Analysis of contamination propagation in groundwater systems using the finite element method

GGU-CONTAM-FE

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1   Preface

The GGU-CONTAM-FE program allows analysis of contaminant transport on the basis of horizontal, vertical and axis-symmetrical groundwater systems modelled with GGU-SS FLOW2D using FEM.

For evaluation and presentation of analysis results, the GGU-PLGW programs are available. They enable impressive, time-dependent animation or presentation of concentrations along sections through the system.

Data input is in accordance with WINDOWS conventions and can therefore be learned almost entirely without the use of a manual. Graphic output supports the True-Type fonts supplied with WINDOWS, so that excellent layout is guaranteed. Colour output and Bitmap graphics are supported.

It is not the task of this manual to give an introduction to contaminant propagation analysis using finite-element methods. For details, please refer to the literature. The program system has been used in a large number of projects and has been thoroughly tested (using analytical solutions and in comparison with other finite-element programs). No faults have been found. Nevertheless, liability for completeness and correctness of the program system and the manual, and for any damage resulting from incompleteness or incorrectness, cannot be admitted.

The following general remarks are important:

- The basis for groundwater flow analyses is given by data sets from analyses with the GGU-SS FLOW2D program.
- Triangular elements are used.
- Concentrations are calculated at every node. Concentration distribution is linear within the triangular elements.

2   Installation

For installation and subsequent registration of GGU Software, please refer to the information in the "Installation notes for GGU Software", which are provided with the program.

3   Program concept

In order to analyse contaminant propagation, the flow field is required (velocities with magnitude and direction). These data are recovered by the GGU-CONTAM-FE program from a data set (e.g. PLGW.DA1) generated during a previous analysis using the GGU-SS FLOW2D program. It is therefore necessary to load this file first after opening the program. The flow field

contained in this file remains constant for subsequent calculations.

Besides the flow field, the GGU-CONTAM-FE program requires information on the initial contaminant distribution conditions at time t = 0. These so-called initial concentrations can be arbitrarily defined. If you do not define any values, the program will assume an initial concentration of "0" at all nodes.

Apart from the flow field, the PLGW.DA1 file also includes the effective pore space n_{eff}, upon which steady-state modelling is based. This "steady-state" soil property (n_{eff}) cannot be altered in GGU-CONTAM-FE. If editing of these values were allowed, the flow field would no longer "fit" the calculated potentials and contaminant transport analysis would produce nonsensical results. However, you must enter additional soil properties that are required for contaminant transport analysis.

Further to additional soil properties, you can also define time-dependent boundary conditions. You must enter boundary values (concentration or concentration source) as a function of time, by means of polygon courses. These polygon courses can then be assigned system nodes, either individually or in groups. Soil properties (contaminant transport analysis) and polygon courses, as well as their allocations to system nodes, can be saved in a separate file (so-called boundary values), in order to make them available again for later analyses.

Unsteady-state data **cannot** be evaluated using the GGU-CONTAM-FE program. Three evaluation programs are designed for this purpose (see below).

Generally, when analysing unsteady-state groundwater systems, a flood of result values is generated. The analysis results are saved in a file (generally PLKO.DA1) by the program. The program is able to evaluate these results.

The GGU-CONTAM-FE program is opened by conventional WINDOWS operations. The program is equipped with a large number of "error" queries. Even highly nonsensical input will usually be detected by the program and an error message will be displayed on the screen. Independently of this you should, for security reasons, intermittently save extensive input to disk or hard drive, if only to save renewed input in the case of a power cut.
After opening the program you will see a start-up screen with a coordinate system.

The start-up screen shows two **menus** at the top edge.

- **File**
- **?**

After clicking on the "File" menu, a groundwater flow system can be loaded by means of the "Load GW data" menu item. After selecting the system, the menu bar will show seven menus:

- **File**

- **Editor**
- **Boundary values**
- **Calculation**
- **View**
- **Page**
- **?**

After clicking on one of these menus, the so-called menu items roll down, allowing you to access all program functions.

The program works on the "What you see is what you get" principle. This means that the screen presentation represents, on the whole, what you will see on your printer. In the last consequence, this would mean that the screen presentation would have to be refreshed after every alteration you make. For reasons of efficiency, and as this can take several seconds for complex screen contents, the GGU-CONTAM-FE screen is not refreshed after every alteration. If you would like to refresh the screen contents, press either the [F2] key, or the [Esc] key. The [Esc] key will additionally set the screen presentation to A4.

