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GWHRT – A finite element solution to the coupled ground water flow and heat transport problem in three dimensions

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Stockholm, Sweden May 1983

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GWHRT - A FINITE ELEMENT SOLUTION TO THE COUPLED
GROUND WATER FLOW AND HEAT TRANSPORT PROBLEM IN
THREE DIMENSIONS

Description of HYPAC - A program package for
pre- and post processing finite element data

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**GWHRT - A finite element solution to the
coupled ground water flow and heat trans-
port problem in three dimensions**

Description of HYPAC - A program package for
pre- and post processing finite element data

Bertil Grundfelt
Kemakta Consultant Company, Stockholm

SUMMARY

A program package for modelling ground water flow with the Finite Element Method (FEM) is presented. The package, that comprises programs for pre- and postprocessing data for the FEM-model, has been extensively used together with the GWHRT-model developed by Roger Thunvik.

Thunvik's hydraulic model is one-, two- or threedimensional. It solves the ground water pressure distribution and the temperature distribution in the modelled domain using the Finite Element Method. Also saturated/unsaturated flow can be modelled.

The calculations performed in the KBS-3 study are three-dimensional steady state calculations for isothermal conditions. Such a calculation typically involves the following steps:

- Generation of the finite element mesh.
- Assigning boundary conditions and material properties to the domain.
- Solving for the hydraulic pressure distribution.
- Checking the results.
- Presenting the results.

In the program package HYPAC these steps are implemented. This report deals mainly with the type of calculations made in the KBS-3 study although the program package in principal can handle also other types of calculations like for instance transient saturated-unsaturated flow.

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1 INTRODUCTION

1.1 BACKGROUND

In the context of nuclear waste disposal one of the most essential problem areas in a repository performance assessment is to understand the movements of ground water around the repository. Because of the time spans involved and the limited possibilities to perform direct measurements of the ground water movements one is restricted to using mathematical models for predicting flow rates and flow paths. In the KBS-3 study a model, GWHRT, developed by Roger Thunvik et al /1/ was used for this purpose. This report will present a program package developed by KEMAKTA Consultants Co to prepare the input for GWHRT model and to present the results. For completeness also GWHRT is presented briefly.

The development was sponsored by SKBF/KBS and performed with active moral and scientific support from Roger Thunvik.

1.2 SUMMARY

Thunvik's hydraulic model (GWHRT) is one-, two- or threedimensional. It solves the ground water pressure distribution and the temperature distribution in the modelled domain using the Finite Element Method (FEM). Also saturated/unsaturated flow can be modelled.

The calculations performed in the KBS-3 study are three-dimensional steady state calculations for isothermal conditions. Such a calculation typically involves the following steps:

- Generation of the finite element mesh.
- Assigning boundary conditions and material properties to the domain.
- Solving for the hydraulic pressure distribution.

- Checking the results.
- Presenting the results.

In the program package HYPAC these steps are implemented as shown in the schematic representation in figure 1-1. The contents of the boxes in figure 1-1 are further developed in the subsequent chapters. This report deals mainly with the type of calculations made in the KBS-3 study although the program package in principal can handle also other types of calculations like for instance transient saturated-unsaturated flow.

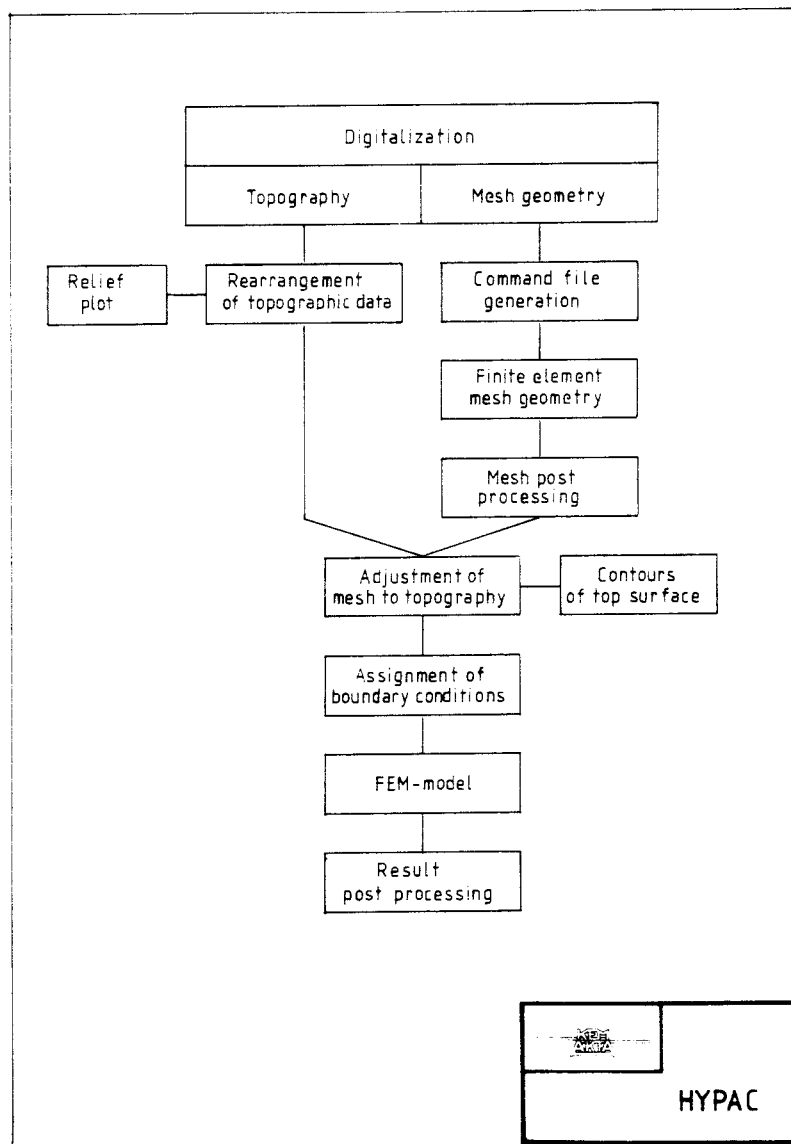


Figure 1-1: Flow-sheet of the program package HYPAC for pre- and post processing Finite Element data.

2.1 PRINCIPAL INPUT TO A FEM-RUN

The primary input to a FEM-calculation can be summarized as:

- Geometry description
- Boundary conditions
- Material properties

In ground water flow modelling in crystalline rock the geometry to be described typically involves fracture zones and the topography of the site. In the KBS-3 calculations the topography of the ground water table was used in place of the site topography in order to facilitate boundary condition assignment.

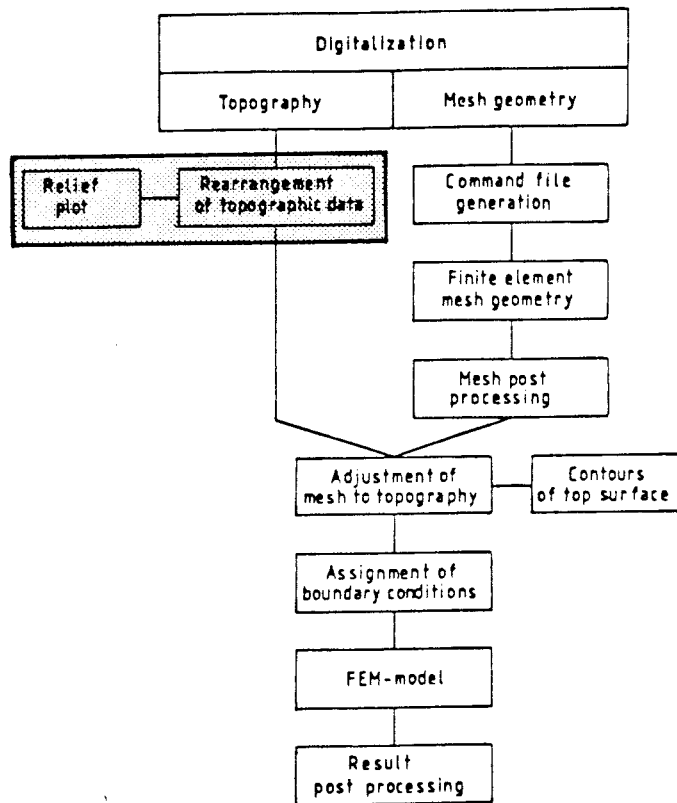
The boundary conditions used in the KBS-3 study are a prescribed pressure at the ground water table ($p = 0$) and non-flow boundaries at the vertical boundaries and at the bottom of the mesh. The latter condition is the natural boundary condition for the FEM formulation used in GWHRT.

