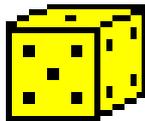Modelling of contamination propagation in
groundwater systems using the random walk method

GGU-CONTAM RW

VERSION 3

Contents:

1   Preface

The GGU-CONTAM RW program allows you to model contaminant transport in horizontal, vertical or axis-symmetrical groundwater systems according to the random walk method. A dataset containing the basic steady-state data must have been previously generated using the GGU-SS FLOW2D program (formerly GW2).

The GGU-PLGW program is available for evaluation and presentation of analysis results. It enables 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. DXF files can also be imported by means of the integrated Mini-CAD module (see Mini-CAD manual).

It is not the aim of this manual to introduce contaminant propagation modelling methods. For details, please refer to more advanced 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 FEM applications). No faults have been found. Nevertheless, liability for completeness and correctness of the program and the manual, and for any damage resulting from incompleteness or incorrectness, cannot be accepted.

The following general remarks are important:

- The data forming the basis for groundwater flow are datasets generated during analysis with the GGU-SS FLOW2D program.

- Modelling is based on a rectangular array.

2   Installation and language selection

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

GGU-CONTAM RW (International version) is a bilingual program. You may choose to work in German or English. The international version is delivered with English as the default menu and graphics language.

If you would like to work with GGU-CONTAM RW (international version) in German, start the program and click on "File / New" in the initial menu bar. An expanded menu bar appears. Click on the "?" menu and there on the menu item "International version" and deactivate the switch for translating the menus and graphics (see also Section 13.4).

3   Program concept

There are a number of numerical methods available for contaminant transport modelling:

- finite-element method,

- finite-difference method,

- particle tracking method (and in particular the random walk method).

The finite-element method is the most powerful of these, not only due to the flexible mesh design. This gives rise to the most basic question: why use particle tracking at all (here the random walk method in particular)? The reason is numerical dispersion, which is not related to physical dispersion. Numerical dispersion occurs where the finite-element method and the finite-difference method are used. The reason for numerical dispersion is the generally linear approximation approach within an element. The contaminant front "smears", an effect similar to physical dispersion and which is therefore known as numerical dispersion.

Particle tracking methods do not suffer from this problem. The particle tracking method is the simplest method. This method is incorporated in the GGU-SS FLOW2D steady-state application in the shape of flow lines. The particle tracking method cannot consider either dispersion or diffusion effects. Only convection can be taken into consideration (movement of particles at groundwater speed). If, in addition, you wish to consider dispersion, diffusion, etc., the random walk method is generally used. The analytical solution of simple flow processes with contaminant transport leads to functions that correspond to a Gaussian distribution. This function can be modelled with a random generator, if sufficient attempts are made. This mathematical effect is utilised by the random walk method (random path method). The method first assumes propagation at groundwater flow velocity. This underlying velocity is superimposed upon by a dispersion (diffusion) velocity, the direction of which is determined by a random generator integrated in the application. In order to model the Gaussian curve mentioned above adequately, it is no longer sufficient to simply consider one contaminant particle. Rather, a multitude of particles is started and their courses recorded. This also has the result that the accuracy of the analyses increases with the number of started particles. Because of the integrated random generator, you will not get exactly the same result for any two different runs.

For contaminant propagation modelling a flow field is required (velocity magnitude and direction). GGU-CONTAM RW gets this data from a dataset (e.g. GW2-Vertical.DA1) generated in a previous analysis using the GGU-SS FLOW2D application. It is therefore necessary to load this file first after opening the program. The flow field contained in this file remains constant for subsequent analyses.

Also typical for the random walk method is that analyses must be based on a rectangular mesh. This requirement does not conform to the flexibility of the triangular elements used in FEM (GGU-SS FLOW2D), which forms the basis of the flow data for modelling. GGU-CONTAM RW solves this problem by placing a rectangular array over the whole FEM mesh. It is possible to edit the rectangular array subdivisions within broad limits. In this system of triangular mesh and rectangular array, you now define the initial concentrations and any contaminant sources. The definition of time-dependent changes, such as performed in GGU-CONTAM FE (formerly KON) by means of polygon courses, is not possible using the random walk method. Once the initial concentrations have been defined, you must still specify how many particles to start. The program then assigns each particle a corresponding partial concentration. Now, during analysis, the paths of the contaminant particles are traced and the number of particles found in each rectangular cell counted for each time step. The summation of all partial concentrations within a cell then provides the total concentration that applies for that cell. These explanations demonstrate,

- that numerical dispersion cannot occur with this procedure,

- that the accuracy of the analysis is increased with the number of started particles.

