
Extension and Refinement of the Aquamod Computer Software

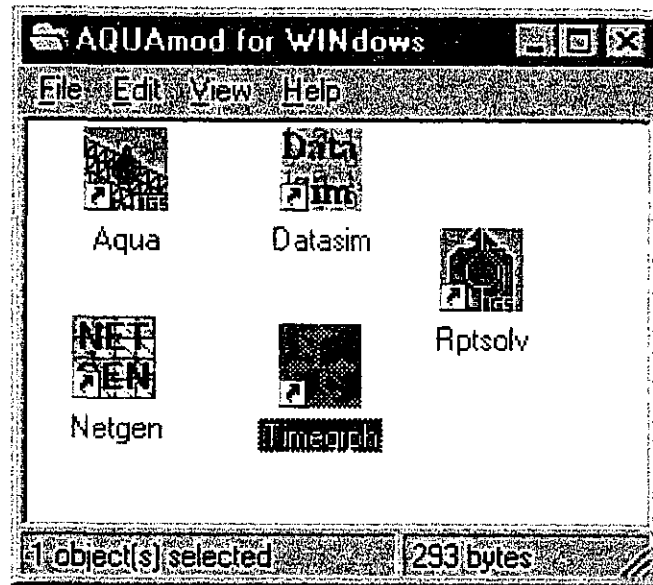
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by the
Institute for Groundwater Studies
University of the Free State

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EXTENSION AND REFINEMENT OF THE AQUAMOD COMPUTER SOFTWARE



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EXTENSION AND REFINEMENT OF THE AQUAMOD COMPUTER SOFTWARE PACKAGE

The Steering Committee who directed the project consisted of the following persons:

Mr AG Reynders	WRC (Chairman)
Mr H Maaren	WRC
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1. Prof. Wolfgang Kinzelbach of Germany for supplying to us his inverse code.
2. Dr. V.E. Cogho for the initiation of the first project regarding management models.
3. Dr. Hugo van Rensburg for programming the Monte Carlo Risk models (as part of his Ph.D. study).
4. Dr. D.B. Bredenkamp for development and refinement of the CRD-method.
5. Mr. Johan Verwey for coding the pump-test analysis program.

EXECUTIVE SUMMARY

1. INTRODUCTION

The purpose of the project, as stated in the contract with the Water Research Commission, was as follows:

- (i) to make the current AQUAMOD computer package user-friendly; and
- (ii) to extend the computer package to include groundwater quality management aspects.

The work on the project began in January 1994 and ended in October 1996.

During a previous project, entitled: "The development of management and risk techniques for Southern African Aquifers", most of the AQUAMOD computer software was developed. This program, however, was not very user-friendly, and the main objective of the follow-up project was to fulfil this objective.

The AQUAmod for WINdows (short: **AQUAWIN**) program is the result of this objective.

2. COMPUTER STRUCTURE OF AQUAWIN

AQUAWIN is a 2D-triangular finite element Groundwater Modelling Package, consisting of five programs: namely Network Generator, **NETGEN**, the Groundwater Modelling program, **AQUA**, **DATASIM** for the graphic presentation of the modelling results, **TIMEGRPH** for the display of time-dependent data and **RPTSOLV**, a pumping-test procedure for fractured-rock aquifers. Figure 1 shows the layout of AQUAWIN.

PROGRAM NETGEN (GRID GENERATOR)

NETGEN generates a finite triangular mesh between a finite set of user-defined data points.

PROGRAM AQUA

This program consists of eight subprograms, namely:

AQUAWIN MODELING PACKAGE

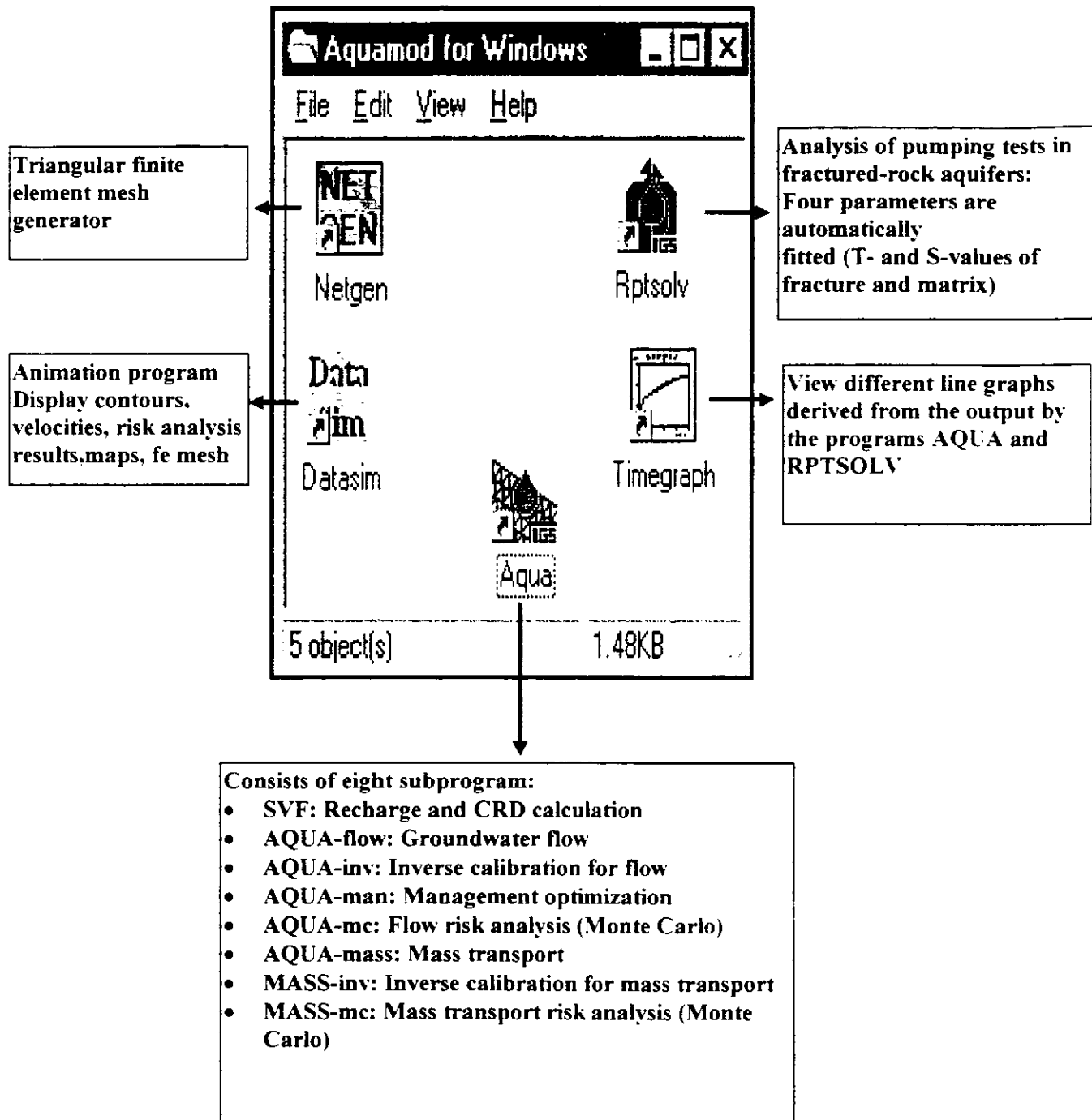


Fig. 1 AQUAWIN layout

AQUA-FLOW: (FLOW PROGRAM)

AQUA-FLOW solves the Galerkin finite element method in two dimensions for groundwater flow.

Special features of AQUA include the ability to specify:

- (i) variable pumping rates;
- (ii) time-dependent recharge values as percentage of monthly rainfall; and
- (iii) a confined or water-table aquifer.

The output of AQUA yields:

- (i) monthly simulated water levels at each node (e.g. for contouring purposes) or water levels at specific user-defined nodes;
- (ii) groundwater velocities in the centre of each element (optional); and
- (iii) a groundwater balance.

PROGRAM AQUA-INV (INVERSE PROGRAM FOR FLOW)

AQUA-INV is an automated parameter identification program which uses the flow program AQUA and the Marquardt optimization algorithm to obtain the following choice of parameter combinations for zones in an aquifer which simultaneously produce the best fit between observed and simulated historical water-level data:

1. T- and S-variables
2. T
3. S
4. Recharge
5. T and recharge
6. Neumann inflow flux at boundary
7. T, S and inflow flux at boundary.

PROGRAM AQUA-MASS

This program solves the convection diffusion equation in two dimensions for mass transport problems.

PROGRAM MASS-INV (INVERSE MASS TRANSPORT PROGRAM)

This program is the equivalent of the AQUA-INV program, and can be used for the automated calibration of the mass transport problem. The parameters which could be inverse are the T-values and the longitudinal and transversal dispersivities.

PROGRAM AQUA-MAN (MATHEMATICAL OPTIMIZATION)

AQUA-MAN links the distributed parameter groundwater flow simulation model, AQUA, with mathematical optimization methods using a technique known as the response matrix approach. Linear programming formulation of the management problem is solved by a simplex routine obtained from Kinzelbach (1986).

PROGRAM SVF (RECHARGE ESTIMATION)

This program estimates the groundwater recharge of an aquifer with the aid of the SVF-method and was originally programmed for the WRC-project of Kirchner *et. al.* (1991). It is also possible to calculate cumulative rainfall departures (CRD) with this program (Bredenkamp *et. al.*, 1995).

PROGRAM AQUA-MC AND MASS-MC

Two program modules (AQUA-MC and MASS-MC) were added to the AQUAMOD package to cover the aspects of groundwater flow and pollution risk respectively. The programs are based on the Bayes approximation which requires the specification of probability density functions (p.d.f.) for the different variables. The p.d.f. approach is much less complicated and less time-consuming than the geostatistical approach and can be performed with ease on a PC.

Program MASS-MC utilizes Monte Carlo simulations in the determination of pollution risk using a Bayes approximation.

PROGRAM RPTSOLV

Bredenkamp and co-workers (Bredenkamp, 1992, and Bredenkamp *et. al.*, 1995) demonstrated that the calculated S-values in fractured-rock aquifers (if analysed with the Theis-model or any analytical fractured model, e.g. Moench) are a function of the distance between the abstraction and observation boreholes (the larger the distance, the smaller the estimated S-values).

Prof. Wolfgang Kinzelbach suggested that a 2D-radial flow model might be the solution to the problem. The necessary software, RPTSOLV, was written and is included as part of the AQUAWIN software suite.

PROGRAM DATASIM AND TIMEGRPH

Datasim is an animation program and can be used for the display of contours, velocities, maps and finite element meshes, while program Timegrph is a line graph viewer.

3. CONCLUSIONS AND RECOMMENDATIONS

The AQUAmod for WINdows program is the result of five years of research and programming and can be used with great benefit for the management of our aquifers. After getting acquainted with all the input files and menu structures, the work of a groundwater modeller will definitely be made easier.

There are, however, shortcomings in the program. It is recommended that the following modules must be added to the software:

- a module for pathline calculations;
- a module for capture zone calculation; and
- a module for calculating salt balances at specific nodes and zones.

AQUAWIN is a 2D finite element program. It is recommended that the program must be converted to a quasi-3D program (like MODFLOW).

A workshop on the usage of the AQUAWIN modelling package was held during September 1996 at the Institute for Groundwater Studies. The presentation of more workshops on AQUAWIN is recommended.

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1. INTRODUCTION

1.1 GENERAL

During a WRC-project entitled: The development of risk analysis and groundwater management techniques for Southern African aquifers , Section 1: The development of groundwater management techniques (Van Tonder *et. al.*, 1994), the AQUAMOD computer package was developed which can be used for:

- constructing a finite element mesh;
- automated calibration of the aquifer parameters (inverse problem);
- obtaining an estimate of natural groundwater recharge;
- optimization and groundwater flow simulations; and
- mass transport solutions.

The main objective with the current project was to convert these programs into a Windows environment.

Following a decision to carry out all programming in Windows, the first step was to evaluate different programming languages and develop tools for Windows. It became evident that programming Windows with the standard Windows application programmers interface (API) function calls using the C programming language, is a tedious and complicated task. Every option investigated for developing Windows programs pointed towards object orientated programming.

Object orientated programming can be said to be a set of techniques that can be used to make programming more efficient, while improving the reliability of resulting programs. The main objective of object orientated programming is to develop different objects or classes for performing different tasks. These objects are based on and constructed around the data on which the program operates. Without getting further into the more technical aspects of object orientated programming, it can, without any doubt, be said that they differ conceptually in many ways from linear programming.

Microsoft introduced Visual C++ with the Microsoft Foundation Classes (MFC) which is fully object orientated. The MFC encapsulates most of the standard windows API function calls and thus simplifies programming for Windows. Visual C++ has different tools to enable the programmer to visually construct menus, dialogs, push-buttons

and icons which enables the programmer to see exactly how the program is going to look. After deciding to use Microsoft VisualC++, immediate steps had to be taken in getting acquainted with the new language and the new environment.

Following an introduction to object orientated C++, it became clear that re-writing the software for Windows, would set the project back by at least seven months.

The introduction of Windows 95 during October 1995, led the way for the final programs to be in a Windows Environment.

1.2 ANALYSIS AND INTERPRETATION OF PUMPING-TESTS IN FRACTURED FORMATIONS

Bredenkamp and co-workers (Bredenkamp, 1992, and Bredenkamp *et. al.*, 1995) demonstrated that the calculated S-values in fractured-rock aquifers (if analysed with the Theis-model or any analytical fractured model, e.g. Moench) are a function of the distance between the abstraction and observation boreholes (the larger the distance, the smaller the estimated S-values).

Prof. Wolfgang Kinzelbach (1995, personal communication) suggested that a 2D-radial flow model might be the solution to the problem. The necessary software, RPTSOLV, was written and is included as part of the AQUAWIN software suite.

2. COMPUTER PROGRAM STRUCTURE OF AQUAMOD FOR WINDOWS

Aquamod for Windows is part of a Groundwater Modelling Package, consisting of five programs; namely Network Generator, **NETGEN**, the Groundwater Modelling program, **AQUA**, **DATASIM** for the graphic representation of the modelling results, **TIMEGRPH** for the display of time-dependent data and **RPTSOLV**, a pumping-test procedure for fractured-rock aquifers.

The programs interact with one another through a set of files which must all have the same name with different fixed extensions.

The Groundwater modelling program, **AQUA**, is subdivided into the following eight subprograms:

- Subprogram **SVF**: Recharge and CRD
- Subprogram **Aqua-Flow**: Groundwater Flow
- Subprogram **Aqua-inv**: Inverse calibration for flow
- Subprogram **Aqua-man**: Management optimization (response matrix procedure)
- Subprogram **Aqua-mc**: Flow risk analysis (Monte Carlo Method)
- Subprogram **Aqua-mass**: Mass transport
- Subprogram **Mass-inv**: Inverse calibration for mass transport
- Subprogram **Mass-mc**: Mass transport risk analysis (Monte Carlo Method)
-

2.1 PROGRAM NETGEN (GRID GENERATOR)

NETGEN generates a finite triangular mesh between a finite set of user-defined data points. It uses an algorithm developed by Watson (1982). This algorithm constructs triangles by subdividing an initial triangle that encloses all the data points. Data points are introduced one at a time and triangles are formed, so that no node lies within another triangle's circumcircle. Where this happens, these triangles are deleted and new ones are formed including this new data point. On completion of this process, the triangles with connections to the initial triangle are deleted. Triangles which are situated outside the boundary are deleted simultaneously. This triangulation scheme complies with the Delaunay criteria and may therefore be classified as a Delaunay triangulation.

After the triangulation, the band-width can be reduced considerably with a built-in option. It builds a level structure from the connectivities of the nodes. An initial starting node with lowest connectivity (degree) is listed in the first level. All nodes

connected to this node are listed in the second level. For each of the nodes in the second level, all nodes connected to this node that were not listed before, are listed in the third level. The same is done for the third level and levels to follow, until all nodes are listed in the level structure.

This level structure is then reduced to have a new structure with levels of smaller height. This new structure is then renumbered to give the same network with a smaller band-width.

Marking of zones, hereafter called zoning, is accomplished in a novel manner. An area is enclosed by a few lines (polygon) and all triangles in this area are coloured with the chosen zone colour.

At each generated node, the user has the option to specify certain information about the nodes, e.g. abstraction rate, constant head node, drainage node, observation node, constant concentration node, etc.

2.2 PROGRAM AQUA

This program consists of a eight subprograms, namely:

2.2.1 AQUA-FLOW: (FLOW PROGRAM)

AQUA-FLOW solves the Galerkin finite element method in two dimensions for groundwater flow.

Special features of AQUA include the ability to specify:

- (i) variable pumping rates;
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The output of AQUA yields:

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AQUA-INV is an automated parameter identification program which uses the flow program **AQUA** and the Marquardt optimization algorithm to obtain the following choice of parameter combinations for zones in an aquifer which simultaneously produce the best fit between observed and simulated historical water-level data:

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2. T
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This program solves the convection diffusion equation in two dimensions for mass transport problems.

2.2.4 PROGRAM MASS-INV (INVERSE MASS TRANSPORT PROGRAM)

This program is the equivalent of the **AQUA-INV** program, and can be used for the automated calibration of the mass transport problem. The parameters which could be inverse are the T-values and the longitudinal and transversal dispersivities.

2.2.5 PROGRAM AQUA-MAN (MATHEMATICAL OPTIMIZATION)

AQUA-MAN links the distributed parameter groundwater flow simulation model, **AQUA**, with mathematical optimization methods using a technique known as the

response matrix approach. Linear programming formulation of the management problem is solved by a simplex routine obtained from Kinzelbach (1986).

2.2.6 PROGRAM SVF (RECHARGE ESTIMATION)

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2.2.7 PROGRAM AQUA-MC AND MASS-MC

Two program modules (AQUA-MC and MASS-MC) were added to the AQUAMOD package to cover the aspects of groundwater flow and pollution risk respectively (Van Rensburg, 1995). Although the CSIR also concentrated on risk assessment in flow studies (Elphinstone *et al.*, 1994) and used the Monte Carlo-based risk approach, their approach differed from the approach used in the AQUA-MC program. The CSIR based their approach on a geostatistical one, while the current program is based on the Bayes approximation which requires the specification of probability density functions (p.d.f.) for the different variables. The p.d.f. approach is much less complicated and less time-consuming than the geostatistical approach and can be performed with ease on a PC.

Program MASS-MC utilizes Monte Carlo simulations in the determination of pollution risk using a Bayes approximation. The steps are as follows:

(i) Determine the nature of the investigation and the decision to be taken. (Is the problem one of water supply, contamination-remediation or a geotechnical problem in which hydrogeology plays an important role and what are the alternative actions to be chosen to solve the problem?). Define failure and the cost associated with failure under each design alternatively, e.g. in a water-supply situation, failure will be when the water level in an abstraction borehole is drawn below the last water strike in the borehole (probabilistic cost associated with failing to meet demand might have severe cost implications, if the supply is, for example, to a big city and will have less impact when the supply is for stock-watering). In a contamination problem, failure will be the exceedance of a specified concentration at a predetermined location and the probabilistic cost associated with failure will be the cost to clean up or to remediate the site. In a geotechnical application, failure will be the failure of the side walls in an opencast mine or a slimes dam and the probabilistic cost to rehabilitate the mine or site and the cost of loss of production.

(ii) Identify the uncertainty in input parameters that may have an effect on the decision to be made and construct p.d.f.'s for each of them. In the case of a

water-supply problem, uncertainty in the following parameters will have an impact on the risk of the decision to be taken:

- transmissivity and storativity (storage coefficient or specific yield depending on the type of aquifer) in the case of 2-D flow;
- hydraulic conductivity and specific storativity in the case of 3-D flow; and
- rainfall distribution and recharge as a function of rainfall.

If the problem is one of contamination or remediation, p.d.f.'s in addition to the above must be established for the:

- longitudinal and transversal dispersivities; and
- kinematic porosity.

If the problem is geotechnical of nature where e.g. slope stability is of importance, p.d.f.'s should be established for the shear-strength parameters (cohesion and friction angle) in addition to the input parameters discussed in the water-supply situation.

(iii) Generate stochastically (random) values (100 values should be sufficient) for each of the uncertain input parameters.

(iv) Construct simulation models to predict the probability of failure of the hydrogeological component and/or geotechnical component of the design. During the phase of model construction, useful techniques such as the Bayes water-level interpolation method can be utilized to produce the initial water-level condition in the model.

(v) Use the stochastically generated values (in iii) to simulate response of the hydrogeological components (programs AQUA-MC and MASS-MC). Construct p.d.f.'s for the output parameters (water levels with time at specified location and contaminant concentrations with time at specified location). The probability of failure (risk) can be determined from these p.d.f.'s by integration of the area at or below a certain critical value.

If different decisions are to be compared, perform the following additional steps:

(vi) Multiply the probability of failure with the cost associated with failure to obtain the risk for each alternative in terms of monetary value (Rands).

(vii) Obtain the benefits and costs under each design alternative.

(viii) Utilize the obtained benefits, costs and risks for each alternative in the decision model by taking into consideration the monetary value. Choose the design alternative with the largest net present value (NPV) in the case of a benefit-cost-risk analysis and the design alternative with the smallest NPV in the case of a cost-risk analysis.

2.3 PROGRAM RPTSOLV

The effective management of an aquifer is primarily dependent on how well the aquifer parameters are known. A variety of methods were developed recently to determine these parameters. They include slug tests, packer tests, tomography and even numerical modelling. However, the well-known pumping test is still the preferred method of many geohydrologists (Kruseman and De Ridder, 1991). The reasoning that a pumping test places the same type of stress on an aquifer as a normal production borehole, but in a short, economical way, still holds true. Furthermore, a wealth of interpretation tools exists to analyse this data, often in an automatic, effortless way.

These interpretation methods all use analytical solutions of the groundwater flow equation, dependent on certain assumptions, including homogeneity. However, in a fractured porous medium, especially at the scale of a pumping test, this assumption is violated. The mixture of horizontal movement in the fractures and vertical leakage in the surrounding matrix, cannot be accounted for in the analytical solutions. Therefore incorrect and unrealistic values, for especially the storativity of the aquifer, are calculated.

The unrealistic values obtained by interpreting pumping test data in aquifers in the Karoo formations have been addressed in previous publications (Kirchner *et. al.*, 1991). A particular problem was in the estimated value for the storativity. Pumping tests in the Dewetsdorp and De Aar regions revealed values for S as low as 10^{-6} while water balance studies, specifically the SVF method (Kirchner *et. al.*, 1991), showed values of S in the order of 10^{-3} .

A series of pumping tests was conducted, in typical Karoo formations, at the Test Site at the University of the Free State. These data were analysed with the program AQTESOLV (Duffield and Rumbaugh, 1991). The values obtained for the transmissivity were typical for Karoo aquifers, and corresponded with the yields of the boreholes. However, the values of the storativity showed no physical meaning. The observation boreholes were situated almost randomly around the pumping borehole and provided an opportunity to investigate the dependence of the storativity on the radial distance from the pumping borehole. This decrease in S with distance (the pumping tests were analysed with the classical Theis-method), is documented in more than twenty cases in South Africa, all in secondary aquifers.

This distance dependence of the storativity does not occur in homogeneous aquifers. Geological and geohydrological investigations of the boreholes at the Test Site

suggest a region of highly fractured sandstone, situated in a less fractured region. However, it is very difficult to distinguish between these two zones. In fact, the theoretical approach to these fractured porous aquifers is to consider them as multi-porous, multi-permeable regions (Bai *et. al.*, 1993). A simplified, three-dimensional conceptual model was therefore developed, consisting of two porous layers, of which the hydraulic properties differ considerably.