4   Short description

Since I know from personal experience that reading user-manuals is quite a chore, there will now follow a short description of the main program functions. After studying this section you will quickly be in a position to analyse contaminant transport based on steady-state groundwater flow. You can learn about the details of the program in the later chapters.

- Open the GGU-CONTAM-FE program and select the menu item "File / Load stationary GW data", in order to load the desired data set of a flow system analysed using GGU-SS FLOW2D.

- Using the "Editor" menu you can define your "soil characteristics". A description of the individual constants can be found in the "Info" function field.

- Using the "Editor / Boundary condition polygons" menu item, you specify the temporal changes in concentration as polygon courses. This is initially independent of location. By clicking on the menu item you will see a dialogue box within which, by clicking the "New" field and then "Edit polygon course", you can specify the number of polygon points, i.e. the number of temporal changes in your concentrations.

- The initial system concentration is specified via the menu item "Boundary values / Initial concentrations". It is possible to set the concentration individually for specific nodes, or for several nodes in section.

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- Contaminant transport analysis is started by selecting "Calculation / Start".

Specify the desired end time at which the calculations are to cease. Subsequently, checks are carried out by the program (Peclet and Courant criteria). The Courant criterion determines the maximum permissible time step for your system. Before actual analysis begins, you will see this value in a dialogue box. You can edit this value. The Peclet criterion principally concerns the element size; if this criterion is not satisfied, you will generally have no other choice but to analyse with a finer mesh (GGU-SS FLOW2D).

- With the assistance of the evaluation program GGU-PLGW you can evaluate and display the analysis results. To do this, load the file generated by GGU-CONTAM-FE into one of the programs (generally PLKO.DA1).

5   Contaminant propagation theory

5.1   Overview

The primary aim of contaminant transport analysis is the prognosis of future conditions on the basis of given initial data and, on occasion, pre-specified counter-measures.

Using a numerical analysis approach, even complicated systems can be investigated and assessed. Precise modelling of the natural conditions is difficult, due to the multitude of initial parameters required and the inhomogeneity of aquifers. Before any contaminant analysis, you should therefore ensure that your initial data justify this.

5.2   Mechanisms relevant to contaminant transport

Five important mechanisms describe contaminant transport in groundwater and must be entered as initial data for propagation simulation:

- **Convection**
  is the migration of contaminants in the direction, and with the apparent flow velocity, of groundwater flow. This transport mechanism is normally dominant in a flowing system, but is superimposed upon and influenced by others. Mathematically, this mechanism enters the differential equation in the shape of the apparent flow velocities u_x and u_y.

- **Dispersion**
  includes the local deviation from the mean flow velocity. One differentiates between dispersion caused by the grain skeleton, which describes, amongst other factors, deviations in the flow course around the grain skeleton, and macro-dispersion, which is the dominant mechanism in wide-area contaminant propagation, e.g. in sand lenses and layering. This mechanism is described by the mathematical values of longitudinal (in flow direction) dispersivity α_L (m) and transverse (perpendicular to flow direction) dispersivity α_T (m).

- **Diffusion**

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This type of transport is determined by the concentration gradient. It is normally only effective in systems with extremely low velocity. In water at 10 °C, the diffusion coefficient D_m is 10^{-9} m/s².

- **Adsorption**
  expresses the inhibition of contaminant migration due to adsorption onto the grain skeleton and is described by the sorption constant sorp (-). The sorption constant is the product of grain density and the adsorption coefficient. Contaminant propagation is retarded by adsorption.

- **Decay**
  As a result of physical, chemical and biological reworking, contaminants are eliminated from the groundwater. This process is described by the decay constant λ (l/s).

A mass balance equation and a space- and time-dependent, analysable differential equation results from these values:

Mass balance:

> Increase in dissolved contaminant mass =
> net input by convection
> + net input by diffusion and dispersion
> + input from contaminant sources
> - extraction from wells
> - loss through decay reactions
> - adsorption onto the grain matrix

5.3 Contaminant transport analysis with FEM models

As you know, FEM allows almost unlimited subdivision of the system into triangular elements. Concentrations are assumed to be linearly distributed across each element. Where the contaminant front is discrete, such an approach is no longer capable of precisely modelling contaminant distribution. The contaminant fronts then become "smeared". This effect is known as numerical dispersion. It occurs predominantly when the proportion of convection is large compared to other mechanisms (dispersion and diffusion). The Peclet criterion serves to check whether a system displays a tendency towards numerical dispersion.