- that the accuracy of contaminant distribution is not increased with the number of rectangular cells.

Because of the discrepancies between the triangular mesh and the rectangular array, the results from the rectangular cells are always converted to fit the triangular mesh. GGU-CONTAM RW therefore generates two datasets:

- **Dataset 1 *_RAS.PLW**
  contains all results from the rectangular array. So, during subsequent evaluation using the GGU-PLGW application, a "rectangular triangle mesh" is displayed.

- **Dataset 2 *_FE.PLW**
  contains the values from the rectangular array recalculated to fit the triangular mesh.

Besides the flow field, the GGU-CONTAM RW 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 GW2-Vertical.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 edited in the GGU-CONTAM RW application. 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 the additional soil properties required for contaminant transport analysis.

Besides additional soil properties the GGU-CONTAM RW application also allows you to assign temporally constant concentration sources to individual nodes.

Soil properties (contaminant transport analysis), as well as the allocation of initial concentrations and concentration sources to system nodes (so-called boundary values), can be saved in a separate file in order to make them available again for later analyses.

Transient data **cannot** be evaluated using the GGU-CONTAM RW program. The GGU-PLGW program is available for this purpose (see below).

Generally, when analysing transient groundwater systems, a flood of result values is generated. The analysis results are saved in a file (generally *_RAS.PLW and *_FE.PLW) by GGU-CONTAM RW. The GGU-PLGW program is able to evaluate these results. For example, it is possible to evaluate the results using isolines, animations, in sections and represented as hydrographs.

The GGU-CONTAM RW program is opened by conventional WINDOWS operations. The program is equipped with a large amount of "error" queries. Even highly nonsensical input will usually be detected by the program and an error message 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.

4   Starting the program

After starting the program you will see two menus at the top of the initial window**:**

- 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

- Concentrations

- Modelling

- Graphic preferences

- Page size + margin

- ?

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

The program works on the principle of "What you see is what you get". This means that the screen presentation represents, overall, 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 RW 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 additionally sets the screen representation back to your current zoom, which has the default value 1.0.

5   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. More detailed information about the program can be obtained from the subsequent chapters as you require it.

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

- By clicking on the "File" menu once again the entry "Load boundary values" can be seen as one of the menu items listed. In this way, you can load and process previously saved concentrations.

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

- The initial concentrations and any concentration sources are defined using the "Concentrations" menu. This is possible individually or in a section. You will be shown an info box with instructions. After being queried on whether you want to assign or delete concentrations, a dialogue box opens in which you must define whether it is an initial concentration or a concentration source. In the first instance, the concentration only applies at time t = 0 and is subsequently displaced, whilst a concentration source displays a constant concentration. If you do not define an initial concentration or a concentration source for any nodes, an initial concentration of "0" will be assumed.

- In "Modelling / Preferences", you can apply preferences for the precision and extent of analysis by specifying the size of the array subdivisions. The smaller the array is defined, the more precise, but also time-intensive, the analysis. Moreover, by activating the analysis with the "Element velocities" option and deactivating the "Exact velocities" box you achieve fast, but less precise, analysis, whilst analysis using "Node velocities" and the additional option of "Exact velocities" will give very precise analysis results.

- Commence contaminant transport modelling for your groundwater system with "Modelling / Run". In the dialogue box that then opens you can enter the name of the output file for the rectangular array, as well as generating a dataset for the FEM mesh if you want an additional analysis based on the triangular array. The program then calculates a number of basic parameters. You then define an end time, the size of the time steps and the number of particles. A large number of particles also means more precise results but longer computing time.

- With the aid of the GGU-PLGW evaluation program, you can evaluate and display the modelling results. To facilitate this, load the file generated by GGU-CONTAM RW (*_RAS.PLW) or the file (*_FE.PLW) with the results recalculated on the basis of the FEM mesh.

6 Contaminant propagation theory

See GGU-CONTAM FE manual (formerly KON).

7 File menu

7.1 "Load GW data" menu item

Using the "Load GW data" menu item, you can load the dataset of a previously calculated groundwater flow model, in order to perform contaminant transport modelling. For reasons of clarity, only files with the ".DA1" extension are displayed in the file selector box. You should therefore only save files in GGU-SS FLOW2D using this extension. An appropriate function box can be found in the "Analysis / Run" menu item in GGU-SS FLOW2D.