An explanation for this behaviour can be found in a combination of the vertical movement of the groundwater, with the propagation of the pressure gradient. Near the pumping borehole, a large gradient develops, because of the effect of the pump. Water flows from the upper layer to the lower layer because of this gradient, resulting in the calculation of S from the upper layer, which simulates the less fractured zone. Further away, a smaller gradient exists, and less leakage occurs. The storativity of the lower layer, simulating the more fractured zone, with the high hydraulic conductivity, is therefore calculated from the distant observation boreholes.

One might be tempted to determine the optimal position of the observation borehole empirically, in order to be able to calculate the storativity of the aquifer matrix from a pumping test. The ability to simulate the field conditions with a numerical model, on the other hand, raises the possibility of determining the aquifer parameters from pumping test data with an inverse, three-dimensional numerical model. However, both these methods prove to be impractical. The first, due to different geological conditions, and the second due to presently excessive computer requirements. In the next section, a solution to this problem will be presented.

The movement of groundwater should, in general, be considered in three dimensions. However, in order to simplify data and computer requirements, one often attempts to eliminate the direction in which negligible movement occurs. Examples of these two-dimensional approximations are the horizontal, regional movement of groundwater, but also the vertical sections to describe groundwater movement in the unsaturated zone. A similar approximation is suggested for the modelling of a pumping test.

In the absence of regional base flow, groundwater flow is towards the borehole during a pumping test. Therefore, flow directions are (1) radially, towards the borehole and (2) in the vertical direction. A section through the aquifer in the form of a wedge-shaped slice takes advantage of this restricted flow, with θ in the direction of no-flow (Rathod and Rushton, 1984; Kinzelbach, 1995). The general three-dimensional groundwater flow equation

$$S_0 \frac{\partial \phi}{\partial t} = K \nabla^2 \phi + N$$

can therefore be integrated in the q -direction, resulting in the two-dimensional equation of unit radial width,

$$rS_0 \frac{\partial \phi}{\partial t} = rK \nabla^2 \phi + \frac{Q \delta(\mathbf{x} - \mathbf{x}_0)}{2\pi}$$

with the symbols having the usual meaning. A slice of angular size θ has, on a distance r , an angular width of $r\theta$. The product of the three-dimensional parameters, that is either the specific storativity, S_0 , or hydraulic conductivity, K with $r\theta$, should not be confused with the horizontal two-dimensional parameters of storativity and transmissivity. These angular parameters, $r\theta S_0$ and $r\theta K$, serve the same purpose of reducing the dimensions of the flow equation, but they are distance related and only of use in this radial numerical model. The user must, if needed, calculate S and T from a predefined thickness of the whole aquifer, or a specific layer of interest.

However, when using this model, the thickness of the aquifer, or different layers, must always be known, because this information is necessary for the development of the numerical model. The advantage of this presentation is that vertical variations in the aquifer can be taken into account, but with a two-dimensional flow model.

A complete description of the model is given in Verwey *et. al.* (1995). This procedure has the potential to become a standard pumping test analysis technique in fractured-rock aquifers.

2.4 PROGRAM DATASIM AND TIMEGRPH

Datasim is an animation program and can be used for the display of contours, velocities, maps and finite element meshes, while program Timegrph is a line graph viewer.

3. GENERAL COMMENTS AND HINTS ON AQUAWIN

3.1 DATA REQUIRED TO DEVELOP A GROUNDWATER MODEL

The first phase of a groundwater modelling exercise consists of collecting all existing geological and hydrological data on the groundwater system in question. This will include information on surface and subsurface geology, water tables, precipitation, pumped abstractions, aquifer characteristics, aquifer boundaries and groundwater quality. If such data do not exist or are very scanty, a program of field work must first be undertaken, for no model whatsoever makes any hydrological sense if it is not based on a rational hydrogeological conception of the system (Boonstra & De Ridder, 1990). All the information is then used to develop a conceptual model of the aquifer.

Developing and testing a numerical model, requires a set of quantitative hydrogeological data that fall into two categories:

- data that define the physical framework of the aquifer; and
- data that describe its hydrological stress.

Boonstra & De Ridder (1990) listed the data required to develop a ground-water model:

Physical framework

1. Topography
2. Geology
3. Type of aquifer
4. Aquifer thickness and lateral extent areas
5. Aquifer boundaries
6. Lithological variations within the aquifer
7. Aquifer characteristics

Hydrological stress

1. Water-table elevation with time
2. Type and extent of recharge areas
3. Rate of recharge
4. Type and extent of discharge areas
5. Rate of discharge

3.2 CALIBRATION OF THE GROUND-WATER MODEL

Before a model can perform its task of predicting the future water-table behaviour, it must be calibrated, which means that a check must be made to see whether the model can correctly generate the past behaviour of the water table, as it is known from historical records. Calibration is the most difficult part of ground-water modelling and requires great skill and team-work.

Useful comments on calibration

1. Select a period in which the water table shows a recession, for which historical records are available. (A period of recession is necessary because it is nearly impossible to calibrate for S and recharge simultaneously.) If, however, the recharge rate is known for each month, any historical period can be selected. Obviously, the longer the period used for calibration, the better the results will be.
2. Many modellers (e.g. Kauffmann & Kinzelbach, 1989) calibrate the flow model, both in steady and non-steady state, by starting with the steady state case. In steady state, the computed heads are compared to the measured and time average areal head distribution. It is important to note that for steady state simulations, at least one constant head node must be used. The steady state solution is only dependent on the areal T -distribution, discharge and recharge rates and boundary conditions (and not on the areal S -distribution). The areal T -distribution obtained from the steady state calibration is then used in the non-steady case to calibrate for the S -distribution in the aquifer.
3. It is important to supply the inverse program (AQUA-INV) with realistic upper and lower bounds on T and S for each zone. To be able to do this, a sound judgement of the parameters in question is necessary, and a possible range of errors in the T - and S -values must be provided. It may happen that some of the calculated water-table elevations cannot be matched with the historical ones, even if the values of the parameters have been varied up to their maximum error percentage. Possible reasons for this include:
 - Wrong zonation of the aquifer.
 - Wrong boundary conditions
 - Wrong recharge estimates.

- Wrong input parameters such as abstraction rates, type of aquifer, etc.

Faced with the situation that the above-mentioned factors are correct, one has no alternative but to return to the field for additional measurements.

4. Proper model calibration depends above all on the integrity of the modeller. It is always possible to "calibrate" a model if one has a free hand in changing the input parameters and disregards the maximum error limits. But then, one is not calibrating the model, but is merely playing with it, which is a dangerous game (Boonstra & De Ridder, 1990).
5. Although not necessary, it is advisable to verify the model after it is calibrated. For verification purposes, another historical period is chosen (preferably the period succeeding the calibration period) and the flow model is run for this period. If the fit between the simulated and actual water-level responses is still "good", the model is regarded to be suitable for future applications.
6. It is important to realize that the parameters that give a good match with the observed data, however, may not be the real parameters for the aquifer (Khan, 1980). Because of this, Labadie (1975) named the calibrated parameters surrogate parameters. It is obvious that to get a suitable model to predict the future behaviour of the aquifer, the surrogate parameters must reflect, as closely as possible, the underlying physical structure of the aquifer.
7. Theory, as well as practical experience (De Marsily, 1978), suggests that in dealing with the inverse problem, it is advisable to work in terms of log transmissivities instead of transmissivities, i.e. $Y = \log T$. If T is log normal, then it can be shown that if a subregion (zone) of the aquifer is made small enough so that the hydraulic gradient over it stays more or less uniform, the transmissivity of the zone can be represented by an effective T -value which is the geometric mean of T_i (Neuman, 1980). This implies that the effective log transmissivity of the zone is simply the arithmetic mean of Y_i .
8. To obtain realistic initial groundwater levels, it is recommended that the Bayes method of interpolation (Program TRIPOL developed at IGS, 1993) must be used to obtain these values. In the Bayes method, the topographic values are used as qualified guesses for the water levels. A number of case studies in South Africa showed that the topography mimics the water levels very closely.

3.3 STAGES OF DEVELOPMENT OF A MODEL

A very good description of the stages and development of a model is given in Berkowitz (1992).

1. Conceptual Model

- determination of cause-effect relationships
- a clear, qualitative, physical representation of how the natural system operates.
- make assumptions

2. **Mathematical Model (limitations)**

- represents groundwater systems through mathematical equations (p.d.e.'s) expressing conservation of mass and momentum
- includes boundary and initial conditions
- if possible/sufficient, make simplifying assumptions and solve analytically (e.g. assume radial flow in an infinite aquifer)

3. **Numerical Model**

- approximate continuous differential equations; replace continuous variables by discrete variables defined at grid nodes
- techniques include finite differences and finite elements
- system of equations solved by matrix methods

4. **Computer code (model)**

- translation of numerical model into computer language
- problem solution via computer

THEN

- comparison of numerical model to historical records
 - * if comparison unsatisfactory, return
- prediction
 - * impose system changes
 - * evaluate system response

Model application requires a feedback approach:

1. data collection
2. data preparation
 - * determine location and type of boundaries, discretize region, aquifer parameters, boundary and initial conditions
 - * (return to 1, if necessary)
3. historical matching - model calibration
 - * (return to 1, if necessary)
4. Forecast/prediction
 - * can run many times under various conditions
 - * perform stochastically Monte Carlo simulations

- * expressed results as probabilities (percentiles) of certainty

Considerations when selecting a suitable computer code or model

- * All models have advantages and disadvantages
 - ⇒ no single model is superior for all applications
- * Possibilities exist for:
 - ⇒ wrong solution to right problem...
 - ⇒ right solution to wrong problem...
 - ⇒ *conceptual errors (including model choice)
 - ⇒ *truncation and round-off errors
 - ⇒ *data errors

When beginning a study, the first question is not:

“Which model should I use?” but rather “ Do I need a numerical model to study this problem?”

To answer this question, consider:

1. What are the objectives?
2. What is known about the aquifer system? (what data are available?)
3. Does the study include plans to obtain additional data?

(If possible, the ideal approach is to integrate data collection and analysis with model study.)

Begin with simple models - and increase complexity if necessary, e.g. before attempting to solve a contamination problem, first ensure that the related flow field can be solved satisfactorily.

Try to avoid:

1. misapplication (conceptual error)
2. “overkill” (e.g. 3D-model chosen when 2D-model is sufficient; data not enough for 3D-model; grid size too fine for available information)
3. inappropriate prediction (e.g. use of confined model on aquifer that becomes phreatic through desaturation)
4. misinterpretations (“blind faith” in results) - expectations

Remember the word GIGO “Garbage In, Garbage Out”

3.4 HINTS ON THE AQUAWIN PROGRAM

It is recommended that the user immediately goes to the sample session and completes the two examples. It will take about three hours to complete these two exercises.

1. Program NETGEN

- Do not create too many nodes (e.g. usually between 1000 and 2000 nodes will be sufficient for most problems).
- Remember to save your work at regular intervals.
- Cancel the colour single element option always with the right mouse button.
- When inserting a new layer (map) with the polygon option, draw the polygons at short distances apart.

2. Program AQUA

- Always starts a new project with the Save As option.
- Always opens an existing project with the open file option.
- If the program comes up with " No solution for D-band routine", the most probable reason is triangles with small angles (less than 15 degrees). Correct this in the NETGEN program by moving the nodes. Another reason may be the assignment of zero T-values.
- Check for the Peclet and Courant criteria when running the mass transport program.

3. Program RPTSOLV

- RPTSOLV is a automated 2D radial finite element model for the solution of pumping tests in fractured-rock aquifers. The solution is thus dependent on a number of parameters e.g. boundary conditions, conceptual model and initial guesses. It may happen that the model reaches a local minimum and not the global minimum if the initial guesses are not good.
- The solution of any numerical model is not completely correct close to an abstraction borehole ($r < 1$ m). It is thus recommended that when analysing pump-test results in an abstraction borehole, that the user use an observation distance between 1 and 5 m.
- RPTSOLV solves for four unknowns, namely T of fracture, T of matrix, S of fracture and S of matrix.

Since there are four aquifer parameters that are to be estimated, the identification process is extremely difficult. It must therefore be investigated whether a unique solution for the unknown aquifer parameters exists (i.e. the problem is *well-posed*), or whether several sets of aquifer parameters are able to explain the observed hydraulic heads (i.e. the problem is *ill-posed*). The more *a priori* information that exists, the more the problem tends to be well-posed.

4. Program SIMPLEX and TRIPOL

SIMPLEX (for optimization) and TRIPOL (for Kriging and Bayes estimation) are two Dos programs which are included on the installation diskette.

Before running Tripol, include the statement: Device:C:\windows\command\ansi.sys in the config.sys file in the root directory (c:\).

If the user wants to change some constraints in the *.sim file after running the management flow program, he can use SIMPLEX to perform the calculations. Simplex, however, requires a *.dat file - so copy the *.sim file to a *.dat file.

The AQUAmod for WINDOWS program is the result of five years of research and programming and can be used with great benefit for the management of our aquifers.

4. CONCLUSIONS AND RECOMMENDATIONS

The AQUAmod for WINdows program is the result of five years of research and programming and can be used with great benefit for the management of our aquifers. After getting acquainted with all the input files and menu structures, the work of a groundwater modeller will definitely be made easier.

There are, however, shortcomings in the software suite. It is recommended that the following modules should be included into the software:

- a module for pathline calculations;
- a module for capture zone calculation; and
- a module for calculating salt balances at specific nodes and zones.

AQUAWIN is a 2D finite element program. It is recommended that the program must be converted to a quasi-3D program (like MODFLOW).

The use of classical groundwater models describing flow in porous media is very questionable in the case of fractured aquifers for the following reasons:

- (1) Most of our aquifers are of the fractured type. Classical groundwater flow models designed for flow in confined or unconfined porous media are not appropriate, since they neglect important aquifer properties that are due to specific fracture flow behaviour. Results obtained from experiments performed at different test sites can only be explained assuming a multi-porosity / multi-permeability system. One must assume at least two distinguishable interacting systems: (1) a highly permeable system with low storativity properties, referred to in the following as the *fracture system*, and (2) a system that can be characterized by very low permeability, but higher storativity. This second system is due to porosity in the matrix between fractures and will be referred to as the *matrix system*.
- (2) A deterministic way of describing groundwater flow in the fractured aquifers would require an extensive data set to account for the inherent heterogeneities. Future groundwater exploitation cannot be based on costly investigation programmes. A **strategy** must be developed that enables the future water manager to get maximum benefit from the limited knowledge of aquifer parameters that is available.

The following specific topics require research on:

1. The amount of water that is pumped out of the aquifer system must not exceed the amount of water that returns to the aquifer by processes, such as natural recharge coming from rainfall or artificial recharge coming from waste water or storm-water run-off infiltration. However, in nature there are dry years when natural recharge will be less than the actual water demand, and there will be wet years, when more recharge occurs than what is actually necessary to satisfy the water demand of the concerned community. A **time period** must be determined, to which long-term sustainable abstraction can be related, such that a balance between recharge and consumption over this time period will occur. This time period, of course, directly depends on the frequency and size of recharge events.
2. The **total amount of recharge** in the pumped aquifer system, given in terms of percentage of annual rainfall, must be determined. This will be a crude guess but will be useful for initial planning and management. For optimized pumping strategies, however, the **estimation of more detailed recharge patterns** is important. Locally detailed information on recharge patterns is of additional importance when catchment zones of pumping wells are investigated.
3. The discovery that horizontally orientated mesofractures are the main conduits of water to a borehole in a Karoo aquifer signals a danger flag: dewatered fractures may be deformed by the overburden and the borehole lost. It may well be that the deformation of the water-bearing fracture in the vicinity of the borehole is irreversible and the borehole dries up. It is thus imperative that these boreholes must not be pumped to an extent that their water-bearing fractures are dewatered. It is very important that the water level in the abstraction borehole never reaches the position of the main fracture, because the yield of the borehole will decrease drastically. Moreover, if the hydraulic head gradient is very steep in the vicinity of the borehole, CaCO_3 can deposit due to the change in partial CO_2 pressure. This calcification, in turn, can block fractures feeding the borehole and decrease the water yield. The **uncertainty in drawdown** therefore is of major importance. A sustainable pumping strategy in terms of probability must ensure that the probability of drawing piezometric head in the pumping well down to the depth of the main water-bearing fracture should be less than e.g. 5%.
4. Major flow in fractured aquifers occurs from the rock matrix to the fracture, which supplies the borehole with water. A highly permeable fracture quickly dewateres when pumped, unless replenished through its surfaces. The rate of replenishment depends on the rate at which water can leak from the surrounding rock matrix to the fracture. A point can be reached when the aquifer cannot supply water fast enough to the fracture, to compensate for the loss through pumping. There is thus a limit to the rate at which the rock-fracture system can supply water to a borehole. The limited yield of a borehole therefore is due less to the limited amount of water stored in the aquifer, than to the finite rate at which water can leak from the matrix to the fracture system. The **uncertainty in the leakage rate** must therefore be investigated. In conjunction with that, an **overall optimized pumping strategy** must be determined that ensures a **reliable long-term water yield** of a pumping well-field. The optimized pumping strategy must include the optimization of **single well pumping rates**, their **recovery times**, as well as the **number and location** of pumping wells. The considered opinion of

the research team is that a better sustainable management strategy is to use more boreholes but to pump at lower abstraction rates.

5. Since the uncertainty of the total amount of water stored in the matrix is related to the **uncertainty of the specific yield of the matrix system**, the uncertainty and the local distribution of the specific yield must be estimated.
6. If the uncertainties derived from pumping strategy, specific yield, water-level drawdown and recharge patterns (quantity as well as location and frequency) are identified, the **uncertainty in the total volume of water that is available** for the typical equilibrium time period, can be estimated. Since stochastic modelling gives ranges and intervals rather than exact numbers, conservative or even worst case scenarios can be performed. Due to the limited and imperfect knowledge of all the hydrological data and aquifer parameters, sustainable water management must be based on conservative or worst case scenarios. In terms of probabilities: the probability that a proposed aquifer management strategy fails to satisfy the communities' need, must be less than e.g. 5%. The commitment to a **failure probability** (e.g. 5%) is not a scientific question alone but requires a social and political consensus and will depend on the money and the efforts that a specific community is willing and able to pay or give.
7. **Recharge** from rainfall to the porous matrix can occur in two ways: One is recharge to the matrix directly via the top soil layers. The second is via vertical fractures, first to the fracture system and then, due to the responding pressure gradient, from the fracture system to the matrix. With present knowledge, which of these recharge mechanisms predominate, is unknown.
8. The importance of **educational efforts** is emphasized and people's awareness of water supply and demand must be focused to more reasonable use, not only in dry years.

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APPENDIX A

AQUAMOD FOR WINDOWS: USER'S GUIDE

This chapter appears as the help-file in the software

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1. INTRODUCTION

1.1 Use of software

The AQUAmod for WINdows (**AQUAWIN**) program is distributed free of charge. You may copy the software to other computers or supply it to other users.

1.2 Disclaimer

The user of this software accepts and uses it at his/her own risk. The authors do not make any expressed or implied warranty of any kind regarding this software. Neither the authors, the WRC nor IGS will be liable for incidental or consequential damages from or arising out of the furnishing, use or performance of this software.

1.3 System Requirements

At least a 80486 IBM PC or compatible with coprocessor, a VGA-graphics card and at least 8 MB RAM.

Software: Windows 95 operating system

Windows 95 and Surfer are registered trade names.

1.4 Installing AQUAWIN

Insert disk 1 of 3 and run the setup program. All the programs will be installed in a directory C:\Aquawin and C:\Aquawin\lex (or on the D-drive). The subdirectory lex contains the example files.

After installing the program, click with the right mouse button on the screen and go to New and then Folder. A new folder will be created. Rename the folder to Aquamod for Windows. Open the folder (double-click) and in the folder click with the right mouse button. Then New, shortcut, browse and click on the Aqua.exe item in the Aquawin directory. Repeat this procedure for programs Netgen.exe, Datasim.exe, Timegrph.exe and Rptsolv.exe.

The newest version of AQUAWIN could be extracted from the following ftp site:

FTP:\IGS-NT.UOVS.AC.ZA

1.5 Input and output files of AQUAWIN:

The following is a list of input and output files used: Program	Input files	Description	Output files	Description
NETGEN	*.brd *.map *.bin *.fix	border file Hydrocom map file Line map (same as Surfer bin file) Fix coordinates (e.g. boreholes positions)	*.wng *.net *.mas *.esi	General Binary safe file Finite element mesh info Mass transport info Time info
AQUA				
Flow and Mass Transport	*.net; *.sel; *.mas *.man *.exp *.wob *.woc *.wop *.cop	Use by flow/transport model Management constraints Exper. Parameter values Measured water levels at boreholes Measured conc. values Initial estimates and lower and upper values for inverse	*.hvt *.xyz *.cvt *.xyc *.wb *.res *.sim *.vel *.sec* *.mc *.aqu	Head vs. time X,Y,WL at all nodes at selected times Conc. vs time X,Y,C at all nodes Water balance Optimization results response matrix velocities at each element Section file Monte Carlo gen. values Project Name
Recharge	*.bwl *.rq *.bnd	monthly measured water levels Monthly Rainfall and abstraction inflow and outflow boundary nodes (optional)	*.vol *.cum *.eqa	monthly saturated volumes CRD values Equal volume results
DATASIM				
	*.brd *.bin or map *.xyz *.xyc *.vel *.hvt *.cvt	border file (compulsory) Optional X,Y,WL from AQUA X,Y,C from AQUA Velocities from AQUA Monte Carlo: Flow Monte Carlo: Mass transport	*.smi	Safe all imported files
TIMEGRPH				
	*.hvt *.cvt *.cum *.vol *.eqa *.res	head vs. time conc vs. time CRD SVF Recharge equal volume RPTSOLV results or inverse results	None	
RPTSOLV				
	*.dat	Pump test data	*.res *.rpt	Measured and fitted data and fit parameters Project name

2. PROGRAM NETGEN

This program requires a border file (coordinates of boundary of domain) as primary input (*.brd). The *.bln, *.map and *.fix files are optional.

Input files:

2.1 Input file *.brd (border file)

- A. Number of x,y values (N)
- B. (x,y) value of point 1
- C. Repeat line 2, N times

Example: file Ex.brd on diskette:

```
5
0 0
5000 0
0 5000
0 5000
0 0
```

2.2 Input file *.fix (borehole coordinates or other markers)

- D. Number of fix points (NF)
- E. (x,y) of point 1
- F. Repeat line 2, NF times

Example: file Ex.fix on diskette

```
6
1650 3050
2700 3050
3900 2150
2700 1550
3300 1550
4350 3200
```

2.3 Input file *.map

(Hydrocom map file)

Example: file Ex.map on diskette

Unit_Type = M

+=Pen control Color Level Quadrant Y-coord X-coord Text (optional)

```
1 2 1 1 2400 5000
1 2 1 1 2400 1700
1 2 1 1 3000 1700
1 2 1 1 3000 5000
```

```

1 2 1 1 2401 5000
2 2 1 1 2401 5000
1 2 1 1 2400 1400
1 2 1 1 2400 0
1 2 1 1 3000 0
1 2 1 1 3000 1400
1 2 1 1 2401 1400
2 2 1 1 2401 1400
1 12 1 1 2050 1600
1 12 1 1 2050 1450
1 12 1 1 2200 1450
1 12 1 1 2200 1600
1 12 1 1 2050 1600
2 12 1 1 2050 1600
1 12 1 1 1420 4000
1 12 1 1 1420 3900
1 12 1 1 1570 3900
1 12 1 1 1570 4000
1 12 1 1 1420 4000
2 12 1 1 1420 4000
1 9 2 1 1350 4960
1 9 2 1 1700 4960
1 9 2 1 1700 4900
1 9 2 1 1350 4900
1 9 2 1 1350 4960
2 9 2 1 1350 4960

```

2.4 Input file *.bln

(alternative for map file- the format is that of a SURFER bln file)

- A. Number of points in first segment
- B. (x,y) of point 1 in first segment: repeat this line for other points to be linked.
- C. Number of points in second segment
- D. (x,y) of point 1 in second segment: repeat this line for other points to be linked.
- E. Repeat 1 and 2 for other segments

Example: file Dyke1.bln on diskette

```

5
2400 5000
2400 1700
3000 1700
3000 5000
2401 5000

```

2.5 Input file for interpolation waterlevels to network node positions

Any file name:

- A. (x,y,wl) of first points
- B. repeat 1 as many times you have information for

3. PROGRAM AQUA

The two primary input files needed by AQUA are generated by the Grid Generator, NETGEN, namely the Network File (.NET) and the Selection File (.SEL). These files contain information on the position of network nodes and elements, as well as the purpose of the node, such as Observation nodes or Discharge nodes. The user must add information on different pumping rates and Rainfall and Recharge Values to the end of the Selection File.

