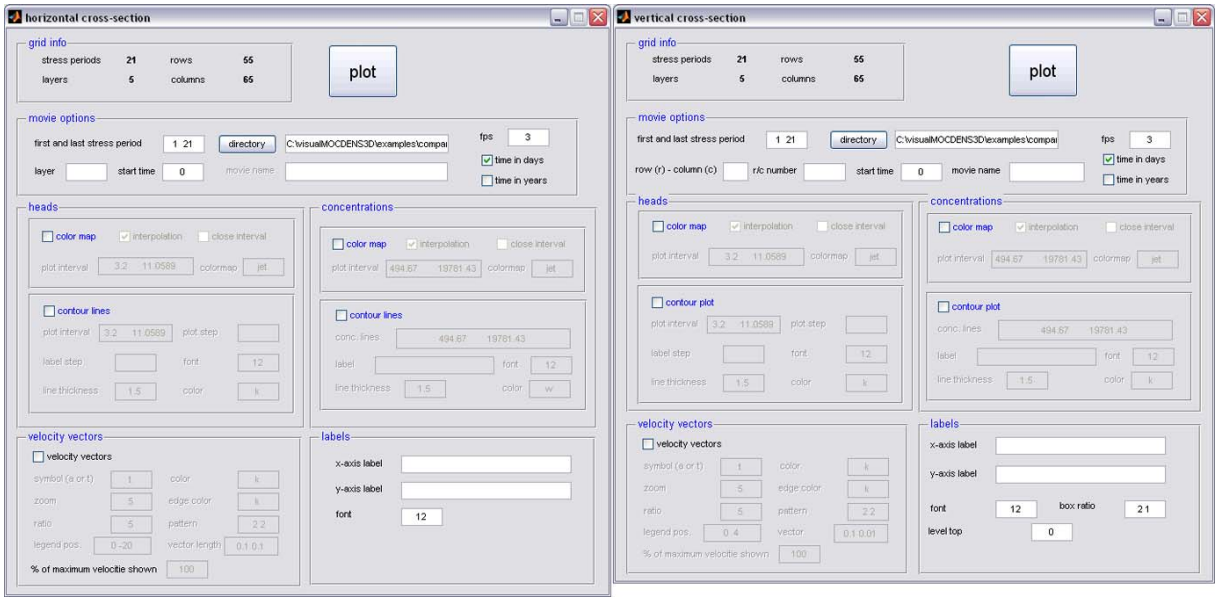


figure 4.26 *GUI's for making movies using horizontal (left) and vertical (right) cross-sections.*

The input GUI's are the same as for the horizontal and vertical cross-sections (see sections 4.2.1 and 4.2.2). Only some additional information must be given to run the movie option, grouped together in the *movie options box*. The GUI's for the two possibilities are given in figure 4.26.

For a horizontal cross-section the layer number and the first and last stress period of the model used for the movie must be given. The model time will be given above the plot. This time can be plotted in days or in years as indicated by the check boxes. The initial time of the model is default set at 0 days or years but can be altered by indicating the start time in the start box. Path and movie name determine were and under which name the movie will be saved. Fps determines the frames per second of the movie.

These options are all the same for a movie with vertical cross-section instead that it must be indicated if a row or column cross-section must be made and which row or column number must be used.

4.10.2 Differences stress periods

With these options a movie is made showing the differences of head or concentration relative to a reference stress period. In this way the evolution of for instance drawdown can be visualised. This movie is in an avi-format. Horizontal as well as vertical cross-sections can be made.

The input GUI's are the same as for the differences in horizontal and vertical cross-sections (see sections 4.3.1 and 4.3.2). Only some additional information (see 4.8.1) must be given to run the movie option, grouped together in the *movie options box*. The GUI's for the two possibilities are given in figure 4.27.

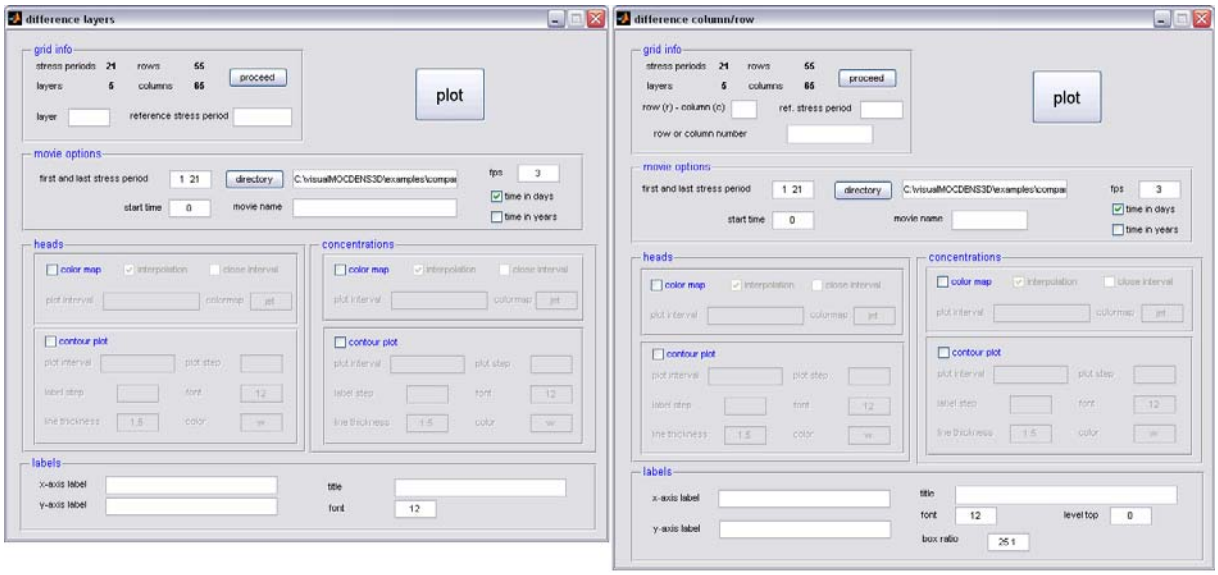


figure 4.27 *GUI's for making movies of differences between stress-periods using horizontal (left) and vertical (right) cross-sections.*

4.10.3 3D cross-sections

This option makes it possible to make a movie of evolution of head or concentrations in function of time, using 3D cross-section (figure 4.28). The 3D cross-section options (see 4.7.1) is here fore used as basis. Only some additional information (see 4.8.1) must be given to run the movie option, grouped together in the *movie options box*.

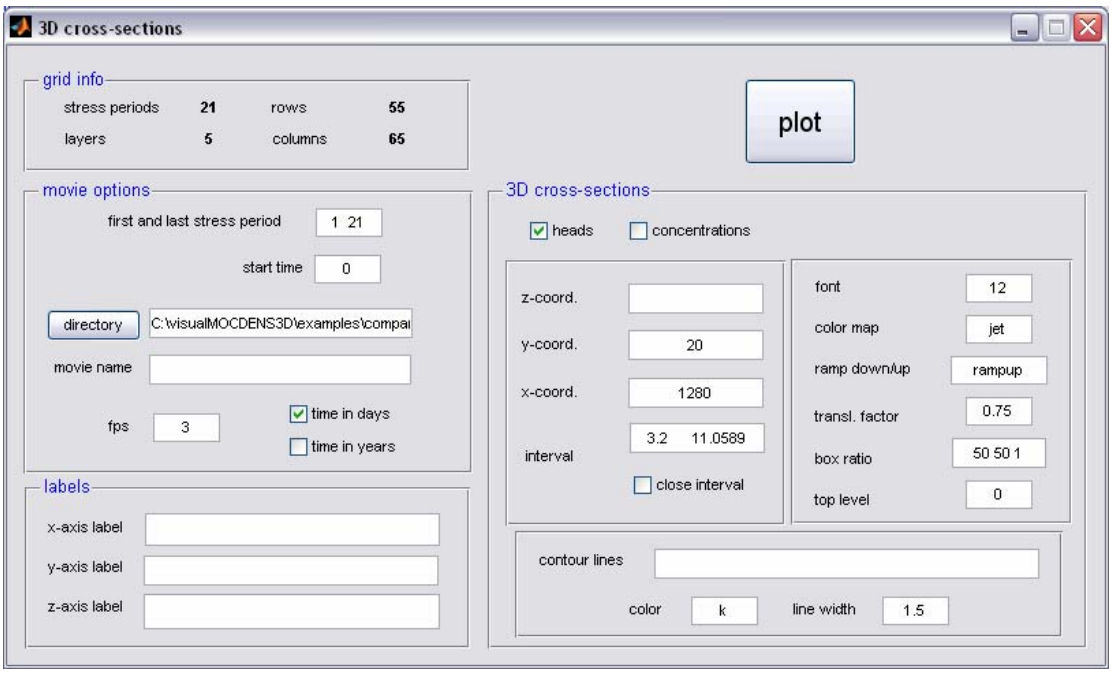
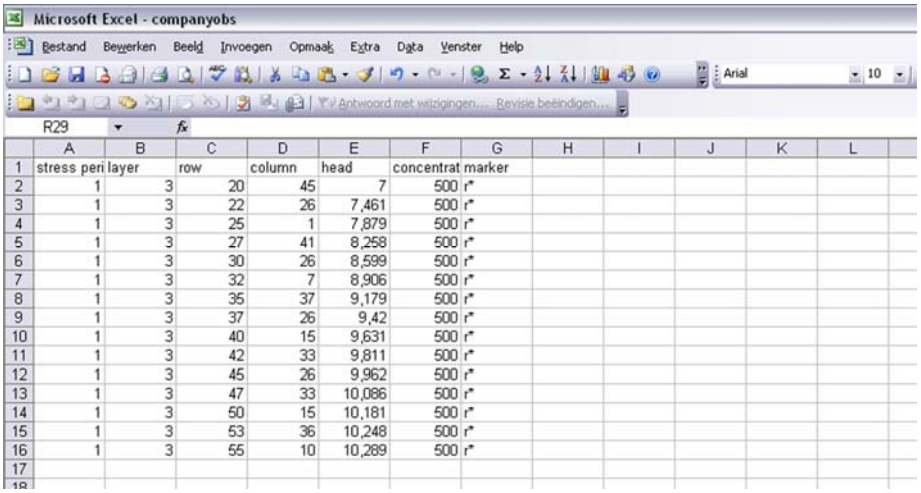


figure 4.87 *GUI's for making movies of 3D cross-sections through the aquifer.*

4.11 Calculations versus observations

4.11.1 Analysis of residuals

This option visualises and helps to analyse the residuals using some statistic properties. Residuals are the observed minus the calculated heads or observations. In the *file input box*, the name of a file listing the observations must be given. This is an excel file and an example is given in figure 4.29. The observations are listed under each other. The stress period of is given in the first column of the excel file, layer in the second, row in the third and column in the fourth. Then the observed fresh water head and concentration are given. A marker lay-out is given in the last column. This consists of a color and a style for the marker and this can be different for every observation. Finally, it must be indicated if head or concentration observations will be analysed.



	A	B	C	D	E	F	G
1	stress peri	layer	row	column	head	concentrat	marker
2	1	3	20	45	7	500	r*
3	1	3	22	26	7,461	500	r*
4	1	3	25	1	7,879	500	r*
5	1	3	27	41	8,258	500	r*
6	1	3	30	26	8,599	500	r*
7	1	3	32	7	8,906	500	r*
8	1	3	35	37	9,179	500	r*
9	1	3	37	26	9,42	500	r*
10	1	3	40	15	9,631	500	r*
11	1	3	42	33	9,811	500	r*
12	1	3	45	26	9,962	500	r*
13	1	3	47	33	10,086	500	r*
14	1	3	50	15	10,181	500	r*
15	1	3	53	36	10,248	500	r*
16	1	3	55	10	10,289	500	r*
17							

figure 4.29 *Example of input of observations for the analysis of residuals option.*

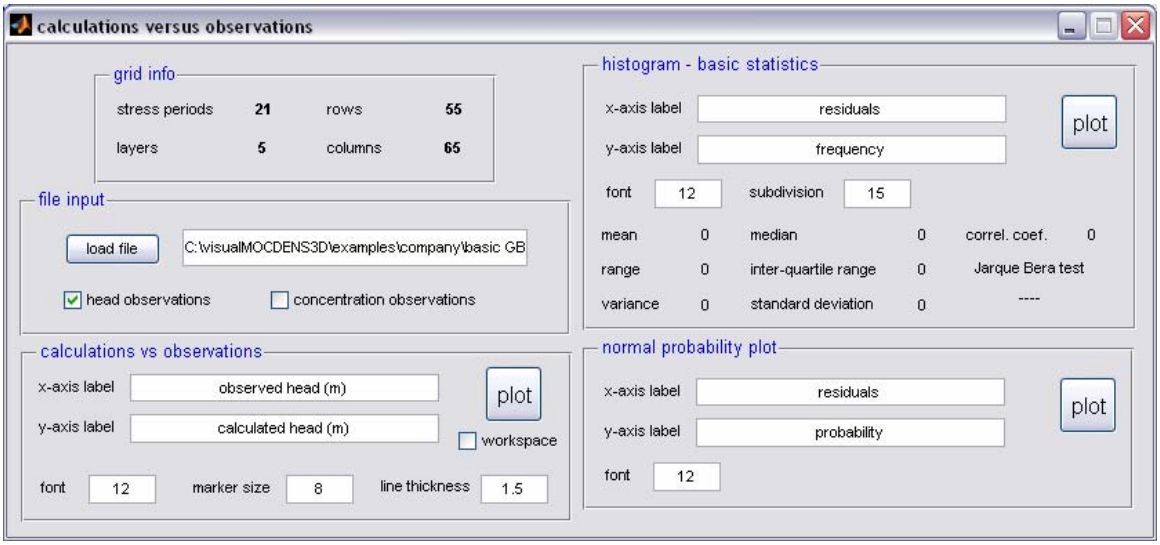


figure 4.30 *GUI helping in the analysis of the residuals.*

Via the *calculations vs observations box*, the former are plotted against the latter. A line indicating a perfect fit is also plotted. Font, marker size and line width can be altered with the appropriate boxes.

Using the histogram – basic statistics box, a histogram of the residuals is made. Labels, font and number of subdivisions for the histogram can be altered. Additionally, a number of statistical parameters are calculated (mean, median, range, inter-quartile range, variance, standard deviation and

correlation coefficient) and the residuals are tested for showing a normal distribution using the Jarque Bera test.

Using the *normal probability plot box*, a normal probability plot is constructed. Font of the plot can be altered.

4.11.2 Observation wells

This option plots observations of fresh water head or concentration versus calculated concentration. This can be done for individual wells (observation wells) or for the net result of concentration pumped up by a number of wells (well battery).

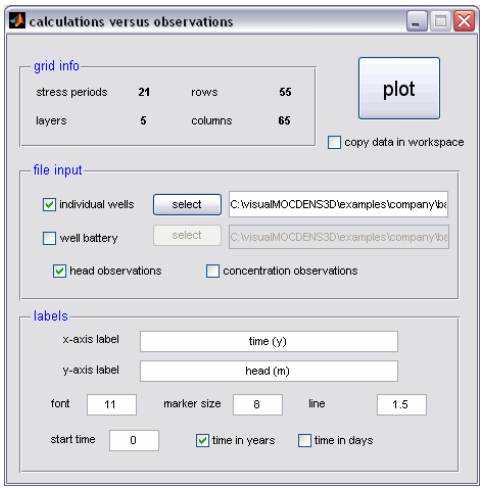


figure 4.31 *Plotting of calculations versus observations GUI.*

Microsoft Excel - Map1

Bestand Bewerken Beeld Invoegen Opmaak Extra Data Venster Help

Arial

Antwoord met wijzigingen... Revisie beëindigen...

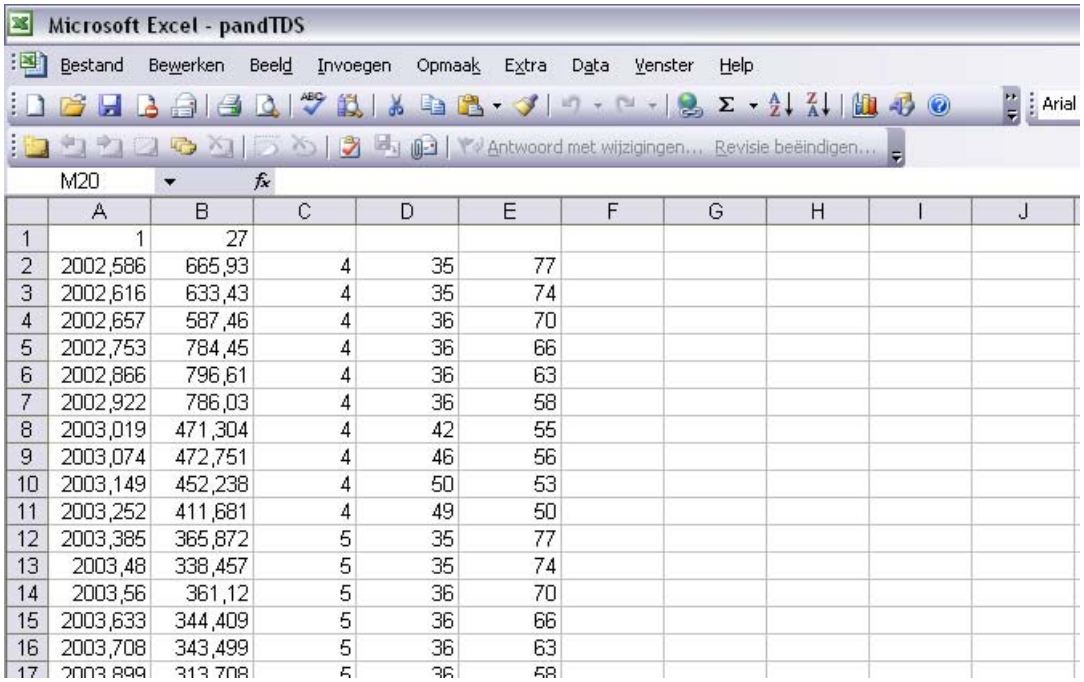
Q20

	A	B	C	D	E	F	G	H	I	J	K
1	time	layer	row	column	head	concentrat	marker				
2	1	2	24	15	7,8	500	r*				
3	2,9	2	24	15	8,9	500	r*				
4	5,3	2	24	15	9,2	500	r*				
5	1	2	24	15	5,8	500	b*				
6	2,9	2	24	15	6,3	500	b*				
7	5,3	2	24	15	7,9	500	b*				
8											

figure 4.32 *Example of input for individual wells.*

In the *file input box*, choice must be made using individual wells or a well battery and if head or concentration observations are used. For a well battery, only concentrations can be compared. The input of observations is via an excel file. An example in case of individual wells is given in figure 4.31. Observation time, layer, row, column, fresh water head, concentration and marker are given in the different columns of the excel sheet. All observations are given under each other. These are automatically sorted according to equal layer, row and column number identifying observations in the same well.

In case of a well battery, the input format is given in figure 4.33. In the first row, the stress periods in which the well battery is active is given. This is in this time from stress period 1 to 27. In the first two columns, from row 2 onwards, the time and concentration observations are given. In the third to fifth column, again from row two onward, the layer, row and column of all wells part of the well battery are given.



	A	B	C	D	E	F	G	H	I	J
1	1	27								
2	2002,586	665,93	4	35	77					
3	2002,616	633,43	4	35	74					
4	2002,657	587,46	4	36	70					
5	2002,753	784,45	4	36	66					
6	2002,866	796,61	4	36	63					
7	2002,922	786,03	4	36	58					
8	2003,019	471,304	4	42	55					
9	2003,074	472,751	4	46	56					
10	2003,149	452,238	4	50	53					
11	2003,252	411,681	4	49	50					
12	2003,385	365,872	5	35	77					
13	2003,48	338,457	5	35	74					
14	2003,56	361,12	5	36	70					
15	2003,633	344,409	5	36	66					
16	2003,708	343,499	5	36	63					
17	2003,899	313,708	5	36	58					

figure 4.33 *Example of input for a well battery.*

In the *label box*, options for plotting the figure are given.

Font: regulates the font of the labels
Marker size: size of the observation markers
Line width: width of the graph line
Start time: start of the time on the x-axis. This must be given in accordance with the time option (years or days), indicated by the check boxes

4.11.3 Map of residuals

This option visualises the residuals (head or concentration) on a map or in 3D. This can provides a help, with the other options described in section 4.11, to track down systematic differences between observations and calculations.

Head and concentration observations are read from an excel file. This is the same file as described in 4.9.1. Reference to this file is given in the *file input box*. A choice must be made if head or concentrations observations will be used.