7.2 "System info" menu item

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

7.3 "Load boundary values" menu item

If, during a previous analysis, you specified boundary values and saved them in a file with the "*.RDW" extension, you can load them again using this menu item.

7.4 "Save (boundary values)" menu item

If you would like to make your defined boundary values available later, you can save the dataset using this menu item. For reasons of clarity, you should use the "*.RDW" extension. If you do not specify an extension, "*.RDW" will be used automatically.

7.5 "Printer preferences" menu item

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

7.6 "Print and export" menu item

This menu item corresponds to the menu item "File / Print and export" in GGU-SS FLOW2D and utilises the same functions. You are therefore referred to the GGU-SS FLOW2D manual for descriptions of these.

7.7 "Quit" menu item

After a confirmation prompt, you can quit the program.

7.8 "1, 2, 3 und 4" menu item

The last four processed files are shown and can be opened here, as an alternative to the "Load GW data" menu item.

8 Editor menu

8.1 "Soil properties" menu item

In this box, you specify important soil properties for contaminant transport. In the example below, one soil has been defined for the system (groundwater modelling with GGU-SS FLOW2D).

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

- **"Info"**

    This item provides information on the meaning of the parameters and the units used by them. Please ensure that you always use the same length and time units as those you applied to the permeability in the steady-state analysis in GGU-SS FLOW2D. You can define the mass dimension at will; you must, however, use the same dimension for all parameters. This also applies to the subsequent definition of initial concentrations and concentration sources.

- **"alph_l"** and **"alph_t"**

    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 transverse 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.

8.2 "Presentation format" menu item

Using the functions provided in this menu item you can alter the system and mesh display according to your wishes. This permits some control, but does not allow manipulation of the analysis.

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

Activate the information you want to have displayed.

9 Concentrations menu

In this menu you will find commands that allow you to assign concentrations to specific points or sections of the system.

9.1 "Define individually" menu item

This menu item first generates the following dialogue box, in which you specify the font size and the number of decimal places.
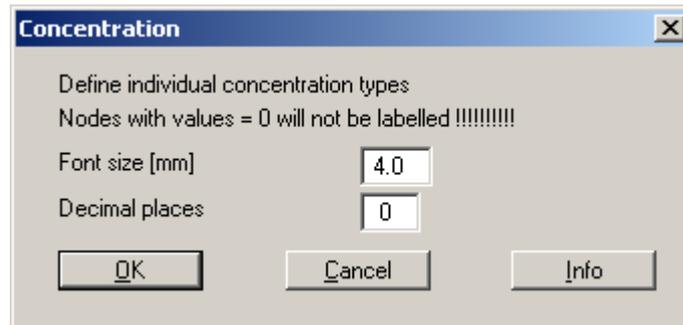
After confirmation you can click on nodes to which you want to assign an initial concentration (> 0.0) or a concentration source, using the left mouse button. A concentration source is constant over time.
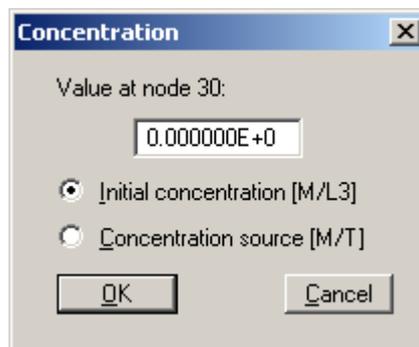
Please ensure that you always use the same length and time units as those you applied to the permeability in the GGU-SS FLOW2D steady-state analysis. You can define the mass dimension at will; you must, however, use the same dimension for all parameters. This also applies to soil properties (see above).

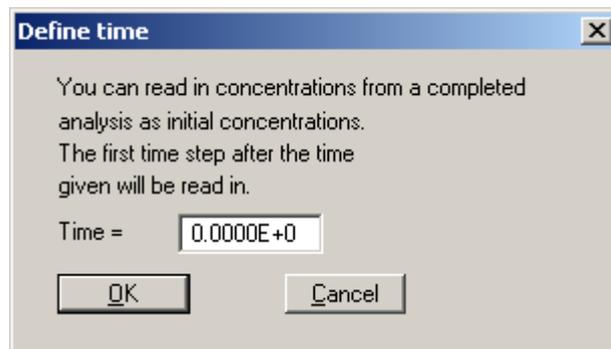These allocations can be deleted with the right mouse button.