Other boundary conditions like a prescribed flux can be applied, but this was not done in the KBS-3 study.

In the equivalent porous medium approach used in GWHRT the governing material property of the geologic medium is the permeability. Taking into account also the properties of the fluid and the gravitational acceleration the hydraulic conductivity can be used as an alternative to the permeability.

In the following subsections, programs for processing topography and mesh geometry are described. The assignment of material properties and boundary conditions will be described later.

2.2 TOPOGRAPHY PROCESSING



In the ideal situation the topography of the site or of the ground water table is defined by a contour map. In the KBS-3 study a digitizer was used to feed the coordinates of such contours to the computer. Such a data set contains typically about 10 000 non-uniformly spread values of the elevation of the ground water table or the ground surface. Figure 2-1 shows an example of a ground water table map used in the KBS-3 study.

As described in figure 1-1 the topography data is used at a later stage for the adjustment of the finite element mesh to the topography. For this reason the data is rearranged in a program called SSF to represent the elevations on a regular grid. This is done using a fifth order polynomial interpolation on a triangulation of the original data /2/. For the practical programming the IQHSCV-routine of the IMSL library /3/ is used.

The number of data points needed to represent a map is usually so large that the working space needed by the IQHSCV routine becomes prohibitive. Therefore only a portion of the modelled area is treated at a time.

The interpolated surface can be presented graphically as in figure 2-2. In this way a visual check that the digitalization and interpolation was successful is obtained.



Figure 2-1: Map of the ground water table at KAMLUNGE (from 157).

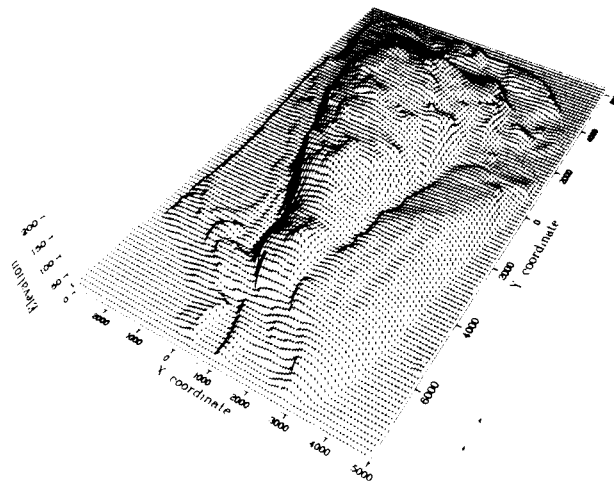
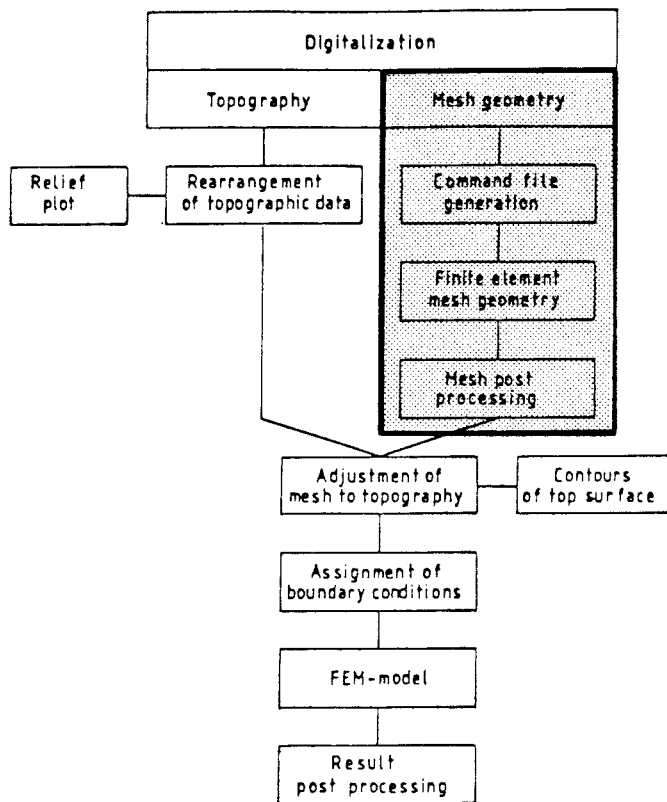


Figure 2-2: Relief of the ground water table at KAMLUNGE.

2.3 MESH GEOMETRY PROCESSING

2.3.1 General

The description of the geometry and the spatial discretization of the modelled domain are of crucial importance to the modelling results. It is also the part of the input to a FEM-calculation that is most tedious to prepare. A typical KBS-3 mesh consists of approximately 2 000 elements defined by up to 20 nodal points per element, in total about 10 000 nodal points. This means that the data needed to define the geometry is something like 2 000 lines of up to 20 nodal numbers and 10 000 lines of nodal coordinates (three coordinates per node).

The generation of these data is automated in three steps:

1. Definition of the geometry of special geological features to be modelled.
2. Mesh generation.
3. Mesh post processing and controle.

In the KBS-3 study the mesh geometry was governed by the regional and sub-regional fracture zones running through the domain. These fracture zones can be either vertical or inclined at arbitrary angles.

The mesh is for simplicity primarily generated with a planar top surface. The adjustment to the topography is taken care of at a later stage (see figure 1-1).

The mesh generating programme used (FEMGEN /4/) is a commercially available code. It is very general and easy to use. It was, however, designed primarily for other applications and can therefore in certain situations generate meshes where the node numbering sequence is hard to control. It can also happen that the same node have different node numbers in different elements. A special programme has therefore been devised in order to check the mesh with respect to element orientation and duplicate node numberings.

The various programs performing these operations are described below.

2.3.2 Definition of the geometry of the domain

In the KBS-3 study the mesh generation is to a great extent governed by the geometry of the fracture zones. The geometry of the fracture zones is defined by tectonic maps like the one in figure 2-3. In order to facilitate the mesh generation the fracture zone pattern is simplified. Figure 2-4 shows such a simplification based on the map in figure 2-3.

The simplified fracture zone map can then be used to feed the coordinates of fracture zone intersections, -bends, -endpoints etc to the computer using a digitizer. Furthermore hill summits and other features of geohydraulic importance can be input to the computer in the same way.

The digitized points are processed in a program (PREFG) to give a command file to the mesh generator (see subsection 2.3.3). During the processing the coordinates of the intersections of the fracture zone "walls" are calculated from the widths and directions of the involved fracture zones as illustrated in figure 2-5. As also illustrated in the figure the points defining an extra element row along the fracture zone can be calculated should that be required.

The program currently operates in an x-y geometry. In a three dimensional case this means that only the situation at the surface or at any given level can be calculated. This is, however, not a severe limitation as the mesh generator can create three-dimensional bodies from two two-dimensional surfaces. Extensions of the PREFG-program to treat full 3D-geometry are possible.