5.3.1 The Peclet criterion

Numerical dispersion, which bears no relation to physical dispersion, causes "smearing" of a discrete contaminant front in the course of propagation. This can be avoided by selecting a denser triangular mesh.

The "Peclet criterion" is required to calculate the necessary mesh density. This criterion is checked by the program after calculations have begun. If it is exceeded, mesh refinement will be required. You will then need to reprocess

the system using GGU-SS FLOW2D. Under certain conditions, however, a very dense mesh is required. If necessary, you can obtain a solution using the RANDOM-WALK method, as this procedure does not recognise the numerical dispersion effect.

5.3.2 The Courant criterion

The precision of all numerical procedures is influenced by the time step Dt. Precise results can be achieved with small time steps, but analysis time increases correspondingly. The optimum time step size can be derived from the "Courant criterion".

After starting analysis, the program examines the Courant criterion and suggests the determined time step.

6 Description of individual menus

In this chapter, the individual menus and corresponding menu items will be explained.

6.1 File menu

6.1.1 "Load stationary GW data" menu item

Using the menu item "Load stationary GW data", you load the data set of a previously calculated groundwater flow model, in order to carry out a contaminant transport analysis. For reasons of clarity, only files with the ".DA1" suffix are displayed in the file selector box. Therefore, you should only save files with this suffix in GGU-SS FLOW2D. Under the menu item "System / Calculate" in GGU-SS FLOW2D, you will find an appropriate function box.

6.1.2 "System info" menu item

By selecting this menu item you will be shown information on the type of system, and the number of elements and nodes.

6.1.3 "Load boundary values" menu item

If, during a previous analysis, you have specified boundary values and saved them in a file with the ".KON" suffix, you can load them with this menu item.

6.1.4 "Save boundary values" menu item

If you would like to make your defined boundary values available at a later time, save the data set using this menu item. For reasons of clarity, use the ".KON" suffix. If you do not specify a suffix, ".KON" will be used automatically.

6.1.5 "Output preferences" menu item

You can edit printer preferences or select another printer in accordance with WINDOWS conventions.

6.1.6 "Start output" menu item

This menu item is completely analogous to the corresponding GGU-SS FLOW2D menu item and offers the same functions. For details, please refer to the GGU-SS FLOW2D user-manual.
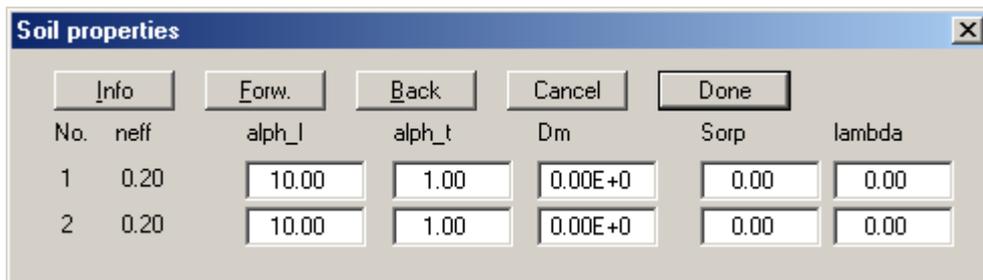

6.1.7 "Quit" menu item

After a confirmation prompt, you can quit the program.

6.2 Editor menu

6.2.1 "Soil properties" menu item

After selecting this menu item, the following dialogue box appears:

In this box, you specify important soil properties for contaminant transport. In the example above, two soils have been defined for the system (groundwater modelling with GGU-SS FLOW2D).

"Info"

This menu item provides some information on the meaning of the properties and their units. Take care to always use the same dimensions, as these are not pre-specified by the program. The result will be given in terms of the dimensions with which you entered your data.

"alph_l" and "alph_t"

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Enter the value of the longitudinal dispersivity alph_l. This is a function of grain size and varies between a few centimetres (laboratory tests in sand) and over 100 metres (jointed rocks).

The transversal dispersivity alph_t is generally a magnitude smaller than the longitudinal. In field tests, ratios around 0.01 were determined. Values of up to 0.3 are given in the literature.

"Dm"

Enter the value of the diffusion coefficient Dm. This value only influences contaminant distribution at very low flow velocities. For water at 10°C, this value is 10^{-9} m/s².