In the *options box*, first the stress period of which the residuals will be plotted must be given. Then choice must be made between residuals per layer or on a 3D plot. In the former case, the *layer* number must be given, in the latter case, the level of the top of the model must be given. Finally, some lay-out options an be changed.

Marker symbol: symbol whit which residuals will be plot
Marker unit: the larger the absolute value of the residuals, the larger the marker symbol will be. The relative size of the symbol can be altered by varying the marker unit number
Marker color: gives the colors of the markers. Two colors must be given, one for negative residuals and one for positive residuals
Font: regulates the font of the labels

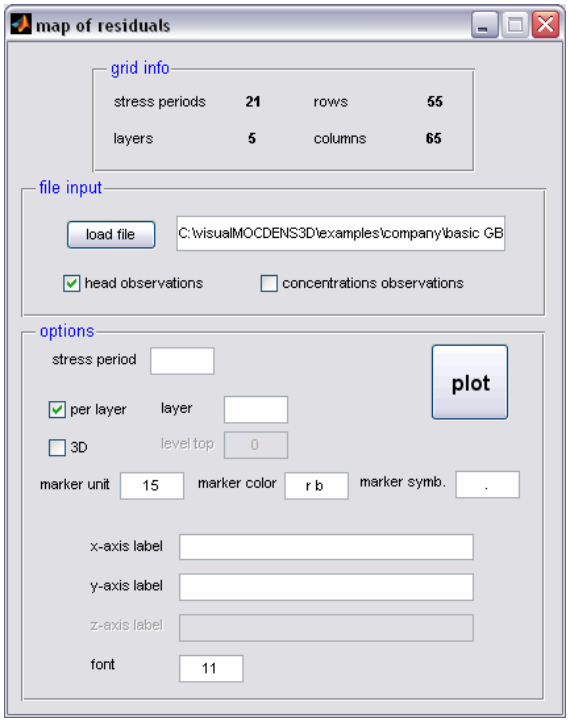


figure 4.34 *GUI for plotting residuals on a map or in 3D.*

4.12 Extra

4.12.1 Stress periods

This option visualises the number and length of stress periods. Two options are possible:

- Bar plot of all stress periods (indicate "length of stress periods" box)
- Length of stress periods in function of model time (indicate "divisions in time" box)

Days or years (d or y): choose between days or years for the time
Start of model: start date of the model
Color: color of the plot
Font: font of the plot

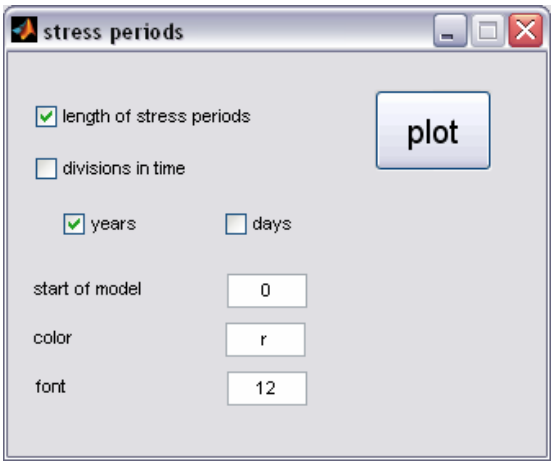


figure 4.35 *Stress periods GUI..*

5 ParTrack module

5.1 Flow paths, capture zones and travel times

The ParTrack module visualises flow paths (or streamlines) and calculates capture zones and travel times using a steady state or transient state flow pattern of a MOCDENS3D model. To calculate these, particle tracking is used.

To calculate a flow path, a particle is placed at a certain position which is the beginning of the flow path. This particle is characterised by its x-, y- and z-coordinates in the model grid. Then, the particle is followed during a time T. Therefore, the time T is subdivided in n time increments Δt. Its position x^{n+1}, y^{n+1}, z^{n+1} at time step n+1 is:

$$x^{n+1} = x^n + v_x \Delta t \qquad y^{n+1} = y^n + v_y \Delta t \qquad z^{n+1} = z^n + v_z \Delta t \tag{1}$$

where x^n, y^n, z^n are the coordinates at time step n and v_x, v_y and v_z are the effective groundwater flow velocities in the coordinate directions. These effective velocities are calculated using the velocity field of the MOCDENS3D model. If a steady state flow field is chosen, the stress period must be indicated. Otherwise, when a transient state flow field is chosen, the stress period in which the flow path starts must be indicated. Based on the time increment and length of the different stress periods in the model, the appropriate velocity field is selected to calculate particle movement.

The calculation of capture zones is also based on this concept. Throughout the model domain, particles are placed. These are again characterised by their coordinates. The pathways of all these particles are followed until they arrive in a cell where they disappear from the model for instance because of a pumping well or a river or drainage system is present. The time needed to travel from the starting point to the point where each particle disappears from the model is registered and these are used to map the capture zones.

As explained in the section on MOCDENS3D stability criteria (section 2.2.4), the time increment must be chosen carefully. The distance a particle moves during a time increment is equal to (or approximately so in case where particles cross a cell face and the adjacent cells have different properties) the velocity at the location of the particle times the length of the time increment (equation 1). In effect, this constitutes a linear spatial extrapolation of the position of a particle from one time increment to the next. Konikow and Bredehoeft (1978) note that where streamlines are curvilinear, the extrapolated position of a particle will deviate from the streamline on which it was previously located. This deviation introduces an error into the numerical solution that is proportional to the time increment. Thus for a given velocity field and grid (the latter also determines the streamlines), some restrictions must be placed on the size of the time increment to assure that the distance a particle moves in the x-, y- and z-direction does not exceed some critical distances. These critical distances can be related to the grid dimensions by

$$\Delta t V_{x(p)} \le \gamma \Delta x \qquad \Delta t V_{y(p)} \le \gamma \Delta y \qquad \Delta t V_{z(p)} \le \gamma \Delta z \tag{2}$$

where γ (or CELDIS in the input files) is the fraction of the grid dimensions that particles will be allowed to move (normally, $0 < \gamma < 1$). From equation 2 the smallest time increment can again be determined.

5.2 Flow paths

Different GUIs are available to calculate and plot flow paths for a 3D and a 2D model. In case of a 3D model distinction is made if starting points are placed via a regular pattern or via a specific (irregular) user defined pattern.

5.2.1 Flow paths with 3D cross-sections as background

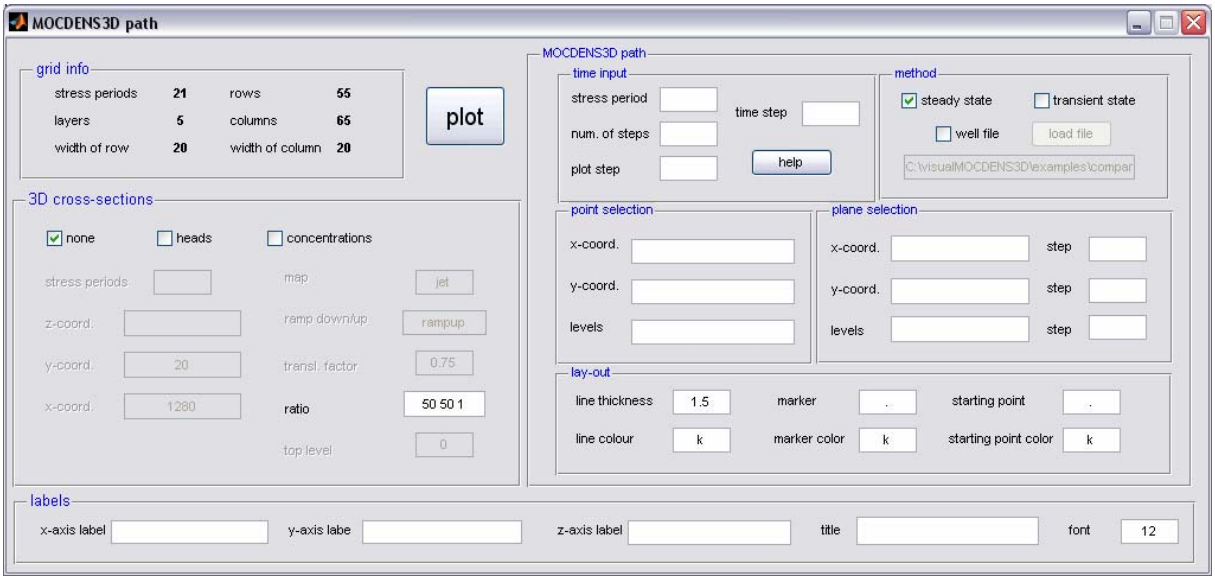


figure 5.1 *Flow path GUI. Flow paths are plotted with 3D cross-sections of heads or concentrations as possible background.*

This option visualises flow paths with head or concentration cross-sections as possible background.

The *grid info box* summarises the grid sizes of the model

The *3D cross-sections box* regulates the input for the cross-sections. These cross-sections can be drawn with slices through the aquifer for which heads or concentrations can be plotted with color maps.

First, indicate by using the check boxes if heads or concentrations are plotted. Choose then the cross-sections by indicating the levels (z-coordinates, in m), the x-coordinates (in m) and the y-coordinates (in m). By default, cross-sections according to the last column and first row are given.

Stress period: give stress period for which the cross-sections will be plotted
z-coord.: give the levels for horizontal cross-sections, in m
y-coord.: give the y-coordinate of the vertical cross-section, in m
x-coord.: give the x-coordinate of the vertical cross-section, in m
Map: give the colour map, standard MATLAB colour maps are used. If an 'i' is given after the regular MATLAB colour maps, the colour map is inverted.

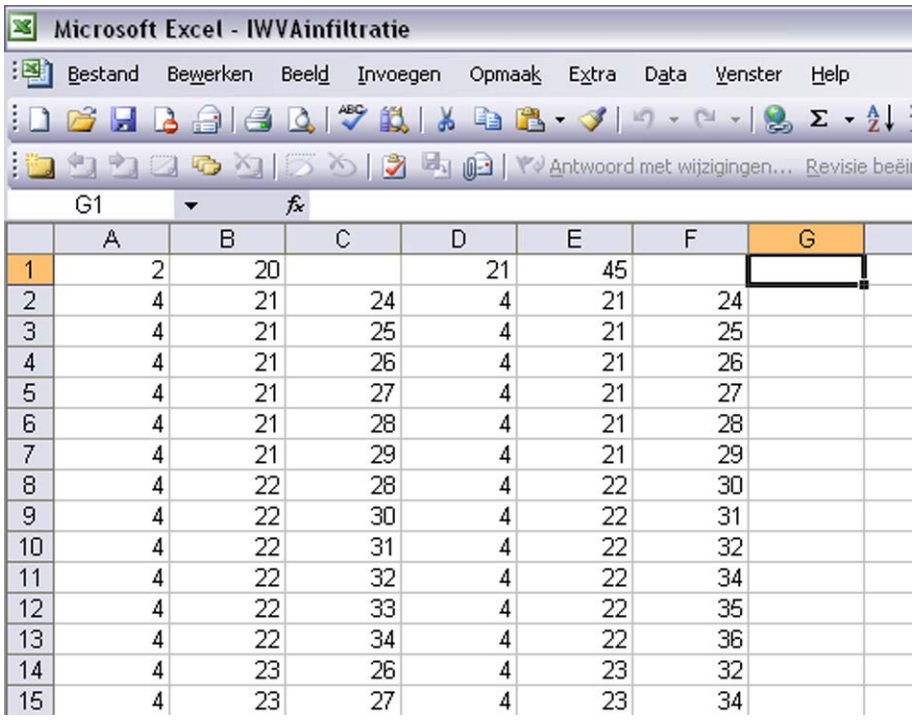
Ramp down/up: choose between the rampdown or rampup MATLAB option
Trans. Factor: factor determines the translucency of the cross-sections
Ratio: give ratio of between the x-, y- and z-directions
Level top: indicates the level of the top of the model in mTAW

If the option 'none' is chosen, only a box is made in which the flow paths will be plotted.

The *MOCDENS3D path box* regulates the input for the calculations of the flow paths. The time input box regulates the time increment and number of steps and particle tracking algorithm.

Stress period: the stress period of which velocities are used, calculating steady state flow paths, or the stress period used as starting point calculating transient state flow paths
Number of steps: number of steps with length as given by the time step
Plot step: number of step after which a marker is plotted
Time step: length of time step (d). If the 'help' button is pushed, a help for choosing this time step is provided. The time step is suggested based on the maximum velocities according to the rows, columns and layers and a percentage of a cell that can be moved in one time step (the so called celdis (%)).

The *method box* regulates if steady state or transient state flow paths are plotted. If a well file is present, the well file box must be indicated and the right path where this file is found must be indicated. The well file must be an excel file. An example is given in figure 5.2.



	A	B	C	D	E	F	G
1	2	20		21	45		
2	4	21	24	4	21	24	
3	4	21	25	4	21	25	
4	4	21	26	4	21	26	
5	4	21	27	4	21	27	
6	4	21	28	4	21	28	
7	4	21	29	4	21	29	
8	4	22	28	4	22	30	
9	4	22	30	4	22	31	
10	4	22	31	4	22	32	
11	4	22	32	4	22	34	
12	4	22	33	4	22	35	
13	4	22	34	4	22	36	
14	4	23	26	4	23	32	
15	4	23	27	4	23	34	

figure 5.2 *Example for the input of well or extraction (drainage, rivers, etc.) points..*

The first line gives the intervals of the stress periods for which a well configuration applies. In the example, two well configurations are used, the first between time step 2 to 20, the second from time step 21 to 45. No wells are active in the first stress period. For every such period, the layer, row and column are given from the second line onward. These are thus given in columns A, B and C for the first period, in columns D, E and F for the second period etc.

Flow paths can be plotted in two ways. If a selection of specific starting points is preferred, then the point selection option must be chosen.

x-coordinate: x-coordinates (m) of the different points
y-coordinate: y-coordinates (m) of the different points
levels: levels (m) of the different points

Starting points can be grouped in planes. These are given in the plane selection section.

x-coordinate: x-coordinates (m) of vertical planes parallel with YZ-plane, thus according to the columns
y-coordinate: y-coordinates (m) vertical planes parallel with XZ-plane, thus according to the rows
levels: levels (m) horizontal planes parallel with XY-plane, thus according to the layers
step: step (m) in the two directions by which the starting points are set.

The lay-out box is used to define the lay-out of the flow paths.

Line width: width of the flow paths
Line colour: colour of the flow paths
Marker: symbol of a marker, standard MATLAB symbols are used
Marker colour: colour of a marker, standard MATLAB colours are used
Starting point: symbol of the starting point, standard MATLAB symbols are used
Starting point colour: colour of the starting point, standard MATLAB colours are used

Label on the x-axis, y-axis and legend can be plotted via the *labels box*. Font regulates the font of the axes, labels and title.

By using the 'rotate 3D' button in the figure window, the box can be rotated in every possible direction to view better the flow paths. Also the flow paths can be projected in the XY, XZ or YZ plane.

5.2.2 Flow paths with isosurfaces as background

This option visualises flow paths with head or concentration isosurfaces as background.

The *grid info box* summarises basic grid input. Also a choice must be made of head or concentration isosurfaces or isocaps will be plotted for a given time step.

Stress period: give stress period of which the isosurface(s) will be plotted

By pushing the 'proceed' button, minimum and maximum values are given in the limits section of the *isosurfaces or isocaps box*.

The *isosurfaces or isocaps box* gives the options for plotting the surfaces. Indicate by clicking on the appropriate box if isosurface or isocaps are to be used.

Surface value: give the value of the surfaces. By using isosurfaces, more than one value can be chosen. By using isocaps, only one value can be chosen.
Colours: give the colours of the surfaces. By using isosurfaces, more than one value can be chosen. By using isocaps, only one value can be chosen.
Limits: repetition of the limits which can be chosen.
Ratio: give ratio of between the x-, y- and z-directions
Level top (mTAW): indicates the level of the top of the model in mTAW
Trans. Factor: factor determines the translucency of the cross-sections

The *MOCDENS3D path box* regulates the input for the calculations of the flow paths. The time input box regulates the time increment and number of steps and particle tracking algorithm.

Stress period: the stress period of which velocities are used, calculating steady state flow paths, or the stress period used as starting point calculating transient state flow paths
Number of steps: number of steps with length as given by the time step
Plot step: number of step after which a marker is plotted
Time step: length of time step (d). If the 'help' button is pushed, a help for choosing this time step is provided. The time step is suggested based on the maximum velocities according to the rows, columns and layers and a percentage of a cell that can be moved in one time step (the so called celdis (%))

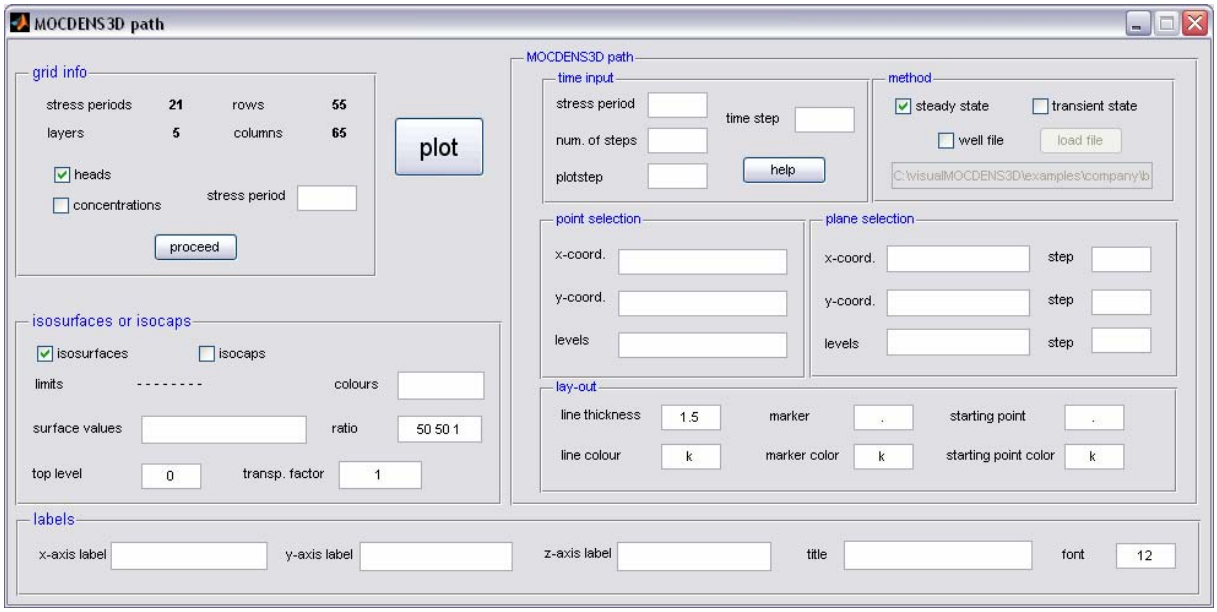


figure 5.3 *Flow path GUI. Flow paths are plotted with isosurfaces as background.*

The *method box* regulates if steady state or transient state flow paths are plotted. If a well file is present, the well file box must be indicated and the right path where this file is found must be indicated. The well file must be an excel file. An example is given in section 5.2.1.

Flow paths can be plotted in two ways. If a selection of specific starting points is preferred, then the point selection option must be chosen.

x-coordinate: x-coordinates (m) of the different points
y-coordinate: y-coordinates (m) of the different points
levels: levels (m) of the different points

Starting points can be grouped in planes. These are given in the plane selection section.

x-coordinate: x-coordinates (m) of vertical planes parallel with YZ-plane, thus according to the columns
y-coordinate: y-coordinates (m) vertical planes parallel with XZ-plane, thus according to the rows
levels: levels (m) horizontal planes parallel with XY-plane, thus according to the layers
step: step (m) in the two directions by which the starting points are set.

The *lay-out box* is used to define the lay-out of the flow paths.

Line width: width of the flow paths
Line colour: colour of the flow paths

Marker: symbol of a marker, standard MATLAB symbols are used
Marker colour: colour of a marker, standard MATLAB colours are used
Starting point: symbol of the starting point, standard MATLAB symbols are used
Starting point colour: colour of the starting point, standard MATLAB colours are used

Label on the x-axis, y-axis and legend can be plotted via the *labels box*. Font regulates the font of the axes, labels and title.

5.2.3 Selected flow Paths

In the former two options, starting points of flow paths must be placed in a regular order (according to a plane) or if points were selected, the exact coordinates must be given. This option provides a way to plot flow paths in a more dynamic way: selection of starting points is done by clicking on a map. Figure 5.4 shows the input GUI for horizontal cross-sections, figure 5.5 shows the GUI for vertical cross-sections.