If you open the AQUA program for the first time and want to start with a new project, always start with the **Save As** item under the **File** menu and give your file a name (without extension - use the same name as that given in NETGEN, e.g. Ex - a project **Ex.aqu** will be created).

3.1 Input file *.SEL (Selection file)

The dimensions of the program are set according to the following parameters:

(Each value is increased with 10 in the program dimensions)

- MNB: Maximum number of Fixed Neumann Boundaries
- MND: Maximum number of Drainage Nodes
- MNO: Maximum number of Observation Nodes
- MNA: Maximum number of Abstraction Points
- MNP: Maximum number of Pumps that change rates
- MNT: Maximum number of Times that rates change
- MRV: Maximum number of Rainfall Values

1. Heading 1

2. Heading 2

3. "Neuman Boundaries"

3.1 nnb.-.nnb: number Neumann boundaries

3.2 nnn fqq

- nnn: number of Neumann nodes,
- fqq: Flux

3.3 n1, ..., nnnn - Neuman Nodes

Repeat lines 3.1 and 3.2 for all Neuman Boundaries

4. "Drainage Nodes"

4.1 ndn - number Drainage Nodes

4.2 nodes, drain value repeat this line ndn times

5. "Observation Nodes"

5.1 nobs - number Observation Nodes

5.2 nodes(1-nobs)

6. "Abstraction Nodes"

6.1 nbor - number Pump nodes

6.2 node and initial rate (repeat nbor times)

7. "Changing rates"

7.1 nbch - number changing rate boreholes, nt - number times

7.2 time(1-nt)

7.3 pump node, rates(1-nt) repeat for all pump nodes

8. "Monthly Rainfall and recharge"

8.1 nrain - number rainfall values

8.2 month number, rainfall(mm), recharge for each zone

(Repeat for each month)

9 XXXXX - End mark

Example: File Ex.sel on diskette:

Generated by NetGen

Example

Drainage Nodes

4

15 200

18 230

21 210

34 330

Observation Nodes

6

388

626

636

772

904

999

Abstraction Nodes

2

636 0.000000
 999 -2500.000000
 Neuman Boundaries
 1
 4 1000
 1 2 3 4
 Changing rates
 2 3
 30 60 90
 636
 -591 -400 -560
 999
 -971 -780 -930
 Monthly Rainfall and recharge
 3
 1 20 3 2
 2 29 3 2
 3 12 3 2
 XXXXX

3.2 Input file *.NET (generated by NETGEN)

1. Comment line
2. NN,NE,NB,IWAT,NZONE

Where:

NN=number of nodes

NE=number of elements

NB=halfband width

IWAT= type of aquifer (0=confined; 1=water table)

NZONE=number of zones

3. K,X,Y,Z,ITYPE,TH

Where:

K=node number

X=x-coordinate of node K

Y=y-coordinate of node K

Z=water level

ITYPE=type of node (1=constant head; 0=No flow)

TH=Thickness of aquifer at node K

4. L,IN1,IN2,IN3,T,S,POR,IZ

where

L=element number

IN1, IN2 and IN3 = element incidences (anti-clock wise)

T=transmissivity in m²/d

S=storage coefficient

POR= effective porosity

IZ=zone number

Example of *.net file: File Ex.net on diskette:

Generated by NetGen:Example

```
1156 2178 36 0 2
  1  0.000 5000.000  0.000 0  30.000
  2  0.000 4848.485  0.000 0  30.000
continue until node 1156
1156 5000.000  0.000  0.000 0  30.000
  1  36  1  2 100 0.005 0.100 1
  2  36  35  1 100 0.005 0.100 1
continue until element 2178
2178 1156 1155 1121 100 0.005 0.100 1
```

Menu: NETWORK

Items included under this menu are:

Network Information

Time Settings

Discharge

Recharge

Update Network

Interpolation

Network Information

Different options could be set here, e.g. options to activate the drainage nodes, observation nodes, specify abstraction, step discharge and specify recharge.

Time Settings

Different output time selections are performed here. If a value of zero is used, the steady state solution is calculated.

Discharge

Different discharges can be specified here for the abstraction points.

Recharge

Either annual recharge (mm/a) or monthly recharge could be specified here. If both are specified, the annual recharge will be used. The annual recharge is specified for each zone.

Update Network

Initial heads in the .NET file, can be replaced with output values from AQUA (the .XYZ file), TRIPOL (the .DAT file) or a constant value.

T and S values in the .NET file, can be multiplied with the values computed by AQUA-INV, in the .RES file

Interpolation - Preparing input files for program TRIPOL

1 - Interpolate Guesses to network nodes

If Bayes interpolation is preferred the guesses, usually topography values, are read from the .TOP file and the .DFL file created to obtain guesses at all network nodes. When the .NET file is updated after Interpolation these guesses are written to the .NET file, to be used by the option 2 as qualified guesses at the network nodes.

2 - Prepare for Bayes interpolation from Heads

The Coordinates and Water Levels of boreholes in the .BHL file as well as the nodal coordinates and guesses from the .NET file are used to create the TRIPOL.DFL file.

3 - Prepare for interpolation without Bayes

The Coordinates and Water Levels of boreholes in the .BHL file as well as the nodal coordinates from the .NET file are written to the TRIPOL.DFL file.

INPUT file: .BHL (Initial Heads)

1 Heading

2 number Boreholes

3 Borehole number, Borehole coordinates and Observed Water Levels

INPUT file: .TOP (Guesses)

1 NUMBER OF Guess Points

2 Number, Guess coordinates and Value

After each TRIPOL run, the .NET file must be updated to write the initial nodal values to the .NET file.

Menu: Groundwater Flow

Items included are:

Recharge Calculation

Flow Simulation

Inverse Calibration

Management
Risk Analysis

3.3 Subprogram: Recharge Calculation

3.3 1 INPUT file: .RQ

1 number of monthly rainfall values

2 RVAL Q

RVAL: Monthly Rainfall (mm)

Q: monthly discharge (expressed in m³/day)

Example:

34

103.1 130.

75.5 126.

120.7 146.

66.5 123.

etc. (continue up to month 34)

3.3.3 INPUT file: .BWL

1 number of Boreholes

2.LABEL X Y WLEV

LABEL: Name (6 characters only)

X Y: coordinates X and Y (2F11.0)

WLEV: Water level for each month (free format)

Example:

72

00011 -29353. -270367.

1466.70 1467.00 1468.20 1468.40 1468.70 1467.80 1468.40 1468.30 1468.20

1468.00 1467.50 1467.00 1467.00 1467.00 1466.30 1467.00 1467.00 1467.50

1468.00 1468.00 1468.00 1468.10 1468.00 1468.10 1468.00 1468.00 1468.50

1468.90 1469.00 1472.30 1473.00 1471.50 1470.50 1470.00

00012 -29330. -270354.

1467.00 1467.00 1467.50 1468.00 1468.60 1467.80 1468.00 1468.00 1468.20

1468.00 1468.00 1468.00 1468.00 1468.00 1468.00 1468.00 1468.00 1468.00

1467.80 1468.00 1468.00 1468.10 1468.00 1467.80 1468.00 1468.00 1468.40

1468.90 1469.00 1472.20 1472.00 1471.30 1470.50 1469.90

(etc. repeat up to borehole 72)

3.3.3 INPUT file: .BND

(only if necessary)

1. number of INFLOW and OUTFLOW nodes
2. INFLOW node numbers
3. OUTFLOW node numbers

3.4 Subprogram: Flow Simulation

INPUT files: .NET and *.SEL (from NETGEN)

Results

.HVT = HEADS VERSUS TIME AT SELECTED NODES
.XYZ = WATER LEVELS FOR SELECTED TIMESTEPS
.VEL = VELOCITIES if calculated
.SEC = SECTION VALUES AT SELECTED NODES
.WB = WATER BALANCES FOR EACH TIME

3.5 Subprogram: Inverse for Flow Calibration

The following combinations of parameters are possible: The numerical value in brackets shows the number of unknowns if you have 2 zones and say 1 Neumann boundary.

1. T and S (4)
2. T (2)
3. S (2)
4. Recharge (2)
5. T and recharge (4)
6. Neumann flux (1)
7. T,S and Neumann flux (5)

3.5.1 INPUT file: .WOP

1. NUMBER OF UNKNOWNNS.
2. INITIAL GUESSES.
3. LOWER LIMITS ON VARIABLES.
4. UPPER LIMITS ON VARIABLES.

Example on diskette: Ex.wop

4

5 5 5 5
.1 .1 .1 .1
10 10 10 10

Comment: The first 2 values in each line are multipliers for the first parameter (T in this case) and the last 2 values are multipliers for the second parameter (S in this case).

3.5.2 INPUT file: .WOB

Contains : Water level Observations

1. Heading
2. number of Observations, number of Times
3. node numbers of observation points
4. node number, time, drawdown (or head)

Example: file Ex.wob on diskette:

Example

6	12				
388	626	636	772	904	999
388	30.000000	-6.557612E-02			
388	60.000000	-1.718347E-01			
388	90.000000	-2.928706E-01			
388	120.000000	-4.185463E-01			
388	150.000000	-5.463508E-01			
388	180.000000	-6.759791E-01			
388	210.000000	-8.074892E-01			
388	240.000000	-9.408771E-01			
388	270.000000	-1.076043			
388	300.000000	-1.212834			
388	330.000000	-1.351071			
388	360.000000	-1.490577			
626	30.000000	-4.211327E-03			
626	60.000000	-2.972648E-02			
626	90.000000	-9.225335E-02			
626	120.000000	-1.973439E-01			
626	150.000000	-3.430471E-01			
626	180.000000	-5.243283E-01			
626	210.000000	-7.356218E-01			
626	240.000000	-9.718279E-01			
626	270.000000	-1.228563			
626	300.000000	-1.502137			
626	330.000000	-1.789461			
626	360.000000	-2.087940			
636	30.000000	-4.841715			

636	60.000000	-5.843868
636	90.000000	-6.407103
636	120.000000	-6.862899
636	150.000000	-7.282359
636	180.000000	-7.686131
636	210.000000	-8.081675
636	240.000000	-8.472050
636	270.000000	-8.858615
636	300.000000	-9.241985
636	330.000000	-9.622412
636	360.000000	-10.000000
772	30.000000	-9.390032E-01
772	60.000000	-1.680875
772	90.000000	-2.316520
772	120.000000	-2.911215
772	150.000000	-3.487585
772	180.000000	-4.053697
772	210.000000	-4.612668
772	240.000000	-5.165690
772	270.000000	-5.713179
772	300.000000	-6.255219
772	330.000000	-6.791772
772	360.000000	-7.322774
904	30.000000	-6.394013E-01
904	60.000000	-1.402590
904	90.000000	-2.139348
904	120.000000	-2.837013
904	150.000000	-3.505441
904	180.000000	-4.153481
904	210.000000	-4.786628
904	240.000000	-5.407993
904	270.000000	-6.019308
904	300.000000	-6.621560
904	330.000000	-7.215343
904	360.000000	-7.801043
999	30.000000	-5.618153
999	60.000000	-6.870546
999	90.000000	-7.783280
999	120.000000	-8.588018
999	150.000000	-9.339630
999	180.000000	-10.058510
999	210.000000	-10.754020
999	240.000000	-11.431100
999	270.000000	-12.092710

999	300.000000	-12.740740
999	330.000000	-13.376550
999	360.000000	-14.001130

Results

.RES = OPTIMIZATION RESULTS

.HVT = HEADS VERSUS TIME AT SELECTED NODES

.XYZ = WATER LEVELS FOR SELECTED TIMESTEPS

3.6 Subprogram: Management for flow optimization

3.6.1 INPUT file: *.MAN

1. NP, NCON, 1

NP: number of Pumps

NCON: number of Constraints

1 1 for simplex maximization (-1 is minimization)

2. CONSTRAINTS (Label </=> Value)

3. COEFFICIENTS (1 to NP).

Example: File Ex.man on diskette

```

2 8 1
388 < 2.5
626 < 2.5
636 < 10.0
772 < 10.0
904 < 10.0
999 < 14.0
Q1 < 1000.
Q2 < 2500.
1.000000
1.000000

```

3.6.2 INPUT file: *.SIM created by AQUA-MAN

1. NP, NCON

NP: number of Pumps

NCON: number of Constraints

2. COEFFICIENTS.

3. Response Matrix

RESULTS

.SIM = RESPONSE MATRIKS FOR SIMPLEX ALGORITHM

3.7 Subprogram: Flow Risk Analysis

3.7.1 INPUT file: .MC

1. NUMBER OF MONTE CARLO RUNS
2. COMMENT LINE
3. Random T, S and Recharge for each zone

Example: File Ex.mc on diskette:

```
10
Random Values for Risk Analysis
111.841 .726024 .486909E-02 .503168E-02 25.0880 21.9094
139.710 .326483 .502256E-02 .486646E-02 18.0142 16.9012
97.1343 1.00898 .490961E-02 .493739E-02 10.2222 23.6355
75.8542 .558063 .502092E-02 .485007E-02 33.2644 24.9317
58.1095 1.55627 .480621E-02 .504783E-02 17.4198 29.4699
100.425 2.19904 .504059E-02 .505371E-02 25.0039 21.0884
107.740 1.62218 .509970E-02 .508278E-02 22.0860 21.7447
121.561 .830029 .528037E-02 .506509E-02 3.03853 21.9663
111.620 1.70457 .485791E-02 .496681E-02 17.9963 16.7942
101.762 1.10479 .507718E-02 .483010E-02 15.0388 20.7261
```

3.7.2 INPUT file: .EXP (real data values)

- LINE 1. NT NS NR: NUMBER OF Random values for S, T and R
- LINE 2.1. Zi Ni: zone number and number of T values,
- LINE 2.2. Ti: values for zone (Repeat lines 2.2 and 2.3 for all Zones)
- LINE 3.1. Zi Ni: Zone number, number of S values
- LINE 3.2. Si: S values for zone (Repeat lines 3.4 and 3.5 for all Zones)
- LINE 4.1. Zi Ni: Zone number, number of R values
- LINE 4.2. Ri: Recharge for zone (Repeat lines 4.6 for all Zones)

Example:

```
5 5 0 (Meaning of zero=use mean for paramer 3)
1 3
110 90 100
```

2 6

1.4 6 1.5 1.0 1.1 .9

1 4

.005 .003 .007 .004

2 4

.004 .003 .001 .003

1 5

5.0 2.3 4.6 7.8 4.0

2 5

1 3 2 6 3

RESULTS

.HVT = HEADS VERSUS TIME AT SELECTED NODES

Menu: Mass Transport

Items appearing under this menu are:

1. Parameters
2. Transport Simulation
3. Inverse Calibration
4. Risk Analysis

3.7.3 INPUT file: .MAS created by program NETGEN

Contains NODAL CONCENTRATIONS

1 Heading

2 i, C0, Input Volume, Input Concentration, Type(0/1)

Where:

i= node number

C0= initial concentration (mg/l or any relative number)

Input volume: Only positive Q could be specified

Input volume = $+Q/nD$ must be specified, where n= porosity and D= thickness of aquifer.

Input concentration: concentration of input in mg/l (or any relative number)

Type: 1 for constant concentration, else zero.

Example: File Ex.mas on diskette:

Example:Generated by NetGen

1 0.000 0.000 0.000 0

...etc. up to node 348 and at constant concentration node the following:

```
348 100.000 0.000 0.000 1
```

..etc.

```
500 100.000 0.000 0.000 1
```

..etc. up to last node (i.e. 1156)

```
1156 0.000 0.000 0.000 0
```

3.7.4 INPUT file: .XYZ created by the Flow Program AQUA

Contains node number,X,Y, Heads, time from flow program.

RESULTS

.CVT = CONCENTRATION VERSUS TIME AT SELECTED OBSERVATION POINTS

.XYC = X,Y,CONCENTRATIONS AT SELECTED TIMESTEPS

.VEL = VELOCITIES AT CENTRE OF EACH ELEMENT

.SEC = SECTION VALUES AT SELECTED NODES

Parameters

The following parameter values should be entered here:

Anisotropic factor; Longitudinal dispersivity, transverse dispersivity, Molecular diffusion (1e-6), recharge concentration and transport type. If transport with retardation is to be calculated, put the retardation coefficient to a value greater than 1.

3.8 Subprogram: Mass Transport

File needed is the *.mas file created by NETGEN

3.9 Subprogram: Inverse Calibration Mass Transport

3.9.1 INPUT file: .COP

1. NUMBER OF UNKNOWNNS.
2. INITIAL GUESSES.
3. LOWER LIMITS ON VARIABLES.
4. UPPER LIMITS ON VARIABLES.

Example: the same as for the .wop and .wob files of flow

3.9.2 INPUT file: .COB

Contains Concentration observations for all times, or just the last time

1. 1 Heading
2. 2 number of Observations, number of Times
3. 3 node, time, concentration

RESULTS

.RES = OPTIMIZATION RESULTS

.CVT = CONCENTRATION VERSUS TIME AT OBSERVATION NODES

.XYC = CONCENTRATIONS FOR SELECTED TIMESTEPS

3.10 Subprogram: Risk Analysis for Mass transport

3.10.1 INPUT file: .MC

1. NUMBER OF MONTE CARLO RUNS
2. COMMENT LINE
3. Random T (for each zone) ,Porosity (for each zone) and ALFA L (LONGITUDINAL DISPERSIVITY- only 1 value for all zones)

3.10.2 INPUT file: .EXP

LINE 1. NUMBER OF Random values for T, P and ALFA L

LINE 2.1. zone number, numT

LINE 2.2. T values for zone (Repeat line 2.2 and 2.3 for all Zones)

LINE 3.1. zone number, numP

LINE 3.2. Porosities for zone (Repeat line 3.4 and 3.5 for all Zones)

LINE 4.1. 0, numAL,

LINE 4.2. LONG. DISPERSIVITY values

RESULTS

.CVT = CONCENTRATION VERSUS TIME AT SELECTED NODES

4. PROGRAM TIMEGRPH

With the TIMEGRPH program the user can view different line graphs derived from the output by the programs AQUA and RPTSOLV.

5. PROGRAM DATASIM

With the DATASIM program, contours, velocities, risk analysis results, maps and the finite element mesh can be displayed (contours with time).

6. PROGRAM RPTSOLV

RPTSOLV is a two-dimensional radial finite element model and can be used for the analysis of pumping tests in fractured-rock aquifers. When analyzing pumping test results with the Theis model or any other fractured-rock model (e.g. the Moench method), the calculated S-values will show distance dependency - the larger the distance between the observation borehole and the abstraction borehole, the smaller the estimated S-value. With RPTSOLV, the aquifer is divided into two sub-systems, e.g. an upper matrix part and a lower fractured part, the calculated S-values show no distance dependency.

Four parameters are automatically fitted using the non-linear Marquardt method, namely:

T_f and T_m and S_f and S_m , where the subscripts f and m denote fracture and matrix respectively. Usually T_f is much larger than T_m and S_m is much larger than S_f .

Because RPTSOLV is a numerical model, either a no-flow and constant head boundary condition could be specified.

Prediction after a specified time could also be performed.

6.1 Input file *.dat

1. Comment line
2. Comment line
3. Number of values
4. Comment
5. Time, Drawdown
6. Repeat 5 for all data values

Example: File UO16.dat on diskette

```
PUMP UO5 AT 2 L/S
measurements at UO16 (r=14 m)
10
TSDATA
2      1.41
5      1.7
10     2.14
15     2.51
20     2.82
25     3.10
30     3.35
40     3.83
50     4.23
60     4.43
```

7. HINTS ON THE AQUAWIN PROGRAM

It is recommended that the user immediately goes to the sample session and completes the two examples. It will take about 3 hours to complete these two exercises.

I. Program NETGEN

- Do not create too many nodes (e.g. usually between 1000 and 2000 nodes will be sufficient for most problems).
- Remember to save your work at regular intervals.
- Cancel the colour single element option always with the right mouse button.
- When inserting a new layer (map) with the polygon option, draw the polygon at short distances apart.

II. Program AQUA

- Always starts a new project with the Save As option.
- Always open an existing project with the open file option.
- If the program comes up with " No solution for D-band routine", the most probable reason is triangles with small angles (less than 15 degrees). Correct this in the NETGEN program by moving the nodes. Another reason may be the assignment of zero T-values.
- Check for the Peclet and Courant criteria when running the mass transport program (Peclet < 2 and Courant < 1).

III. Program RPTSOLV

- RPTSOLV is a automated 2D radial finite element model for the solution of pumping tests in fractured-rock aquifers. The solution is thus dependent on a number of parameters e.g. boundary conditions, conceptual model and initial guesses. It may happen that the model reaches a local minimum and not the global minimum if the initial guesses are not good.
- The solution of any numerical model is not completely correct close to an abstraction borehole ($r < 1$ m). It is thus recommended that when analysing pump-test results in an abstraction borehole, that the user use an observation distance between 1 and 5 m.
- RPTSOLV solves for four unknowns, namely T of fracture, T of matrix, S of fracture and S of matrix.

Since there are four aquifer parameters that are to be estimated, the identification process is extremely difficult. It must therefore be investigated whether a unique solution for the unknown aquifer parameters exists (i.e. the problem is *well posed*), or whether several sets of aquifer parameters are able to explain the observed hydraulic heads (i.e. the problem is *ill posed*). The more *a priori* information that exists, the more the problem tends to be well posed.

4. Program SIMPLEX and TRIPOL

SIMPLEX (for optimization) is a Dos programs which are included on the installation diskette.

If the user wants to change some constrains in the *.sim file after running the management flow program, he can use SIMPLEX to perform the calculations. Simplex, however, requires a *.dat file - so copy the *.sim file to a *.dat file.

TRIPOL is an interpolation (Kriging and Bayes) program for Windows. See the example at the end of the section.

8. Sample Session

8.1 EXAMPLE 1: Pump test analysis

The following data were collected on the UFS-pump testing site. Borehole UO15 was pumped at 2 l/s and measurements were made in UO16, which is 14 m from UO15. The Theis model yields the following estimates: $T=9 \text{ m}^2/\text{d}$ and $S=0,0002$

Analyse the data with program RPTSOLV and compare the results with the Theis model.