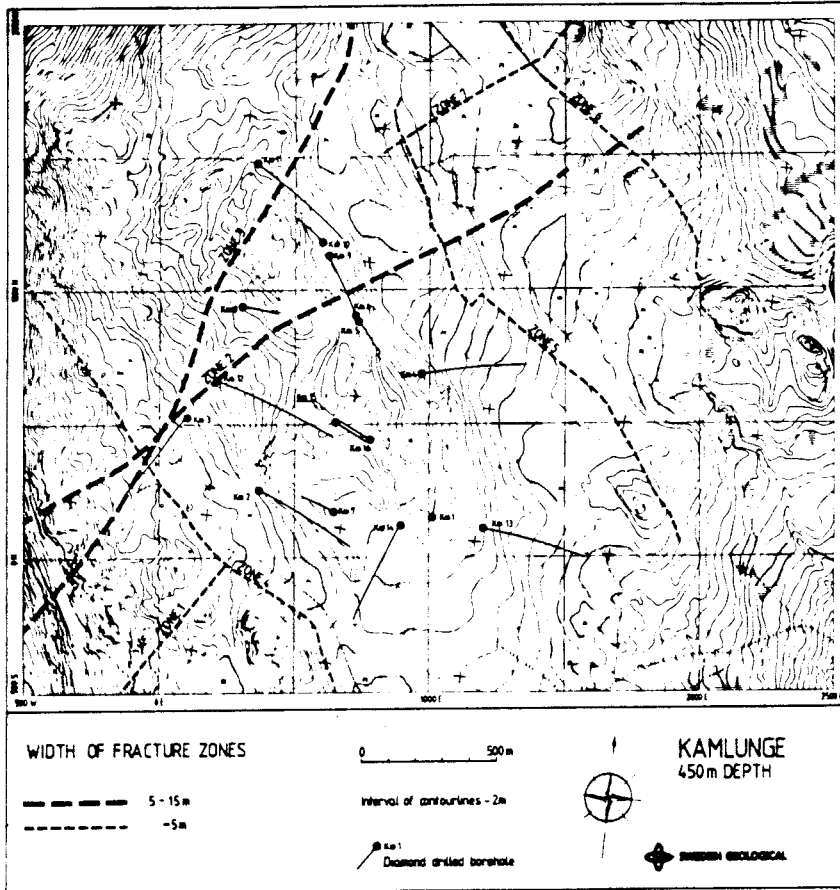


Figure 2-3: Tectonic map showing the identified fracture zones at KAMLUNGE (from 157).

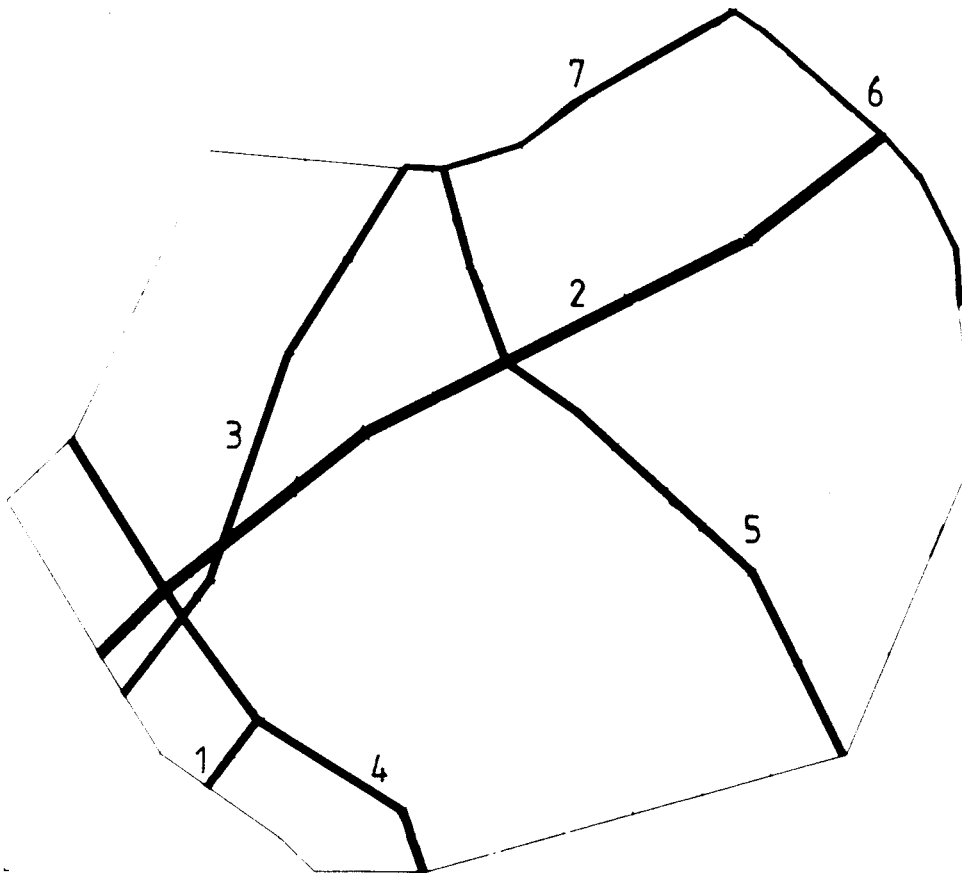


Figure 2-4: Simplified fracture zone pattern at KAMLUNGE.

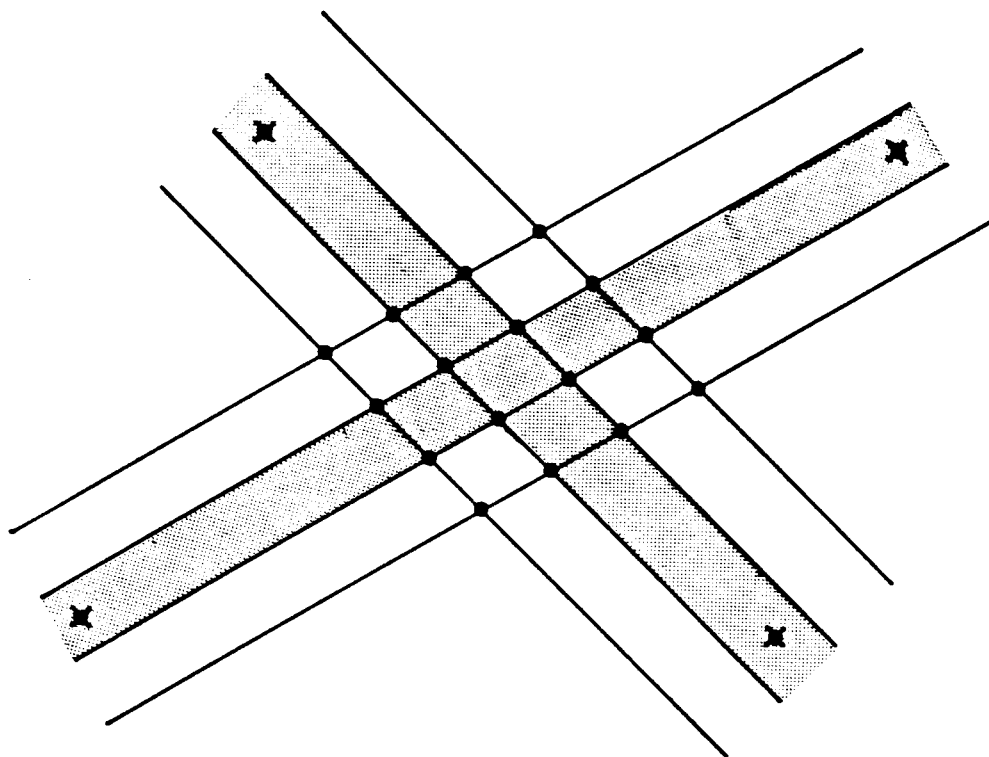


Figure 2-5: Illustration of the operation of the PREFG program. The digitized points (x-marked) and fracture zone widths are used to compute the coordinates of fracture wall intersections (dot-marked). The fracture zones are shaded. Optionally an extra element layer can be included as seen in the figure.

2.3.3 Mesh generation

For mesh generation the FEMGEN code /4/ developed at Lund's computer central in Sweden has been used. This is an interactive program that allows the geometry to be defined by points, lines, surfaces and bodies. The actual discretization is governed by a division parameter in the line command.

The FEMGEN program includes interactive plotting routines and graphic input facilities. Figure 2-6 shows a plot of the top surface of the mesh used to describe the local area at Kamlunge in the KBS-3 study.

The discretization of ground water flow domain is often very irregular due to nature's irregularity. The required amount of input to describe the domain is therefore significant. Part of the input is generated automatically as described in the previous section whereas part of the data has to be typed to the computer manually.