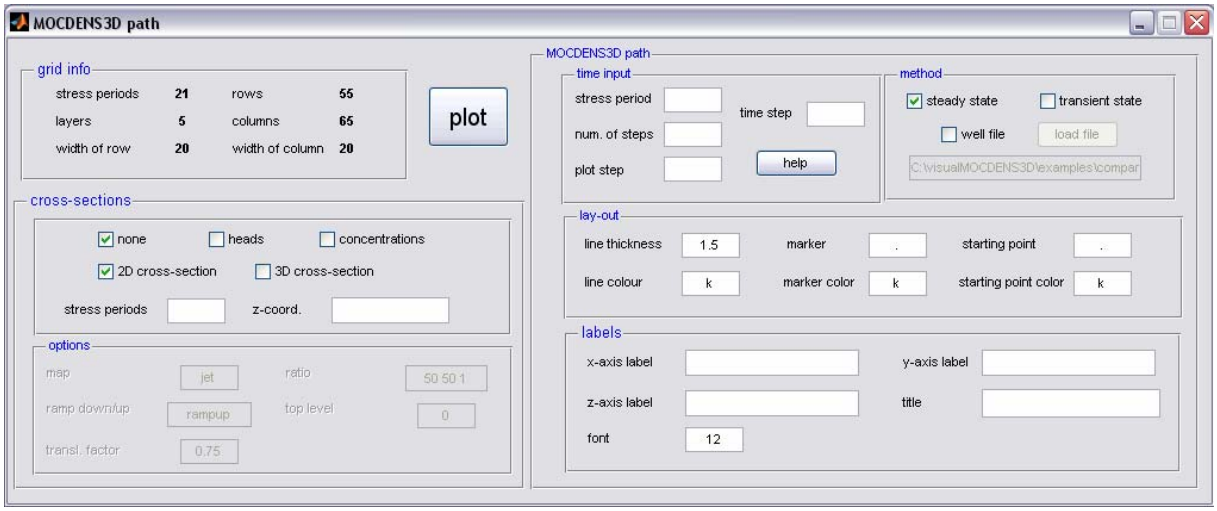


figure 5.4 *GUI for selected flow paths on a horizontal cross-section. Flow paths points which are determined by the user by clicking on a map are calculated*

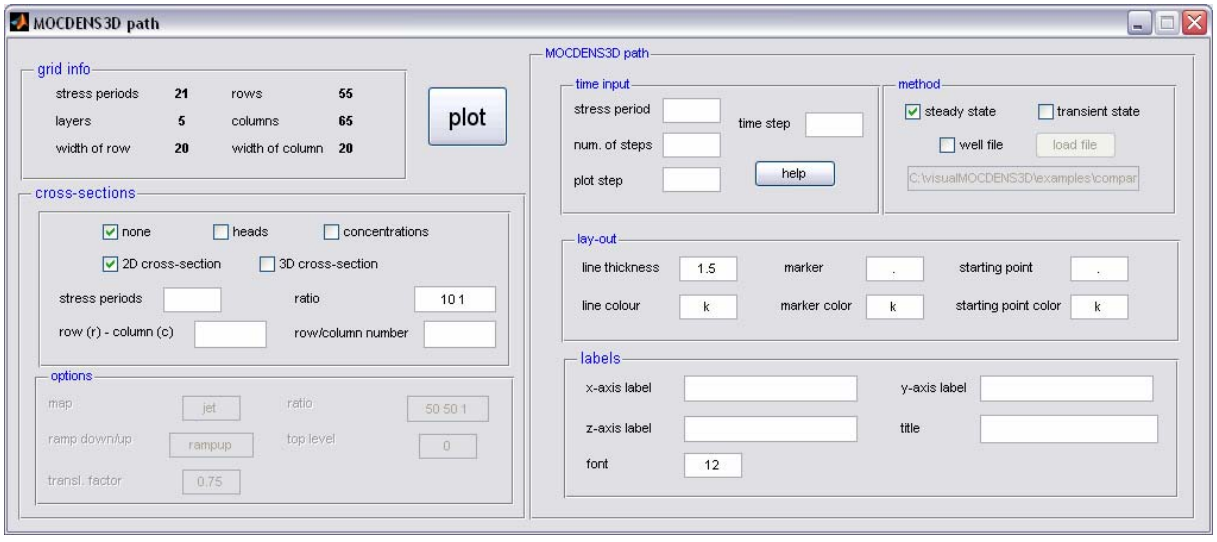


figure 5.5 *GUI for selected flow paths on a vertical cross-section. Flow paths points which are determined by the user by clicking on a map are calculated*

This GUI is similar to the one shown in figure 5.1. In the *cross-section box*, it is first indicated if a background of hydraulic heads or concentrations are used. It can also be opted to use no background (none). The resulting flow paths can be plotted in a 3D-box, like the preceding options, or projected in a horizontal (2D) cross-section. Thereupon, the stress period for head or concentration background and the z-coordinate of the particles must be given for a horizontal cross-section. For a vertical cross-section it must be indicated if a cross-section of a column of row will be made and the number of column of row must be given. Also the ratio for the vertical cross-section must be given.

In case it is opted to use a 3D visualisation following option must be filled in:

Map: give the colour map, standard MATLAB colour maps are used. If an 'i' is given after the regular MATLAB colour maps, the colour map is inverted.
Ramp down/up: choose between the rampdown or rampup MATLAB option
Trans. Factor: factor determines the translucency of the cross-sections
Ratio: give ratio of between the x-, y- and z-directions
Level top: indicates the level of the top of the model in mTAW

The *MOCDENS3D path box* regulates the input for the calculations of the flow paths. The time input box regulates the time increment and number of steps and particle tracking algorithm.

Stress period: the stress period of which velocities are used, calculating steady state flow paths, or the stress period used as starting point calculating transient state flow paths
Number of steps: number of steps with length as given by the time step
Plot step: number of step after which a marker is plotted
Time step: length of time step (d). If the 'help' button is pushed, a help for choosing this time step is provided. The time step is suggested based on the maximum velocities according to the rows, columns and layers and a percentage of a cell that can be moved in one time step (the so called celdis (%))

The *method box* regulates if steady state or transient state flow paths are plotted. If a well file is present, the well file box must be indicated and the right path where this file is found must be indicated. The well file must be an excel file. An example is given in section 5.2.1.

The *lay-out box* is used to define the lay-out of the flow paths.

Line width: width of the flow paths
Line colour: colour of the flow paths
Marker: symbol of a marker, standard MATLAB symbols are used
Marker colour: colour of a marker, standard MATLAB colours are used
Starting point: symbol of the starting point, standard MATLAB symbols are used
Starting point colour: colour of the starting point, standard MATLAB colours are used

Label on the x-axis, y-axis and legend can be plotted via the *labels box*. Font regulates the font of the axes, labels and title.

If these options are filled in correctly, the plot button can be pushed. In first instance a map made according to your choices (heads or concentrations for chosen stress period and z-coordinate or a blank map) appears. Now you can click with the mouse on the map to select the starting points for the flow paths. If you selected all the starting points you press "enter" and the flow paths are calculated.

5.2.4 Flow paths in a 2D model

This option visualises flow paths for 2D models with head or concentration cross-sections as possible background. In contrast with a 3D model positioning of starting points according to a regular pattern or selected user defined pattern is combined in one GUI (figure 5.6).

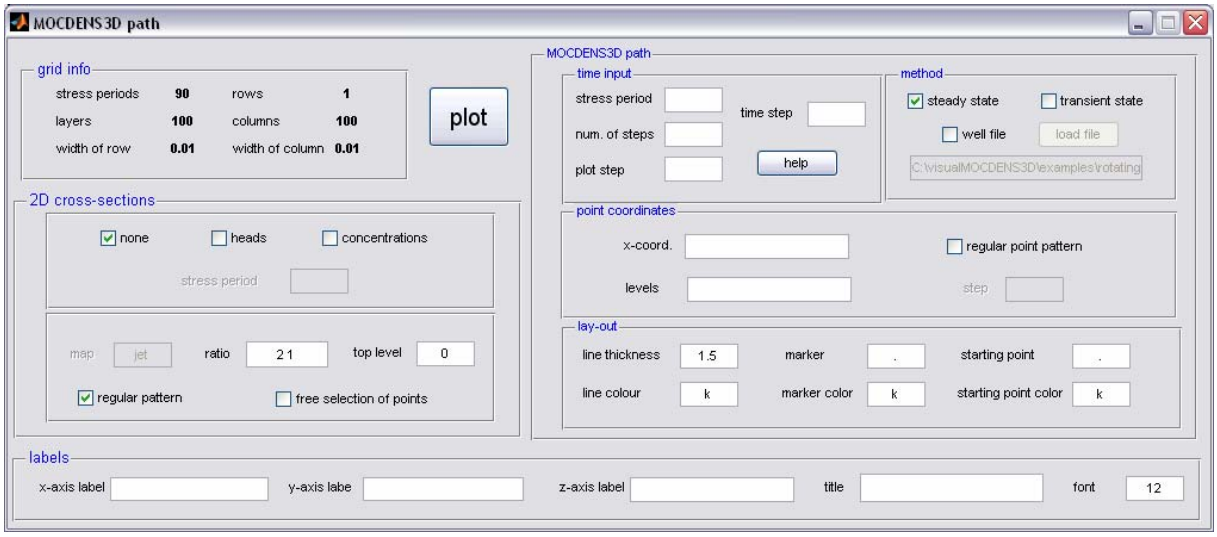


figure 5.6 *Flow path GUI for a 2D model. Flow paths are plotted with 2D cross-sections of heads or concentrations as possible background.*

The *grid info box* summarises the grid sizes of the model

The *2D cross-sections box* regulates the input for the cross-sections. First, indicate by using the check boxes if heads or concentrations are plotted.

Stress period: give stress period for which the cross-sections will be plotted
MATLAB colour maps, the colour map is inverted.
Ratio: give ratio of between the x- and z-directions
Level top: indicates the level of the top of the model in mTAW

If the option 'none' is chosen, only a box is made in which the flow paths will be plotted.

Then choose if you want to define the locations of the starting points with a regular grid or want to define a free selection of points by clicking on the cross-section.

The *MOCDENS3D path box* regulates the input for the calculations of the flow paths. The time input box regulates the time increment and number of steps and particle tracking algorithm.

Stress period: the stress period of which velocities are used, calculating steady state flow paths, or the stress period used as starting point calculating transient state flow paths
Number of steps: number of steps with length as given by the time step
Plot step: number of step after which a marker is plotted
Time step: length of time step (d). If the 'help' button is pushed, a help for choosing this time step is provided. The time step is suggested based on the maximum velocities according to the rows, columns and layers and a percentage of a cell that can be moved in one time step (the so called celdis (%)).

The *method box* regulates if steady state or transient state flow paths are plotted. If a well file is present, the well file box must be indicated and the right path where this file is found must be indicated. The well file must be an excel file. An example is given in figure 5.2.

If you have chosen to define the starting points by clicking on the map, you can no push the plot button to start the calculation and plotting of the flow paths.

Otherwise you have to continue with filling in the *points coordinates box*. In this case flow paths can be plotted in two ways. If a selection of specific starting points is preferred, then the point selection option must be chosen.

x-coordinate: x-coordinates (m) of the different points
levels: levels (m) of the different points

A regular pattern of points can be given by selecting the regular point pattern checkbox and by filling in the step (m) in the two directions by which the starting points are set.

The lay-out box is used to define the lay-out of the flow paths.

Line width: width of the flow paths
Line colour: colour of the flow paths
Marker: symbol of a marker, standard MATLAB symbols are used
Marker colour: colour of a marker, standard MATLAB colours are used
Starting point: symbol of the starting point, standard MATLAB symbols are used
Starting point colour: colour of the starting point, standard MATLAB colours are used

Label on the x-axis, y-axis and legend can be plotted via the *labels box*. Font regulates the font of the axes, labels and title.

5.3 Capture zones

5.3.1 Horizontal cross-sections

In this option capture zones are calculated and visualised with horizontal cross-sections. The *grid info box* summarises basic grid input.

The *MOCDENS3D path box* options for the calculation and visualisation of the capture zones must be given. The time input box regulates the time increment, number of steps and particle tracking algorithm.

Stress period: the stress period of which velocities are used, calculating steady state flow paths, or the stress period used as starting point calculating transient state flow paths
Number of steps: number of steps with length as given by the time step
Time step: length of time step (d). If the 'help' button is pushed, a help for choosing this time step is provided. The time step is suggested based on the maximum velocities according to the rows, columns and layers and a percentage of a cell that can be moved in one time step (the so called celdis (%))

The method box regulates if steady state or transient capture zones are calculated. A well file, giving the locations of locations were water is removed from the model (e.g. wells, rivers, drainage systems, etc.) is needed. The right path to where this file is found must be indicated. The well file must be an excel file. An example is given in section 5.2.1.

In the option box, the window for which a capture zone will be calculated must be indicated. This exists of the number of the layer and the first and last column and row of the model in which particles

will be placed. The step is the increment in the column (or x) and row (or y) direction with which particles are placed and this is expressed in meter. Further a choice must be made if the capture zones will be given in days or in years.

figure 5.7 *GUI for the visualisation of capture zones, horizontal cross-sections.*

The second part of the box regulates the figures of the capture zones. There are two possibilities: a plot with contour lines or a plot with filled contours.

For the contour plot, information needed is:

Font: font of the labels
Line width: line width of the contour lines
Color: color of the contour lines
Contour lines: enumeration of the contour lines which will be plotted
Contour labels: enumeration of the labels which will be plotted with the contour lines

For he filled contour plot:

Color map: color map of the filled contours

Label on the x-axis, y-axis and legend can be plotted via the *labels box*. Font regulates the font of the axes, labels and title.

5.3.2 Vertical cross-sections

In this option capture zones are calculated and visualised with vertical cross-sections. The *grid info box* summarises basic grid input.

The *MOCDENS3D path box* options for the calculation and visualisation of the capture zones must be given. The time input box regulates the time increment, number of steps and particle tracking algorithm.

Stress period: the stress period of which velocities are used, calculating steady state flow paths, or the stress period used as starting point calculating transient state flow paths
Number of steps: number of steps with length as given by the time step
Time step: length of time step (d). If the 'help' button is pushed, a help for choosing this time step is provided. The time step is suggested based on the maximum velocities according to the rows, columns and layers and a percentage of a cell that can be moved in one time step (the so called celdis (%))

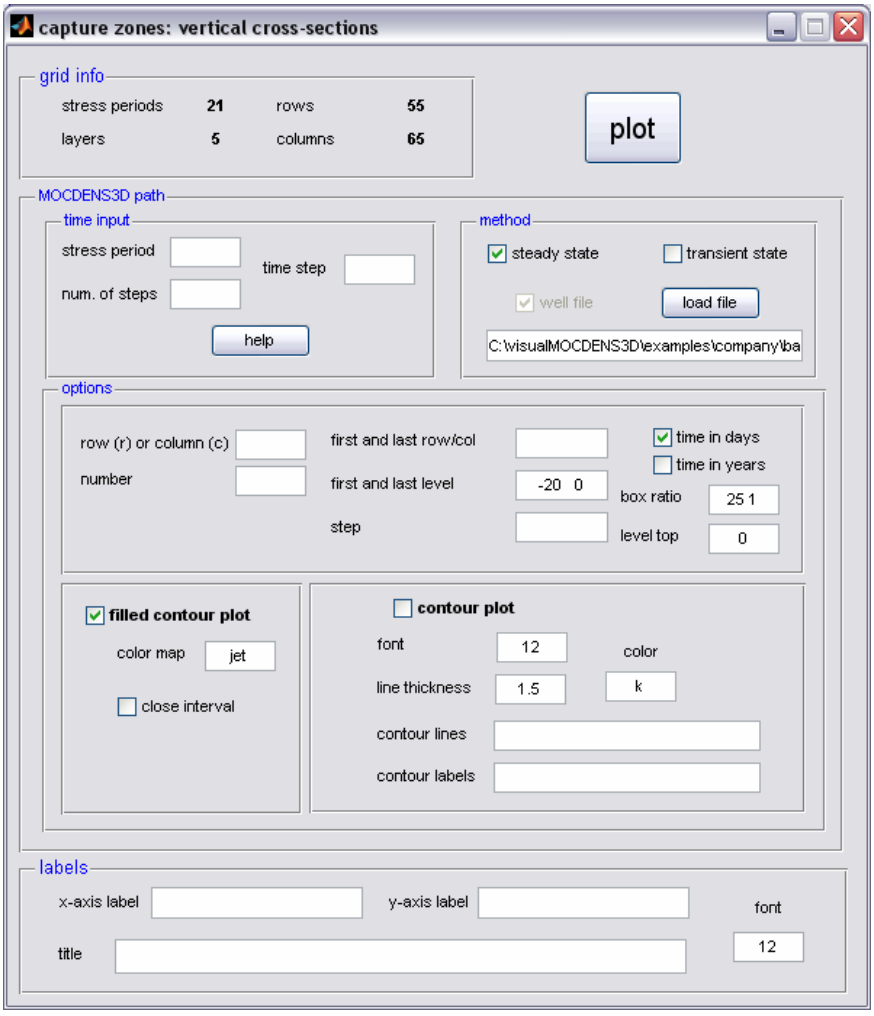


figure 5.8 *GUI for the visualisation of capture zones, vertical cross-sections.*

The *method box* regulates if steady state or transient capture zones are calculated. A well file, giving the locations of locations were water is removed from the model (e.g. wells, rivers, drainage systems, etc.) is needed. The right path to where this file is found must be indicated. The well file must be an excel file. An example is given in section 5.2.1.

In the option box, the window for which a capture zone will be calculated must be indicated. This exists of the number of the row or column and the first and last column and row of the model in which particles will be placed. The step is the step in the column (or x) and row (or y) direction with which particles are placed and this is expressed in meter. Further a choice must be made if the capture zones will be given in days or in years.

The second part of the box regulates the figures with the capture zones. There are two possibilities: a plot with contour lines or a plot with filled contours.

For the contour plot, information needed is:

Font: font of the labels
Line width: line width of the contour lines
Color: color of the contour lines
Contour lines: enumeration of the contour lines which will be plotted
Contour labels: enumeration of the labels which will be plotted with the contour lines

For he filled contour plot:

Color map: color map of the filled contours

Label on the x-axis, y-axis and legend can be plotted via the *labels box*. Font regulates the font of the axes, labels and title.