Thickness of aquifer = 20 m

Fracture at 21 m

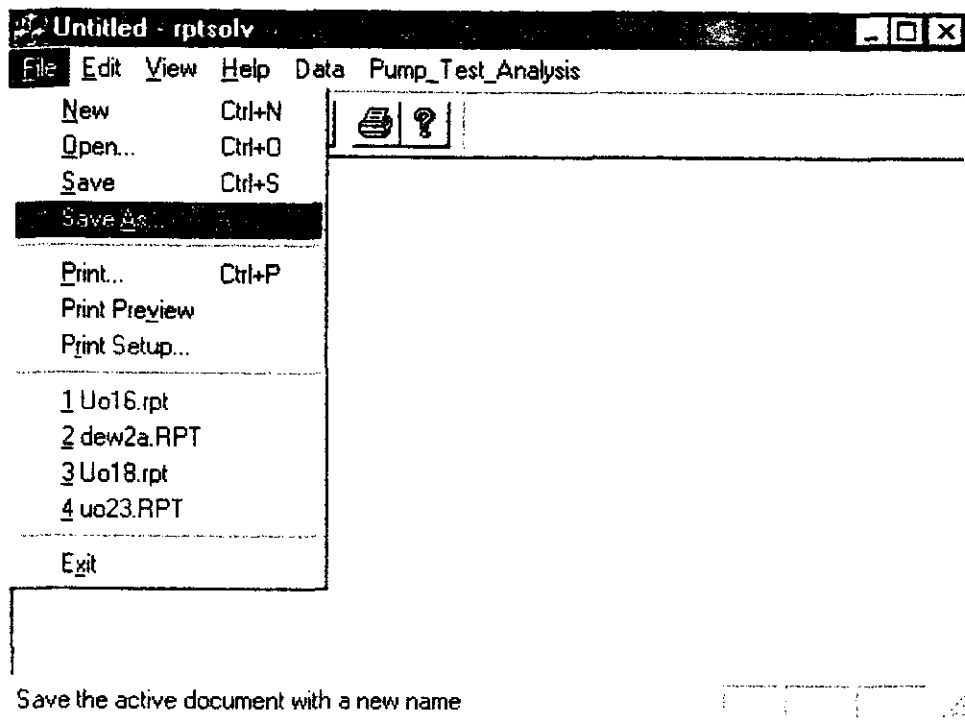
Time (min)	Drawdown (m) in UO16
2	1,41
5	1,70
10	2,14
15	2,51
20	2,82
25	3,10
30	3,35
40	3,83
50	4,23
60	4,43

(Results from RPTSOLV: $T = 10 \text{ m}^2/\text{d}$ and $S=0,003$.)

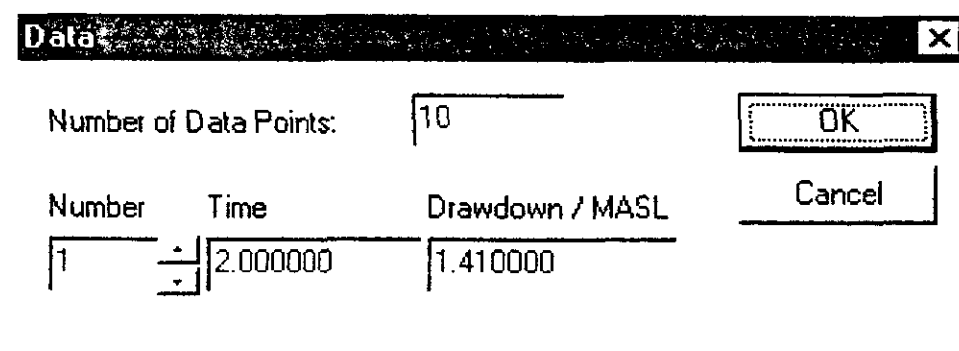
The T-values compare favourably with the Theis estimate, but the S is ten times larger than the Theis estimate.

Solution:

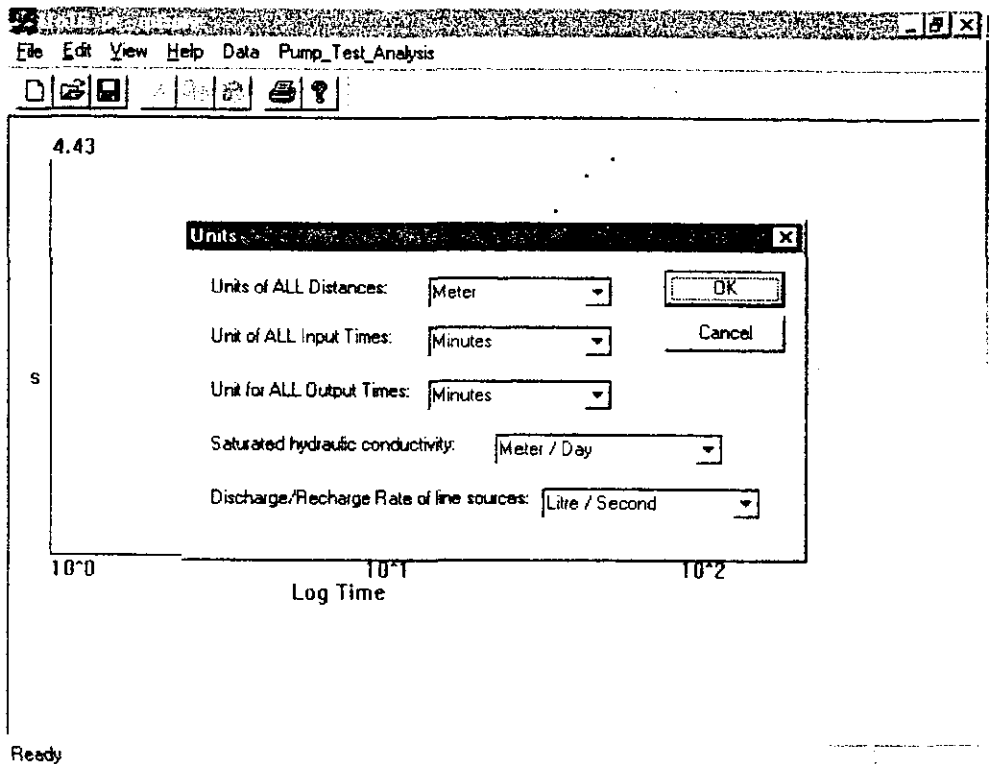
1. In the **Main Program Folder**, double-click on the **RPTSOLV** icon.
2. Open a new project name: Go to the **File** menu and click on **Save AS** and call it UO16.



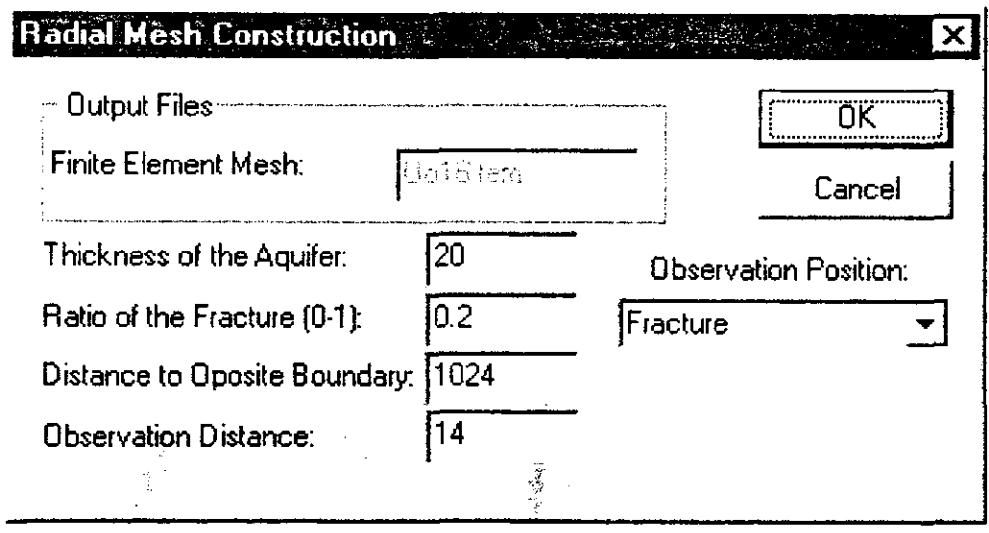
3. Go to the **Data** menu and enter the data



4. Go to the Pump_Test_Analysis menu and click on Units and enter the values.



5. Then click on Mesh Construction and enter the required values.



6. Click on the Parameter item and enter the values:

Parameters [X]

Input Files
 Pump Test Data: Uo16.dat

Output Files
 Observation File: Uo16.obs
 Parameter File: Uo16.par

Data Selection
 Use Subset
 Number of Times to Select: 0

Discharge Rates
 Number of Pump Steps: 1

Step	Time	Rate
1	0.000000	2.000000

Pump Position
 Fracture

Opposite Boundary
 No Flow
 Constant Head

Water Level Observations
 Drawdowns
 Meter above sea level

OK
 Cancel

7. Click on the Analysis item and enter the values:

Pump Test Analysis [X]

Input Files
 Observation File: Uo16.obs
 Parameter File: Uo16.par

Output Files
 Result File: Uo16.res
 Simulation File: Uo16.sim

Optimization
 Fixed Time
 Prediction

OK
 Cancel

RESET Parameters
 SET Boundaries

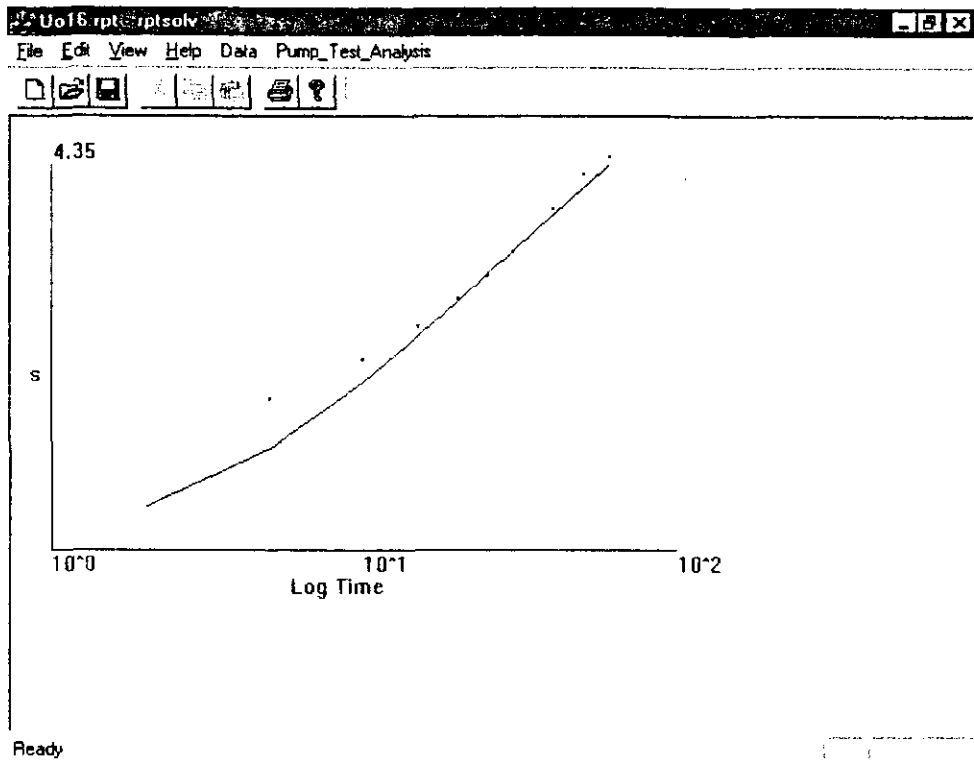
Optimization
 Use All Points
 Number of Initial Points to Ignore: 6
 Minimum Fit Requirements (RMSE): 0

Prediction
 Simulation Time (Days): 0
 Number of Timesteps: 0

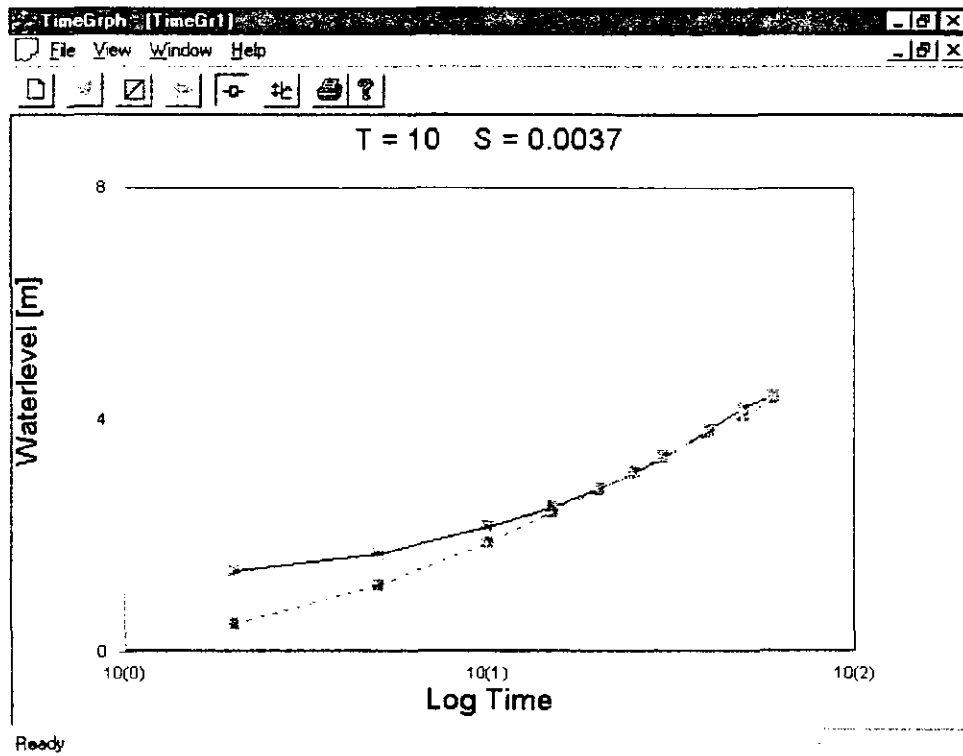
Aquifer Parameters

	Minimum	Guess	Maximum
Transmissivity (fracture):	15	30	120
Transmissivity (matrix):	1e-007	0.001	1
Storativity (fracture):	1e-010	1e-006	1e-005
Storativity (matrix):	3e-006	0.003	0.3

8. The following curve fit will be displayed after running the program:



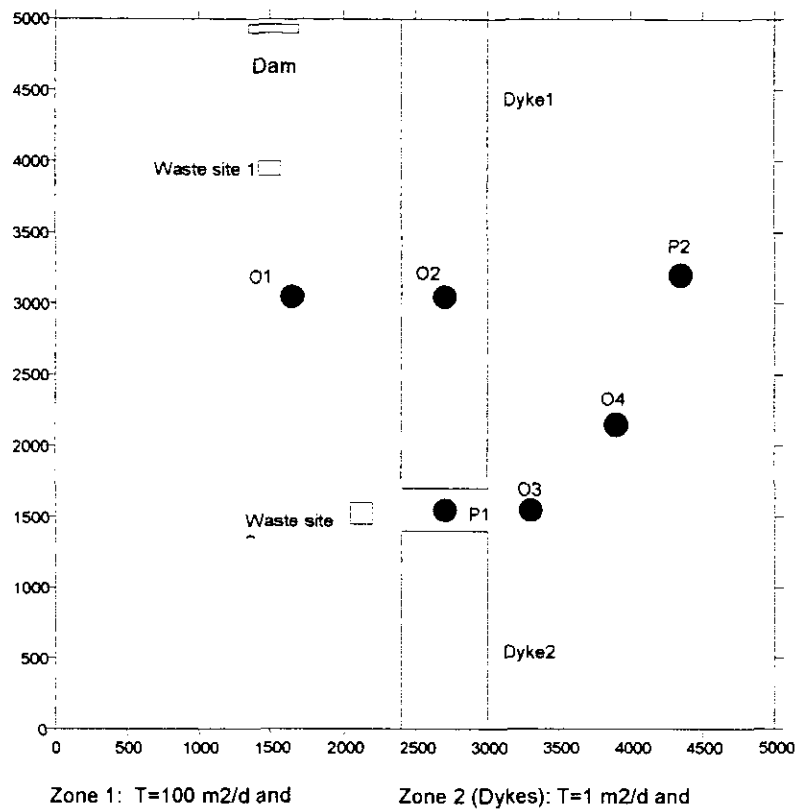
9. With the TIMEGRPH program the fit looks as follows:



8.2 EXAMPLE 2: Flow and Mass Transport

Consider an aquifer (5000 m x 5000 m) bounded by impervious boundaries except at the position of a surface water dam (constant head boundary).

The position of the 2 abstraction boreholes (P1 and P2), 4 observation boreholes (O1 to O4), 2 dykes and 2 waste sites (with constant relative concentrations of 100%) are shown on the figure below. The thickness of the aquifer is equal to 30 m and the porosity is equal to 0,1.



Tasks

1. Generate a steady state flow field for the situation where 2500 m³/d water is abstracted from P2.
2. Use this steady state flow field and display the movement of pollutants from the two waste dumps after every 360 days up to 3 600 days. (Longitinal dispersivity = 80 m and transversal dispersivity = 10 m, molecular diffusivity = 0)
3. Obtain the maximum abstraction rates of boreholes P1 and P2 after 360 days of pumping such that the following constraints are not violated (use zero initial water levels at each node; no recharge):

Drawdown at O1 < 2.5 m

Drawdown at O2 < 2.5 m

Drawdown at O3 < 10 m

Drawdown at O4 < 10 m

Drawdown at P1 < 10 m

Drawdown at P2 < 14 m

Max Q of P1 < 1000 m³/d

Max Q of P2 < 2500 m³/d

(Solution: P1 = 591 and P2 = 971 m³/d)

4. File Ex.wob contains supposed measured drawdowns (generated with the T and S values given in the figure) of the 6 boreholes at 30 day intervals for 1 year.

Start with initial guesses of:

Zone 1 : T = 500, S= 0.025 and Zone 2 : T = 5 and S=0.025

(i.e. multipliers of 5 for each parameter)

Run the inverse solution to obtain the correct T and S-values (if Multipliers 1.00 for all 4 unknown parameters are reached, the correct solution is obtained).

5. Perform a risk assessment using a mean T = 100 (variance =20) for zone 1 and T=1 (variance = 0.5) and S= 0.005 (variance =0.0001) for both zones. Use mean Long. dispersivity = 80 (variance = 20) and mean porosity = 0.1 (variance = 0.05). Generate 10 values and calculate the pollution distribution (80 percent percentile) at the 6 boreholes after 720, 1800 and 3600 days of abstracting water at borehole P2 =-2500 m³/d. Use the steady flow field.

(Furthermore a risk analysis on the flow could be performed: e.g. what are the possibilities that the drawdown constraints are to be violated with the abstractions of 591 and 971 m³/d?). (if you want to perform this you must enter P1=-591 and P2=-971, and generate 10 random values according to the parameters above. Use times of 90, 180 and 360 days for output of risk file (ex.hvt). Then run the flow risk program). If you want to save the result file, copy ex.hvt to say, flowrisk.hvt.

A. Finite element mesh construction

The following files are available on the installation diskette:

Ex.brd = border file

Dyke1.blm = position of first dyke

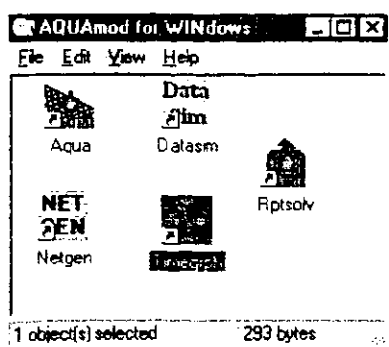
Dyke2.blm = position of second dyke

Mas.blm = position of two waste sites

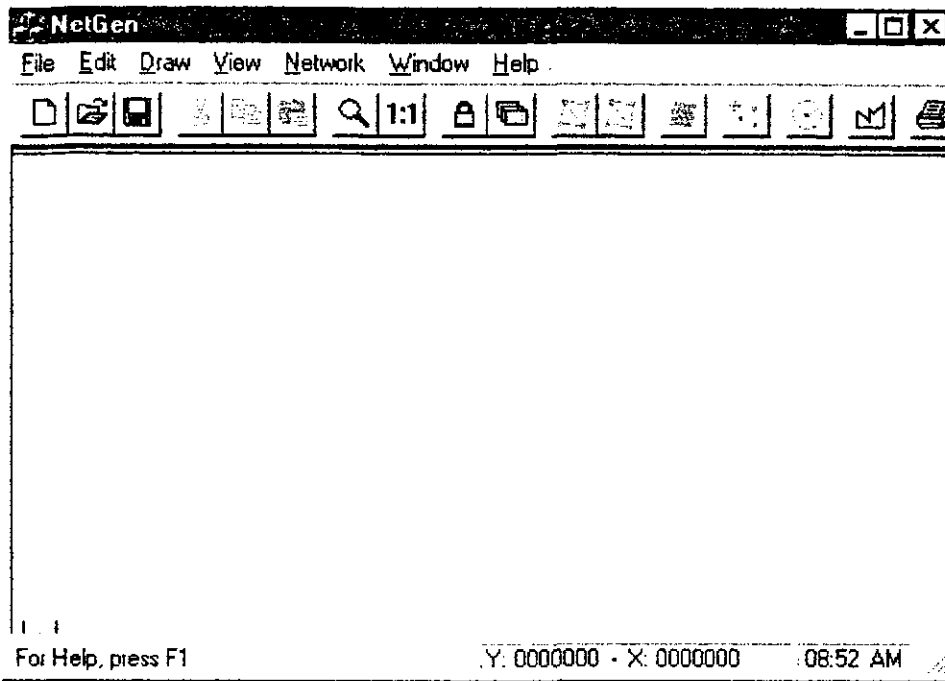
(Ex.map is the equivalent Hydrocom map file of the *.blm files)

Ex.fix = position of 6 boreholes

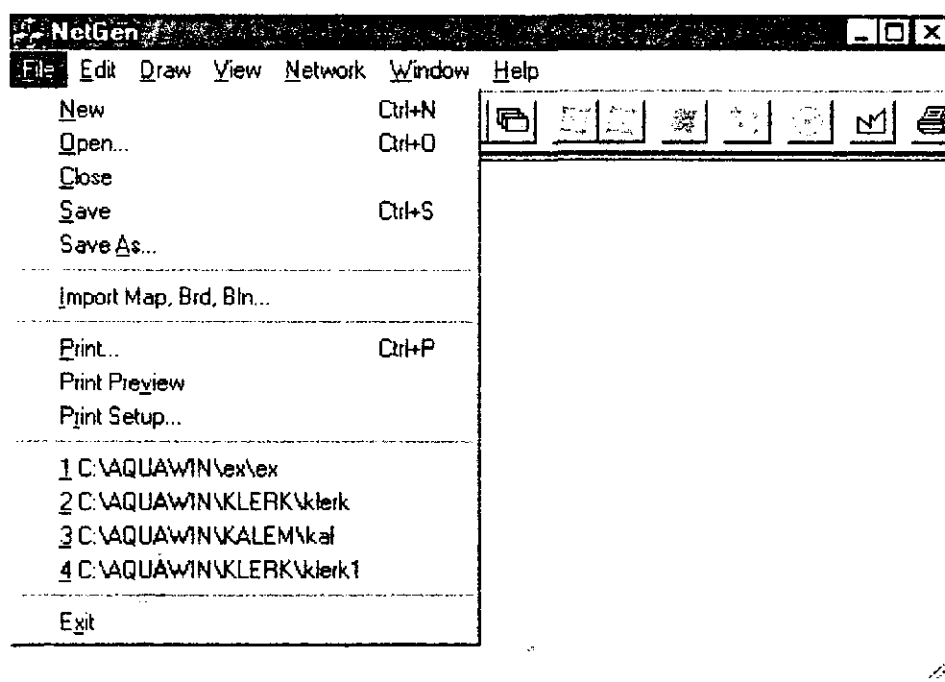
- (a). Start the **NETGEN** program by double-clicking on the **Netgen** icon in the **Main Program Folder**:



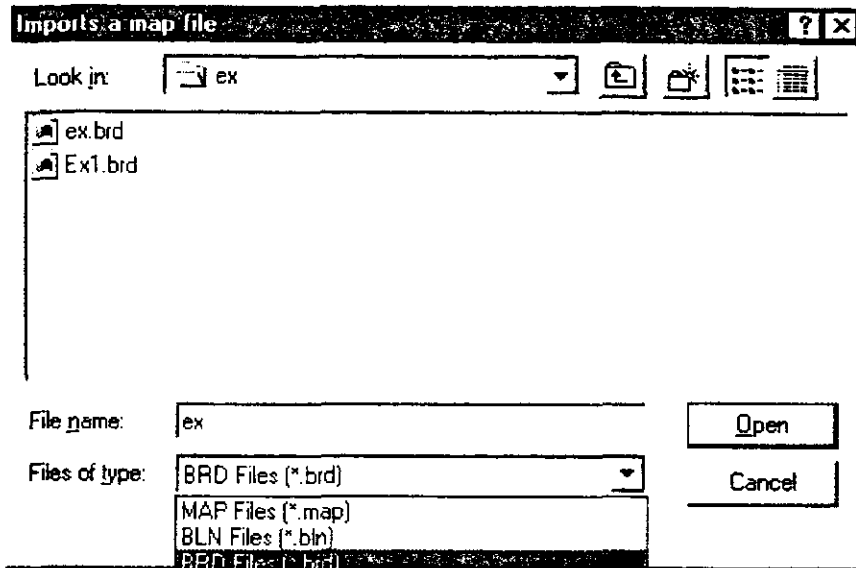
The following window will appear



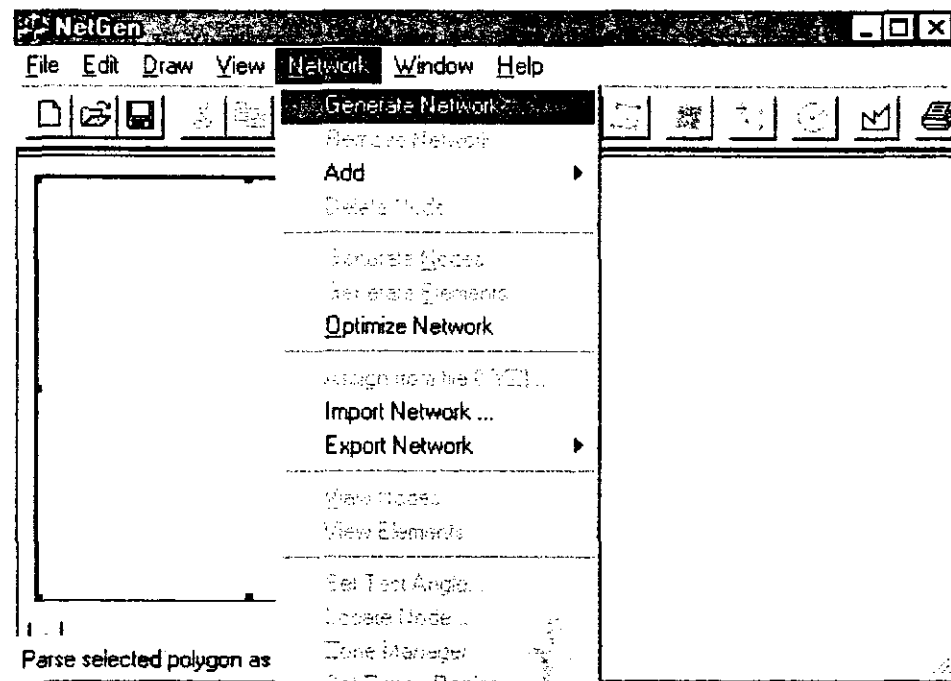
- (b) On the menu bar click on the File menu: then click on the Import Map, brd, bln item:

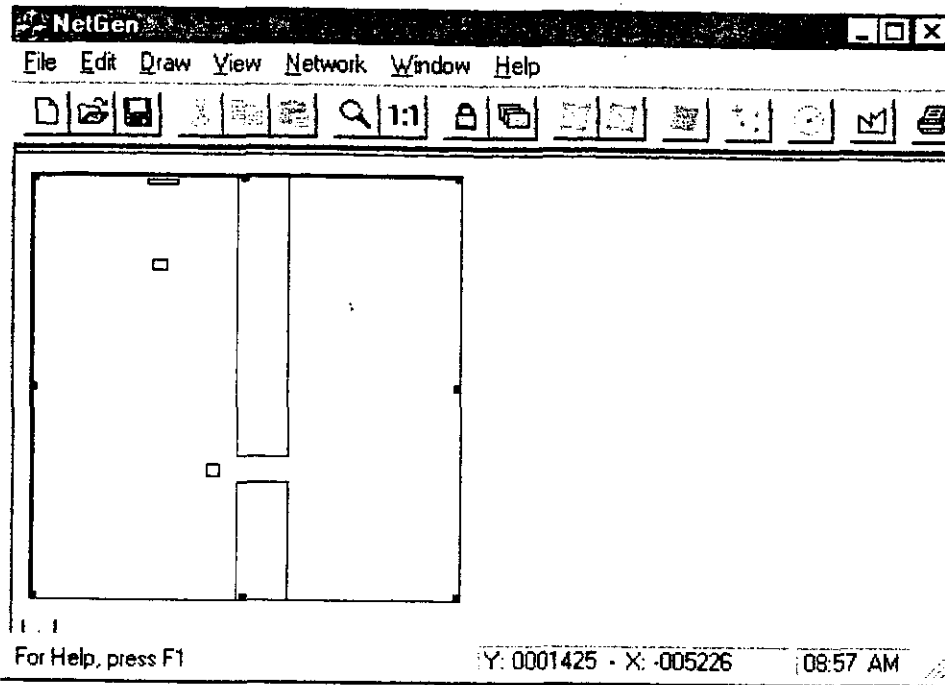


- (c) Import the Ex.brd file by double clicking on it. Also import the *.bln files (or just the Ex.map file).

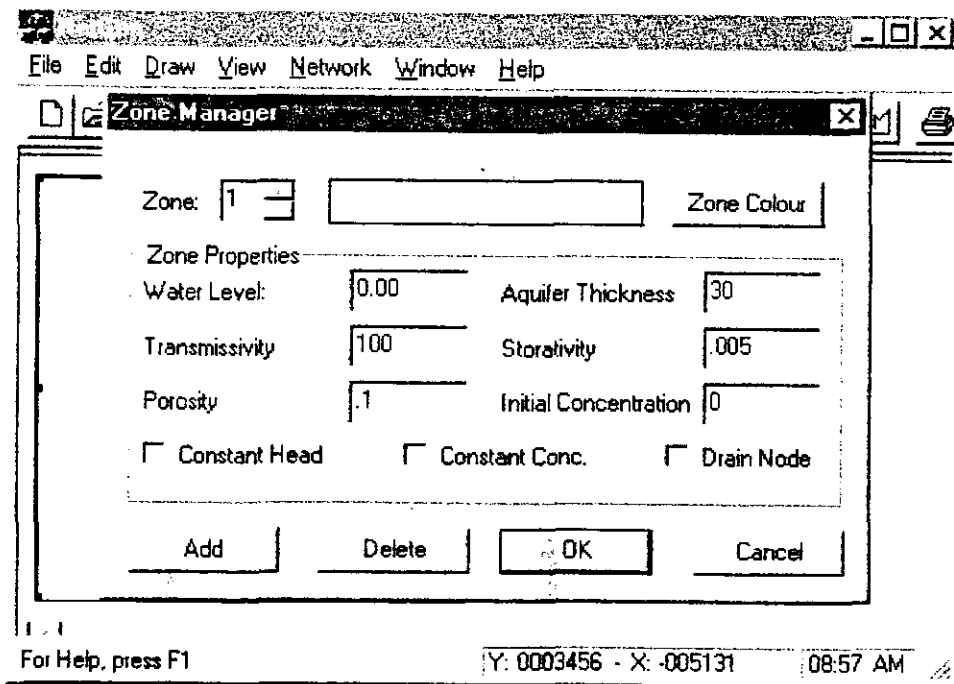


- (d) Select the border file by clicking the mouse on the border. Click on the Network menu and click **Generate Network**.

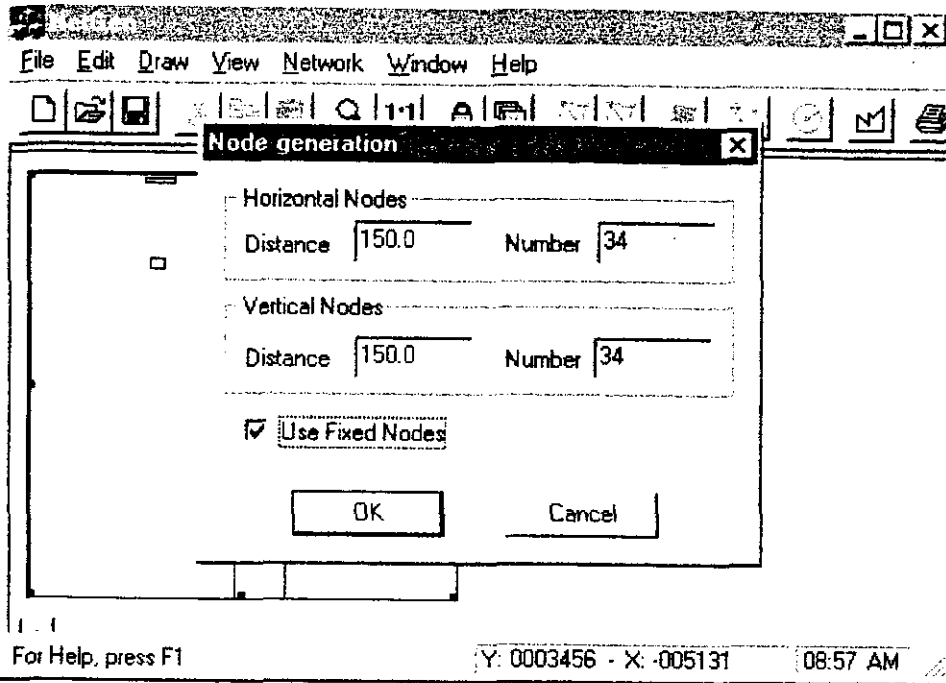




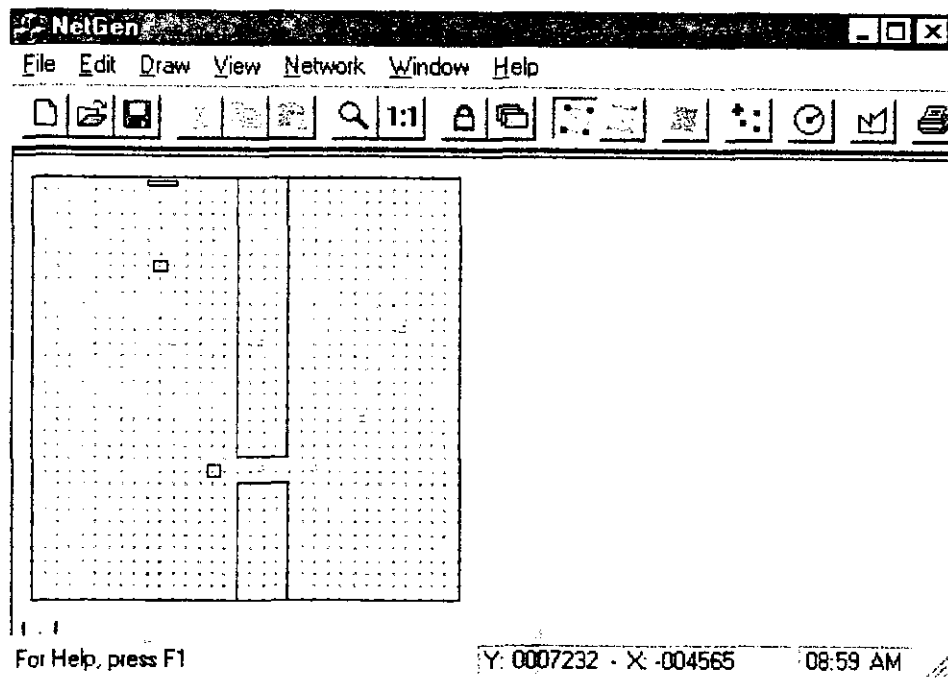
(e) Enter the parameters values and click **OK**.



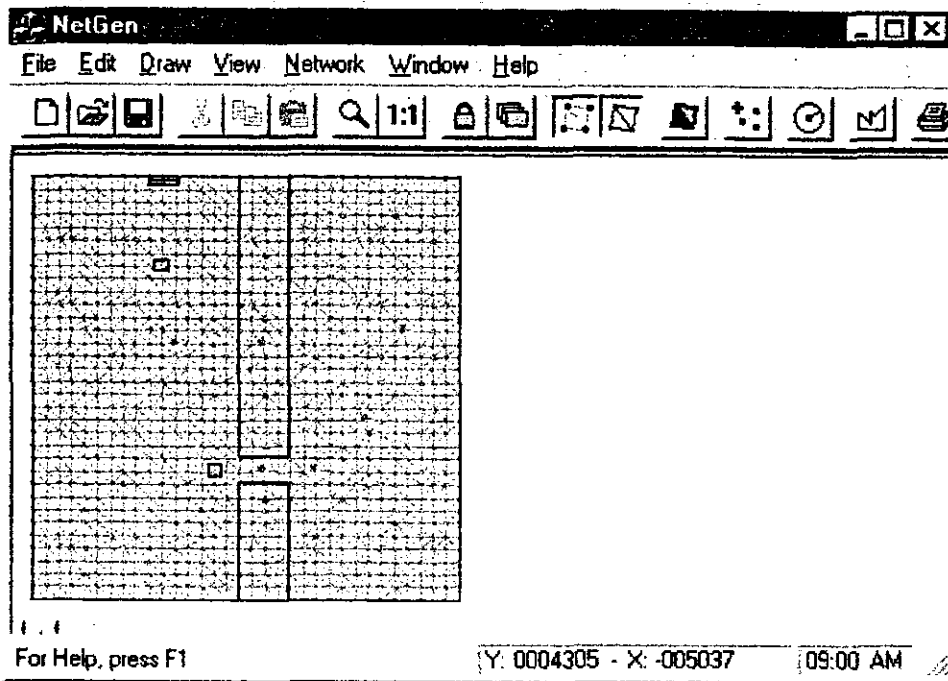
(f) Leave the distance 150.00 in both horizontal and vertical cases and click on the **Use Fixed Nodes** button. Import the Ex.fix file.



You will see the following generated nodes:

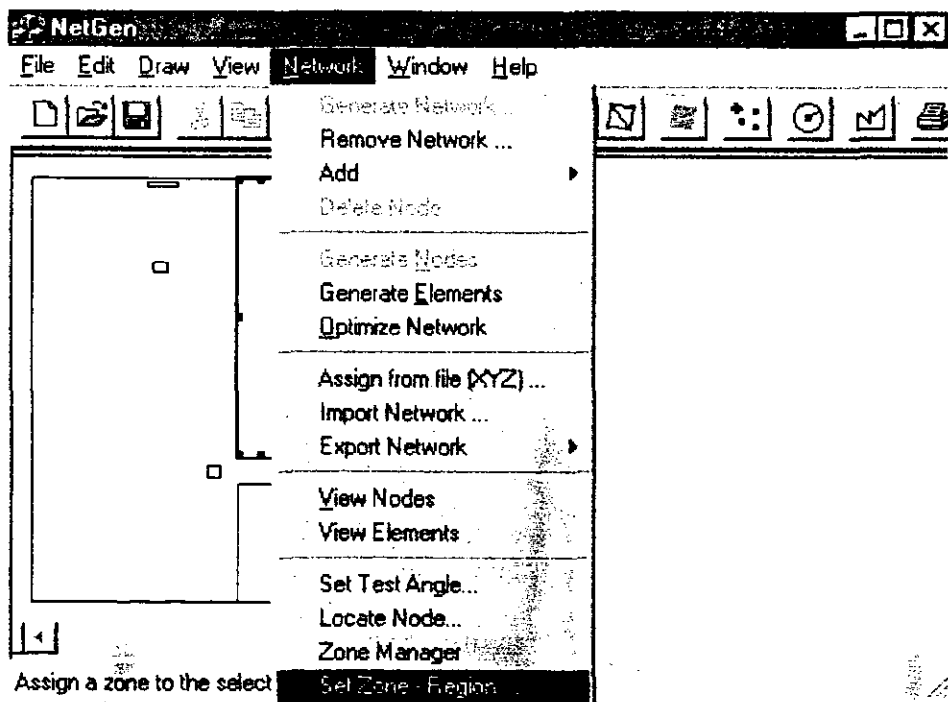


- (g) Go to the **Network** menu. Click on **Generate elements** and thereafter on **Optimize Network**.

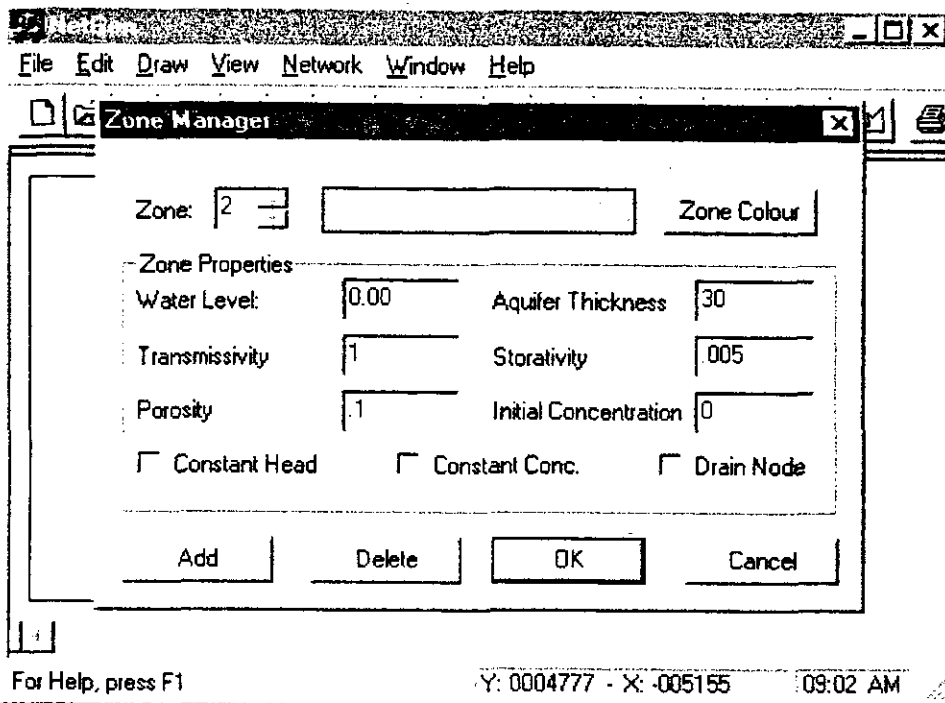


Click on **view nodes** and then on **view elements** (they will appear depressed).

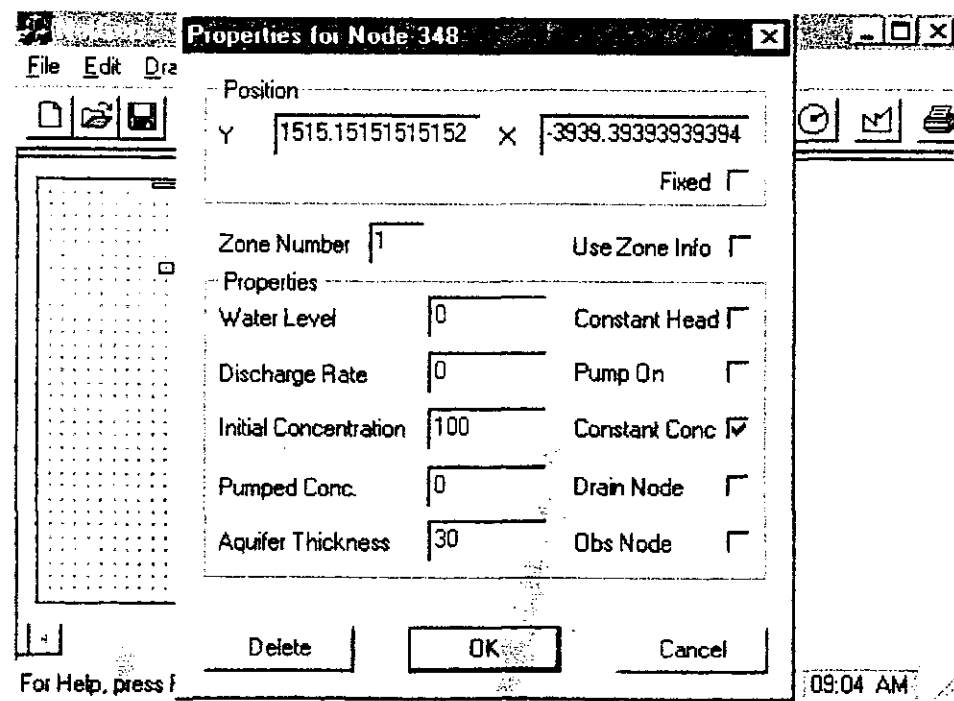
(h) Select the first dyke with the mouse and Under the **Network** menu, click on the **Set Zone-Region** item.



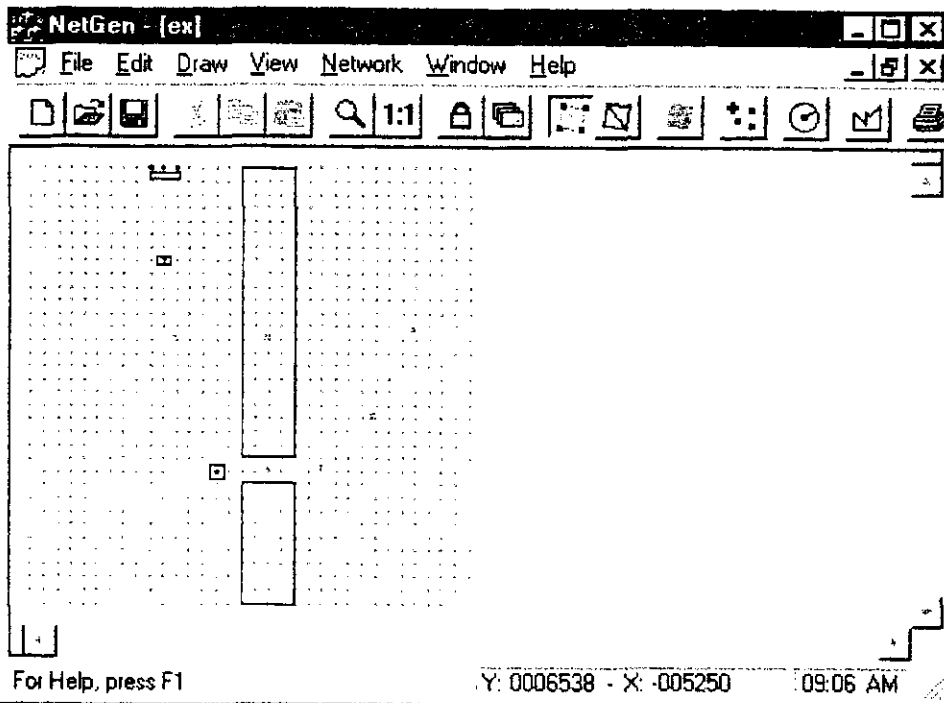
(i) Add a zone and enter the parameter values for zone 2. Repeat for second dyke.