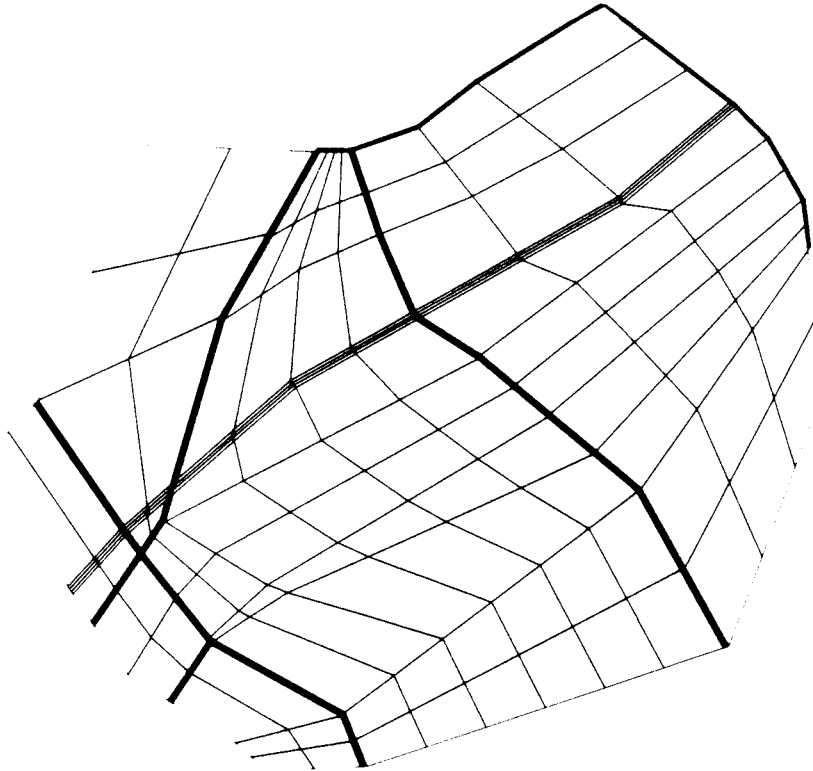


Figure 2-6: The top surface of the mesh used to model the local area at KAMLUNGE in KBS-3.

2.3.4 Post processing the mesh

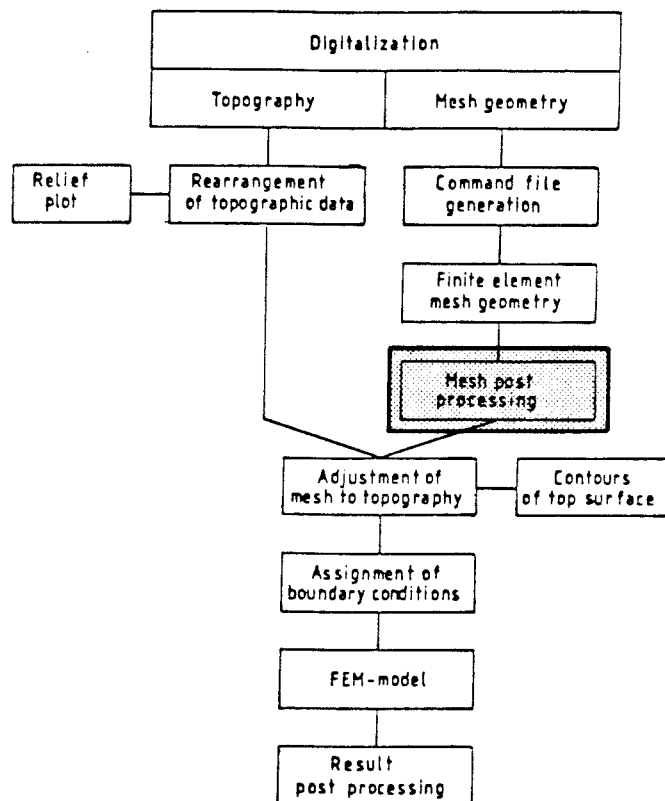
The mesh as created by FEMGEN is stored on a data base format that can be read only by some user accessible routines in the FEMGEN system. A special program POSTFG was devised to convert the data base to a sequential file that can be easily read by any computer code.

Apart from converting the file format the POSTFG code performs the following tasks:

- Checks for duplicate numbering of nodes. Duplicate node numbering, i.e. the same node has two or several different numbers when referred to in different elements, might occur because input sequences that were not foreseen when FEMGEN was written have been proven practical to use when describing irregular geometries.
- Checks for element orientation, i.e. the node numbering sequence. This is done by checking the sign of the determinant of NDIM edge vectors setting up the element (NDIM is the dimensionality of the element, i.e. either 2 or 3).
- Checks for excessive element distortions by checking the sign of the Jakobian matrix determinant at all Gaussian quadrature abscissae for both volume and surface integration.

The mesh after a POSTFG run is topologically correct and should also not be too geometrically distorted. However, the numbering of the nodes and elements might, or rather is most probably not, optimal with respect to the effort in solving the equation system in the finite element model. The mesh furthermore still has a planar top surface that must be adjusted to the topography or to the ground water situation. These two later steps are described below in sections 2.4 and 2.5.

2.4 OPTIMIZATION OF THE EQUATION SYSTEM



In the Finite Element Method the differential equation is integrated to give an algebraic equation system. In the formulation of the ground water flow problem used in GWHRT the unknowns of the equation system are the ground water pressures at the nodal points. Recalling what was mentioned earlier that a mesh in the KBS-3 study contained typically 10 000 nodes one realizes that the effort needed to solve the equation system can be substantial. The numbering order of equations and unknown's is therefore crucial to minimize computational costs. A program called OPT was designed to optimize the mesh numbering. As GWHRT has options for including both a banded matrix solver and frontal solver both the band width and the front width are minimized in OPT. In fact the method used for minimizing the front width requires that the band width is first optimized.

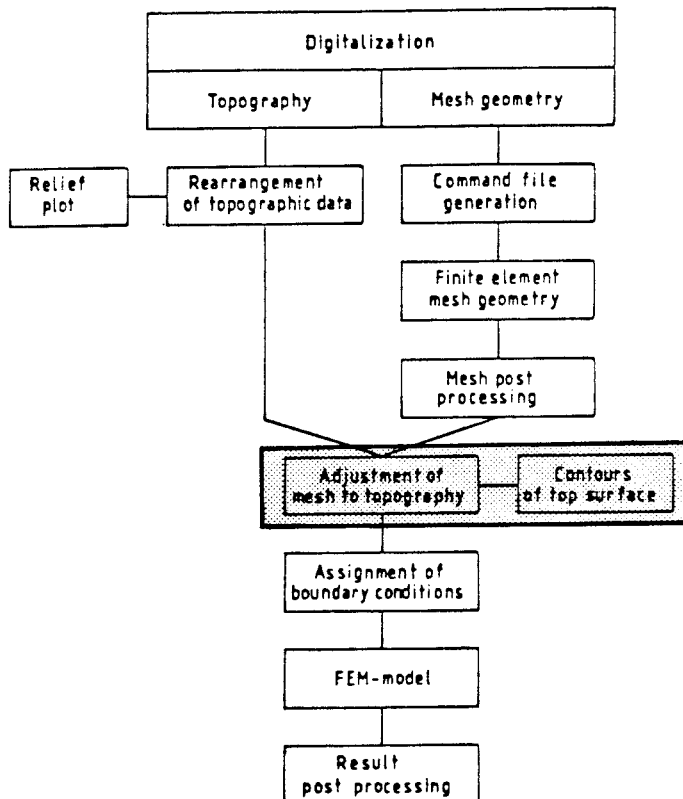
The band width of the equation system is minimized using the GPS- (Gibbs, Poole and Stockmeyer) method /6/. This method has been deemed to be the most efficient in several comparisons /7, 8/.

The GPS-method is a graph-theoretical method that runs through the following principal steps:

1. Find the endpoints of a pseudo diameter.
2. Minimize the level width of the graphs rooted at the endpoints of the pseudo diameter.
3. Renumber the nodes level by level, i.e. topologically perpendicular to the pseudo diameter.

The front width is minimized using a method proposed by Razzaque /9/. The method utilizes the fact that the elements, in order to obtain optimal front width, should be numbered in the same direction as the nodes are numbered to yield minimal band width. This means that the results from the band width optimization are directly utilized to renumber the elements.

2.5 ADJUSTMENT OF THE MESH TOP SURFACE TO THE TOPOGRAPHY



When the mesh has been generated by FEMGEN and processed by the POSTFG and OPT programs it is topologically correct and has near

to optimal numberings of the nodal points and the elements. However, it remains to adjust the top surface to the topography of either the ground surface or the ground water table. This is done using the program AMT.

AMT uses a bi-cubic spline interpolation as implemented in the IMSL-routine IBCIEU /3/ to calculate the elevation of the surface nodes from the topography description generated by the SSF-program (see section 2.1).

In order to avoid creation of excessively distorted elements by applying the AMT algorithm the nodes down to a given level are also adjusted vertically in proportion to vertical movement of the top surface nodes.