5.4 Travel time statistics

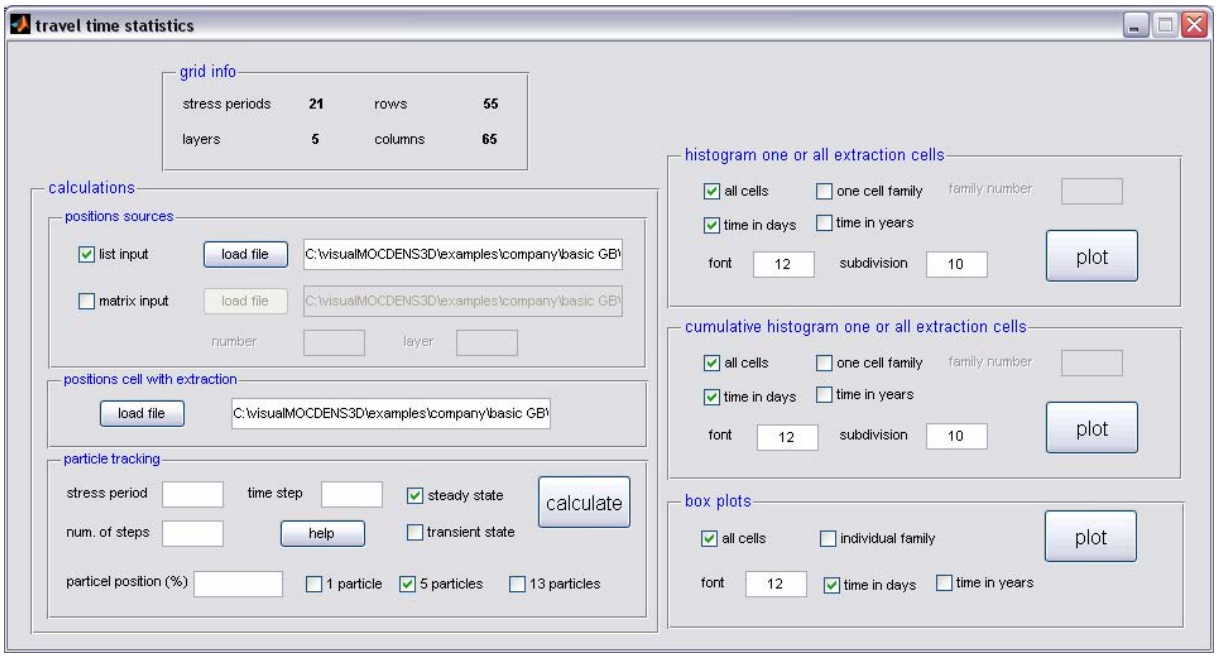


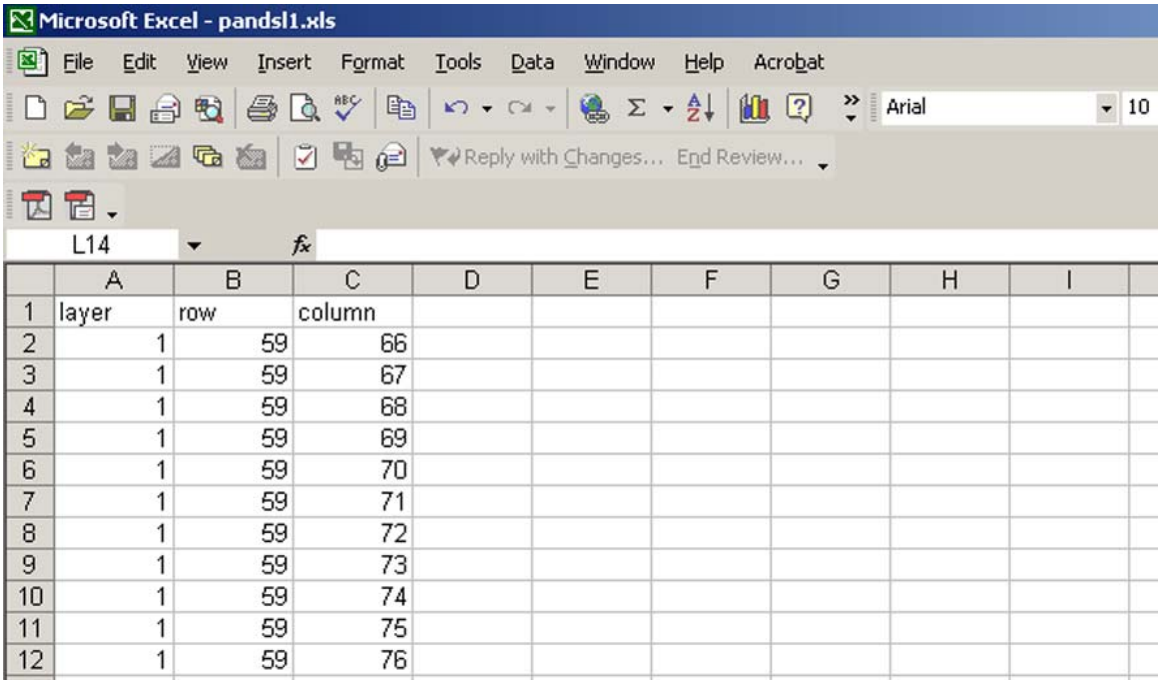
figure 5.9 *GUI for the analyses of travel times.*

The travel times to extraction points in the model (these are wells, rivers, drainage systems, etc.) are analysed using this option. A statistic is made of the travel times of particles coming from a source location and which are captured in a cell which represents a well, river, drainage system etc. For instance cells which represent a pond where water infiltrates are the sources. This water moves

towards a number of pumping wells and the question is how long it takes for the infiltration water to reach the wells. Therefore, a number of particles are placed in the cells representing the pond and these are followed until they reach the wells. Not all particles arrive in the wells at the same time and thus a statistic of the arrival times can be made. This can be done for instance for individual wells, or the arrival times of all wells can be analysed together. Therefore histograms, cumulative histograms and box plots are used.

The *grid info box* summarises basic grid input.

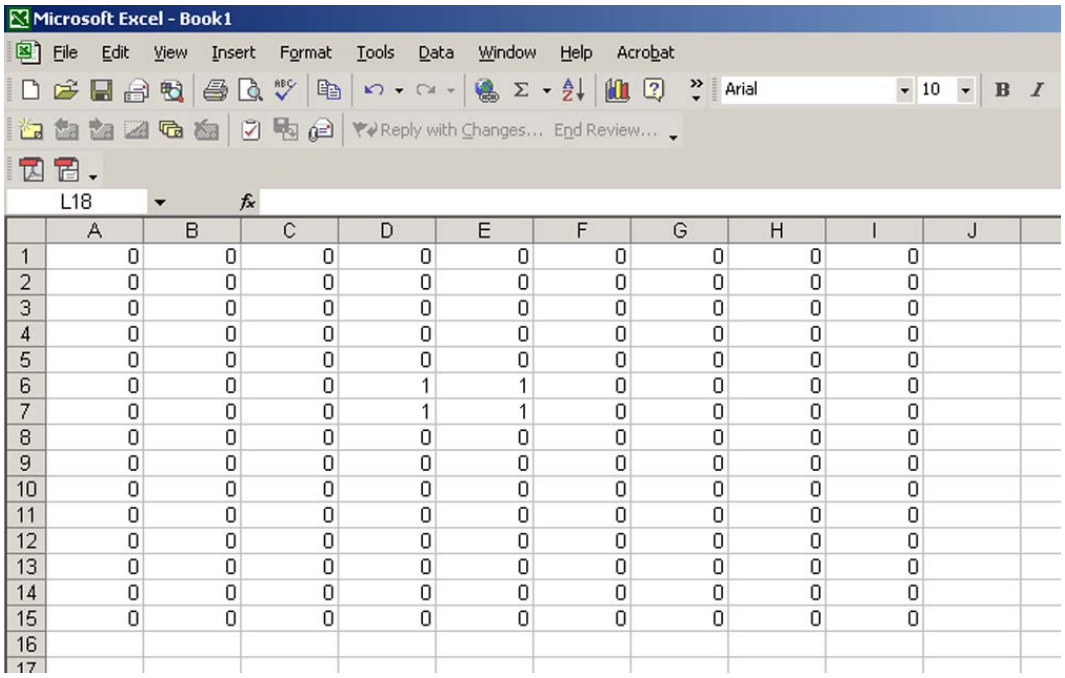
The first step is the performance of calculations, using the *calculations box*. The locations of the sources are given via an input file. This can be a list of cell locations or a matrix of cell locations. In case of list of source locations an excel file must be made as exampled in figure 5.10. This gives for all the source cells the layer, row and column.



	A	B	C	D	E	F	G	H	I
1	layer	row	column						
2	1	59	66						
3	1	59	67						
4	1	59	68						
5	1	59	69						
6	1	59	70						
7	1	59	71						
8	1	59	72						
9	1	59	73						
10	1	59	74						
11	1	59	75						
12	1	59	76						

figure 5.10 *Input example for the source cells via list input.*

Additionally, the input of source cells can also be done using a matrix. This matrix is given via an excel file or via a text file (txt extension). An example of an excel file is given in figure 5.11. The dimensions of the matrix are number of rows times number of columns. Different cells are indicated via different numbers, in the example the source cells are indicated by 1 and the other cells by 0.

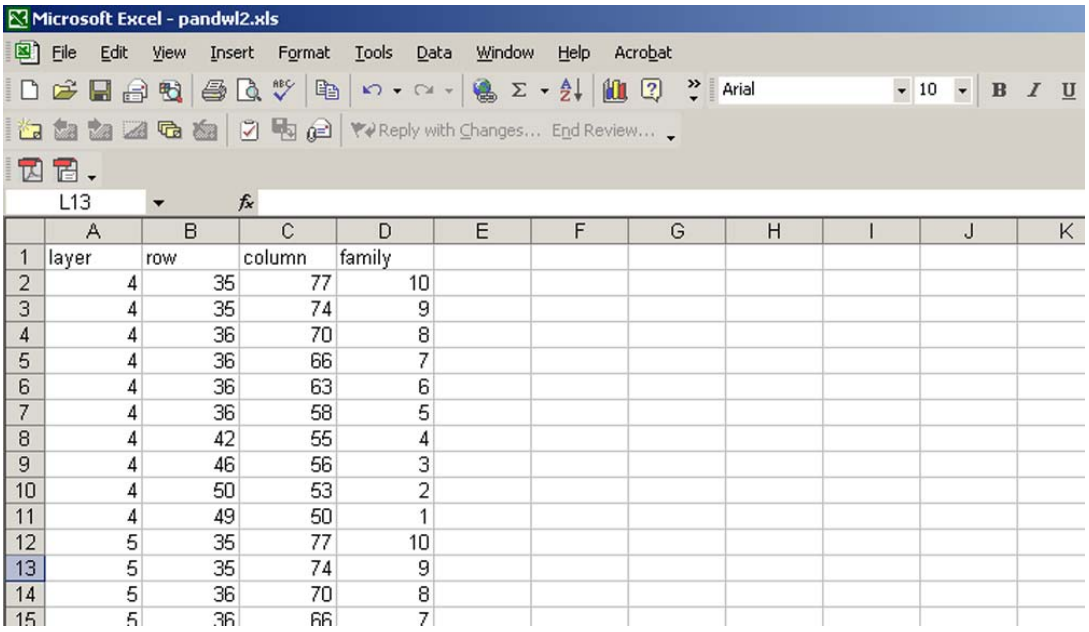


	A	B	C	D	E	F	G	H	I	J
1	0	0	0	0	0	0	0	0	0	
2	0	0	0	0	0	0	0	0	0	
3	0	0	0	0	0	0	0	0	0	
4	0	0	0	0	0	0	0	0	0	
5	0	0	0	0	0	0	0	0	0	
6	0	0	0	1	1	0	0	0	0	
7	0	0	0	1	1	0	0	0	0	
8	0	0	0	0	0	0	0	0	0	
9	0	0	0	0	0	0	0	0	0	
10	0	0	0	0	0	0	0	0	0	
11	0	0	0	0	0	0	0	0	0	
12	0	0	0	0	0	0	0	0	0	
13	0	0	0	0	0	0	0	0	0	
14	0	0	0	0	0	0	0	0	0	
15	0	0	0	0	0	0	0	0	0	
16										
17										

figure 5.11 *Input example for the source cells via matrix input.*

The input via a matrix is given for on specific layer. Therefore, this layer must be given. Additionally, the number in the matrix representing the source (for instance 1 in the example here) must also be given.

Thereafter, the positions of the extraction points must be given via an excel file. An Example is given in figure 5.112. In the first three columns, the layer, row and column number is indicated. In the fourth column of the excel file, the family number of the cell is given. This makes it possible to group cells together in one family. For instance one well which is present in different model layers or all cells from one river receive the same family number to group them together and distinGUIsh them from other wells or rivers.



	A	B	C	D	E	F	G	H	I	J	K
1	layer	row	column	family							
2	4	35	77	10							
3	4	35	74	9							
4	4	36	70	8							
5	4	36	66	7							
6	4	36	63	6							
7	4	36	58	5							
8	4	42	55	4							
9	4	46	56	3							
10	4	50	53	2							
11	4	49	50	1							
12	5	35	77	10							
13	5	35	74	9							
14	5	36	70	8							
15	5	36	66	7							

figure 5.12 *Input example for the input file with positions of wells, rivers, drainage systems etc.*

Finally, the options for the particle tracking must be defined:

Stress period: the stress period of which velocities are used, calculating steady state flow paths, or the stress period used as starting point calculating transient state flow paths
Number of steps: number of steps with length as given by the time step
Time step: length of time step (d). If the 'help' button is pushed, a help for choosing this time step is provided. The time step is suggested based on the maximum velocities according to the rows, columns and layers and a percentage of a cell that can be moved in one time step (the so called celdis (%))

Choice between steady state or transient state calculations must be made. The positions of the wells, however, remain the same and can not be changed in function of time in case of a transient state calculation.

The particles are initially set in a horizontal plain in the source cells. The level of this plain is given in the particle position box and is expressed as a percentage. 0% is on top of the cells, 100% at the bottom of the cells and 50% is in the middle of the cells. Finally a choice must be made between 1, 5 or 13 particles per source cell.

Then the calculate button must be pressed to calculate the particle tracking. A warning will be given if this is finished and one can proceed with the analyses of the travel times. This can be done using three options.

First, the histogram of the travel times of particles in one or all extraction cell can be calculated. Choice must be made if a histogram of travel times in all extraction cells together will be made or in one particular family of cells. In the latter case, the number of the family must be given. Arrival times can be expressed in days or in years be designating the appropriate box. Finally, the font and the number of subdivisions of the histogram can be altered.

Secondly, a cumulative histogram of the arrival times can be made. The same options as for the histogram apply.

Finally, a box plot of the travel times for all families together or for all individual families can be made. The font and if travel times will be expressed in days or years, can be altered.

6 Examples

6.1 Artificial recharge ponds: CBTM

6.1.1 Problem formulation

The possibilities of the different Visual MOCDENS3D modules are first illustrated with a relatively simple example. A company extracts water from an aquifer using one pumping well with a screen of 12 m length at the base of the aquifer. This water is used by the company and thereafter artificially recharged using two ponds. These ponds have a diameter of 50 m and are 250 m from each other. The production water is first transported to the most western pond which has an overflow pipe. This leads extra water to the eastern pond. In the western pond, mean infiltration rate is 80 m³/d whereas this is 70 m³/d for the eastern pond. Salt content of the water has decreased from 500 mg/l in the pristine water to 20000 mg/l in the recharge water.

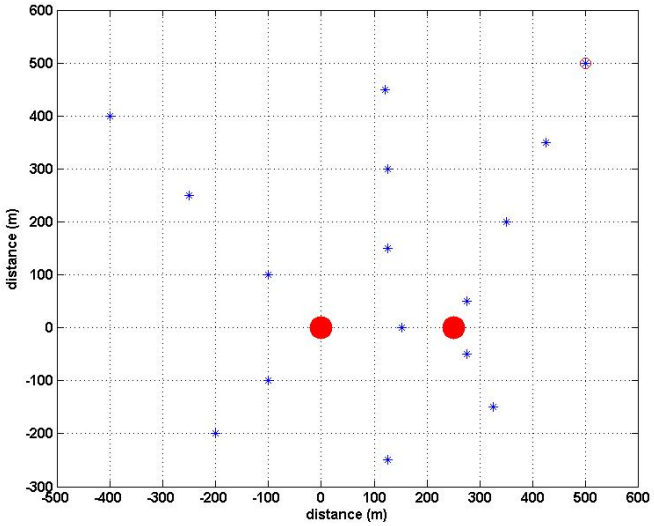


figure 6.1 *Overview of the area showing the positions of the pumping well (o), infiltration ponds (•) and observation wells (*).*

The company has already extracted during 5 years water from the pumping well with a mean discharge rate of 150 m³/d. The aquifer consists of sandy deposits with a mean horizontal hydraulic conductivity of 2.5 m/d and an effective porosity 0.3. The aquifer is bounded below (level -10 m) by clay which can be considered impervious in this study. Annual natural recharge is 200 mm/y.

In the area, 14 observation wells are present where the hydraulic head was measured before the start of the pumping. The observation wells have screens between 0 and -4 m. Also, a measurement in the pumping well was made. These are given in table 6.1.

The purpose of the modelling is to study the effect of the groundwater extraction and the artificial recharge on the groundwater flow and quality. Special attention must go to the question if the recharge of salt waste water will affect the extraction of water in the future.

table 6.1 *Head measurements in the observation wells and pumping well before the start of the pumping. X and Y coordinates refer to figure 6.1.*

X	Y	Head (m)	X	Y	Head (m)
500	500	7.000	-100	100	9.631
125	450	4.461	275	50	9.811
-400	400	7.879	125	0	9.962
425	350	8.258	275	-20	10.086
125	300	8.599	-100	-100	10.181
-250	250	8.906	325	-150	10.248
350	200	9.179	-200	-200	10.289
125	150	9.420			

Input files for this model can be found in the directory "c:\visualMOCDENSD3D\examples\company". In this directory, three maps are present 'basic GB', 'advanced GB' and 'VBTM'. In the two first maps, the input files are present for the model described below, respectively constructed via the basic and advanced grid options. Input file given in the folder 'VBTM' illustrates this option and is described in section 6.2.

6.1.2 Model schematisation

With a mean annual recharge of 200 mm/y and a discharge rate of 150 m³/d, the pumping draws water from an area with a radius of 295 m towards the well. The model boundaries must be at a minimum distance of 295 m from the pumping well to minimise influences of these boundaries.

A model area of 1300 to 1100 m² is used with 55 rows and 65 columns, each with a width of 20 m. the aquifer is subdivide in five layers with a thickness of 4 m each. From the head measurements in table 1 it can be seen that the groundwater flow before start of the pumping and infiltration is strictly north-south oriented. Therefore, the west and east boundaries are no flow boundaries and the north and south boundaries are constant head boundaries.

The pumping well is present in layers 3 to 5, row 20 and column 45. The infiltration ponds are present in four cells in the uppermost layer.

The model is a constant boundary type model (CBTM). The input files are made with the Grid Builder module, basic grid option. Figure 6.2 shows the bas and bcf input GUI. An initial constant head for the northern boundary is 6 m whereas this is 11 m for the southern boundary. 21 stress periods of a half year each are used. The first stress period serves to calculate the groundwater flow before the start of the pumping and to calibrate the model. The 20 other stress periods calculate the evolution of the solute transport for the past and future 5 years of water extraction. The hydraulic conductance is calculated with a vertical hydraulic conductivity of 0.25 m.

Figure 6.3 shows the moc and wel input GUI. Initial concentration for all layers is 500 mg/l, longitudinal dispersivity is 0.2 m, horizontal transversal dispersivity is 0.02 m and vertical transversal dispersivity is 0.002 m. In the well file, natural recharge of 0.219 m³/d per cell is used (0.2 mm/y) and discharge/infiltration rates of the well and ponds is given via an excel input file.

Also a densin.dat and company.sip file are made as are the two name files (infile.nam aned comp_moc.nam, notice that a file name can only have 8 characters!).