"Sorp"

Enter the value of the sorption constant sorp. The sorption constant is dimensionless and is the product of grain density and the adsorption coefficient.

"lambda"

Enter the value of the decay constant lambda.

6.2.2 "Boundary condition polygons" menu item

With the help of this menu item you specify the temporally variable (unsteady) boundary conditions of the system, i.e., you enter the concentrations for the specified time intervals. This is initially location-independent. By clicking the **"New"** function box in the dialogue box, the following dialogue box, appears:
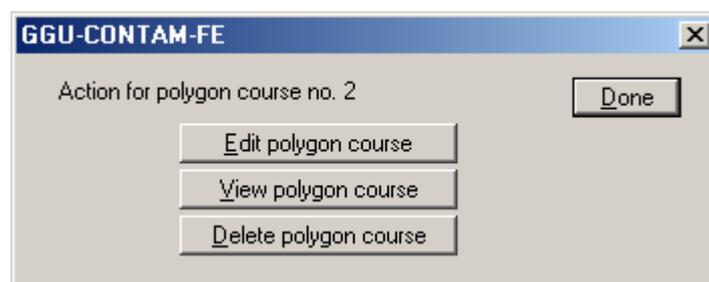

"Edit polygon course"

The following dialogue box appears:
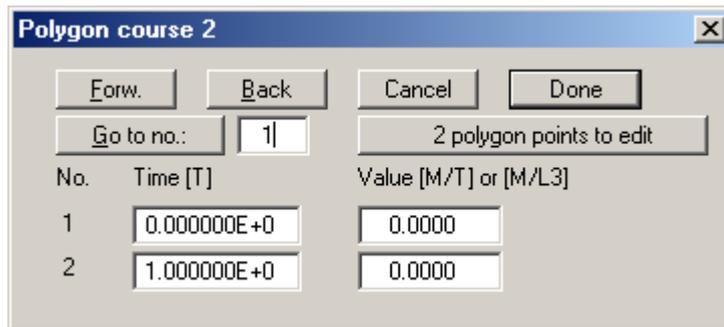
Using the function box "2 polygon points to edit", you specify the number of variations within your boundary conditions. It is possible to define up to 100 polygon points. Once you have done this, a further dialogue box appears, in which you can define the temporal course with the corresponding boundary condition value.

This dialogue box shows an example:
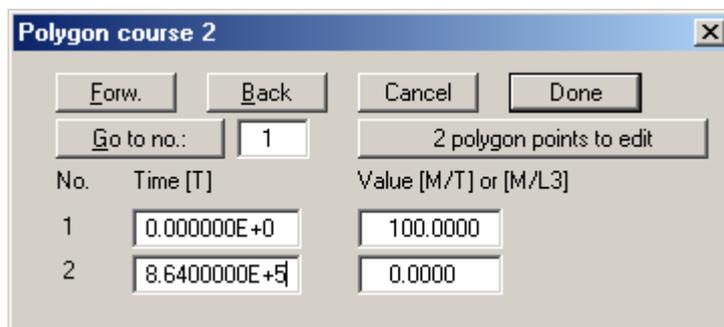
The GGU-CONTAM-FE program works with true dimensions. Times must therefore be given in the time dimension used for permeability. For example, if permeability was entered in m/s, times must be entered in seconds. The polygon value must be entered in mass/time (e.g. mg/s) for concentration sources, or mass/length³ for concentrations. The length dimension must also coincide with the permeability length dimensions.

After clicking on the "Done" box, you will return to the initial dialogue box. If you then click on "Done" and "New" once again, you can specify a further polygon course.
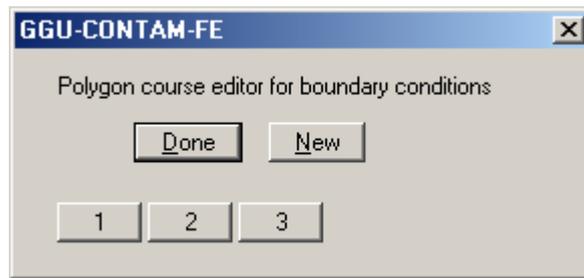
"View polygon course"

With this command it is possible to have your polygon course presented in a diagram for viewing.

"Delete polygon course"

By clicking this box you can delete the current polygon course after a confirmation prompt.

For example, after defining three boundary condition polygons, the following

dialogue box appears:

By clicking on a number box you can view, edit or delete the corresponding boundary condition polygon.