The topography of the mesh top surface can be contoured to permit a comparison with the original map. The contouring is done using the actual shape functions of the elements. This means that the contours describe without smoothing the topography actually used for the modelling. The same contouring algorithm is used also for result post processing and therefore described in that context in chapter 5. An example is shown in figure 2-7.

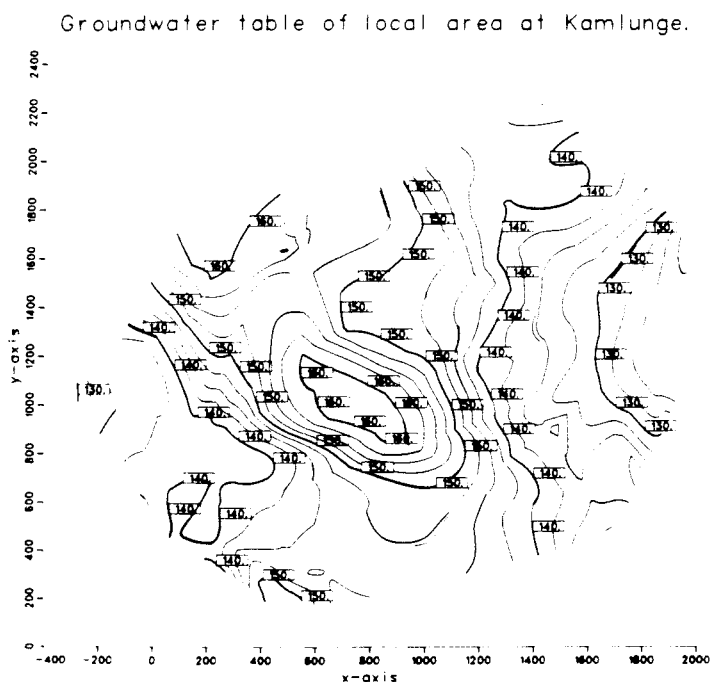
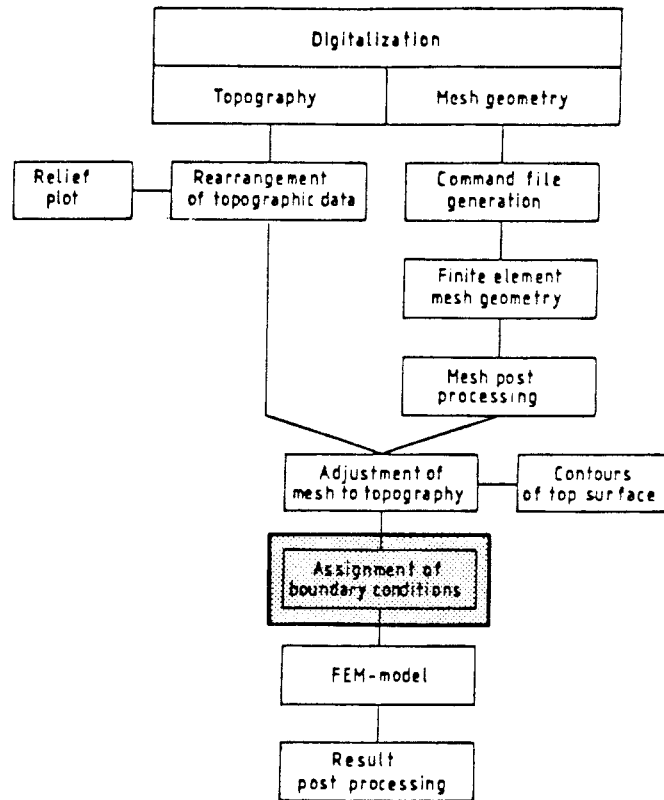


Figure 2-7: Contour map of the top surface of the mesh for the local area at KAMLUNGE. The values correspond to the head applied as top surface boundary condition.

3

ASSIGNMENT OF BOUNDARY CONDITIONS AND MATERIAL PROPERTIES

The natural boundary condition for the finite element model is a non-flow boundary:

$$(\bar{\nabla}p + \rho\bar{g}) \cdot \hat{n} = 0 \quad (3-1)$$

This boundary condition will automatically be used for all boundaries where no other condition is specified.

Other boundary conditions that are possible are a fixed head (pressure) or a fixed flux condition:

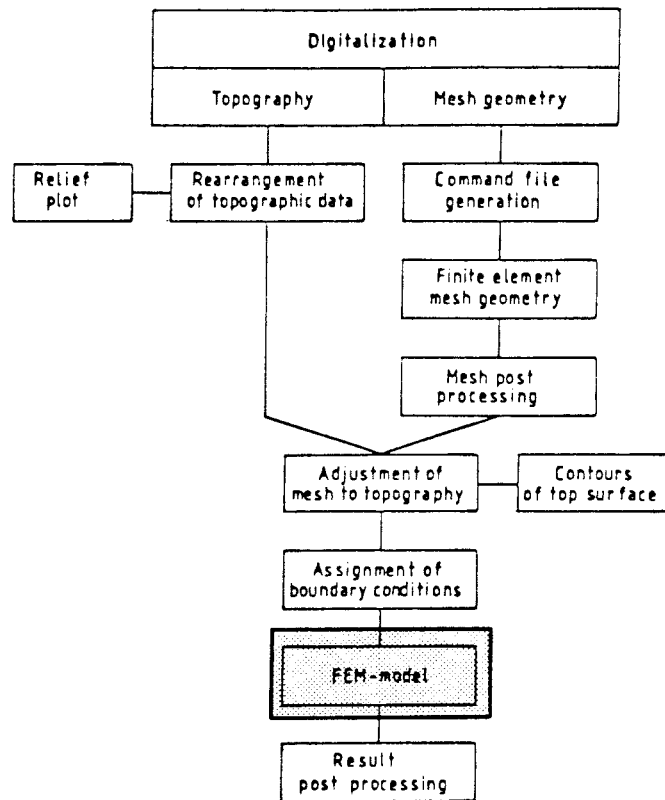
$$p = \text{const.} \quad (3-2)$$

or

$$\rho \frac{\bar{k}}{\eta} (\bar{\nabla}p + \rho\bar{g}) = \text{const.} \quad (3-3)$$

The assignment of these boundary conditions requires the identification of the nodal points located at the boundaries. A family of subroutines have been devised for this purpose. At present these routines are dependent on the naming of surfaces, bodies etc used for FEMGEN in the mesh generation (see section 2.3.3).

The subroutines mentioned above are incorporated in a couple of interactive programs that are also used for assigning material properties, i.e. hydraulic conductivities or intrinsic permeabilities, to the various parts of the mesh. Material properties can be assigned to either the elements or to the nodal points. The system in principle allows for full anisotropy with arbitrary main axes of anisotropy. At present, however, not all combinations of assignment techniques and anisotropy are implemented.

THE FEM-MODEL

The interface between the pre- and postprocessing programs in HYPAC and the actual ground water flow model is a number of files. These files are written by easily replacable subroutines which means that in principle any Finite Element code could be interfaced with HYPAC. However, HYPAC was developed primarily to facilitate the use of GWHRT developed by Roger Thunvik /1/.

GWHRT can handle a wide variety of modelling situations covering:

- Transient and steady state flow
- Saturated/unsaturated flow
- Coupled heat- and ground water flow in porous and fractured media.

The equations are given below for these situations.