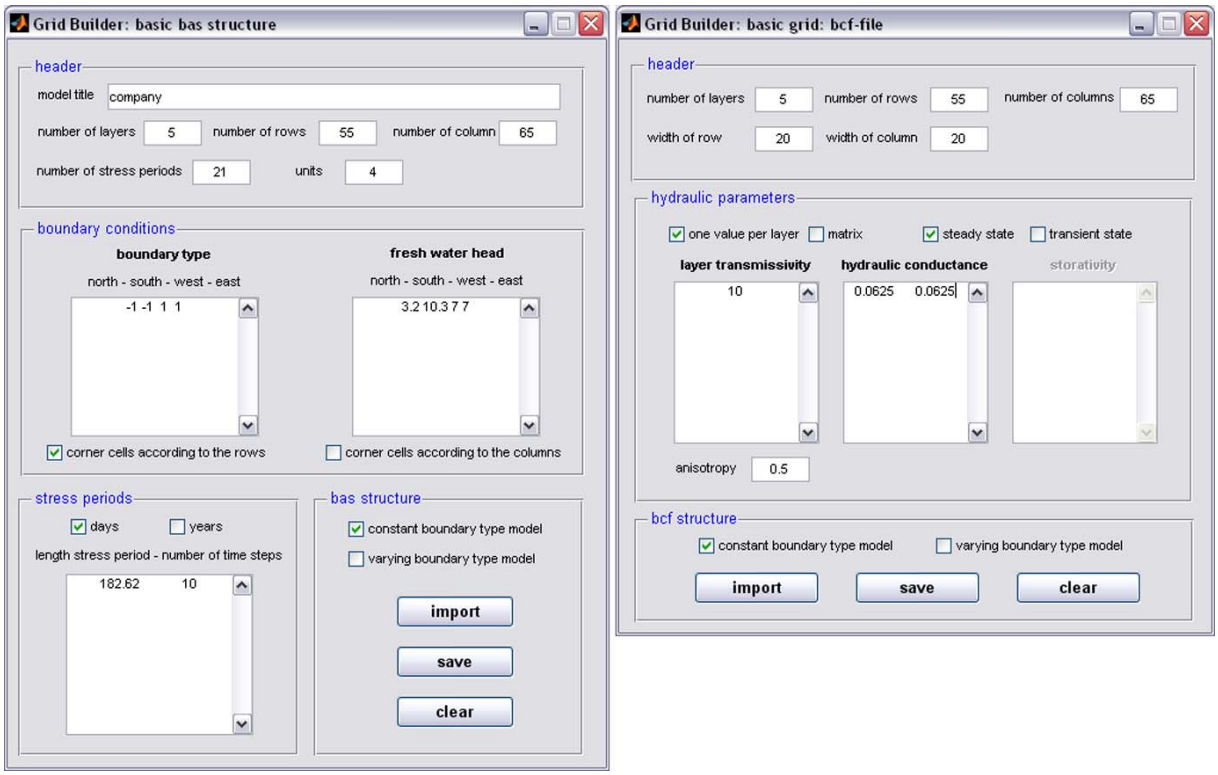


figure 6.2 *Bas and bcf input GUI.*

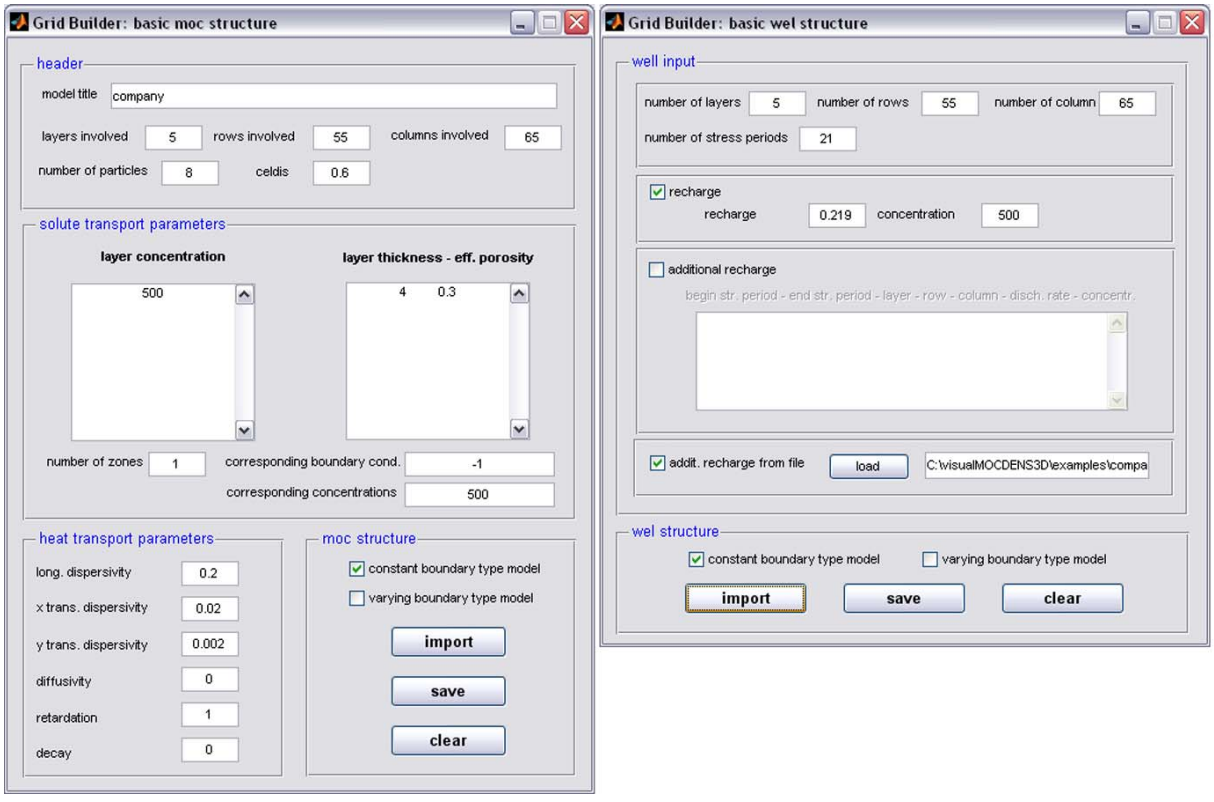


figure 6.3 *Moc and wel input GUI.*

6.1.3 Model calibration

A first calculation is performed with the parameters and boundary conditions given in the previous sections. The model can be calibrated based on the hydraulic head observations of the natural occurring groundwater flow. The result of this is shown in figure 6.4. The hydraulic heads and groundwater flow pattern shows a general flow from south to north.

The positions and head values of the observation wells are given in the file *companyobs.xls* and this is used with the calibration module to validate model fit. The comparison between observed and calculated heads shows that the latter are systematically to large. Table 6.2 gives some statistics about the distribution of the residuals and figure 6.4 further gives a histogram and a normal probability plot of the residuals. In figure 6.5, a map is shown with the position of the observation wells and a representation of the residuals. The larger the marker, the larger the residuals.

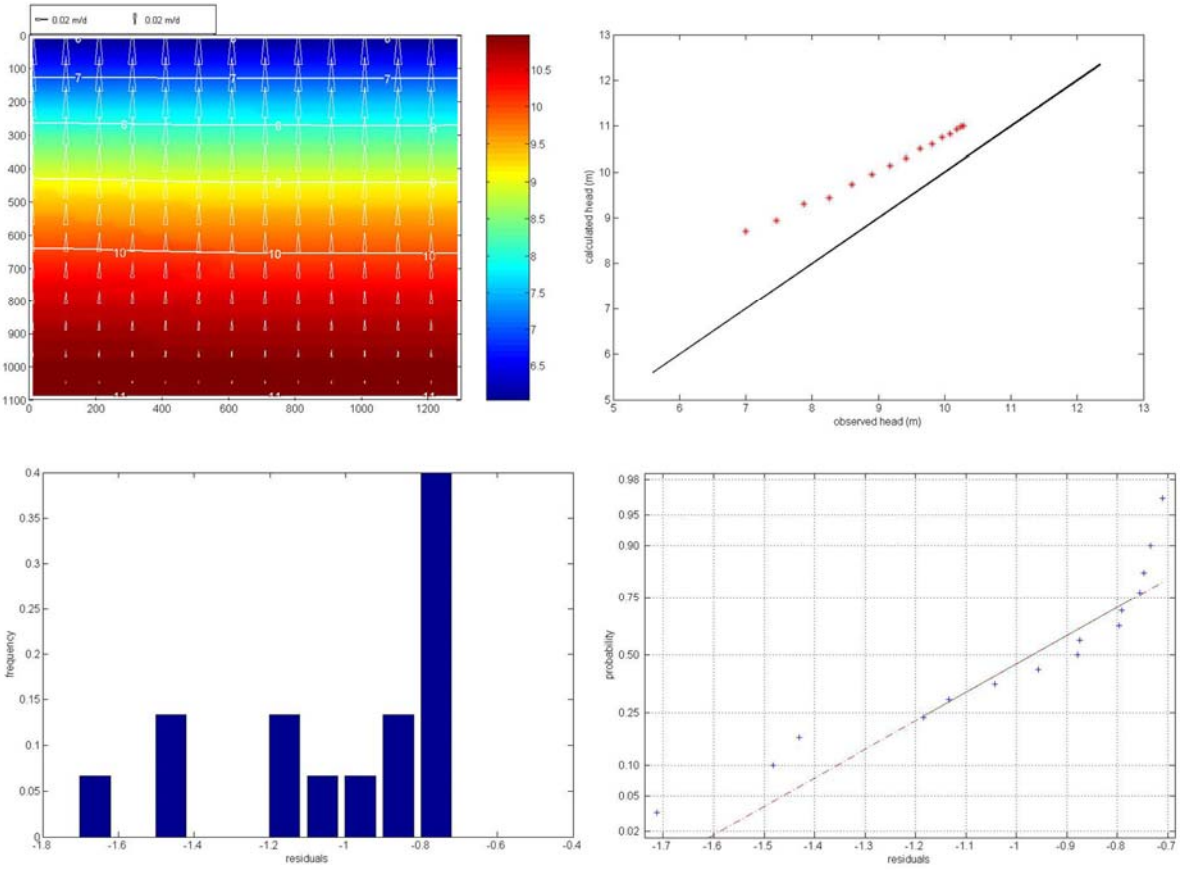


figure 6.4 *Upper left figure shows the hydraulic heads in layer 3 using the initial boundary conditions. The upper right figure shows a comparison between observed and calculated hydraulic heads. A histogram of the residuals I given in the lower left figure whereas the lower right figure gives a normal probability plot of the residuals. The horizontal cross-section option (MOCDENS3D module) and analyses of residuals (calibration module) are used.*

Table 6.1 *Statistics of the residuals obtained in the calculation with the initial parameters and boundary conditions. Analyses of residuals (calibration module) is used.*

mean m	-1.015	inter quartile range iqr	0.4075
median M	-0.879	variance s^2	0.097
correlation coef. C	0.998	standard deviation s	0.312
range r	1.001		

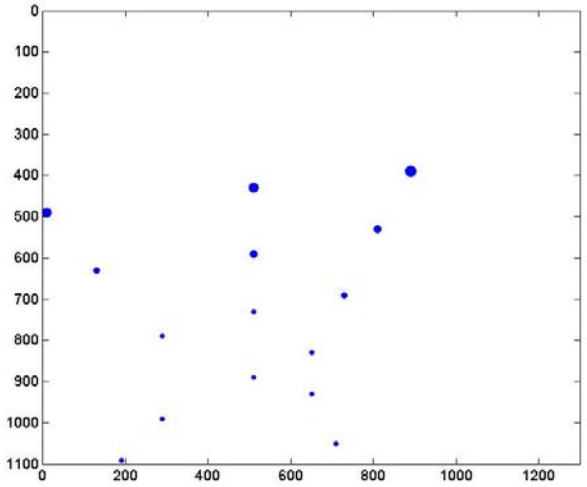


figure 6.5 *Map showing the distribution and magnitude of the residuals. The latter is indicated by the magnitude of the markers. This map is drawn using the residual mapping function of the calibration module.*

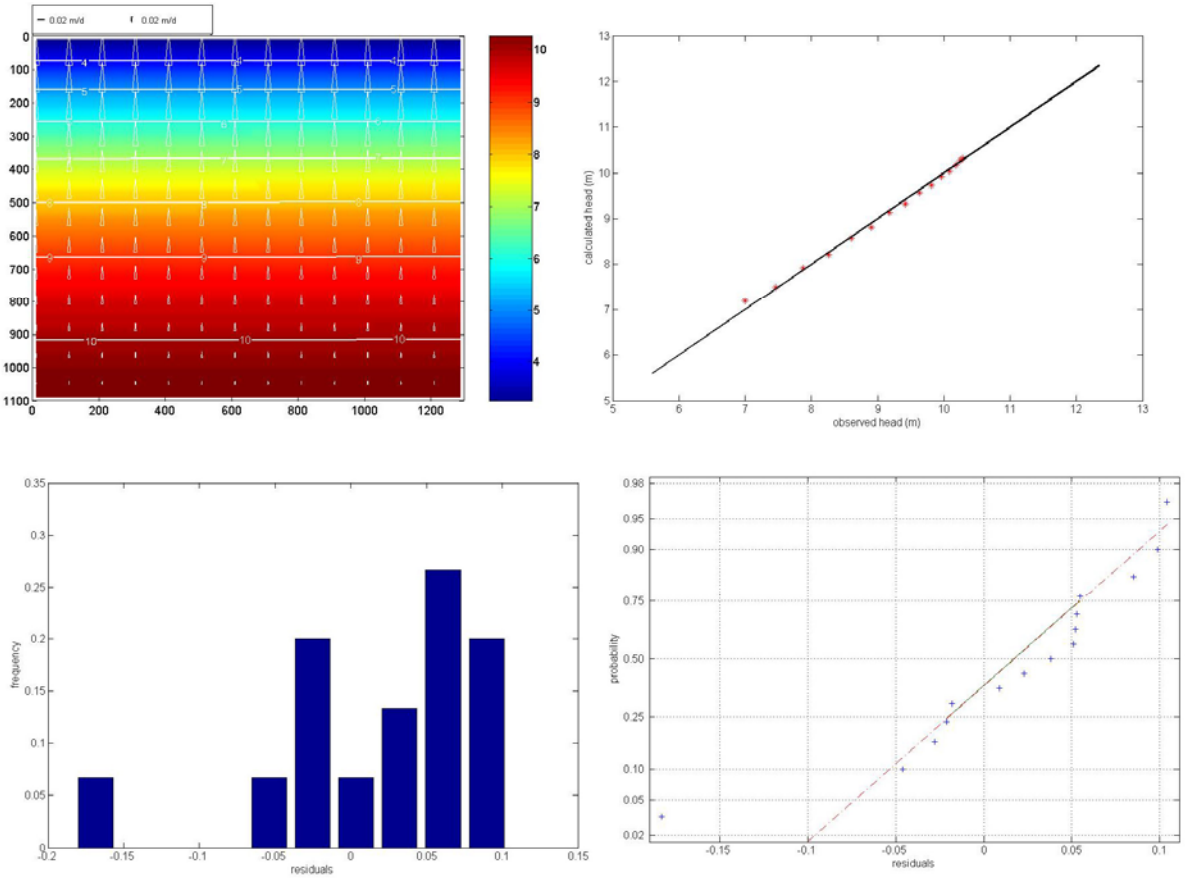


figure 6.6 *Upper left figure shows the hydraulic heads in layer 3 of the calibrated model. The upper right figure shows a comparison between observed and calculated hydraulic heads. A histogram of the residuals I given in the lower left figure whereas the lower right figure gives a normal probability plot of the residuals.*

From figure 6.4 and 6.5, it can be seen that the higher hydraulic heads (towards the south) show larger residuals. Since the hydraulic conductivity and the infiltration rate are known, the only parameters which can be changed are the constant heads on the southern and northern border. These are changed until a good fit between observations and calculations is obtained. From the above analyses it is clear that the constant head of both boundaries must be decreased, the northern border must have a larger

decrease than the southern. A good fit between observations and calculations is obtained with a constant head of 3.2 and 10.3 for both boundaries (figure 6.6). Statistical parameters are given in table 6.2. Mean and median are now close to 0 and there is an almost perfect correlation between observations and calculations. The latter was also the case table 6.1 but the mean and median were much larger.

Table 6.2 *Statistics of the residuals obtained in the calculation with the initial parameters and boundary conditions.*

mean m	0.018	inter quartile range iqr	0.075
median M	0.038	variance s^2	0.005
correlation coef. C	0.998	standard deviation s	0.072
range r	0.287		

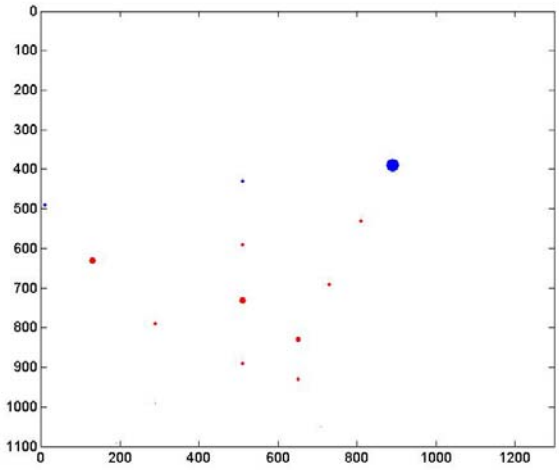


figure 6.7 *Map showing the distribution and magnitude of the residuals. The latter is indicated by the magnitude of the markers.*

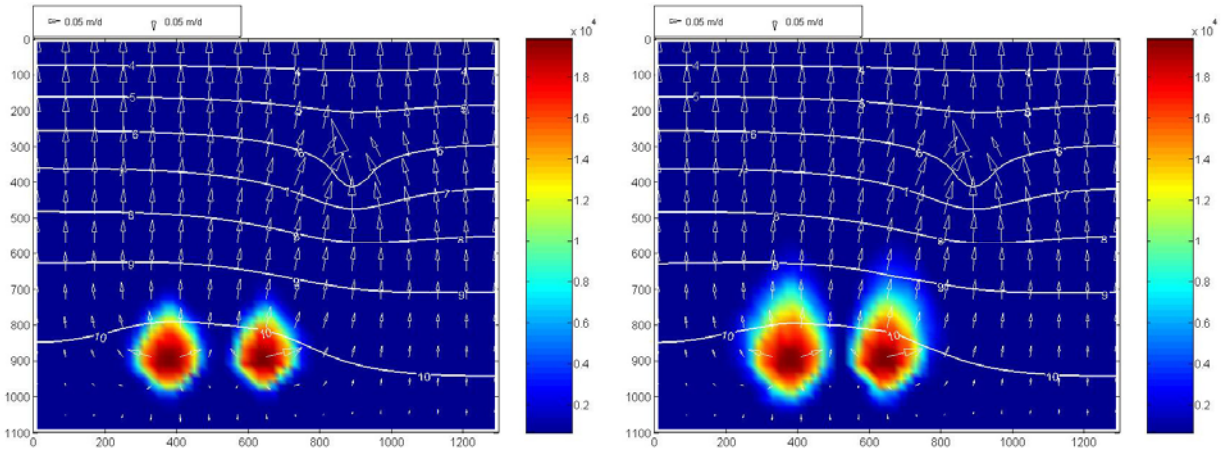


figure 6.8 *Horizontal cross-section through the aquifer (layer 1) showing contour lines of the hydraulic heads whereas the colors represent the TDS. Left figure is the current situation (5 years of infiltration) and the right figure shows the situation after another 5 years.*

6.1.4 Model visualisation

Some of the options to visualise the calculation results are illustrated in the figures 6.8 to 6.16.

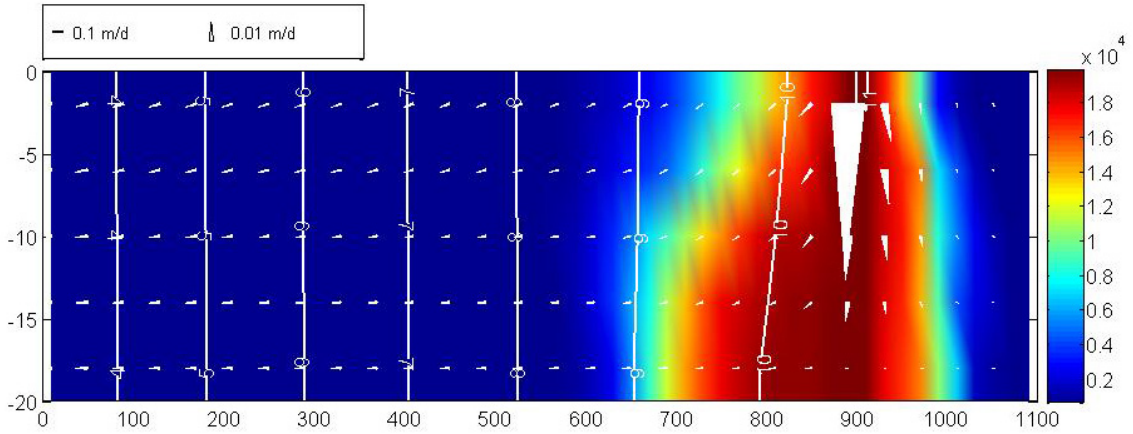


figure 6.8 *Vertical cross-section according to column 33 showing contour lines of the hydraulic heads whereas the colors represent the TDS. Cross-section shows the situation 5 years in the future.*

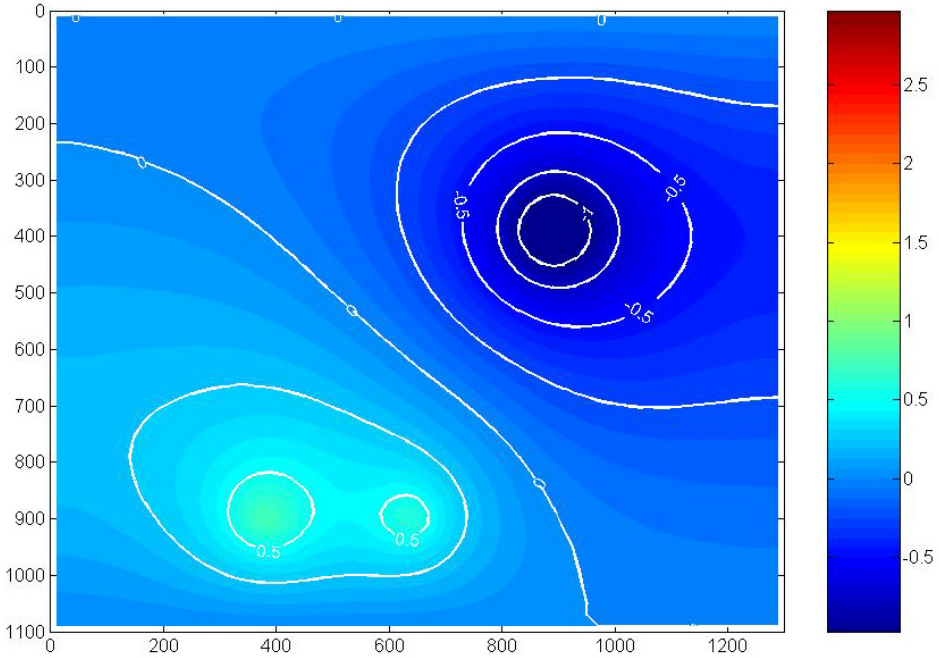


figure 6.9 *Difference between the fresh water heads in layer 3 of stress period 2 and stress period 1. This shows the drawdown due to the pumping or increase in head due to the infiltration.*