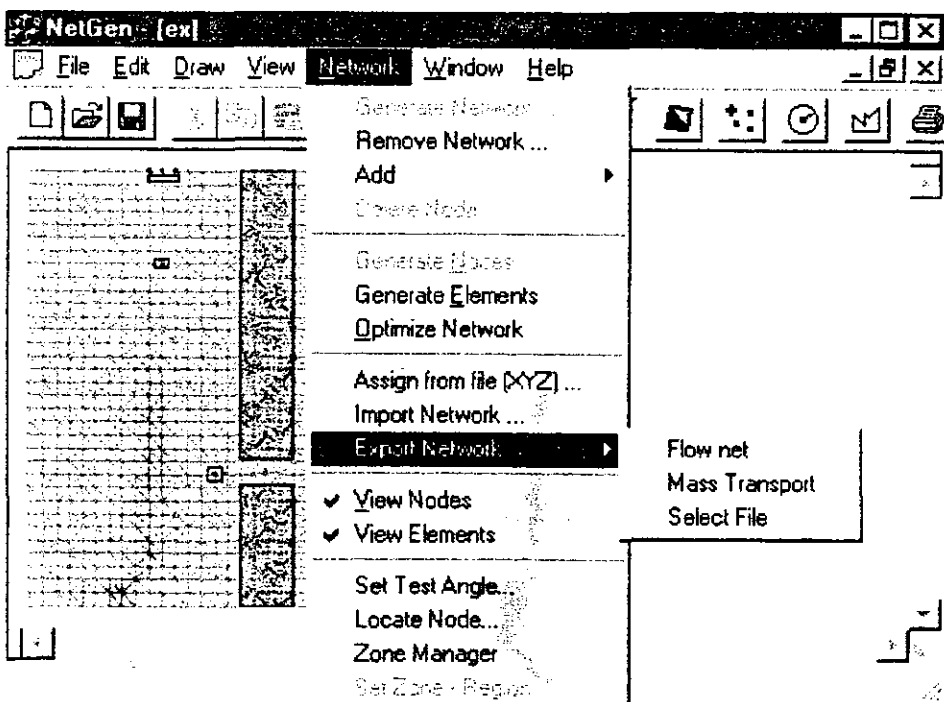
- (j) Click the **right button** of the mouse close to the position of the first waste site and set the parameters as follows (Initial C = 100 with Constant Conc): (Repeat procedure at second waste site).



- (k) Go to the fix nodes (borehole positions), click on the **right mouse** button and set the boreholes as observation points (O1 to O4; i.e. nodes 388, 626 772 904)) and P1 and P2 (nodes 636 and 999). Set the abstraction rate at node 999 as - 2500 m³/d and at node 636 as zero. Set the 3 nodes at the dam as constant head nodes.



- (l) Under the **Network** menu choose **Export network**. Export the flow net, mass transport and select files under any name (e.g. Ex).
- (m) Under the **File** menu, click the **Save As** item and save all information in the Ex.wng file by just typing the name Ex.



Other icons on the toolbar:

The icons on the tool bar after the 1:1 (full size) icon and the lock map icon are as follows:

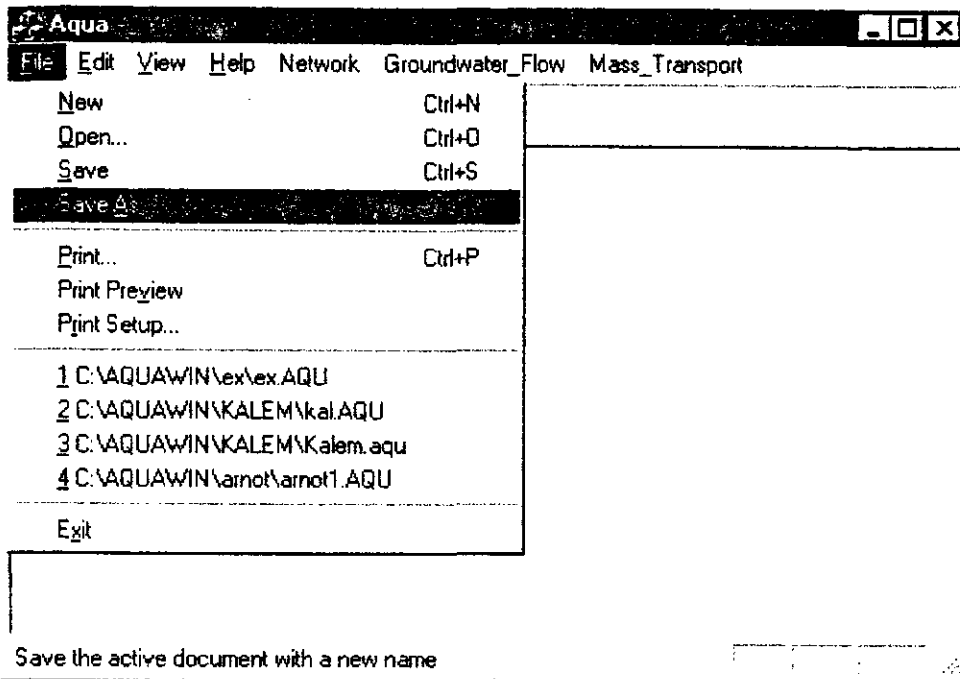
- (l) layers

- (ii) View nodes
- (iii) view elements
- (iv) color single elements
- (v) Insert nodes
- (vi) Insert nodes distance
- (vii) Draw a region on the map (for zoning e.g.)
- (viii) Print network

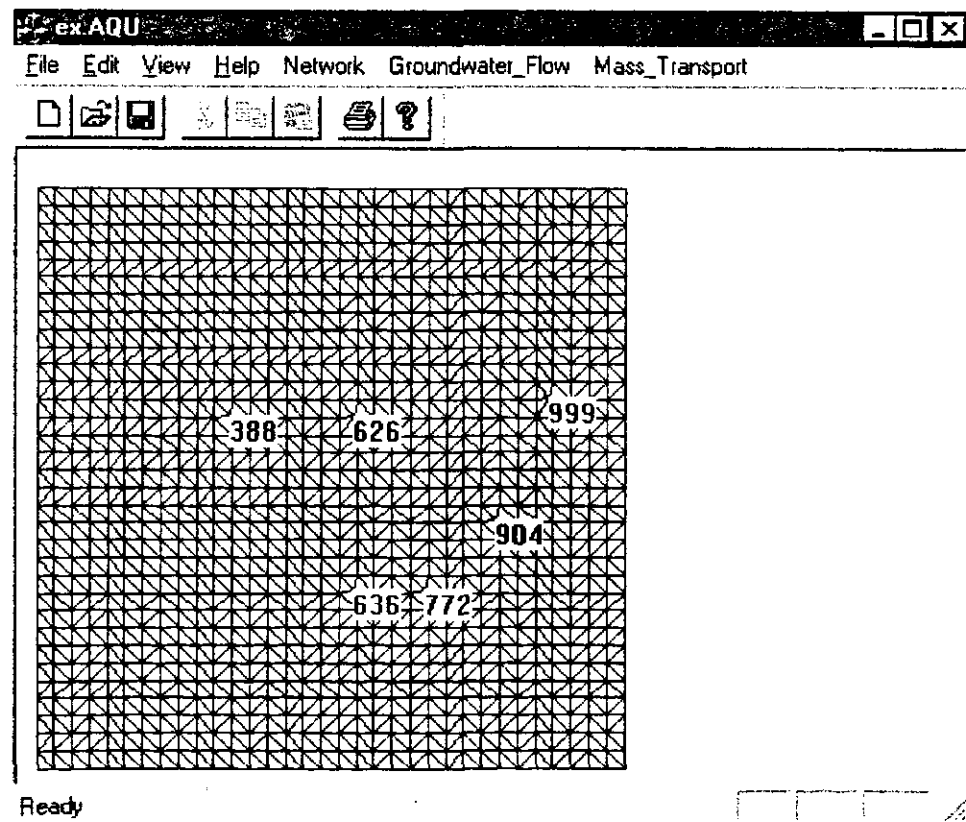


B. Finite element model (AQUA)

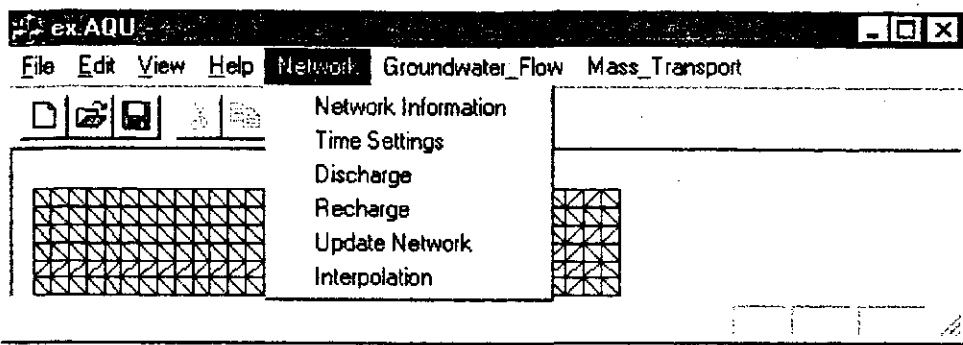
Exit the program NETGEN and go to the **Main Program Folder** (AQUAmod for WINDOWS) and double-click on the **AQUA** icon. Under the **File** menu, click on the **Save AS** item and choose the name Ex (or the name you have given to the export files). A new project with the name Ex.aqu will be created:



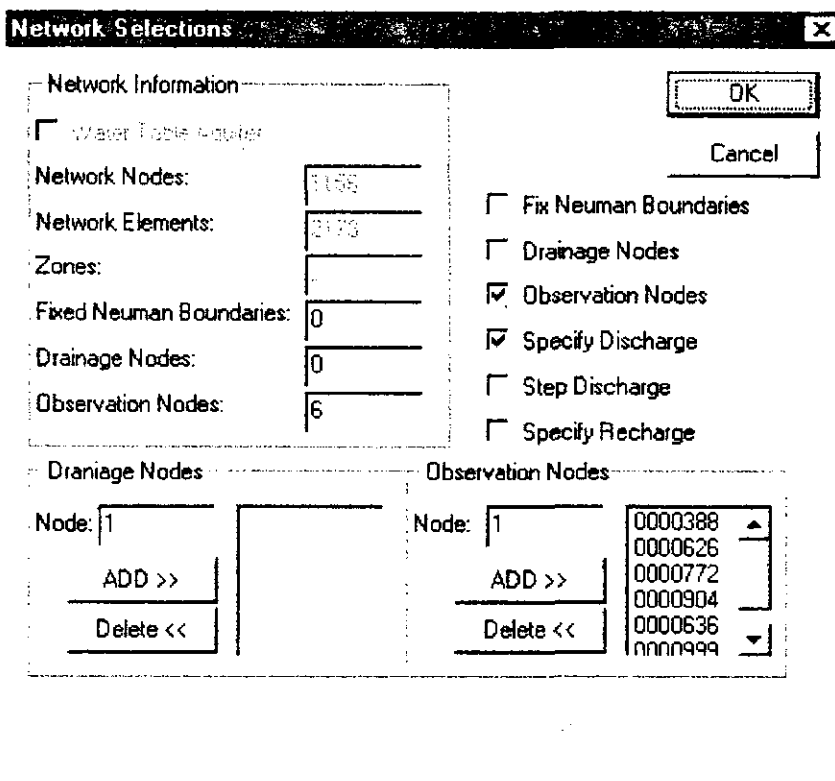
(b) The following window will appear. Observation nodes appear as blue numbers and abstraction nodes as pink numbers.



(c) Choose the menu **Network**



(d) Choose **Network Information**: select **Observation Nodes** and **Specify Discharge** options.



(e) Go to **Network** menu, choose the **Time Settings** and type at maximum time the value zero in (steady state flow). Add results after 30 days as below:

Time Parameters [X]

Simulation Time

Maximum Time (days):

Start Time (days):

Incremental Time Multiplier:

OK

Cancel

Output Times

Output Time Increment:

Output Times Specified:

Time to add (days):

Specified Time (days):

Delete <<

ADD >>

(f) Select the **Discharge** option to look at the abstraction rates: (only node 999 has an abstraction rate)

Discharge [X]

Discharge Nodes

Discharge Nodes:

Changing Rate Nodes:

Times rates changes:

OK

Cancel

Node	Rate (Cubic m/day)
1	0000636
	0000999

ADD >>

Delete <<

Number	Node	Rate (Cubic m/day)
Discharge: 2	999	-2500
Time (days): 1	0.000000	0.000000

(g) Go to the **recharge** option (no information will be entered here because we suppose no recharge). If you want to specify recharge choose the annual recharge option and enter values of recharge for each zone.

Recharge [X]

Monthly Recharge

OK

Cancel

Annual Recharge

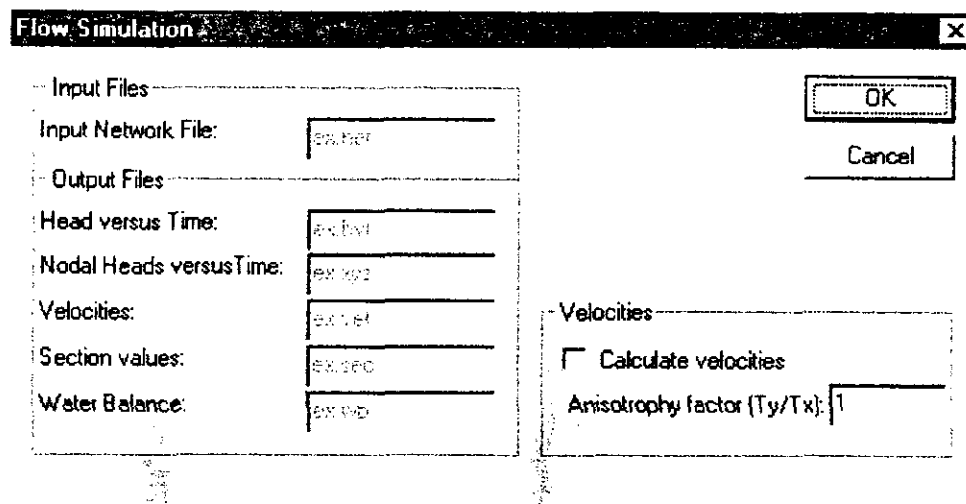
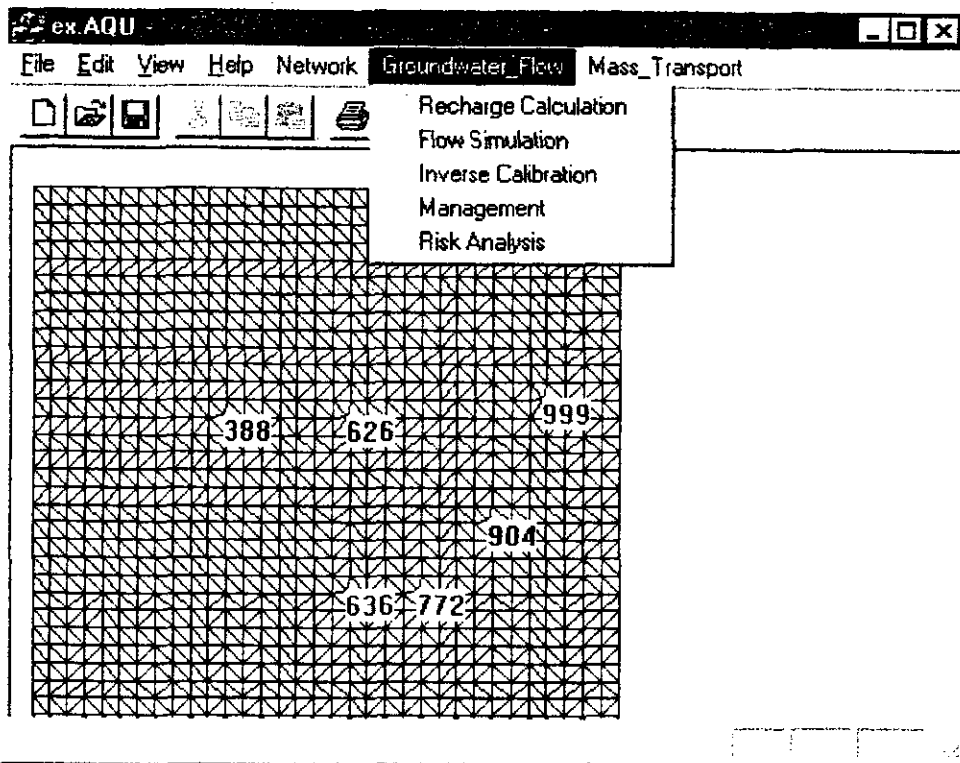
Zone	Recharge (mm./annum)
1	0.000000

Monthly Rainfall and Recharge

Months:

Month	Rainfall (mm.)	Zone	% Recharge
1	0	1	0.000000

- (h) Under the **Groundwater Flow** menu, select the **Flow Simulation** option and run the program.



- (i) If you want to import the steady state solution go to the Update Network option under Network menu and import the last flow values. **We do not need it here.**

Update Network File Values [X]

Replace Initial Heads with

- Last Flow Values
- Interpolation Values
- Constant Value

Constant Water Level:

Replace Aquifer Parameters

- Transmissivity
- Storativity
- Porosity

Constant Value:

OK
Cancel

Multiply Aquifers Parameters

- T and S with Inverse Results
- T with Inverse Results
- S with Inverse Results

Replace Aquifer Parameters per Zone

Zone	Transmissivity	Storativity	Porosity
1	0.000000	0.000000	0.000000

(j) The item **Interpolation** is not used for this example but looks as follows:

Prepare for TRIPOL Interpolation [X]

Input Files

Initial Heads at Boreholes:

Topography at Guess points:

Network file:

Output Files

Tripol input file:

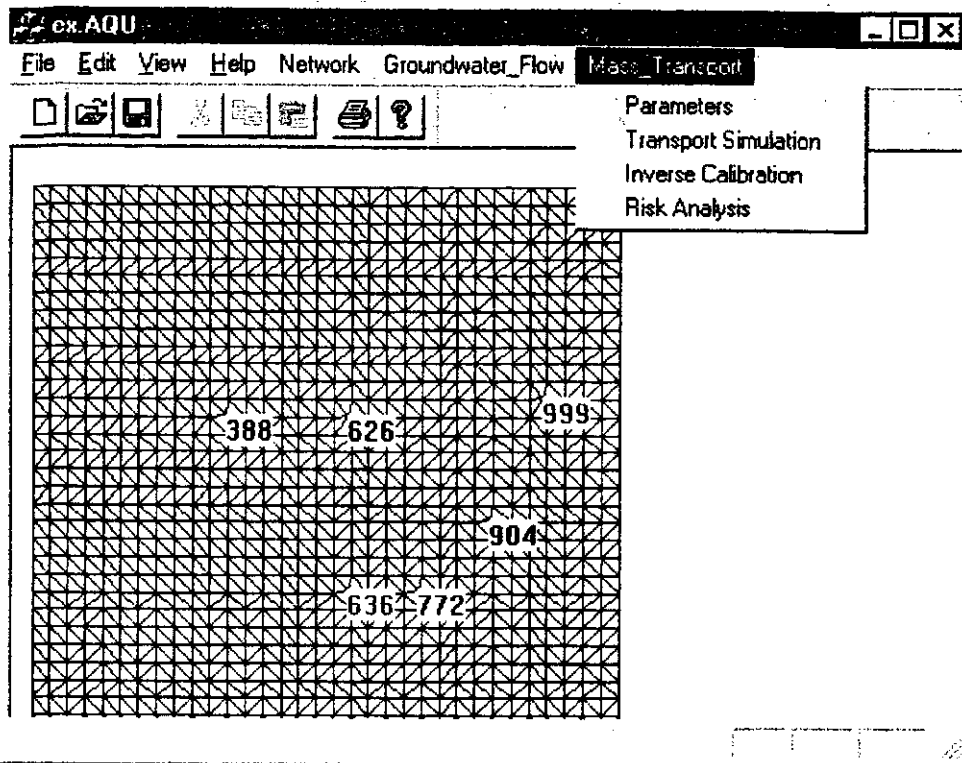
Type of Interpolation

- Guesses to Network Nodes
- Bayes Interpolation
- Interpolation without Guesses

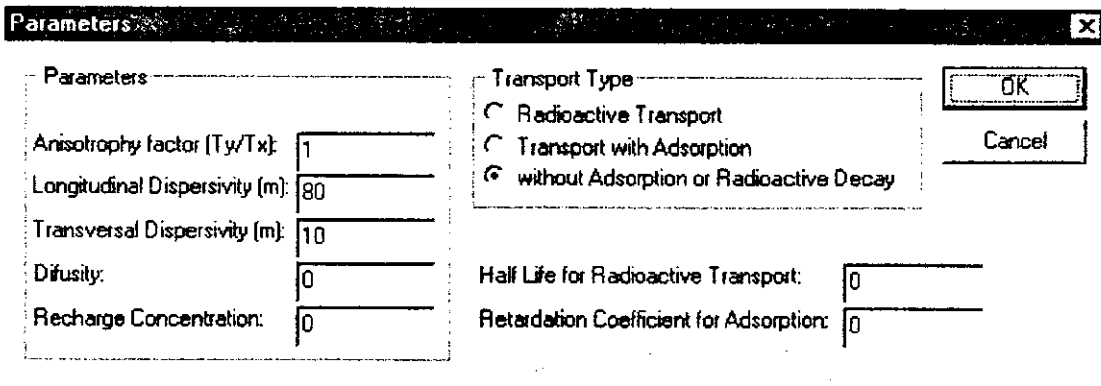
OK
Cancel

(k) Go to the **Network** menu and select **Time Parameters** and change the time to 3600 with the output time increment set to 12 (meaning that concentration at each node will be written to a file *.xyc after every 360 days).