Transient and steady state flow:

$$\epsilon\rho(c^f + c^r) \frac{\partial p}{\partial t} - \bar{\nabla} \cdot \frac{\rho \bar{k}}{\eta} (\bar{\nabla} p - \rho \bar{g}) + Q = 0 \quad (4-1)$$

The compressibilities in Eq. 4-1 are defined as:

$$c^r = \frac{1}{\epsilon} \frac{\partial \epsilon}{\partial p} \quad (4-2)$$

$$c^f = \frac{1}{\rho} \frac{\partial \rho}{\partial p} \quad (4-3)$$

The equation for saturated/unsaturated flow can be written:

$$\epsilon \rho (S (c^f + c^r) + \frac{dS}{dp}) \frac{\partial p}{\partial t} - \bar{v} \cdot \frac{\bar{k}}{\eta} (\bar{v}_p - \rho \bar{g}) + Q = 0 \quad (4-4)$$

In the case of coupled heat- and ground water flow a term including the time derivative of the fluid temperature is added to equations 4-1 and 4-4. Only the complete saturated/unsaturated equation is repeated here since the very easily saturated equation is derived by putting $S=1$. The following equations are solved:

$$\epsilon \rho (S(c^f + c^r) + \frac{dS}{dp}) \frac{\partial p}{\partial t} - \epsilon S \rho \beta \frac{\partial T^f}{\partial t} - \bar{v} \cdot \frac{\bar{k}}{\eta} (\bar{v}_p - \rho \bar{g}) = 0 \quad (4-5)$$

$$\rho = \rho(p, T^f) \quad (4-6)$$

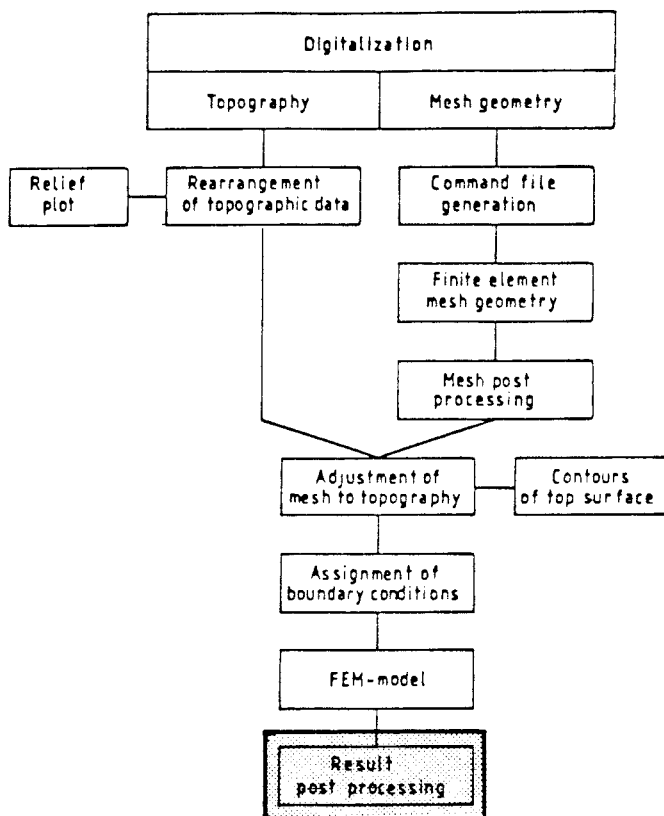
$$\eta = \eta(T^f) \quad (4-7)$$

$$\epsilon \rho C_p^f \frac{\partial T^f}{\partial t} - \bar{v} \cdot \bar{\lambda} \bar{\nabla} T^f + \rho C_p^{f-r} \frac{\partial T^f}{\partial t} + w = 0 \quad (4-8)$$

In the heterogeneous case there is a heat balance for the solid phase (rock) that corresponds to Eq. 4-8:

$$(1-\epsilon) \rho C_p^r \frac{\partial T^r}{\partial t} - \rho C_p^r \epsilon c^r \frac{\partial p}{\partial t} - \bar{v} \cdot \bar{\lambda}^r \bar{\nabla} T^r - w = 0 \quad (4-9)$$

The equations above are solved using the Galerkin formulation of the Finite Element Methods (for details see /1/).

RESULT POST PROCESSING

5.1 GENERAL

The FEM-model gives as a result the ground water pressure and, optionally, the temperature of the ground water and the rock at the nodal points. In studies concerning disposal of radioactive waste one normally wants flowrates and particle travel paths as input to some radionuclide transport model. This requires careful post processing of the FEM-model results. HYPAC contains the following post processing programs:

- CLG/CPL for contouring of hydraulic heads on element faces.
- TRG/TPL for particle tracking. The program can also be used for contouring of heads and flow rates at arbitrary cross sections or for recording heads and fluxes along a line (e.g. a bore-hole or a trajectory).

The post processing also includes programs for checking the relevance of the obtained results. These programs are:

- REC for checking that all calculated heads are within an interval defined by the extremes of the heads assigned as boundary conditions.

- MBC for checking the mass conservatism of the solution. This program can also be used to calculate flowrates across arbitrary element faces.

The programs CLG/CPL, TRG/TPL and MBC are described in more detail below.

5.2 DESCRIPTION OF CLG/CPL

The CLG-program (Contour Line Generator) was written to calculate contours of hydraulic heads (or any other function defined at the nodal points of a finite element mesh) and to write the coordinates of successive points on the contours to a file. The CPL-program (Contour Plotting) then can read this file and present it graphically. This presentation is focused on CLG since CPL is trivial in the sense that it just transforms numerical data to graphical data.

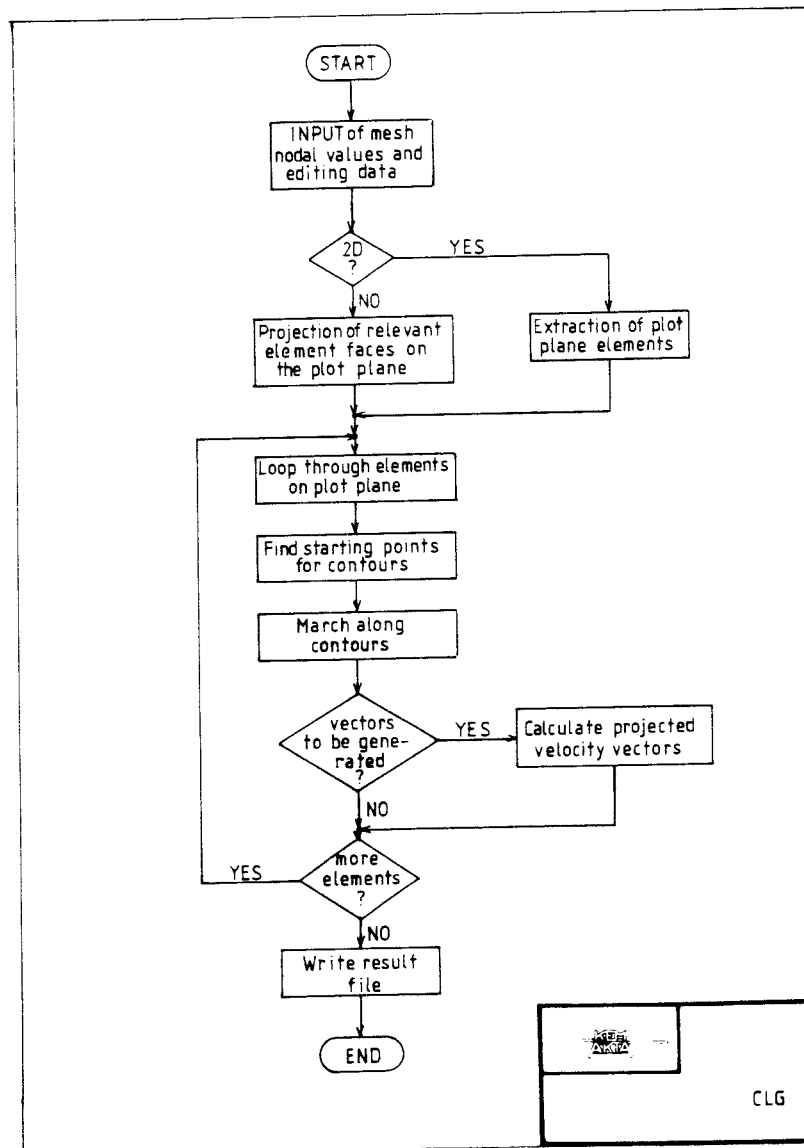


Figure 5-1: Simplified flow-sheet of the CLG-program for contouring on isoparametric surfaces.

A simplified flow sheet of CLG is shown in figure 5-1. The main steps of the program are:

- Definition of a plot plane consisting of a mesh of element faces to be contoured.
- Contouring the mesh element by element.
- Calculation of projected velocity vectors on the element faces.

In the case of 2D calculations a plot plane is defined either by the whole mesh or by a part of it. In presenting results from 3D calculation a plot plane is some cross-section running along element faces. Presently such cross-sections are defined by the aid of FEMGEN-surfaces (see section 2.3.3).

A plot plane can either be straight (horizontal or vertical) or bent at a number of places. In the latter case the plot plane is either projected on one of the principal planes of the coordinate system (x-y-, x-z- or y-z-plane), or straightened out by calculating one or both of the plot plane coordinates as distances in the principal planes.