6.3   Boundary values menu

In this menu you will find commands that allow you to assign initial concentrations or boundary condition polygons to specific nodes or groups of nodes in a section.

If you do not define initial concentrations for any nodes, an initial concentration of "0" will be assumed.

6.3.1   "Individual initial concentrations" menu item

This menu item at first generates a dialogue box in which you specify the number of decimal points for concentrations, and the font size.

If you confirm with "OK", the mesh appears on the screen. Click on the appropriate point with the left mouse button. The current system coordinates of the mouse pointer are shown in the status bar at the bottom of the screen. Enter the desired initial concentration in the following dialogue box.
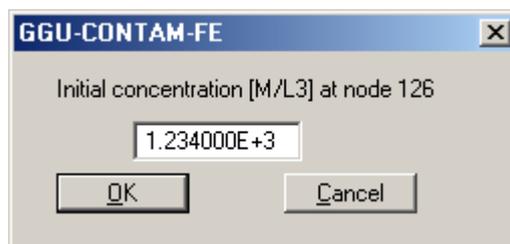
The length dimension must also coincide with the permeability length dimension. If you click on a node with the right mouse button, any current initial concentration will be deleted and the node set to "0".

6.3.2   "In section" menu item

Click on four points in a counter-clockwise direction to define the desired

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section. You will then be asked for the initial concentration you would like to apply to all nodes in the section. Alternatively, you have the possibility of deleting all initial concentrations, i.e. setting them all to "0".

6.3.3 "From file" menu item

You can load concentrations from a previous analysis as initial concentrations. The first time step after the given time will be read.

6.3.4 "Individual boundary conditions" menu item

After asking for the font size, this menu item allows allocation of a boundary condition polygon to a specific node.

Once you have clicked on a node with the left mouse button, the following dialogue box appears:
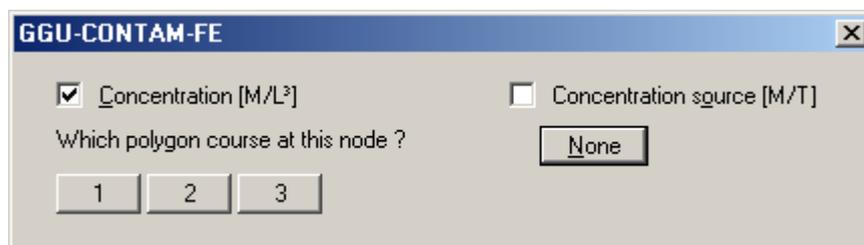
In the example above you can select from three pre-defined boundary condition polygons. Further, you can specify whether the boundary condition is to be a concentration source or a concentration.

If you click on a node with the right mouse button, any current polygon allocation will be deleted.

6.3.5 "Boundary conditions in section" menu item

By selecting this menu item you can assign a boundary condition polygon to a system section. By means of an info dialogue box, you can define a section with the left mouse button, which you can then assign a previously specified polygon course after being asked if you would like to set or delete a condition.

6.4 Calculation menu

6.4.1 "Display mesh" menu item

With this menu item you can choose to display the groundwater flow model without any labelling.

6.4.2 "Start" menu item

After clicking on this menu item several dialogue boxes appear with information and queries about the Peclet and Courant criteria (*cf.* Section 5), which you may accept or edit.

The following dialogue box then appears:
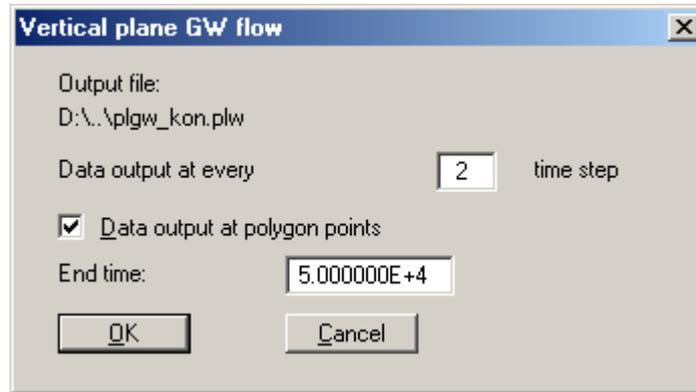
The example shown is for a vertical-plane system. You will see the name of the output file (here plgw_kon.plw). When calculations are complete, this file contains all result data, which can then be evaluated with the GGU-PLGW program.