9.2 "In section" menu item

In a similar manner to the previous menu item, you can assign initial concentrations or concentration sources to sections of the system. This is done by clicking four points in an anti-clockwise direction with the left mouse button. The concentration, which you enter into the following dialogue box, then applies to all nodes within the specified section.

In an intermediate dialogue box you are also given the opportunity to delete the concentrations.

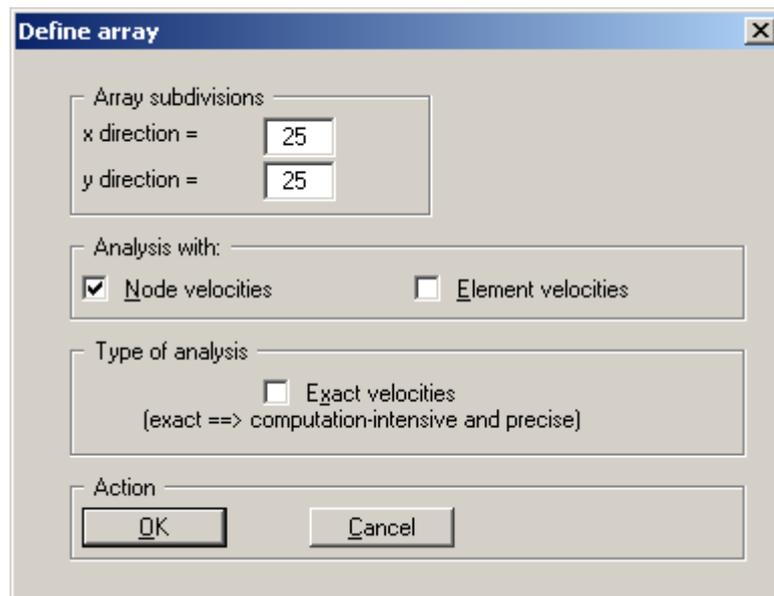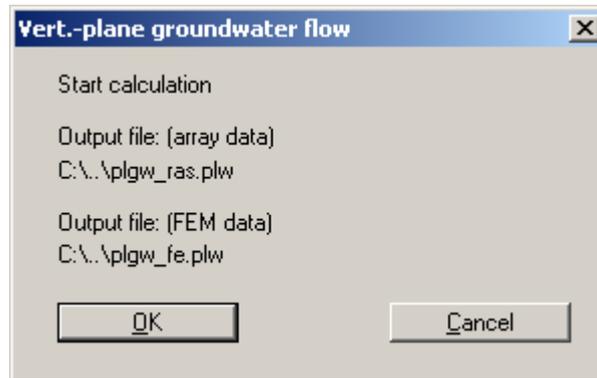The following dialogue box appears, in which you may define a time.

First, define the array subdivisions to stipulate the size of the cells. Read Section 3, "Program concept" to find out what influence the rectangular array has on the analysis.

You can also decide whether the analysis should be based on the node velocities or on the element velocities. Again, the principal difference here is in the analysis precision. The element velocity is constant for each element, whilst the node velocity is calculated from the mean of the velocities in the neighbouring elements. This increases the precision of the analysis, but also the time and effort required.

10 Modelling menu

10.1 "Preferences" menu item

The following dialogue box appears:

By activating the "Exact velocities" option the precision of the analysis is increased yet again. The program then determines the velocity of each contaminant particle at its current location. Otherwise, mean velocities are utilised for the corresponding cell.
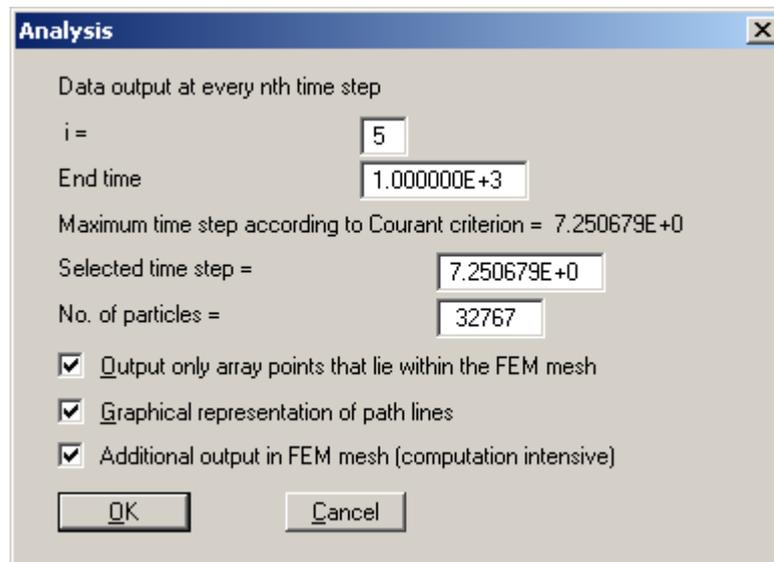
10.2   "Run" menu item