Having defined the plot plane one is left with a two-dimensional mesh which is either a true 2D-mesh or a cross-section of a 3D-mesh. This mesh is run through element by element for contouring and, optionally, calculation of projected velocity vectors.

The actual contouring is done according to the following steps:

- a) find starting points of contours at the sides of the plot plane element,
- b) search for eventual starting points in the interior of the element,
- c) march along the contours.

The steps a) and b) are done solving a non-linear equation system:

$$h = n \cdot Eq. \quad (5-1a)$$

$$(r,s) \in M, M \text{ is a line in the } r,s\text{-plane} \quad (5-1b)$$

The subroutine ZSCNT in the IMSL library is used /3/.

In step a) the line is an element side. In step b) the line is a line from an element corner to an extreme (maximum or minimum) in the element interior which has been found by conventional differentiation of the contoured entity.

The marching along the contour involves is done by solving the equation:

$$\frac{\partial h}{\partial r} dr + \frac{\partial h}{\partial s} ds = 0 \quad (5-2)$$

Euleran stepping is used but, at the endpoint at each step a corrective perpendicular step is taken in order to more closely follow the theoretical contour. The conventional Euleran step is defined by:

$$r_n = r_o + \frac{dL}{V} \frac{\partial h}{\partial s} \quad (5-3a)$$

$$s_n = s_o + \frac{dL}{V} \frac{\partial h}{\partial r} \quad (5-3b)$$

and the corrective move is taken by applying the following:

$$r_c = r_n - \frac{1}{\sqrt{2}} \frac{\partial h}{\partial r} \cdot \Delta h \quad (5-4a)$$

$$s_c = s_n - \frac{1}{\sqrt{2}} \frac{\partial h}{\partial s} \cdot \Delta h \quad (5-4b)$$

$$\Delta h = (h_n - n \cdot Eq) \quad (5-4c)$$

The algorithm is described in /10/.

The calculation of projected velocity vectors is optional. It includes evaluation of velocity vectors at a regular grid on the plot plane element followed, in the 3D case, by the projection of the vector on the element face. The third component of the projected vector is parallel to the normal of the element face.

Figure 5-2 shows a sample plot with projected vectors. Note that some of the contours have sharp bends, especially in the upper part of the plot plane. These bends, that are signs of lacking mass conservatism, would not be visible in a conventional contouring algorithm that involves smoothing of the data. Especially in 3D ground water modelling, where available computer storage normally restricts the fineness of the mesh, discontinuities like those shown in the figure are to be expected. It can thus be concluded that the CLG algorithm is an unusually "honest" way of representing the model output.

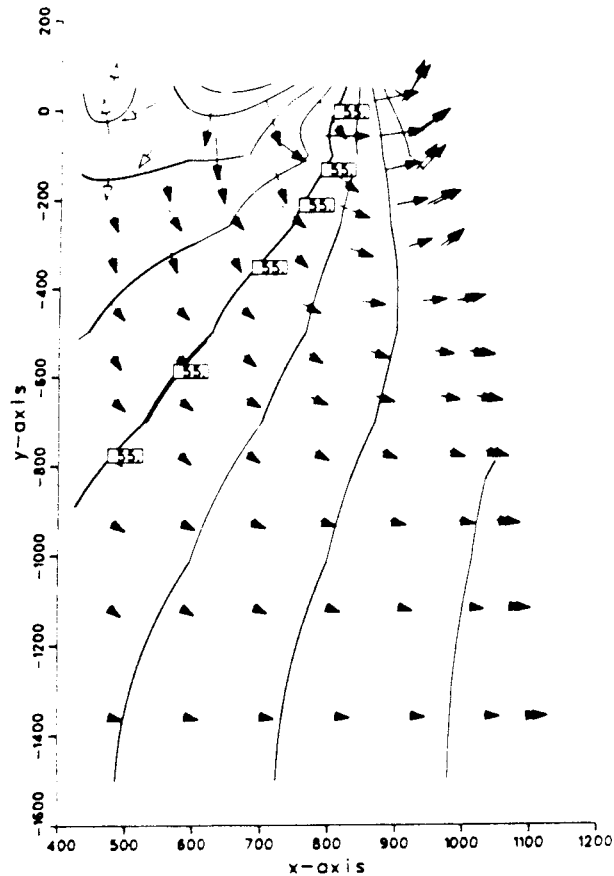


Figure 5-2: Sample contour plot with projected velocity vectors. Filled arrowheads indicate that the third component points towards the reader whereas white arrowheads indicate a third component into the paper. Note that discontinuous gradients appear.

5.3 DESCRIPTION OF TRG/TPL

The TRG program (TRajjectory Generator) was originally devised to track particle pathlines (trajectories) in a field of hydraulic heads defined at the nodal points of a finite element mesh, and to write the coordinates of successive prints along the trajectory to a file. Along with coordinates also the flowrates and the hydraulic heads are written to the file. The TPL-program (Trajectory Plot) then reads the file created by TRG and generates a series of plots. The presentation below is focused on TRG as TPL is merely a data conversion program.

Figure 5-3 shows a simplified flowsheet of the TRG program. The program consists of two main parts dealing with

- locating a point given in global coordinates in terms of local coordinates
- stepping along a trajectory

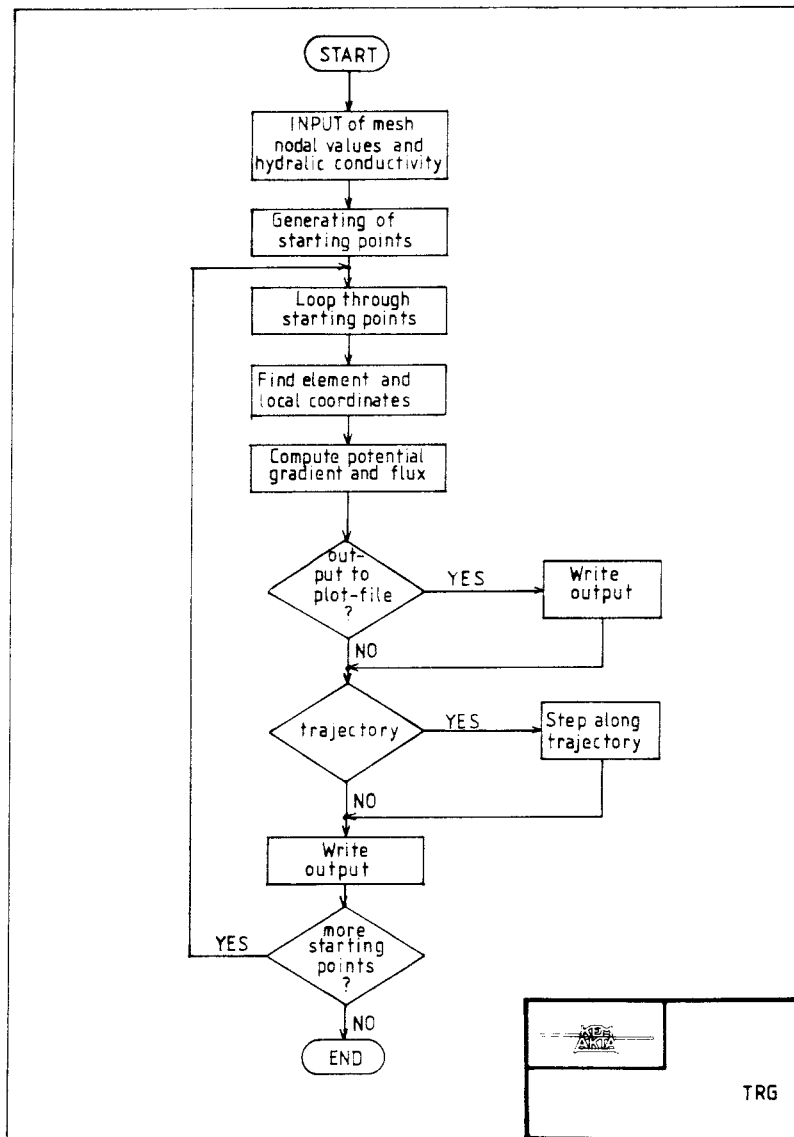


Figure 5-3: Simplified flow-sheet of the TRG-program for particle tracking.

To define the terms of local coordinates an arbitrary point given in global coordinates involves the following steps

- a) locate possible elements
- b) loop through the possible elements to find the local coordinates that corresponds to the given point.