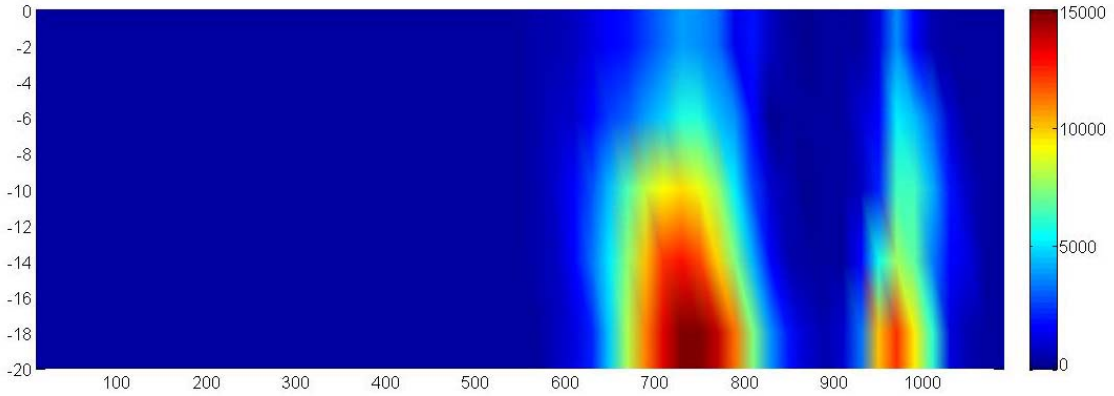


figure 6.10 *Difference between the concentration in cross-section along column 32 of stress period 21 and stress period 11. This shows the expansion of the zone of salt infiltration water over the next 5 years.*

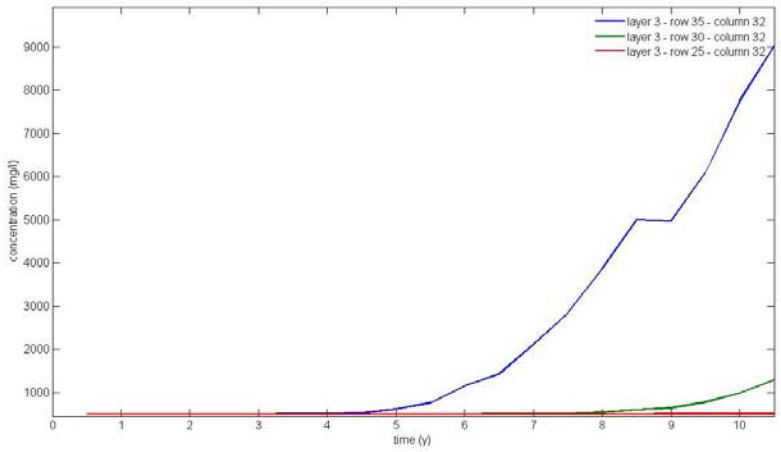


figure 6.11 *Concentration in function of time for a number of positions in the model area.*

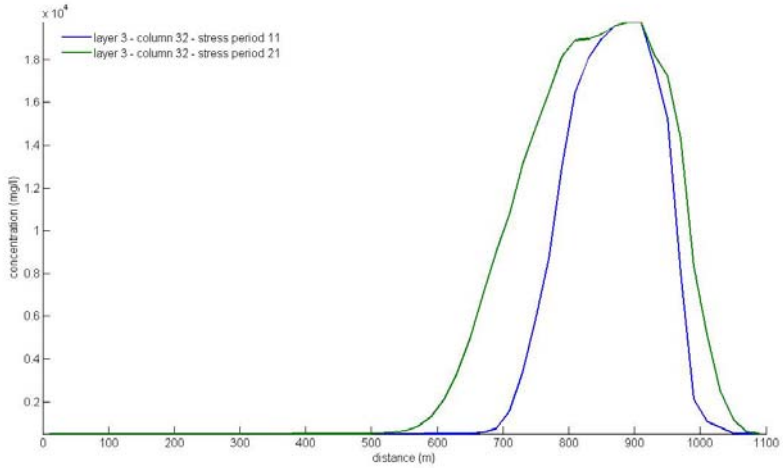


figure 6.12 *Concentration versus distance along a column for a number of stress periods. .*

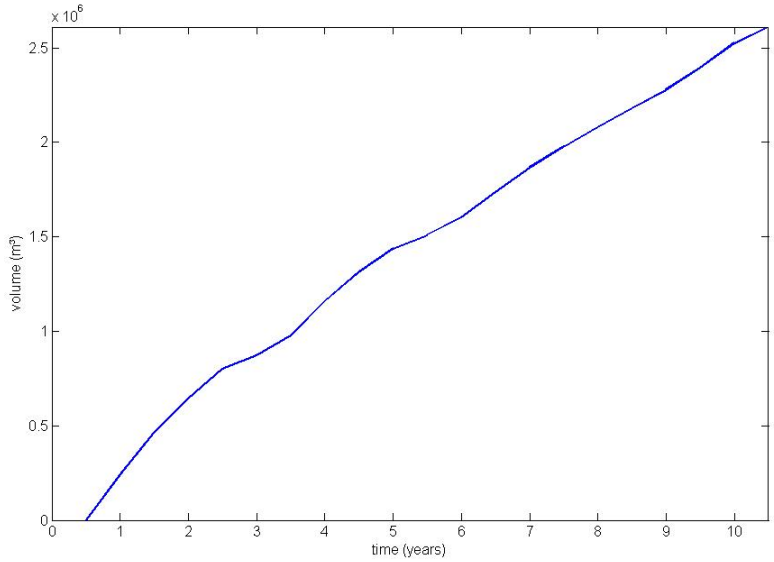


figure 6.13 *Amount of water present in the aquifer with a TDS larger than the background value of 500 mg/l in function of time.*

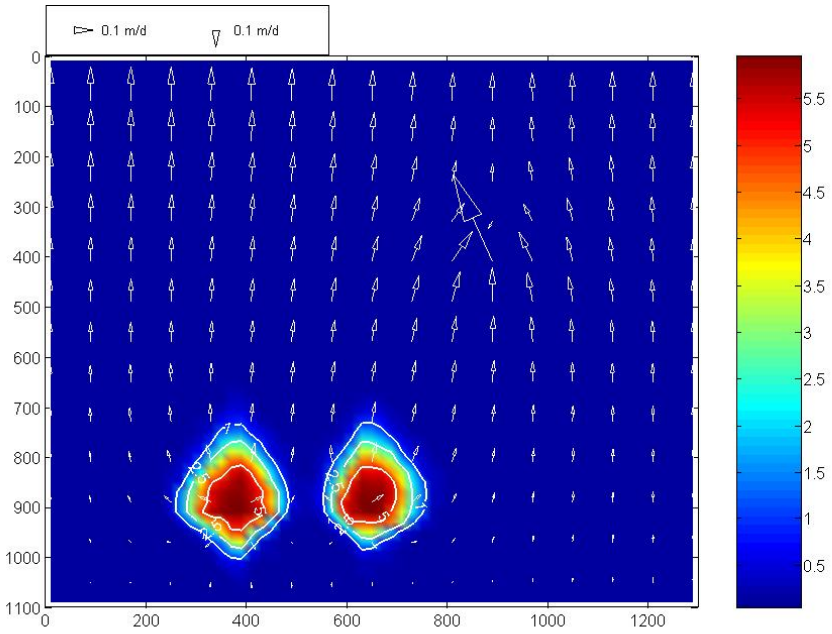


figure 6.14 *Mass expressed as kg per m³ of water present in the aquifer for the current situation in layer **4**.*

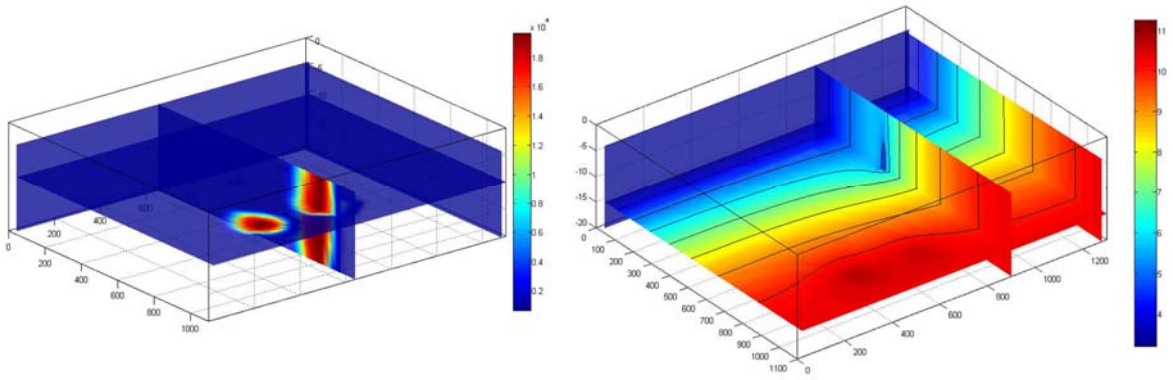


figure 6.15 *3D views of hydraulic heads (right) and concentrations (left).*

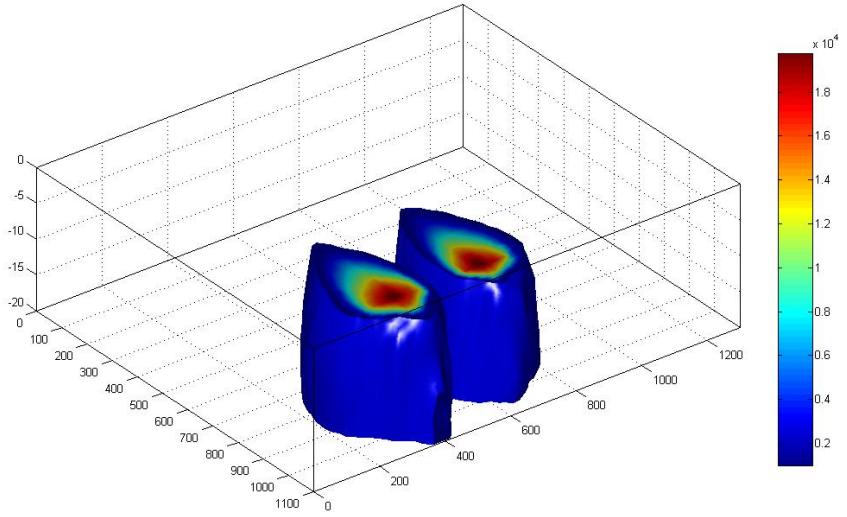


figure 6.16 *3D view using the 1000 mg/l isosurface options (with isocaps).*

6.1.5 ParTrack options

The ParTrack module is used to show flow fields and capture zones.

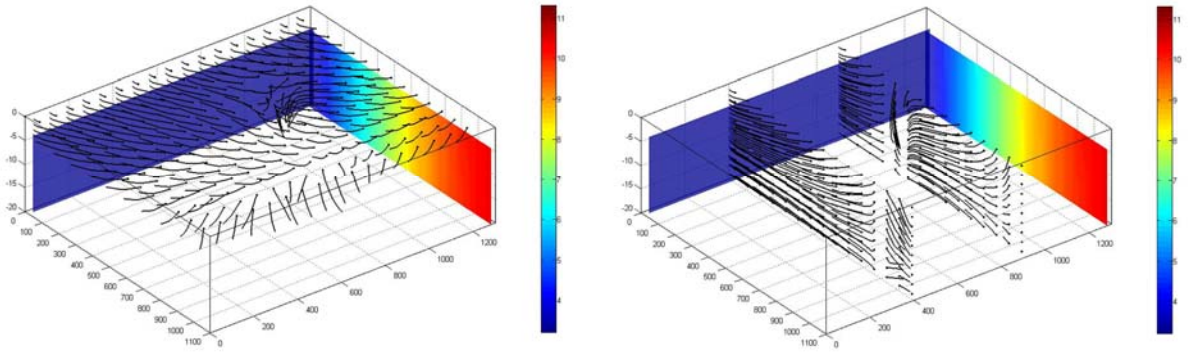


figure 6.17 *Flow paths visualising groundwater flow. The colors represent hydraulic heads.*

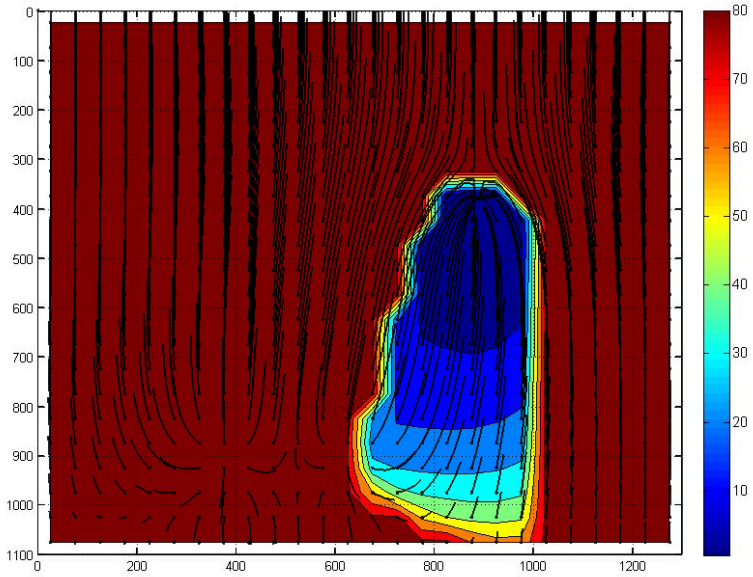


figure 6.18 *Projection of the flowpaths of particles placed in the first layer combined with capture zones (in years) of the well for the recharged water. This visualises flow paths and capture zones of recharge water.*

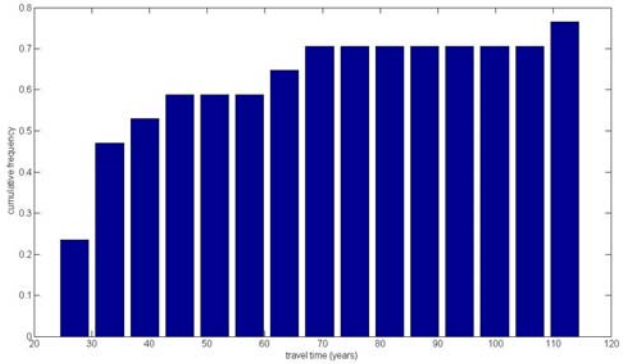


figure 6.19 *Cumulative frequency of the amount of water infiltrated in the ponds at time zero arriving in the pumping well in function of time. Notice that about 25% of the water never reaches the well, whereas the first water arrives after about 25 years.*

6.2 Artificial recharge ponds: VBTM

In the directory "c:\visualMOCDENSD3D\examples\company\VBTM", the model of the artificial recharge is given using the VBTM.

The bas input GUI is shown in figure 6.20. As can be seen five stress periods are considered now for a time span of just over 20 years. The varying boundary type model option is selected and input of boundary conditions and initial heads is via an excel sheet. Take a look at the excel file company_ini.xls. This shows the initial heads. Two periods are considered: stress periods 1 to 3 and stress periods 4 to 5. The northern boundary condition changes between these periods from 3.3 to 2.2 m. The input for bcf, moc, sip and dat can be viewed through the advanced grid builder GUIs.

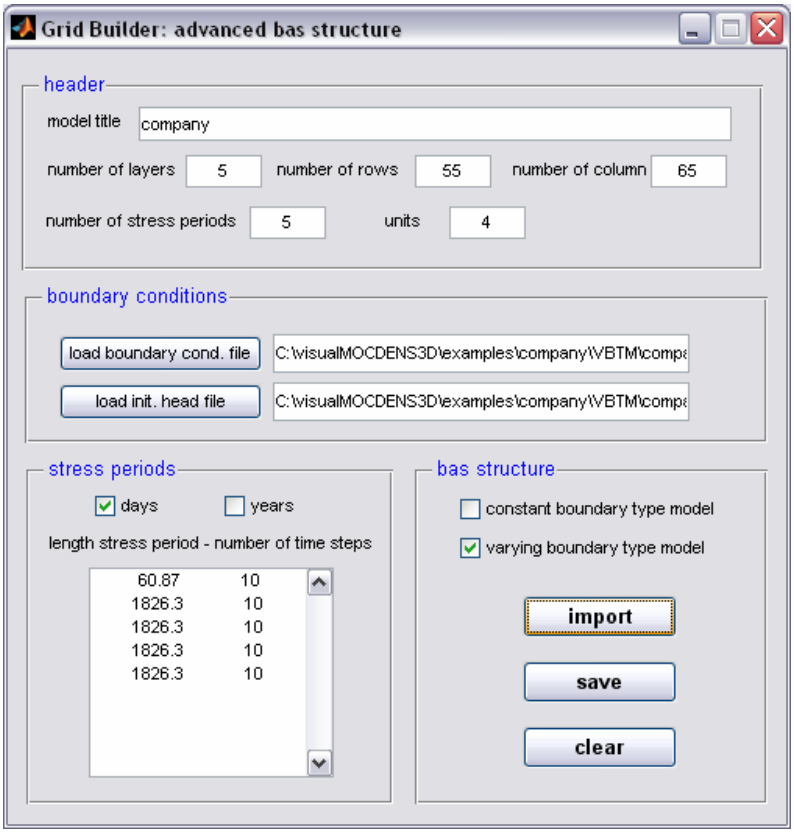


Figure 6.20 *Advanced input GUI for the artificial recharge pond model according to a VBTM.*

Figure 6.21 shows the nam file input GUI. The varying boundary type model option is selected and the name of the input structures is given. The number of stress periods is 5. One change of boundary conditions occurs which means that the 1 stress period (4, the one where the conditions change) is also indicated as variable boundary in selected stress periods.

Figure 6.22 shows the hydraulic heads (colors) and the concentrations (isolines) for stress periods 2 and 4. Notice that the hydraulic head of the northern boundary is indeed 1 m lower during stress period 4 than during stress period 2.