After clicking this menu item a dialogue box opens showing the names of the output files.

```
Vert.-plane groundwater flow                        [x]

    Start calculation

    Output file: (array data)
    C:\..\plgw_ras.plw

    Output file: (FEM data)
    C:\..\plgw_fe.plw

        [   OK   ]              [  Cancel  ]
```

- **Dataset Gwv1_ras.plw**
  contains all results from the rectangular array. So, during subsequent evaluation using the GGU-PLGW application, a "rectangular triangle mesh" is displayed.

- **Dataset Gwv1_fe.plw**
  contains the values from the rectangular array recalculated to fit the triangular mesh (FEM mesh).

Start your analysis by clicking "OK". A number of basic parameters are first calculated. The following dialogue box is subsequently displayed:

```
Analysis                                              [x]

    Data output at every nth time step

    i =                              [  5  ]
    End time                         [ 1.000000E+3 ]

    Maximum time step according to Courant criterion = 7.250679E+0

    Selected time step =             [ 7.250679E+0 ]

    No. of particles =               [   32767   ]

    [✓] Output only array points that lie within the FEM mesh

    [✓] Graphical representation of path lines

    [✓] Additional output in FEM mesh (computation intensive)

        [   OK   ]         [  Cancel  ]
```

Generally, a flood of result values is generated during analysis. You can define an interval (i) for data output. In addition, you must also enter the end time for the analysis.

The precision of all numerical procedures is influenced by the size of the time step. More precise results can be achieved with small time steps, but analysis time increases correspondingly. The maximum allowable time step size can be derived from the "Courant criterion". You can modify this time value, but should not increase the proposed time step.

You then enter the number of particles to be started and whose paths are to be traced.

By activating the "Graphical representation of path lines" option the path lines can be traced on the computer screen during analysis (very impressive, but also increases computation time).

Finally, you have the opportunity of suppressing output of data for recalculation of the array data to the triangular mesh (FEM mesh).

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 the analysis.

The dataset is generated during modelling. If, after commencing modelling, you open the GGU-PLGW program, you can check and evaluate the current results while modelling is still in progress. The "animation" function is particularly impressive here; it can be executed parallel to the running analysis.

11   Graphics preferences menu

The menu items in this menu correspond to the menu items in GGU-SS FLOW2D and utilise the same functions. You are therefore referred to the GGU-SS FLOW2D manual for descriptions of these.

12   Page size + margins menu

12.1   "Auto resize" 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 recompute the coordinates for a complete overview. This function can also be accessed with the [F9] function key.

12.2   "Manual resize (mouse)" menu item

You can alter the image coordinates graphically with the mouse. An info box explains the available options. You can obtain new section coordinates by holding the [CTRL]-key, [Shift]-key and the left mouse button, and marking a region on the drawing.

12.3   "By hand" menu item

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

12.4 "Page size and margins" menu item

When the program is first opened the default page setup is A3. If you prefer different page formats you can define them in this dialogue box.

12.5 "Font size selection" menu item

You can edit font sizes for diagram labelling.

13 ? menu

13.1 "Copyright" menu item

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

13.2 "Maxima" menu item

A box opens with information on the default application maxima.

13.3 "Help" menu item

You will see this manual as a Windows Help file.

13.4 "Translation" menu item

In the international version of GGU-CONTAM RW, this menu item allows you to switch the menus and the graphics from German to English and vice versa. To work in German, activate the two switches "translate dialogs, menus" and "translate graphics".

Alternatively, you can work bilingually, e.g. with German dialogue boxes but with graphic output in English.

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