Before going through step a) a matrix containing the extreme values of the nodal coordinates (x, y and z) for all elements is created. In step a) then this matrix is looped through and all elements that have nodal coordinates bracketing the coordinates of the given point are deemed possible. It should be pointed out that this algorithm is not fool-proof when the elements have non-linear faces. This point is illustrated for a 2D case in figure 5-4. The algorithm would tell that the point is in element 1 but it is really in element 2.

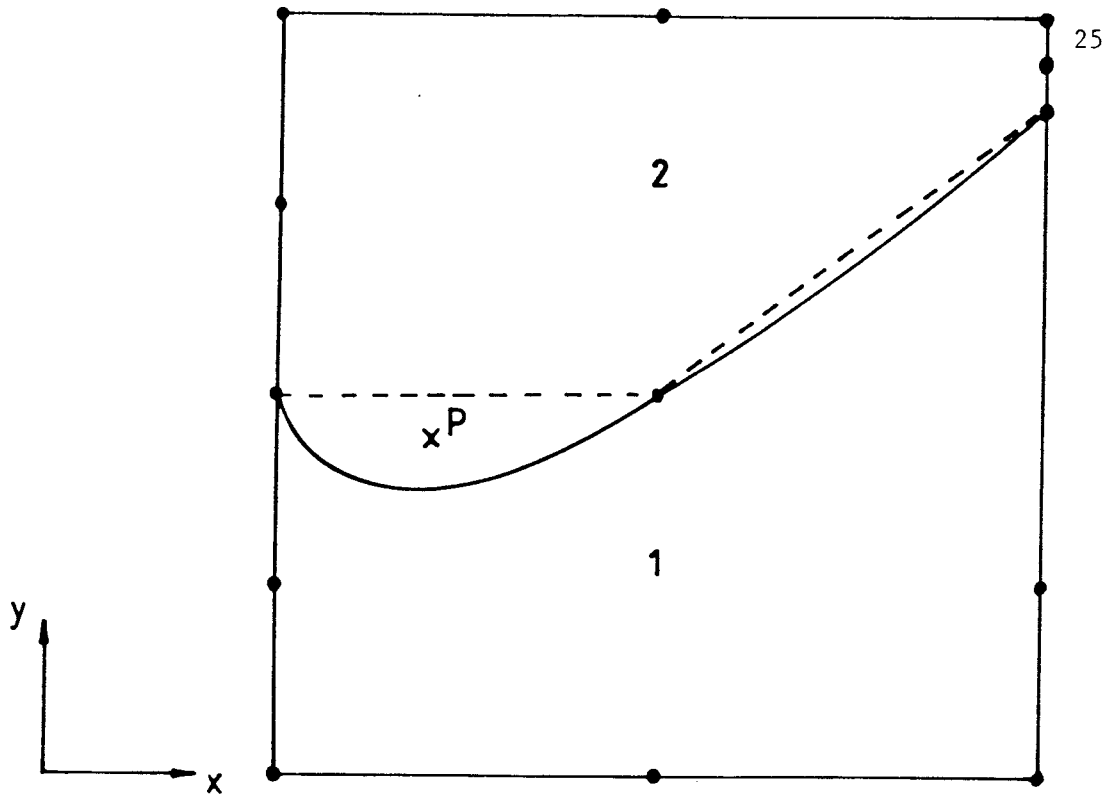


Figure 5-4: Illustration of the difficulty to define quadratic interpolation when used the "home element" of a point. The dashed line illustrates the element extension defined by the nodal coordinates while the full line shows the mathematically true element boundary.

Once the possible elements have been located they are looped through in search for the point P_1 , defined in local coordinates, which is closest to the given point P . This is done using a quasi Newton method to minimize the distance, i.e.:

$$\min \sqrt{(x_1-x)^2 + (y_1-y)^2 + (z_1-z)^2} \quad (5-5)$$

The IMSL-routine ZXMIN /3/ is used. The criteria used to accept a solution, P_1 , from ZXMIN as the local coordinates of point P are that all local coordinates should be within the allowed bounds for the used element type and that the distance between P_1 and P is smaller than an acceptance limit.

The quasi Newton method used requires, for its convergence, that a good enough initial guess is given. For this reason a grid of starting points are defined for each possible element. These starting points are then sorted according to increasing distance to the given point. In this way an efficient search routine package has been designed.

The actual particle tracking starts when the starting point of the trajectory has been located according to the above described procedure. The velocity vector is evaluated and a step is taken in the direction of the vector. The length of the step is given in the program input.

After each step the algorithm to locate the local coordinates is run through for the step endpoint. However, before looping through all possible elements, an attempt is first made to find the new point in the same element as the starting point of the step is made.

The TRG program in principle, because of the point location algorithm, permits the evaluation of any entity defined at the nodal points of a finite element mesh at arbitrary points within the mesh. Advantage has been taken of this fact through the incorporation of options for recording potentials and/or flow rates at given points without initializing the particle tracking. The points can be arranged as single points, along a line or spread over a rectangle.

5.4 DESCRIPTION OF MBC

The MBC-program (Mass Balance Controle) was written to check the mass conservatism of a finite element solution. This is done by, for each face (3D) or side (2D) of each element in the mesh, calculating the following integral:

$$F = \int_S \bar{q} \cdot \hat{n} d\sigma \quad (5-6)$$

The integral 5-6 is solved using Gaussian quadrature.

For each element a massbalance, F_{sum} , and a deviation index, DI, are calculated from the following equations:

$$F_{\text{sum}} = \sum_{i=1}^N F_i \quad (5-7)$$

$$DI = \frac{F_{\text{sum}}}{\sum_{i=1}^N |F_i|} \quad (5-8)$$

The HYPAC program package for pre- and postprocessing finite element meshes and results is a comprehensive package. Although the description of the codes in this report have been focused on the application to a three dimensional steady-state analysis, such as those performed in KBS-3, later developments have made it possible to apply the programmes to transient problems including saturated/unsaturated flow. Due to high degree of modularisation further developments to new application areas can comparatively easily be done. The high degree of automation included in HYPAC proved to be of great utility in connection with the KBS-3 study.

All programmes described in this report are written in FORTRAN (some in FORTRAN 77). Most of them are implemented on an AMDAHL 470 but FEMGEN and POSTFG are run on a CDC CYBER 730/170.

NOTATION

Roman letters

| | | |
|-----------|---|----------------------------------|
| c | compressibility | (Pa^{-1}) |
| C_p | specific heat | $(\text{J}/\text{kg}, \text{K})$ |
| DI | deviation index for mass balance | |
| Eq | equidistance for contouring | |
| F | Flow accross a surface | (m^3/s) |
| g | gravitational acceleration | (m/s^2) |
| h | contoured entity | |
| \bar{k} | permeability tensor | (m^2) |
| L | length | (m) |
| n | integer number | |
| \hat{n} | normal vector of unit length | |
| N | number of element faces/sides | |
| p | ground water pressure | (Pa) |
| P | a point | |
| \bar{q} | specific discharge vector | (m/s) |
| r, s, t | local coordinates in an isoparametric element | |
| S | saturation | |
| T | temperature | (K) |
| w | heat transfer function | (W/m^3) |
| x, y, z | global coordinates | |

Greek letters and special symbols

| | | |
|----------------|---|------------|
| β | thermal expansion coefficient = | (K^{-1}) |
| | $\frac{1}{\rho} \frac{\partial \rho}{\partial T}^f$ | |
| Δ | difference operator | |
| ϵ | porosity | |
| λ | heat conductivity tensor | $(W/m, K)$ |
| η | dynamic viscosity | $(Pa \ s)$ |
| ρ | density | (Kg/m^3) |
| $d\sigma$ | surface differential | (m^2) |
| $\bar{\nabla}$ | gradient operator | |
| ∇ | magnitude of gradient in local coordinates = | |

$$\sqrt{\left(\frac{\partial h}{\partial r^2}\right)^2 + \left(\frac{\partial h}{\partial s^2}\right)^2}$$

Suffixes

| | |
|-----|--|
| 0 | origin of a step along a contour |
| 1 | attempted solution |
| n | end-point of conventional Euleran step |
| c | endpoint of corrective move |
| sum | sum |

Superfixes

| | |
|---|-------|
| f | fluid |
| r | rock |

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