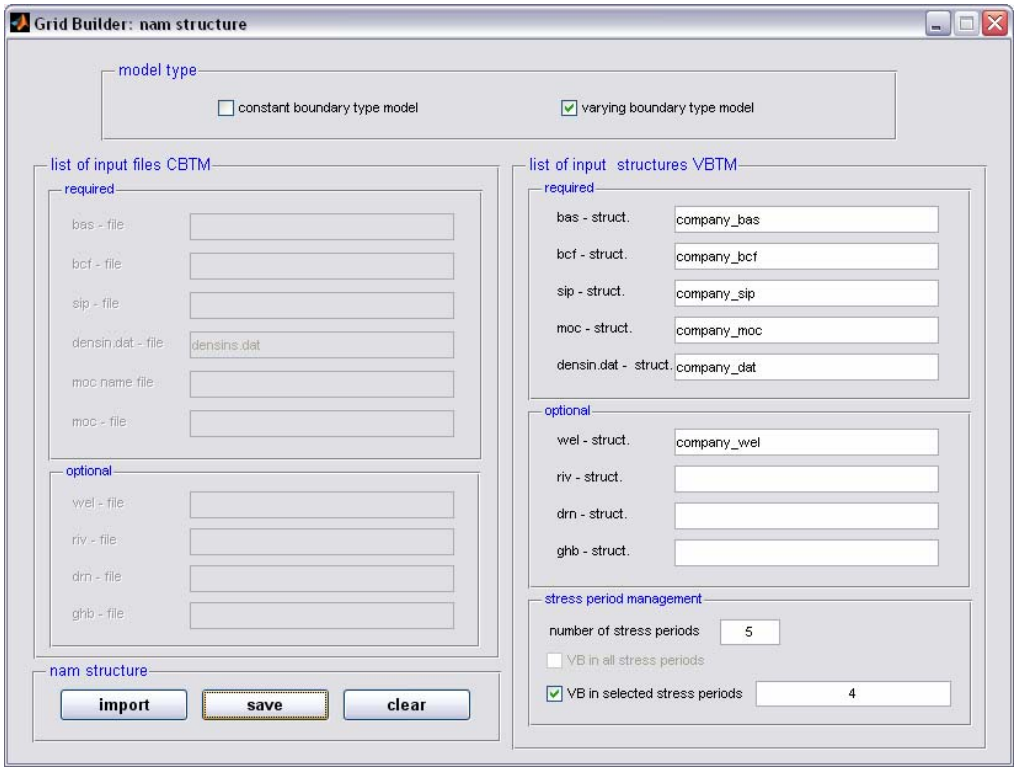


Figure 6.21 *Name input GUI for the artificial recharge pond model according to a VBTM.*

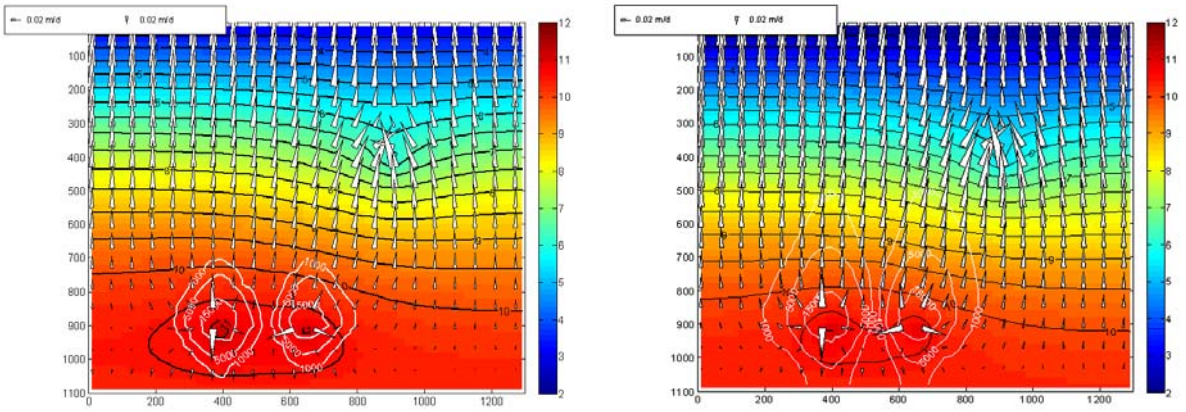


Figure 6.22*Hydraulic heads (colors) and concentrations (lines) for stress periods 2 (left) and 4 (right).*

6.3 Development of a fresh water lens

6.3.1 Problem formulation

In many coastal areas and under islands, fresh water reserves are concentrated in fresh water lenses. These fresh water bodies are surrounded by salt water.

Interesting examples of fresh water lenses can be found in the Belgian coastal plain where they occur under former tidal channels which are now transformed in channel ridges. The relation between quaternary geology, land reclamation and fresh/salt water distribution is very well illustrated here. The necessary intensive drainage and the compaction history of the sediments before and during land

reclamation resulted in the still now observable geomorphology of the area. The drainage of the sandy channel deposits resulted in minor compaction of these sediments. This is in contrast to the clay and peat layers for which compaction can be considerable (for peat, to almost 50% of its thickness for the best-drained parts). Consequently, the old tidal channels formed ridges that stand above the areas where the peat layer occurs. The development of such a fresh water body is modelled here.

6.3.2 MOCDENS3D model

Figure 6.23 shows schematically the model set-up. A 2D model is made of a length of 400 m and a depth of 30 m. In the centre of the model a channel ridge with a width of 200 m is present. In the adjacent areas, the water level is artificially regulated at 5 m. Average infiltration is 280 mm/y. The sediments consist of sand.

figure 6.23 *Conceptual model for the formation of a fresh water lens in a coastal area.*

The model area is subdivided in 40 times 30 elements width a width of 10 m and a thickness of 1 m. Horizontal hydraulic conductivity of every layer is 1 m/d and the ratio of horizontal to vertical hydraulic conductivity is 25. Hydrostatic conditions are present on the east and west border (constant salt water head). Drainage is modelled using the drainage package and the infiltration is given via the well package. 20 stress periods of 5 years are used. Longitudinal dispersivity is 0.2 m, horizontal transverse dispersivity is 0.02 m whereas the vertical transverse dispersivity is 0.002 m. Effective porosity is 0.38.

In the initial situation, the aquifer is filled with salt water. Fresh infiltration water replaces this salt water. Because of the drainage system, no fresh water can enter the aquifer in the adjacent areas to the channel ridge.

6.3.3 Model results

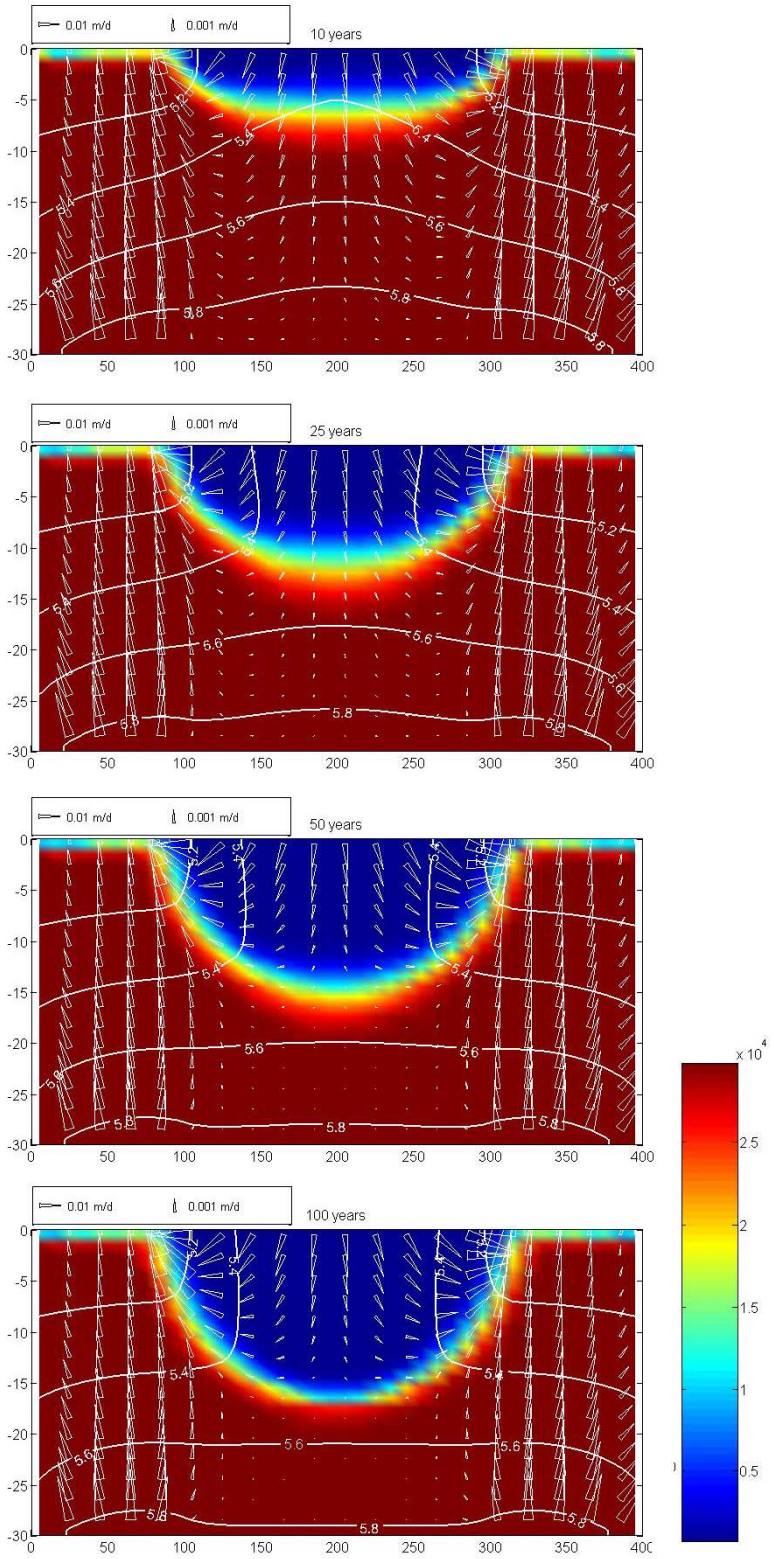


figure 6.24 *Evolution of the fresh water heads (contours) and fresh-salt water distribution (total dissolved solids, mg/l, colors) in function of time. No changes occur after 100 years.*

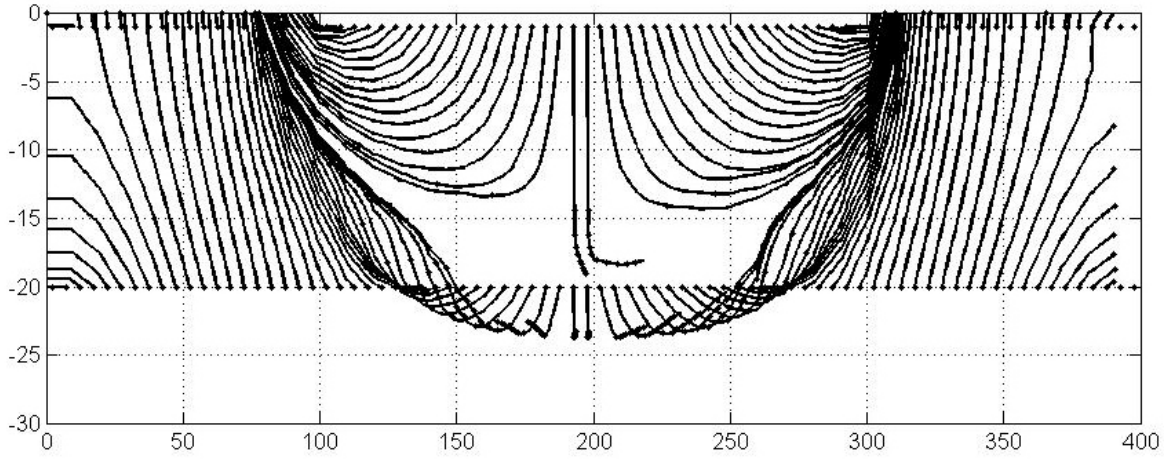


figure 6.25 *Flow paths of particles places at -1 and -20 m. Starting time is the start of the model, thus the start of the freshening of the aquifer and the transient state option is used. It thus shows the flow path of particles during the freshening of the aquifer whereby the velocity field evolves through time.*

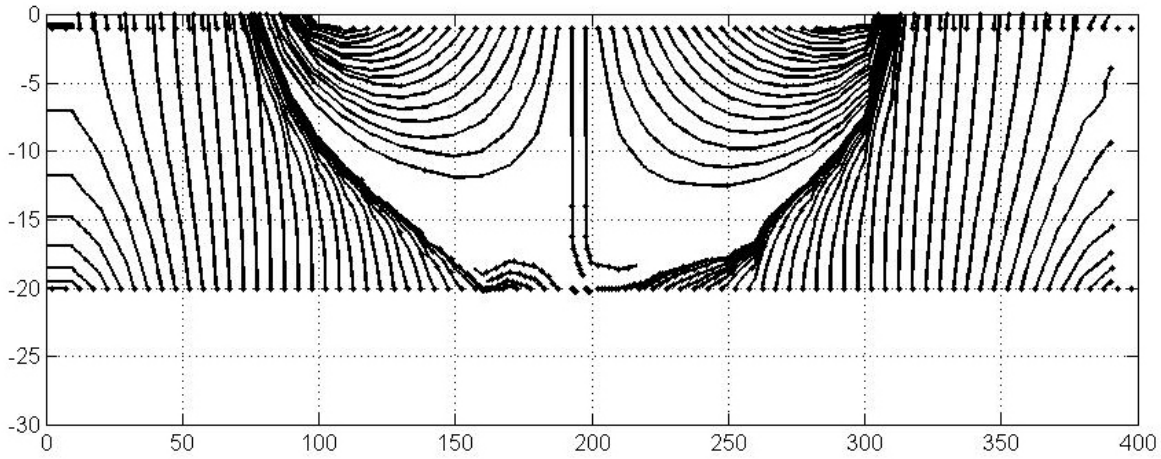


figure 6.26 *Flow paths of particles places at -1 and -20 m. The flow paths are calculated using the velocity field obtained after 100 years simulation. The figure for instance shows what happens to water which infiltrates when the fresh water lens is in an dynamical equilibrium.*

6.3.4 Fresh water exploitation

The influence of a small pumping is simulated. A pumping well is present in the centre of the channel ridge in layers 5, 6 and 7. Extraction rate is 1 m³/d. The pumping starts after the formation of the fresh water lens, thus after the simulation of 100 years shown in figure 6.27.

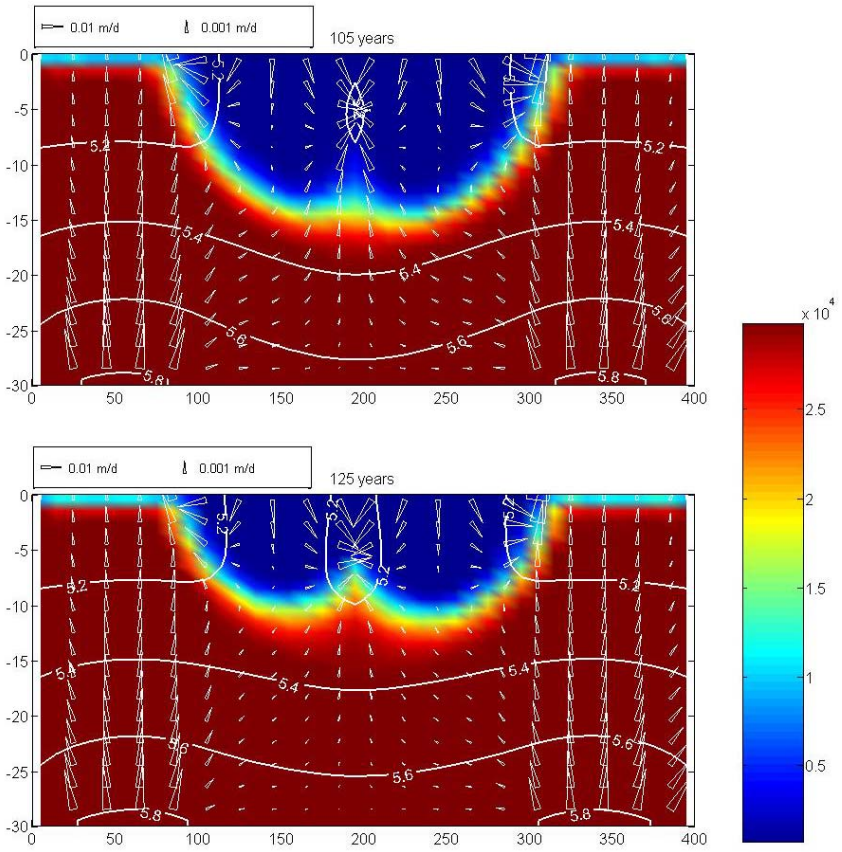


figure 6.27 *Evolution of hydraulic head and fresh-salt water distribution with inclusion of a pumping.*

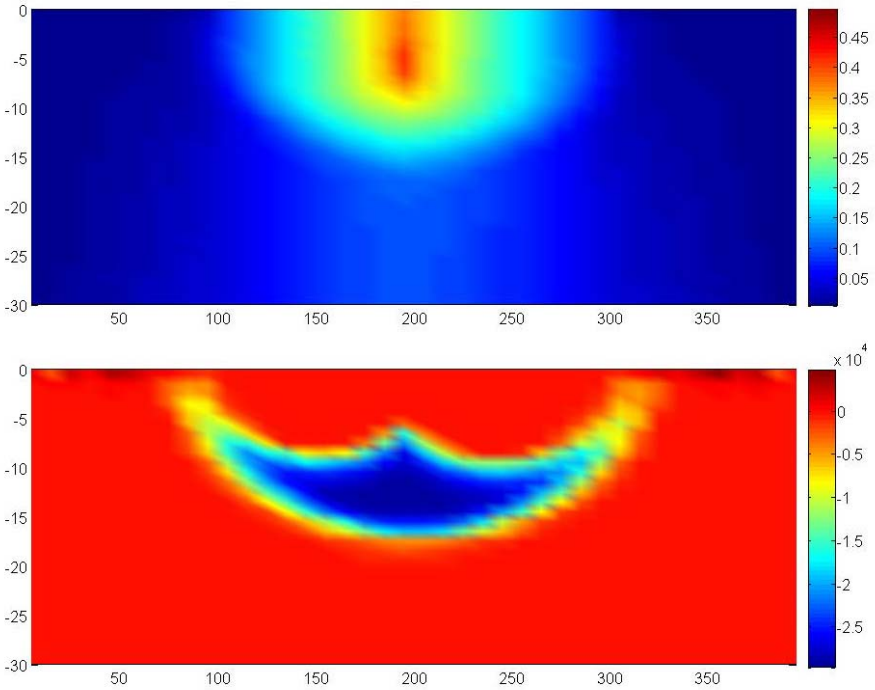


figure 6.28 *Upper figure shows the drawdown (m) due to the pumping. The lower figure shows the difference in total dissolved solids in the aquifer after 50 years of pumping.*

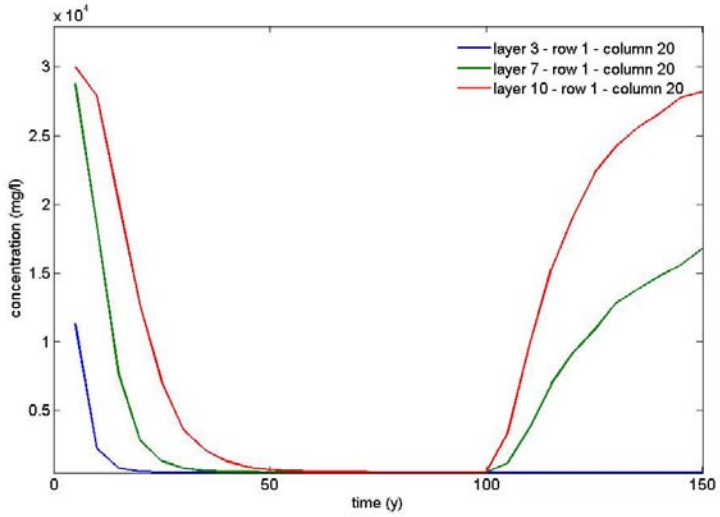


figure 6.29 *Evolution of the concentration at different depths in the centre of the channel ridge..*

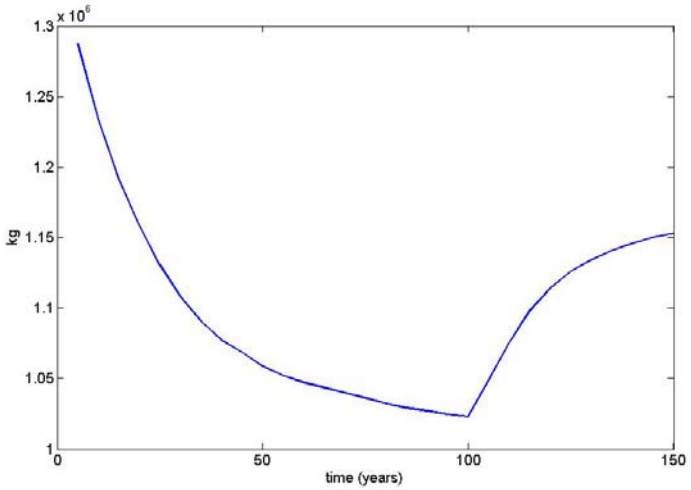


figure 6.30 *Evolution of total salt mass present in the model in function of time.*

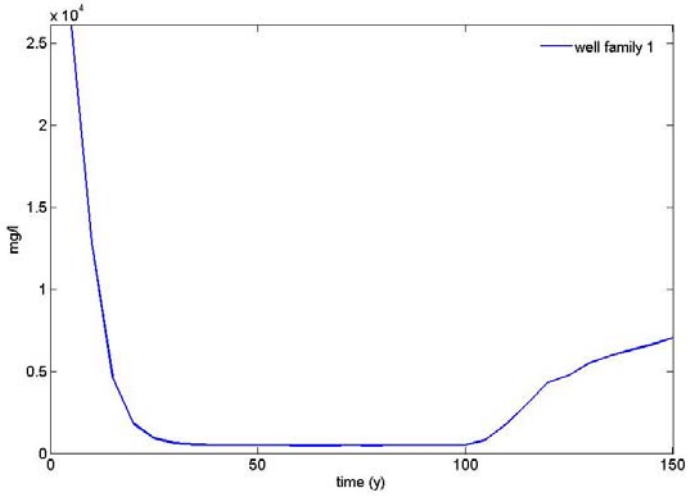


figure 6.31 *Evolution of the mean concentration of the extracted water in function of time.*

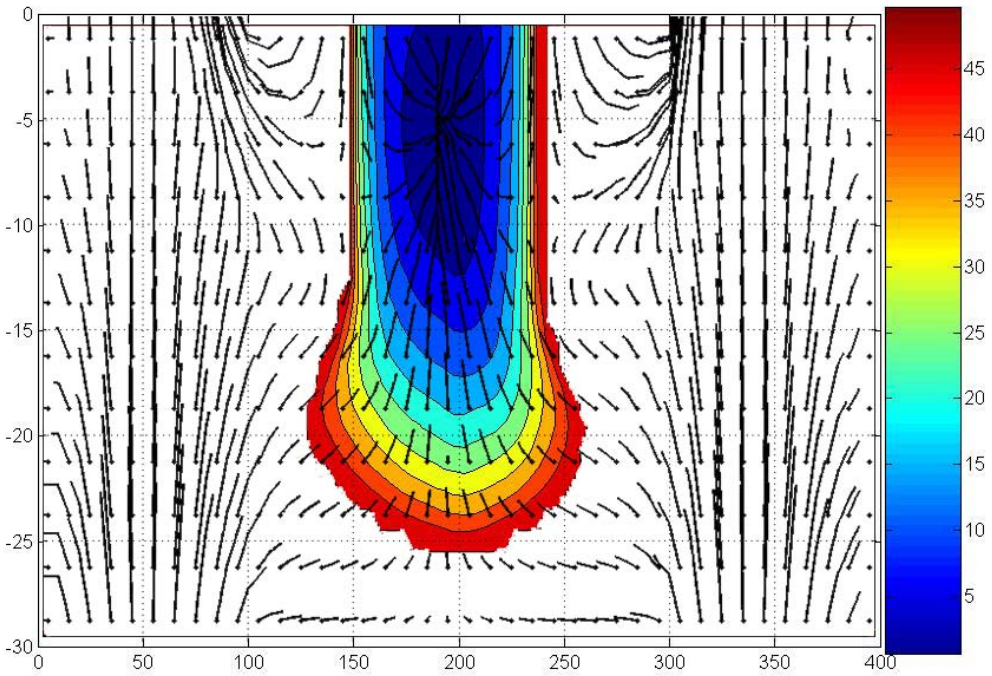


figure 6.32 *Flow paths and capture zones of the pumping.*

6.4 Rotating fresh-salt water interface

6.4.1 Problem formulation

The rotation of a fresh-salt water interface is an academic example illustrating the density dependent groundwater flow. Therefore, consider a box of 1 by 0.5 m containing a porous medium. The right part of the box is filled with salt water (30000 mg/l), the left part with fresh water (500 mg/l) (figure 6.33). This is not a stable density distribution, so the question is to calculate the rotation of the interface.