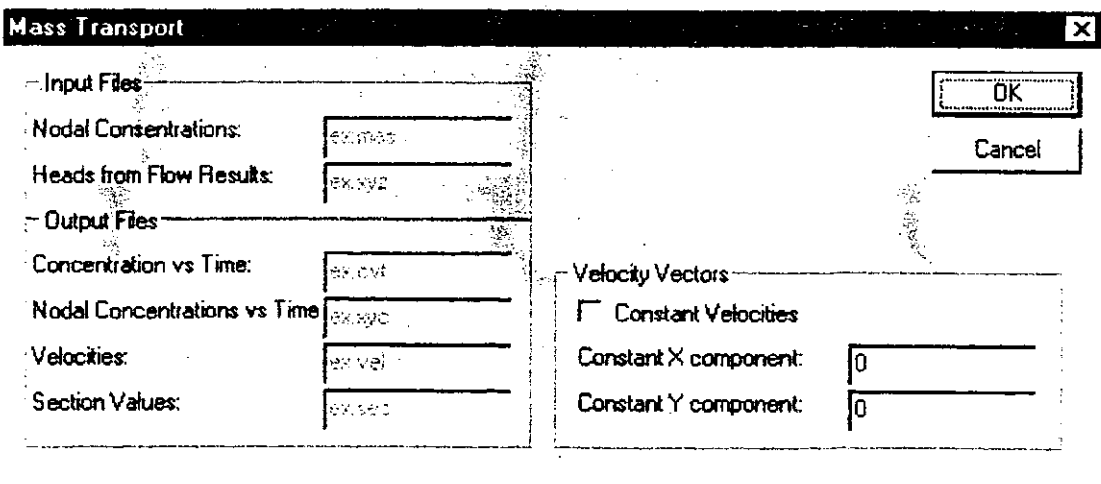
Go to **Mass Transport** Menu and choose **Parameters**:



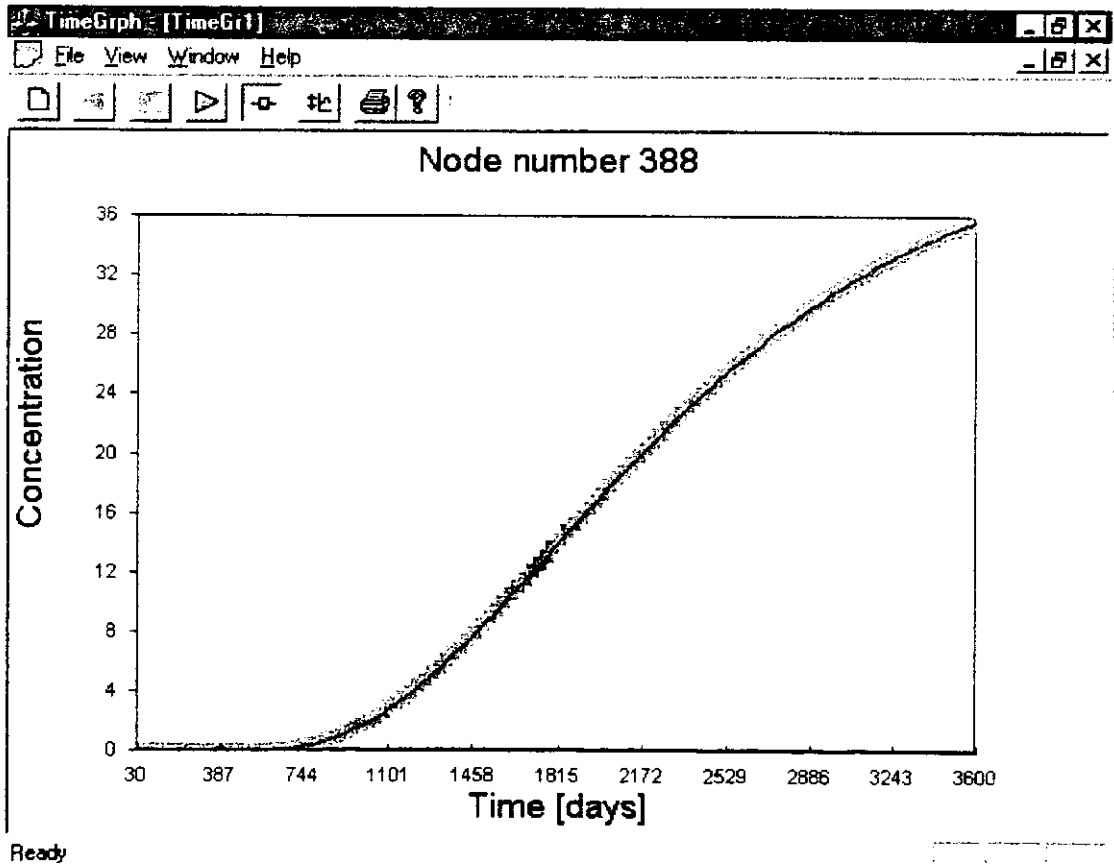
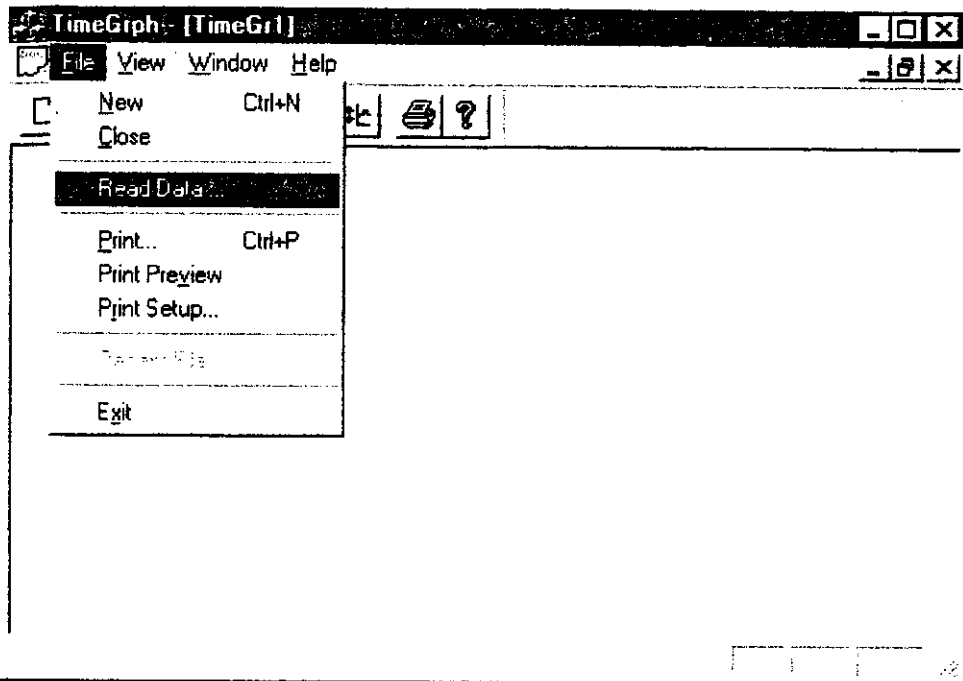
Enter the value 80 for Longitudinal Dispersion and 10 for Transversal Dispersion.



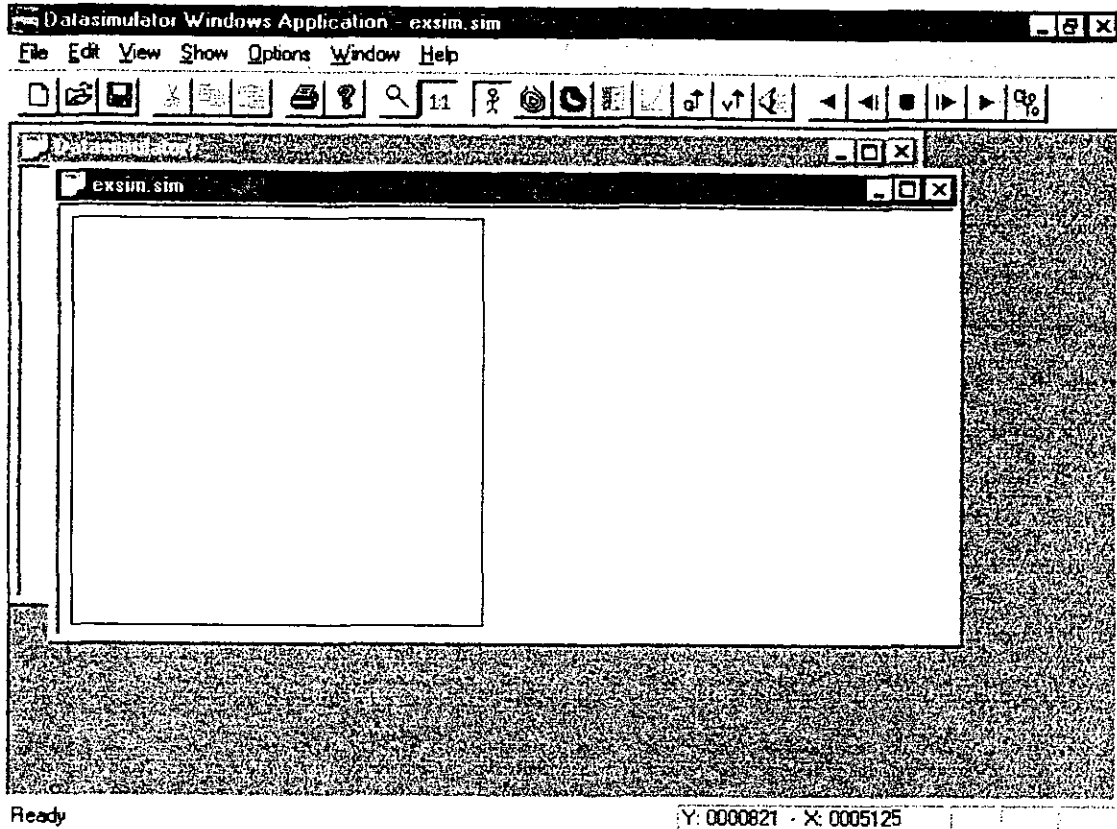
(l) Run the Mass Transport model



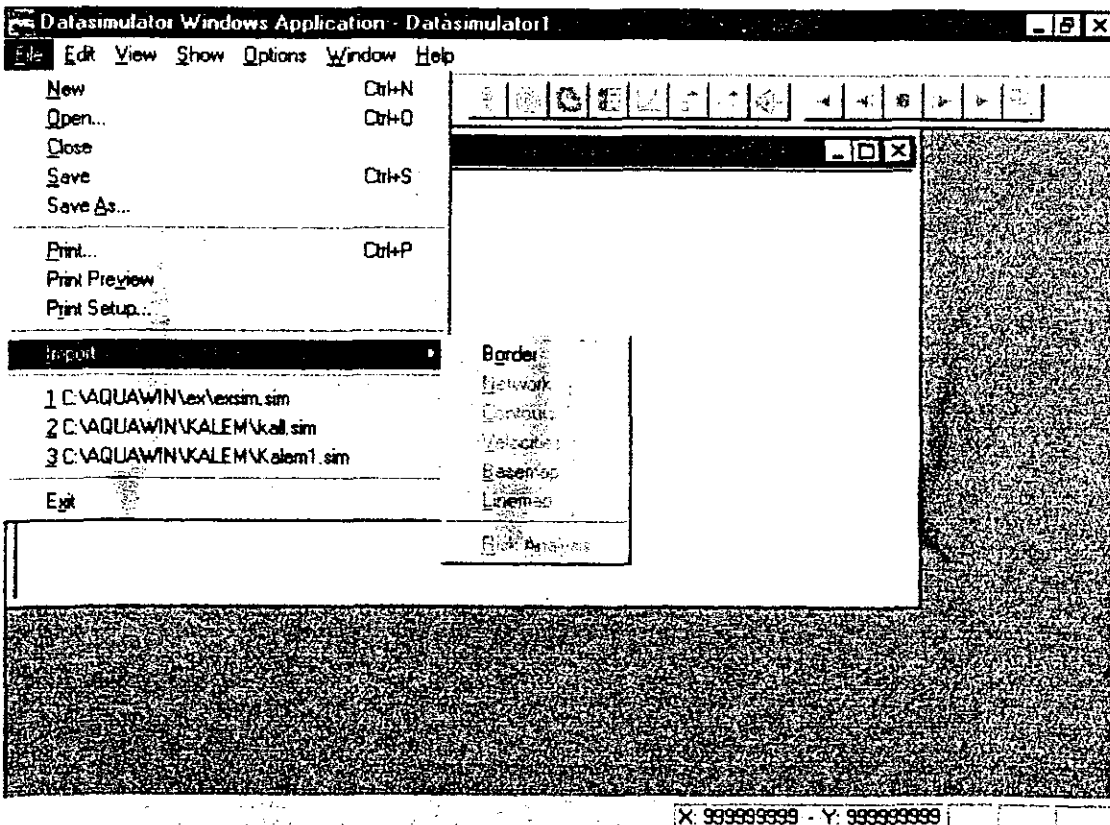
- (m) Save the file under the save option and go to the **Main Program Folder** and click on **Timegrph**. Under the menu **File** click on **Read Data** and enter the file **Ex.cvt** (or the name you choose).

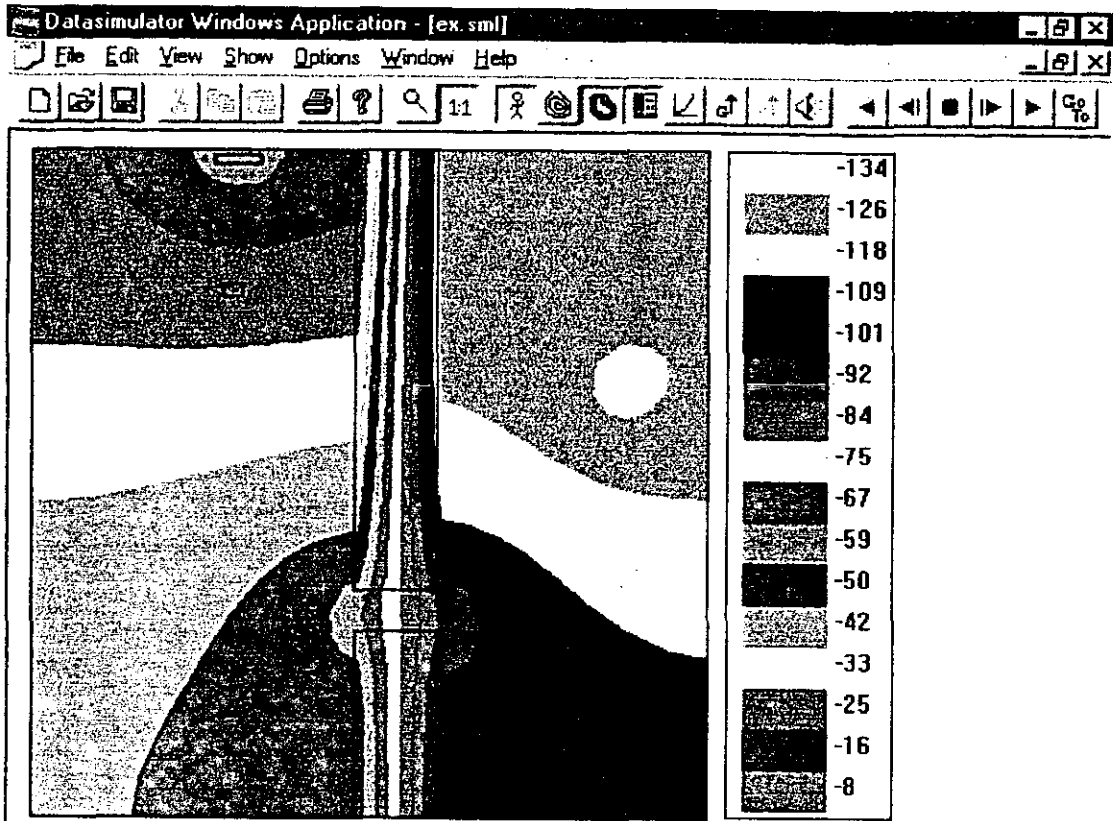


(n) Go to the **Main Program Folder** and click on the **DATASIM** icon.



(o) Under the **File** menu click the **New** option and thereafter **Import** the *.brd, *.net, *.xyz and *.vel files. Display the water levels by clicking on the **color contour bar** after activating the small man (animate) icon.

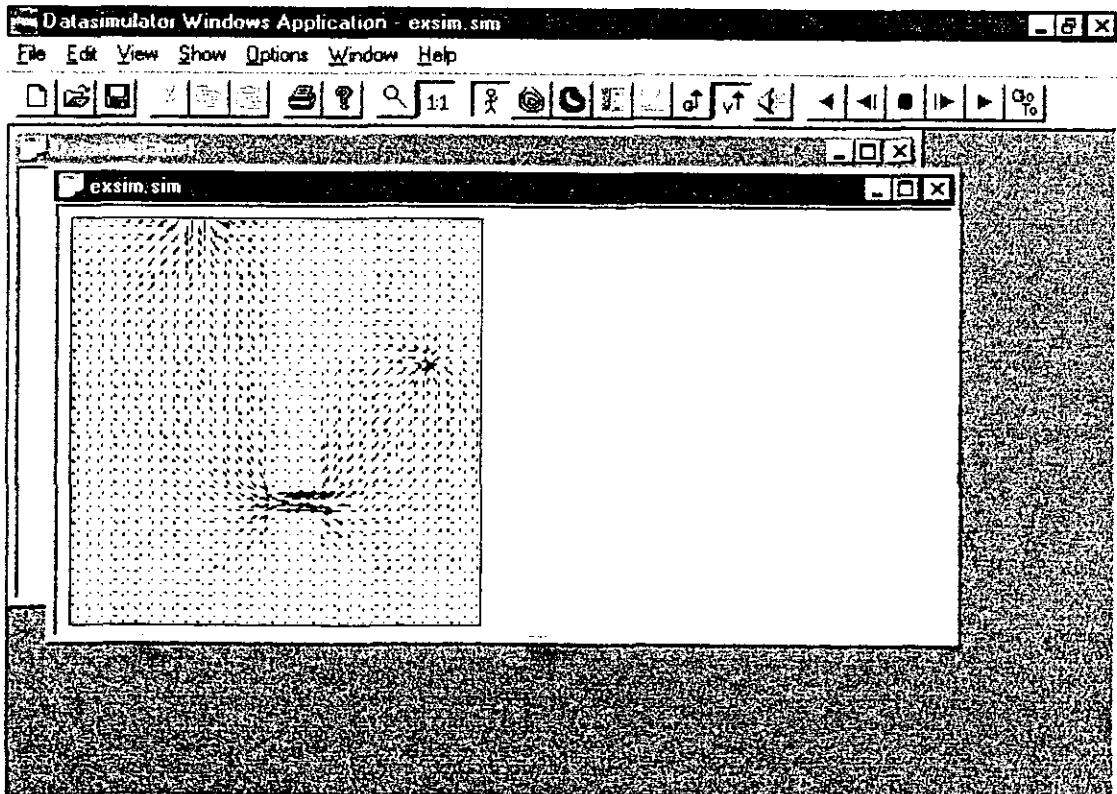




Ready

Y: 0003784 - X: 0005071

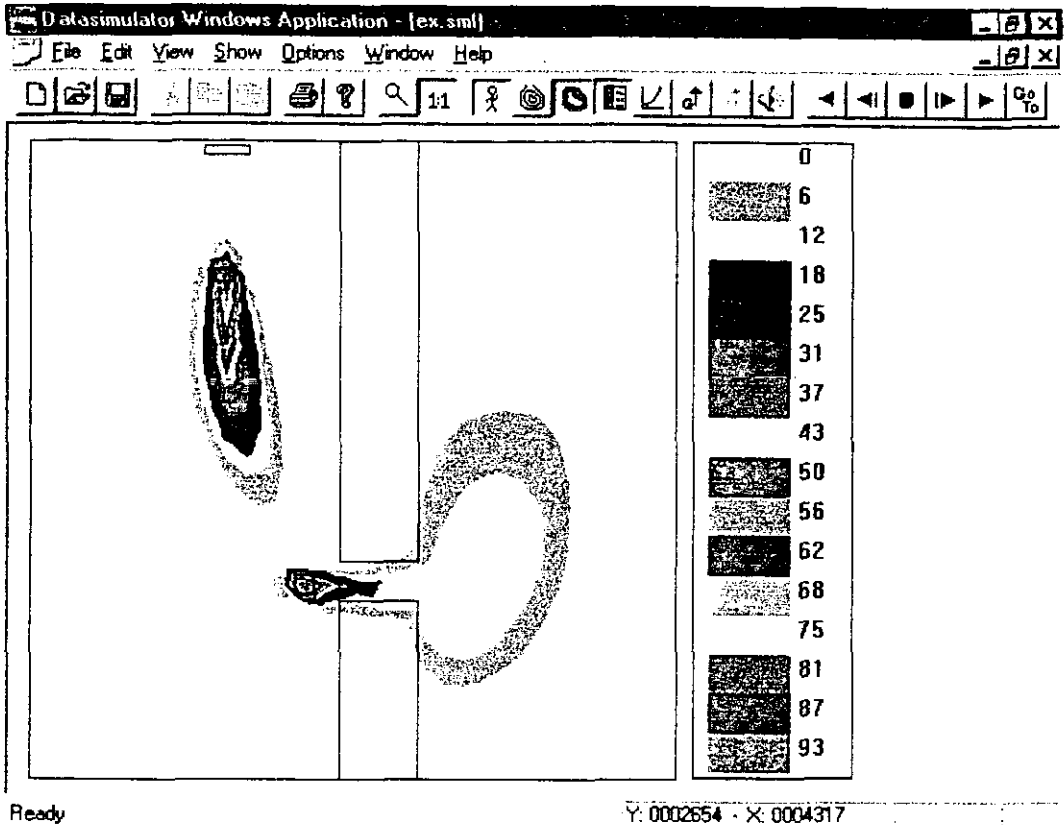
Display the velocities by clicking on the $v\uparrow$ icon:



Ready

Y: 0002929 - X: 0005040

Import the Ex.xyc file (under the **File** menu) and display the results by clicking on the \triangleright icon (e.g. concentration at time 3600 is displayed below).



- (p) Go to the **Main Program Folder**. Open the EX.AQU file (or the name you have used). Go to **Groundwater Flow** menu and click on the **inverse calibration** item: (files Ex.wop and Ex.wob are included on the diskette). If you have used another name (e.g. Extest, you must rename the wop and wob files to Extest.wop and Extest.wob) Click **OK** to run the program. After 13 iterations the required solution for T and S parameters for the two zones (i.e. multipliers = 1,000) will be reached.

Inverse Calibration

Input Files

Water Level Optimization:

Water Levels Observations:

Output Files

Optimization Results:

Head versus Time:

Water Levels versus Time:

Unknowns:

Parameter Type:

Water Level Observations:

Meter above sea level:

Multipliers

Unknown	Minimum	Guess	Maximum
1	0.100000	5.000000	10.000000

OK

Cancel

- (q) A file Ex.man (constraint file) is included on diskette. The idea is to obtain the maximum abstraction rate at the two abstraction boreholes (nodes 636 and 999) such that the constraints at the 6 boreholes are not violated after 360 days of

pumping. Go to the **Network** menu and under the **Time** item specify a time of 360. Go to the **Groundwater Flow** menu and click on the item **Management**. You can look at the constraints by pressing the up move bar. Calculate the **response matrix** and thereafter run the **optimization** part. The optimized abstractions are calculated as -591 and -971 m³/d for nodes 636 and 999 respectively.