A flood of results is usually provided for contaminant transport analyses, with correspondingly large result files. Often, a small time step must be selected in order to achieve sufficiently precise results. You can therefore specify the times at which data output should follow.

Independently of the selected time step, the program automatically proceeds to all times associated with boundary polygons. If you activate the "**Data output at polygon points**" switch, the results for these times will be issued additionally, independent of the previous entry. It is conceivable, for example, to enter a very large value for "**Data output every nth time step**" and to temporally subdivide a boundary condition polygon such that output only occurs at the times specified by you.

Finally, you enter the end time at which analysis is to cease.

After selecting the "OK" button, the program carries out checks. First, the Peclet criterion is checked.
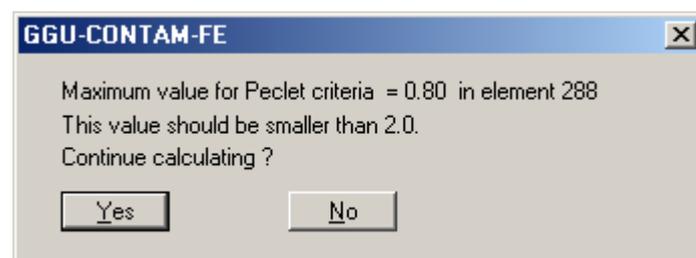
The Courant criterion is then checked and the optimum time step shown
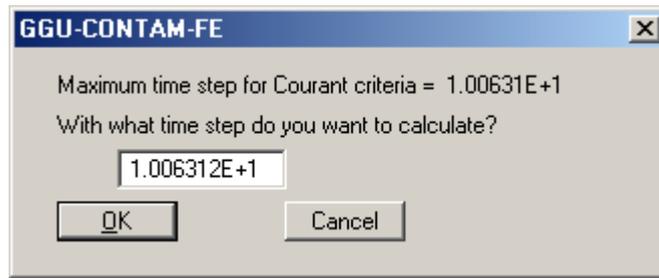
After selecting the "OK" button the calculation proper will begin. A dialogue box with a "Cancel" button will inform you of analysis progress. If you select this button, analysis will not cease immediately, but instead you can edit specific program data and then carry on calculating.
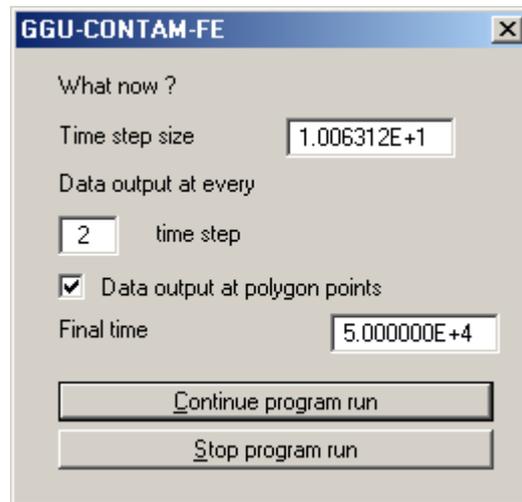
The data set is generated during analysis. If, after starting analysis, you call up the GGU-PLGW program, you can check and evaluate the results while the analysis is still running. The "animation" function is particularly impressive here; it can be executed parallel to the running analysis.

6.5   View menu

The menu items in this menu are completely analogous to those in the GGU-SS FLOW2D program and use the same functions. You are therefore referred to the GGU-SS FLOW2D manual for descriptions of these functions.

6.6   Page menu

6.6.1   "Recalculate coordinates" menu item

If you have altered the image coordinates during use of the program, e.g. by creating sections, you can use this menu item to recalculate the coordinates for

a complete overview. This function can also be accessed with the [F9] function key.

6.6.2 "Coordinates graphically" menu item

You can alter the image coordinates graphically with the mouse. An info box explains the possibilities. You can obtain new section coordinates by holding the [CTRL]-key, [Shift]-key and the left mouse button, and marking an area.

6.6.3 "Coordinates by hand" menu item

You can alter the image coordinates by direct numerical input in the dialogue box.

6.6.4 "Font sizes" menu item

You can edit font sizes for labelling diagrams.

6.6.5 "Page format" menu item

When opening the program an A3 page is set as default. If you prefer different page formats you can define them in this dialogue box.

6.7   ? menu

6.7.1 "Copyright" menu item

You will see a copyright message and information on the program version number.

6.7.2 "Maxima" menu item

In a box you will see the default program maxima for the nodes and elements of the FE mesh.