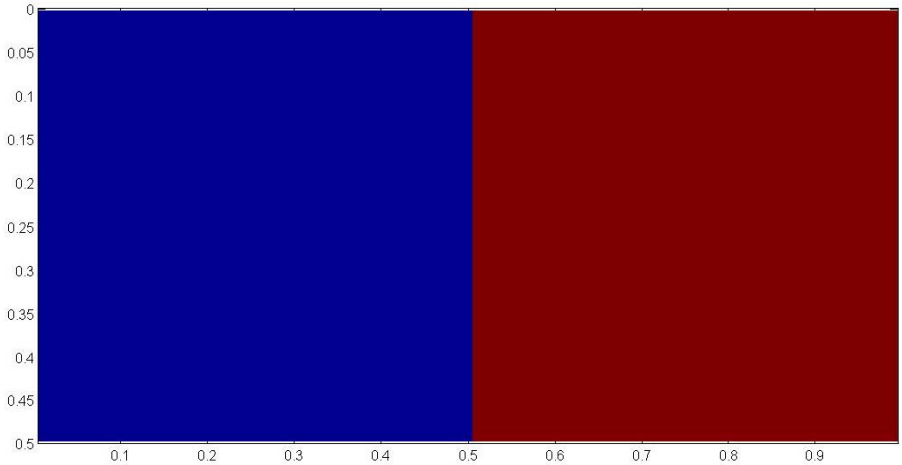


Figure 6.33 *Conceptual model for a box filled with a porous medium and fresh (blue) and salt (red) water.*

6.4.2 Model results

A two-dimensional model is made, consisting of 100 layers (thickness of 0.05 m) and 100 columns (width of 0.1 m). All boundaries are no flow boundaries. 90 stress periods, each of 30 minutes, are used. Buoyancy of the salt water is 0.02 m. Figure 6.34 gives some results of the calculations.

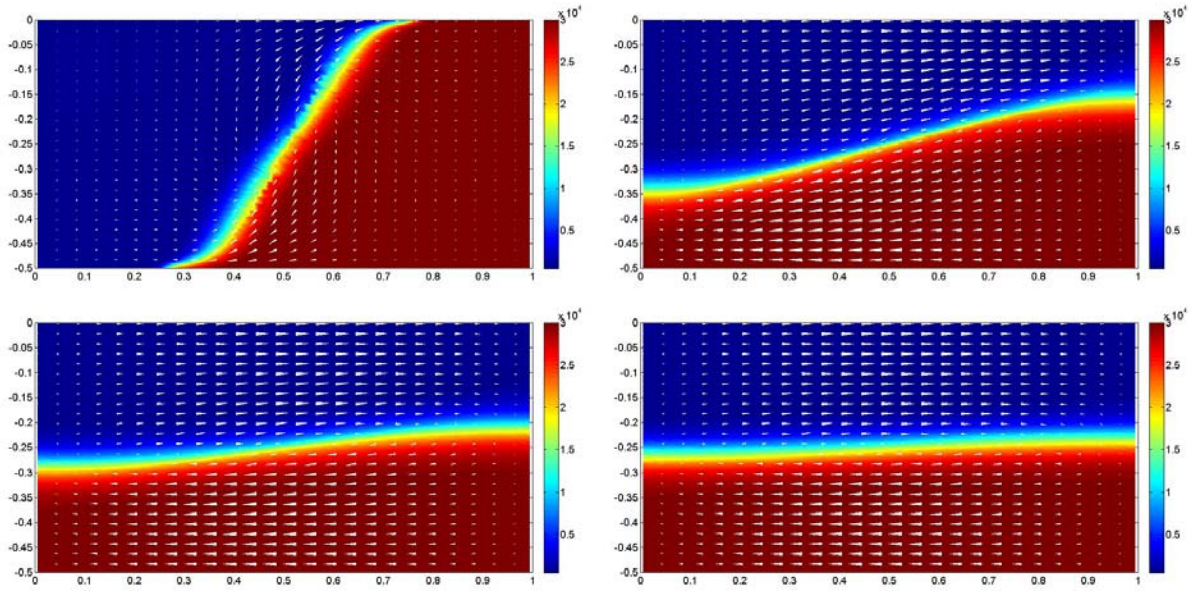


Figure 6.34 *Fresh-salt water distribution at different times (after 0.0208, 0.6240, 1.2479 and 1.8718 days).*

An interesting exercise is to alter the buoyancy. A buoyancy of zero for instance means that two fluids without density difference are present. No rotation of the interface occurs. Change the buoyancy and see what happens. You can also try to alter the length of a stress period or the grid dimensions to see what happens.

Appendix 1: Overview of MOCDENS3D input files

1 (name).bas-file

```
basic grid example
      NLAY      NROW      NCOL      NPER    ITMUNI
         4        50        50         4         4
FREE
         0         1      ; IAPART,ISTRT
        95         1(50I2)                                    3   ; IBOUND 1
-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1 … NCOL
.
.
.
NROW
Repeated for every layer
    9999.00                                                    ; HNOFLO
        95         1(50F7.2)                           1   ; HEAD 1
4.50   4.50   4.50   4.50   … NCOL
.
.
.
NROW
Repeated for every layer
 100.00        10         1     PERLEN, NSTP,TSMULTI
 100.00        10         1     PERLEN, NSTP,TSMULTI
 100.00        10         1     PERLEN, NSTP,TSMULTI
 100.00        10         1     PERLEN, NSTP,TSMULTI
```

Two first lines are comment. The third line gives the number of layers, rows, columns and stress periods as the unit option. Fourth and fifth layer should not be altered. Then the boundary conditions for every layer are given. This starts with a header which gives a file number (must be 95) and a format. This format determines how many numbers and with which format on every line of the following line will be given.

After the matrices of the boundary condition, the head of a no flow cell is given. For use in Visual MOCDENS3D this must be a large number (9999.0) which means it will be recognised as a no flow cell. Afterwards, the matrices with initial heads for every layer are given. The starts again first with a header giving the file number (must be 95) and defining the format.

Finally, for every stress periods, the length of the stress period, the number of time steps and the multiplier are given.

2 (name).bcf-file

The lay-out of an example bcf-file with constant parameter values per layer and for a steady state model:

```
               1         0 0.0 0 0.0 0 0   ISS,IBCFBD     BCF Input
0 0 0 0  LAYCON
         0         1 TRPY
         0     20.0 DELR
         0     20.0 DELC
         0   10.000 TRAN 1
         0    0.0020 VERT/THCK 1
         0    0.500 TRAN 2
         0    0.0020 VERT/THCK 2
         0   15.000 TRAN 3
         0    0.0300 VERT/THCK 3
         0   25.000 TRAN 4
```

The '1' on the first line indicates that a steady state model is used. Otherwise this would be '0'. The other values on the first line are additional flags and must not be changed. The second line gives for every layer the layer type code. Then the ratio of transmissivity in the column direction to row direction and width of row and column are given. Then transmissivity and hydraulic conductance for every layer is listed.
If the hydraulic parameters would be written as matrices, the resulting bcf-file is:

```
               1         0 0.0 0 0.0 0 0   ISS,IBCFBD     BCF Input
0 0 0 0  LAYCON
         0         1 TRPY
         0     20.0 DELR
         0     20.0 DELC
        11       1.0  (50F6.2)                      1    ; TRAN 1
 10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 … NCOL
.
.
.
NROW
        11       1.0  (50F7.4)                      1    ; VERT/THCK 1
 0.0020 0.0020 0.0020 0.0020 0.0020 0.0020 0.0020 0.0020 … NCOL
.
.
.
NROW
Repeated for every layer
```

This is the same format as already explained with the exception that a matrix is given for the transmissivity and hydraulic conductance of every layer. This starts each time with header containing a file number (must be 11) and a format.
The lay-out of an example bcf-file with constant parameter values per layer and for a transient state model:

```
               0         0 0.0 0 0.0 0 0   ISS,IBCFBD     BCF Input
0 0 0 0  LAYCON
         0         1 TRPY
         0     20.0 DELR
         0     20.0 DELC
         0 0.002000 SF 1
         0   10.000 TRAN 1
         0    0.0020 VERT/THCK 1
         0 0.005000 SF 2
         0    0.500 TRAN 2
         0    0.0020 VERT/THCK 2
         0 0.000100 SF 3
         0   15.000 TRAN 3
         0    0.0300 VERT/THCK 3
         0 0.000100 SF 4
         0   25.000 TRAN 4
```

The only difference is the introduction of the storativity values.

In the case a matrix of the parameters for every layer is chosen, the lay-out of the resulting bcf-file is:

```
               0         0 0.0 0 0.0 0 0   ISS,IBCFBD     BCF Input
0 0 0 0  LAYCON
         0         1 TRPY
         0     20.0 DELR
         0     20.0 DELC
        11 1.000000  (50F9.6)                      1    ; SF 1
 0.002000 0.002000 0.002000 0.002000 0.002000 0.002000 0.002000 0.002000 … NCOL
.
.
.
NROW
        11       1.0  (50F6.2)                      1    ; TRAN 1
 10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 10.00 … NCOL
.
.
.
NROW
        11       1.0  (50F7.4)                      1    ; VERT/THCK 1
 0.0020 0.0020 0.0020 0.0020 0.0020 0.0020 0.0020 0.0020 0.0020 0.0020 … NCOL
.
.
.
NROW
Repeated for every layer
```

The only difference is the again introduction of the storativity values.

3 (name).moc-file

```
moc basic grid example

       1       4       1       50       1      50 ISLAY1  ISLAY2  ISROW1 ISROW2  ISCOL1  SCOL2
       0       0       0 NODISP  DECAY   DIFFUSION
       0       8 NPMAX   NPTPND
     0.6    0.05       2 CELDIS  FZERO   INTRPL
       0       3        0        8        0        8       -1 NPNTCL  ICONFM … IVELFM  NPNTDL …
IDSPFM  NPNTBL
  -9999 CNOFLOW
        96       1.0(50F9.2)                      1    ; CONC  1
     0.00     0.00     0.00     0.00     0.00     0.00     0.00 … NCOL
.
.
.
NROW
Repeated for every layer
       1 NZONES
        -1       0.0
         0         1                               ; IGENPT 1
         0         1                               ; IGENPT 2
         0         1                               ; IGENPT 3
         0         1                               ; IGENPT 4
         0      0.50                               ; ALONG
         0     0.050                               ; ATRANH
         0     0.005                               ; ATRANV
         0     1.000                                RF1
         0       5.0                                THICK 1
         0      0.38                                POR 1
         0       5.0                                THICK 2
         0      0.38                                POR 2
         0       5.0                                THICK 3
         0      0.38                                POR 3
         0       5.0                                THICK 4
         0      0.38                                POR 4
```

This file starts with two comment lines. Third line gives the first and last layer, row and column for which solute transport is calculated. Next line indicates if dispersion, decay or diffusion is taken into account. Second number on the fifth line gives the number of particles per cell. First number of the sixth line determines celdis. Next line are flags. Then the concentration of a now flow cell is given. For use in Visual MOCDENS3D this must be a negative number (-9999) which means it will be recognised as a no flow cell. Afterwards, the initial concentrations for every layer are given. This starts with a header containing a file number (must be 96) and a format.

Afterwards, the number of different constant head cells is given (number of zones) and for each zone, the concentration is given. For each layer, a calculation parameter is given. This if followed with the values for dispersivities (if required) retardation and for each layer the thickness and porosity.

4 (name).wel-file

```
      2503          0    AUXILIARY CON  CBCALLOCATE MXWELL,IWELBD
      2503              ITMP (NWELLS)
       1       1       1    1.360       0.0
       1       1       2    1.360       0.0
       1       1       3    1.360       0.0
       1       1       4    1.360       0.0
       1       1       5    1.360       0.0
       1       1       6    1.360       0.0
       1       1       7    1.360       0.0
.
.
.
Number of Wells for this stress period
      -1
      -1
      -1
```

In the first line of this file, the number indicates the maximum number of well cells which are present in one of the stress periods (here 2503). Then for every stress period, the layer, row, column, discharge rate and concentration for every well is given. This is preceded by a header stating how many well cells are active during this stress period. The '-1' at the end of the file, means that for the second to fourth stress period, the wells are identical to the first stress period.

5 (name).riv-file

```
            5          0    AUXILIARY CONC CBCALLOCATE MXRIV,IWELBD
        5               ITMP (NRIVERS)
       1       3       1      2.00     10.00     -2.00    100.00
       1       3       2      2.00     10.00     -2.00    100.00
       1       3       3      2.00     10.00     -2.00    100.00
       1       3       4      2.00     10.00     -2.00    100.00
       1       3       5      2.00     10.00     -2.00    100.00
.
.
.
number of river cells
      -1
        5               ITMP (NRIVERS)
       1       3       1      2.00     10.00     -2.00    100.00
       1       3       2      2.00     10.00     -2.00    100.00
       1       3       3      2.00     10.00     -2.00    100.00
       1       3       4      2.00     10.00     -2.00    100.00
       1       3       5      2.00     10.00     -2.00    100.00
.
.
number of river cells
      -1
```

In the first line of this file, the number indicates the maximum number of river cells which are present in one of the stress periods (here 5). Then for every stress period, the layer, row, column, river stage, river conductance, river bottom and concentration for every river cell is given. This is preceded by a header stating how many river cells are active during this stress period. The '-1' means that for the river cells during this stress period are the same as during the preceding stress period.

6 (name).drn-file

```
        5          0    AUXILIARY CONC CBCALLOCATE MXWELL,IWELBD
        5               ITMP (NDRAIN)
       1       3       1  -1.000    10.0    100.0
       1       3       2  -1.000    10.0    100.0
       1       3       3  -1.000    10.0    100.0
       1       3       4  -1.000    10.0    100.0
       1       3       5  -1.000    10.0    100.0
.
.
.
number of drainage cells
      -1
        5               ITMP (NDRAIN)
       1       3       1  -1.000    10.0    100.0
       1       3       2  -1.000    10.0    100.0
       1       3       3  -1.000    10.0    100.0
       1       3       4  -1.000    10.0    100.0
       1       3       5  -1.000    10.0    100.0
.
.
.
number of drainage cells
      -1
```

In the first line of this file, the number indicates the maximum number of drainage cells which are present in one of the stress periods (here 5). Then for every stress period, the layer, row, column, drainage level, conductance and concentration for every drainage cell is given. This is preceded by a header stating how many drainage cells are active during this stress period. The '-1' means that for the drainaga cells during this stress period are the same as during the preceding stress period.

7 (name).ghb-file

```
        5          0    AUXILIARY CONC CBCALLOCATE MXWELL,IWELBD
        5               ITMP (NGHB)
       1       3       1   5.000    10.0    100.0
       1       3       2   5.000    10.0    100.0
       1       3       3   5.000    10.0    100.0
       1       3       4   5.000    10.0    100.0
       1       3       5   5.000    10.0    100.0
.
.
.
number of ghb cells
      -1
        5               ITMP (NGHB)
       1       3       1   2.500    10.0    100.0
       1       3       2   2.500    10.0    100.0
       1       3       3   2.500    10.0    100.0
       1       3       4   2.500    10.0    100.0
.
.
.
number of ghb cells
       1       3       5   2.500    10.0    100.0
      -1
```

In the first line of this file, the number indicates the maximum number of general head boundary (ghb) cells which are present in one of the stress periods (here 5). Then for every stress period, the layer, row, column, boundary head, conductance and concentration for every river cell is given. This is preceded by a header stating how many ghb cells are active during this stress period. The '-1' means that for the ghb cells during this stress period are the same as during the preceding stress period.

8 (name).sip-file

```
      2500          5     ; MXITER,NPARM                 SIP Input
        1.   1.0E-002          1     0.001 0 ; ACCL,HCLOSE,IPCALC,WSEED,IPRSIP
```

First number on the first line gives the maximum of iterations which are possible. Second number on the second line gives the closure criterion for convergence.

9 Densin.dat-file

```
   30000.0     0.020    CONCD    DVCONC
     0.0    32.5     175     500    1000    2700    CONC.COLORS FOR FILM-OPTION
    5000    7500   10000   15000   20000   27000    CONC.COLORS FOR FILM-OPTION
```

First line gives the maximum concentration with the related buoyancy.

10 (name).nam-files

Infile.nam lists the different files for the calculation of groundwater flow together with an output file. It also refers to the name file for solute transport.

```
List  16 flow.out
BAS   95 test.bas
BCF   11 test.bcf
SIP   19 test.sip
WEL   66 test.wel
CONC  33 test_moc.nam
```

The lay-out of an example (name).nam (moc name file) is:

```
clst    94 test.out
moc     96 test.moc
oba     45 test.oba
data    44 test.obs
```

11 Further reading

For more details, the reader is referred to:

Konikow, L.F., Goode, D.J. and Hornberger, G.Z. (1996). A three-dimensional method of characteristics Solute transport model (MOC3D). U.S. Geological Survey Water-Resources Investigations Report, 96-4267.
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Appendix 2: MATLAB colors, color maps, line styles and marker options

MATLAB colors

b	blue
g	green
r	red
c	cyan
m	magenta
y	yellow
k	black

MATLAB colors maps

jet	hsv
hot	cool
spring	summer
winter	autumn
gray	bone
copper	pink
lines	

adding ‘i’ after the color map name inverts the color map (for instance jeti)

MATLAB line styles

-	solid
:	dotted
-.	dashdot
--	dashed
(none)	no line

MATLAB marker option

.	point
o	circle
x	x-mark
+	plus
*	star
>	arrow
<	arrow
^	arrow
v	arrow
s	square
d	diamond
p	pentagram
h	hexagram

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