Flow Management [X]

Input Files

Management Constraints: [ex:man]

Output Files

Optimization Constraints: [ex:opt]

Stress: [1] [OK] [Response] [Optimization] [Cancel]

Constraints

	Node	Relation	Value
Observation Node:	1	<	2.500000
Pump Node:	1	<	1000.000000
Sum Q		=	0

Maximize

	Pump	Value
Cost / Objective Factor:	1	1.000000

- (r) To perform **risk analysis** (for flow), go to the **Network** menu, and under the **Discharge** option enter the values -591 and -971 at the corresponding nodes. Go to the **Groundwater Flow** menu and under flow management, **generate** 10 random values for the T and S values of zones 1 and 2 by entering the following values (use zero recharge). Click **compute** to generate Monte Carlo values. File Ex.mc will contain the generated values:

Risk Analysis [X]

Input Files

Random values: [ex:rcd] [OK] [Cancel]

Experimental Values: [ex:exp]

Output Files

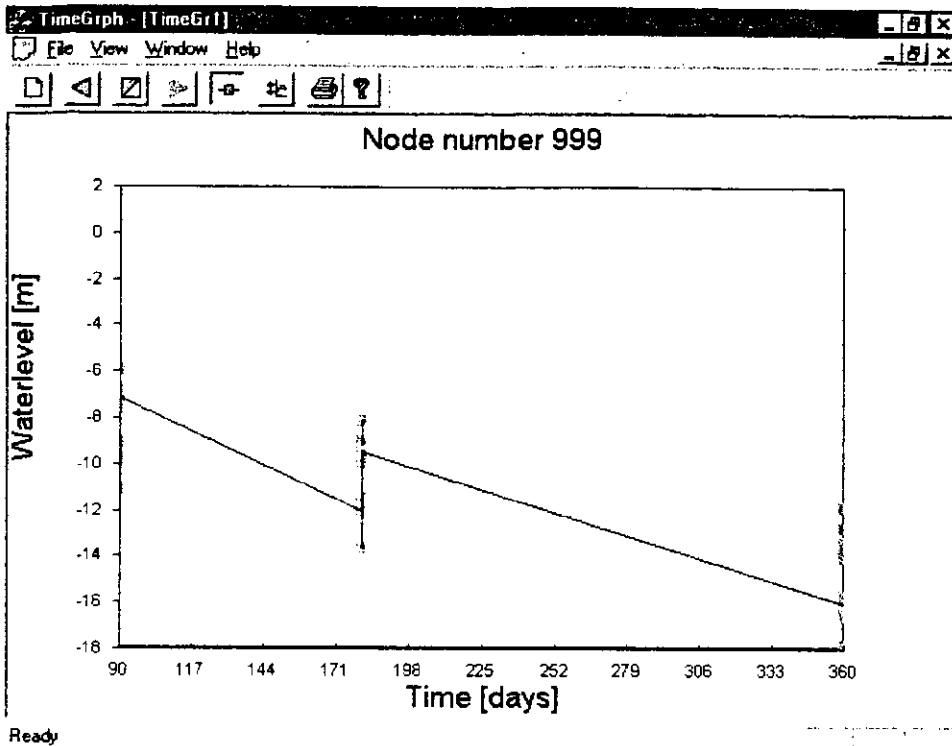
Head versus Time: [ex:hvt]

Random Values

Use Experimental Values [Compute]

	Zone	Number of Values	Mean	Variance
T (m ² /day)	1	10	100	20
Storativity	1	10	.005	.0001
Recharge (mm/ann)	1	10	0.000000	0.000000

Click OK to run the program. The drawdown risk distribution at node 999 (abstraction node) looks as follows if displayed with the **TIMEGRPH** program



The Risk analysis (mass transport) window and parameters look as follows:

Risk Analysis

Input Files

Random values: EX.F05

Experimental Values: EX.E05

Output Files

Concentration versus Time: EX.C05

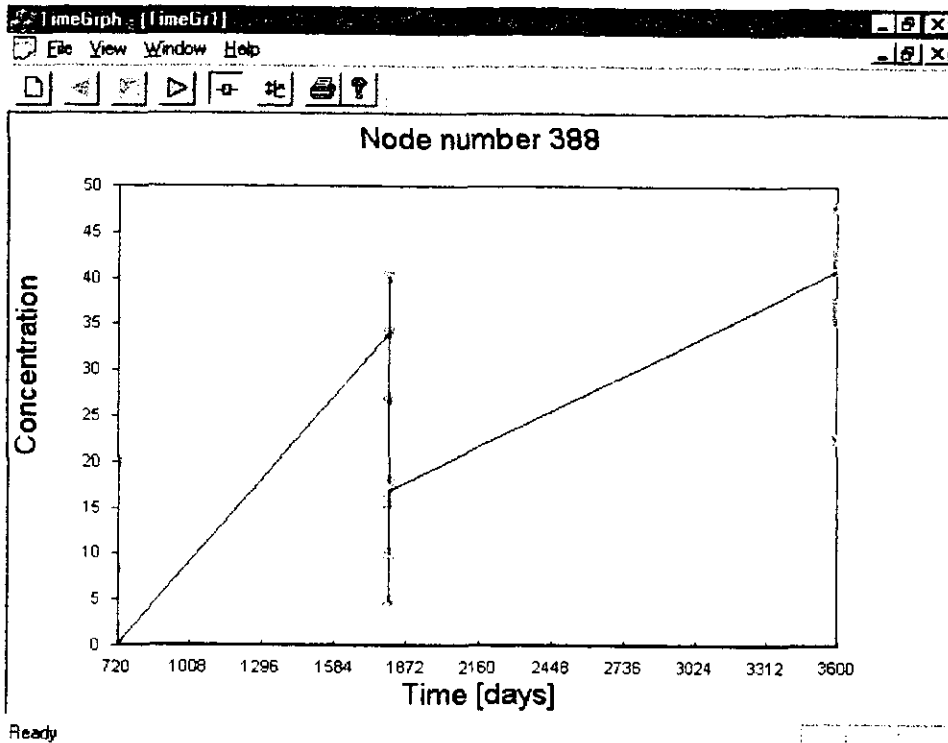
Random Values

Use Experimental Values

	Zone	Number of Values	Mean	Variance
T (m ² /day)	1	10	100	20
Porosity	1	10	.1	.05
Longitudinal Dispervivity (m)		10	80	20

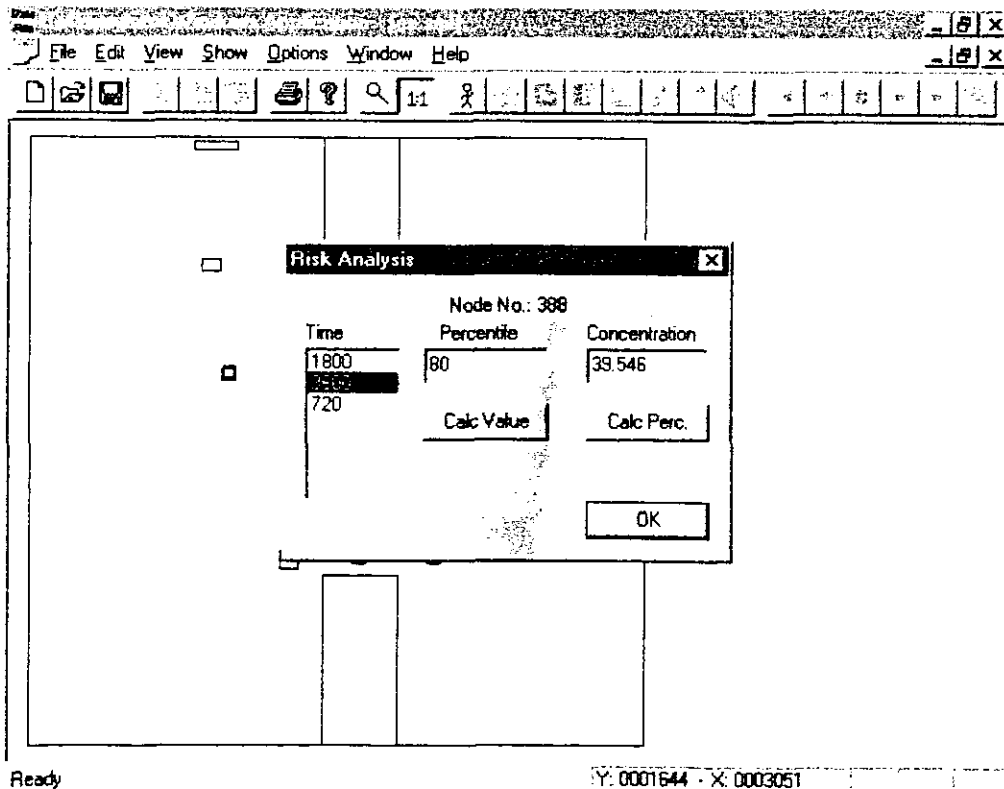
Buttons: OK, Cancel, Compute

The pollution risk distribution at node 388 looks as follows for different times.



The results can be imported in the DATASIM program under risk analysis and displayed together with the percentiles of probability by clicking on the left button of the mouse on a risk point. The result file (ex.cvt) can also be displayed by the TIMEGRPH program as shown above.

With DATASIM the results are displayed as follows:



Mass Transport Inverse calibration Window:

Inverse Calibration [X]

Input Files

Concentration Optimization:

Concentration Observations:

Output Files

Optimization Results:

Concentration vs. Time:

All Concentrations vs. Time:

Unknowns:

Parameter Type:

Multipliers

Unknown	Minimum	Guess	Maximum
1	0.100000	5.000000	10.000000

OK

Cancel

Recharge

Files Dewet.net, dewet.rq, dewet.bwl and dewet.bnd are included on the diskette and can be used to perform recharge calculations and the estimations of the cumulative rainfall departures.

Go to the Groundwater Flow menu and click on recharge. Then calculate the saturated volumes, the probable mean S-value and the equal volume recharge. Remember to enter a T-value of 9 m²/d at the outflow boundary option. Calculate the CRD with a mean cut-off value of 20 mm/month.

Saturated Volume and Recharge Calculation X

<p>Input Files</p> <p>Borehole Water Levels: <input type="text" value="ex.bwl"/></p> <p>Rainfall and Recharge: <input type="text" value="ex.rqd"/></p> <p>In/Outflow Boundaries: <input type="text" value="ex.bnd"/></p> <p>Output Files</p> <p>Saturated Volumes: <input type="text" value="ex.vol"/></p> <p>Saturated Volume / Zone: <input type="text" value="ex.svc"/></p> <p>Equal Volume Recharge: <input type="text" value="ex.evc"/></p> <p>Total Balance Recharge: <input type="text" value="ex.tbc"/></p> <p>Cummulative Rainfall: <input type="text" value="ex.cum"/></p> <p>Rainfall versus Recharge: <input type="text" value="ex.br"/></p>	<p>Calculate</p> <p><input checked="" type="radio"/> Saturated Volume</p> <p><input type="radio"/> Probable Mean Storativity</p> <p><input type="radio"/> Recharge</p> <p><input type="radio"/> Cummulative Rainfall</p> <p style="text-align: right;"><input type="button" value="OK"/></p> <p style="text-align: right;"><input type="button" value="Cancel"/></p>
<p>Recharge Calculation</p> <p>Method: <input type="text" value="Equal Volume Calculation"/></p> <p>Storativity: <input type="text" value="0.005"/></p> <p>Interval Size (months): <input type="text" value="12"/></p> <p>Rainfall -> Recharge Lag (months): <input type="text" value="0"/></p>	<p>Boundary</p> <p><input type="checkbox"/> Inflow/Outflow Boundary</p> <p>Inflow Transmissivity (m²/day): <input type="text" value="0"/></p> <p>Outflow Transmissivity (m²/day): <input type="text" value="0"/></p> <p>Saturated Volume Calculation</p> <p>Maximum Interpolation Distance: <input type="text" value="5000"/></p> <p>Water Levels: <input type="text" value="Meter Above Sea Level"/></p> <p>Cummulative Rainfall Calculation</p> <p>Method: <input type="text" value="Mean Cummulative Rainfall"/></p> <p>Monthly Rainfall Cut-off Value (mm): <input type="text" value="20"/></p> <p>Short Term Memory (months): <input type="text" value="3"/></p> <p>Long Term Memory (months): <input type="text" value="9"/></p>

8.3 Example 3: TRIPOL Interpolation

Data input:

Any file name with the extension *.df1

1. Number of experimental points,N

2. x,y,z,guess

repeat line value N times

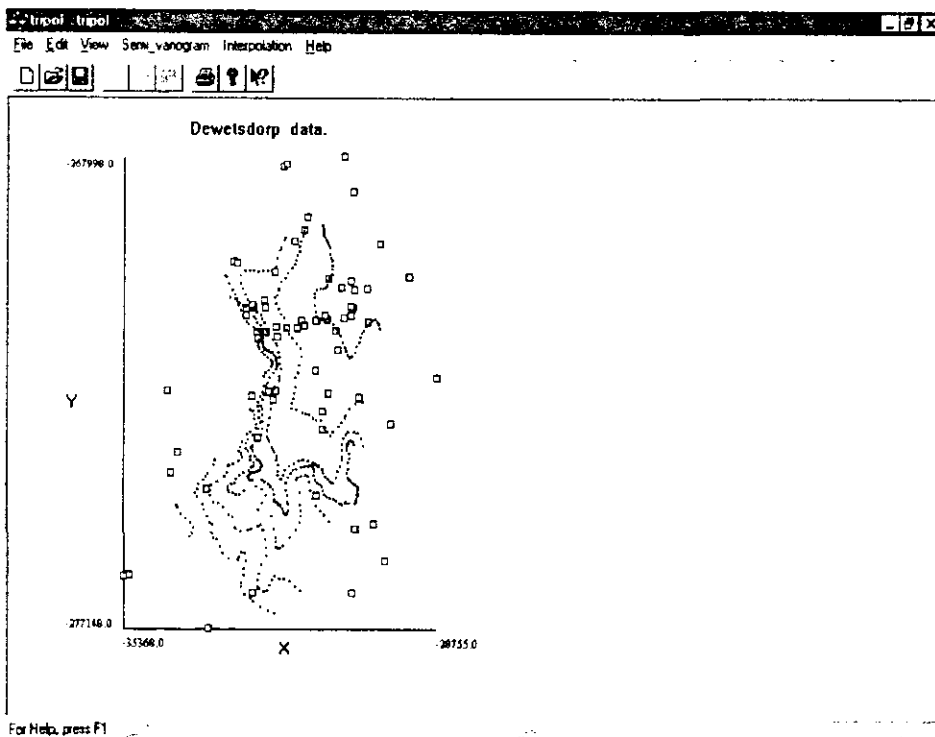
(guess value only necessary for Bayes method)

3. Number of unknown points,NU

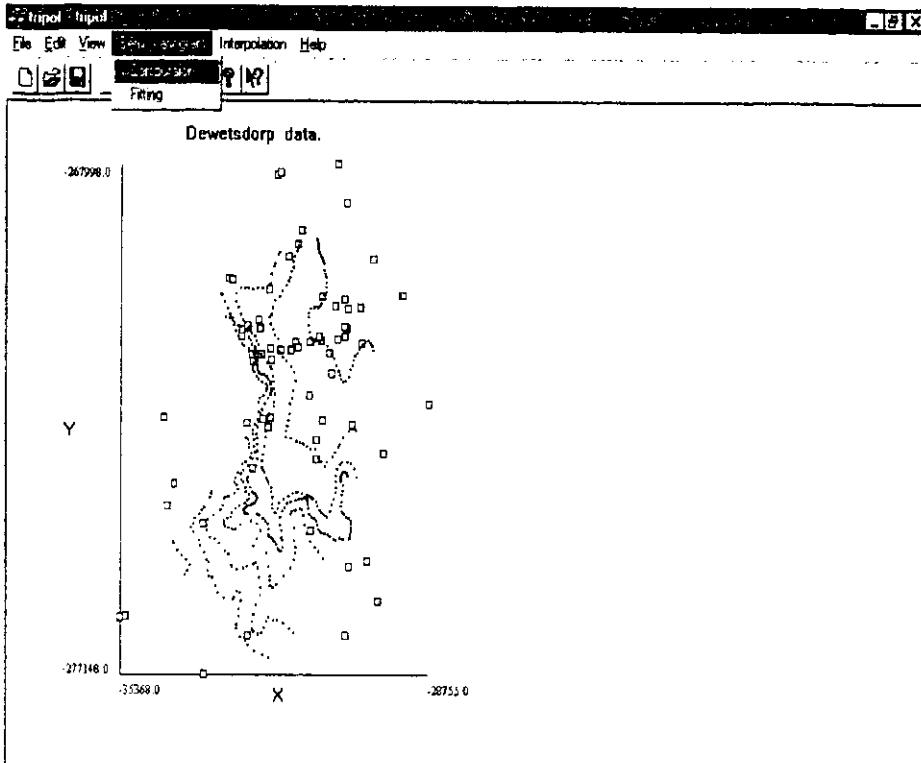
4. x,y,guess (repeat line NU times)

(guess value only necessary for Bayes method)

1. In File menu, Create new and call it tripol (a file tripol.dfl) is included on the installation



2. Semi-variogram calculation: Go to Menu Semi Variogram and click on semi-variogram



Semi Variogram [X]

Input Files

Input Data File: [OK] [Cancel]

Output Files

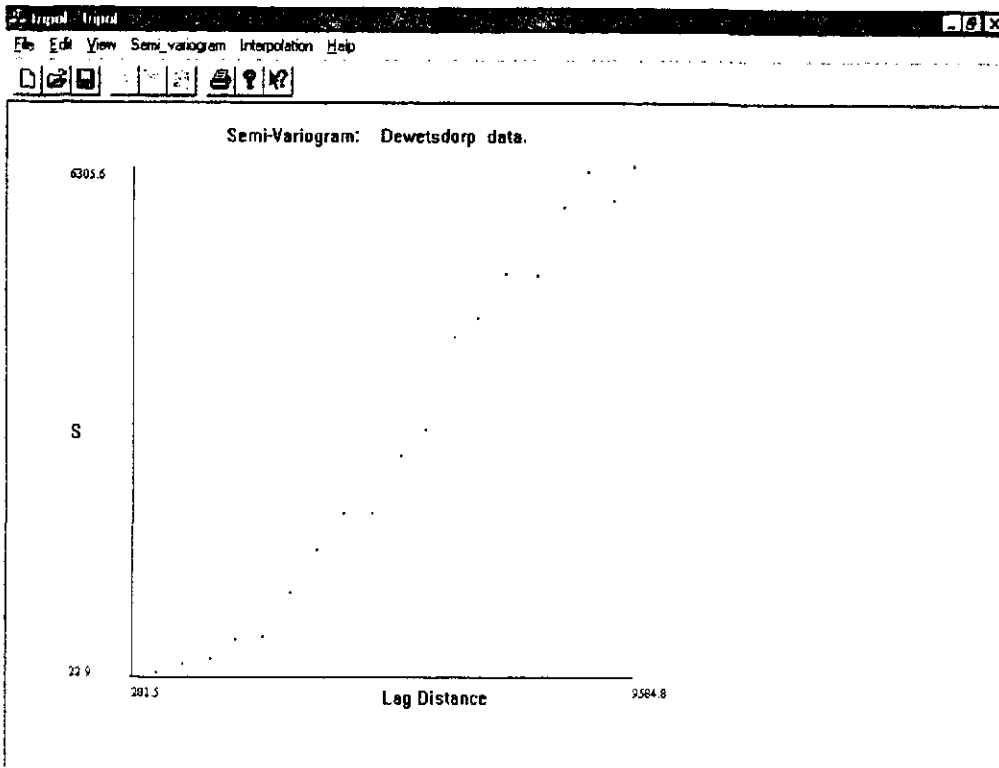
Vario-Gram Results File:

Output file to Fit:

Basic Lag Distance: Logtransform values

Direction: Subtract Values

Direction of Tolerance: Number of Lags:



For Help, press F1

3. Go to fit semi-variogram and click on initialize and run the inverse

Fit Semi Variogram

Files

Input Fit File:

Output Error Analysis:

Number of Lags: Compute best fit

Semi-Variogram Parameters			
	Minimum	Initial	Maximum
B1:	63.056450	6305.645020	63056.449219
B2:	95.847694	9584.769531	95847.695313
B3:	0.000000	22.875700	228.757004

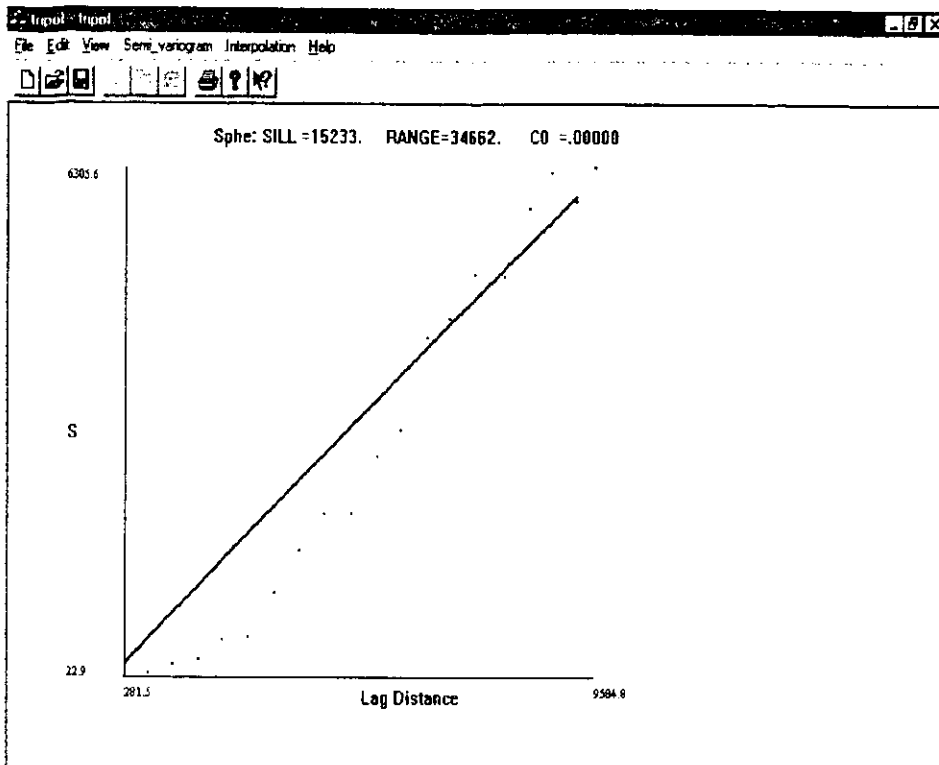
Semi-Variogram Type

- Polynomial
- Spherical
- Exponential
- Gauss
- de Witsjan
- kRho of de Waal

Initialize

OK

Cancel



For Help, press F1

4. Go to menu, click on distance weighting method and Do error analysis
5. Then Kriging and then Bayes

Distance Weighting Interpolation X

<p>Input Files</p> <p>Input Data File: <input type="text" value="input.dfl"/></p> <hr/> <p>Output Files</p> <p>Error Analysis: <input type="text" value="input.lst"/></p> <p>Result Nodes and values: <input type="text" value="input.vals"/></p> <p>Interpolated Values: <input type="text" value="input.fev"/></p> <hr/> <p>Number of Nearest Points: <input type="text" value="4"/></p> <p>Degree of Trendsurface [1-9]: <input type="text" value="2"/></p>	<p> <input checked="" type="radio"/> Do Error Analysis <input type="radio"/> Do Interpolation </p> <p style="text-align: right;"> <input type="button" value="OK"/> <input type="button" value="Cancel"/> </p> <hr/> <p>Interpolation Scheme</p> <p> <input checked="" type="radio"/> 1/d; d=distance between points <input type="radio"/> (1-d/1.1xDmax)^2 / (d/1.1xDmax)^2 <input type="radio"/> exp (-alpha x d) <input type="radio"/> 1 / d^2 <input type="radio"/> exp (alpha x d^2)/(d^2+eps) <input type="radio"/> exp (-d/d^2)/(d^2+eps) <input type="radio"/> Trendsurface </p>
--	--

Kriging [X]

Input Files

Input Data File:

Output Files

Error Analysis:

Result: Nodes and values

Interpolated Values:

Number of Nearest Points:

Order of Kriging [0-2]:

Semi-Variogram Parameters

Sill: C:

a: CO:

Do Error Analysis

Do Interpolation

Logtransform values

Semi-Variogram Type

Polynomial

Spherical

Exponential

Gauss

de Wisjan

OK

Cancel

Bayesian Estimates [X]

Input Files

Input Data File:

Output Files

Error Analysis:

Result: Nodes and values

Interpolated Values:

Number of Nearest Points:

Semi-Variogram Parameters

	kRho of De Waal	Observations	Guesses
Sigma:	<input type="text" value="0.67"/>	Sill: <input type="text" value="1107"/>	<input type="text" value="0"/>
k:	<input type="text" value="43.6"/>	a: <input type="text" value="2000"/>	<input type="text" value="0"/>
Rho:	<input type="text" value="0.79"/>	C: <input type="text" value="1107"/>	<input type="text" value="0"/>
Lag D.:	<input type="text" value="200"/>	CO: <input type="text" value="0"/>	<input type="text" value="0"/>

Do Error Analysis

Do Interpolation

Logtransform values

Scale Guesses

None

Mean Window

Mean

Linear

Semi-Variogram Type

Polynomial

Spherical

Exponential

Gauss

de Wisjan

kRho of de Waal

OK

Cancel

Bayes has given the smallest root mean square error

6. Now one can perform Bayesian estimation to the unknown points.