

DISKMOD: REPRESENTATION OF FAULT ZONES AND DISCONTINUITIES IN HYDROGEOLOGICAL MODELS FOR SAFETY ASSESSMENT OF A DEEP RADIOACTIVE WASTE REPOSITORY

DISKMODtools

Software documentation

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Project leader: **PROGEO, s. r. o. (PROGEO)**

Participant: **Technical University of Liberec (TUL)**

Project head: **Mgr. Michal Polák**

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Author's affiliations: **Technical University of Liberec**

Authors: **Jiřina Královcová, Michal Balatka**

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1 Introduction

This document contains basic information about the GEOTRANtools software. The software is one of the main results of the project, which was financially supported by the **TAČR THETA** program, **project number TK04010207**, the name "***Representation of fault zones and discontinuities in hydrogeological models for the safety assessment of a deep radioactive waste repository***", acronym of the DISKMOD project. The project was handled in the period 01/2022–11/2024. Its leader was the company PROGEO, s. r. o.. (PROGEO), another participant was the Technical University of Liberec (TUL), the application guarantor (AG) is the State Office for Nuclear Safety (SÚJB). The project was focused on researching the influence of discontinuities on the transport of radionuclides (RN) from the deep repository of spent nuclear fuel and highly active waste (DP) into the biosphere.

In the course of the project, as one of the planned main results, software was created at the University of Technology in Liberec to support simulations in the domain containing fault zones as significant discontinuities in hydrogeological models. Software focused on both the preparatory phase and the analysis of the flow and transport model. In accordance with the original intention, it involves the processing of models implemented in the simulation code Flow123D (<https://flow123d.github.io/>), (Březina et al. 2022). The software was developed under the GNU General Public License v3.0.

2 Fundamentals of the software

The DISKMODtool v1.0 software was created to provide support for simulations in the Flow123d simulator (<https://flow123d.github.io/>), (Březina et al. 2022), including a suitable user interface that will enable perform functionalities supported by the software in a uniform way.

Flow123d is developed primarily for the purpose of simulating groundwater flow and transport of solutes in a rock environment. It supports the simulation of other processes, such as heat transport and

the calculation of the stress field due to mechanical loading. Flow123d v4.0 is currently in preparation. This version was not available at the time DISKMODtools was implemented and tested. So DISKMODtools assumes and has been fully tested with Flow123d v3.0.5 and 3.9.0 data formats. The mesh, input and output data "on the mesh" are assumed to be in the MSH format, although Flow123d also supports the VTK format for the given purposes.

One of the basic features of this software is the recording of all activities carried out by the user (protocol), as well as the operations offered for working with the logging. In addition to the basic option of saving the log to a disk file, it is also possible to open/load a file with a saved protocol while simultaneously re-executing all activities recorded in the protocol. The program thus supports the automated repeatability of model data processing. In the case of partial modifications of the recorded protocol, it is thus possible to apply the same data processing to, for example, other variants of the model. In any case, the saved protocol, which contains information about what processing with which data, or what the outputs of the model data processing are, provides a quality record for subsequent documentation of the implemented model, without the user having to record everything manually.

Another key feature of the software is the efficiency of model data processing. We consider models that can be based on meshes with millions of elements. The data files then contain, in addition to the network, several data fields recorded at several times. In particular, files with the results of the transport of several dissolved substances at the same time, the results recorded at several times can reach tens of GB. Working with similar files and data fields is demanding both in terms of the amount of memory and the time required to process/perform partial activities. The implementation had to be approached in such a way that the execution, especially in terms of duration, was as efficient as possible, or so that the execution of long-lasting operations did not hinder the further processing of the data of the given model.

Functionality of logging, re-execution of log actions, parallelization of partial activities, etc. they are based on the design and implementation of our own MWT_GUI library. This library represents a general framework usable also in other applications than the DISKMODtools software is.

3 Installing and running the program

The DISKMODtools software was created in the Python programming language version 3.13. Python version 3.10 was also used for testing. During the implementation, the syntactic elements of the language introduced in version 3.8 were used. The basic effort was to use as many resources as possible that are part of the language itself. Also for this reason, the `tkinter` library is used for the graphical user interface. For some functionalities, it was necessary to use separately installed packages, which are: `numpy`, `PyYAML`, `psutil`, `gmsh`. Regarding the `numpy` package, at least version 2.0 is required.

An installation package is available at <https://omp-cxi-tul.github.io/DiskMod/>. The installation package was created for a 64-bit version of MS Windows. After installation, the DiskMod item is available among the installed programs.

If the computer on which the SW is installed uses a different operating system, or if the installation process cannot be used for any reason, a package (ZIP archive) with all the necessary source files can be downloaded from the above address. After downloading, unzip the archive into a suitable directory. It is necessary to have Python installed including all necessary components. The program can then be run from the command line, e.g. `python DISKMOD.py`. If we start from a different directory, it is necessary to enter the full path to the `DISKMOD.py` files.

The `--options` option can be part of the command line when the program is started in a form `--options:<file>` where `<file>` is the path to the configuration file. The configuration file must be in YAML format. By default, the program is started with the settings in the configuration file `options_default.yaml`, which is in the home directory of the program. In the configuration file,

among other things, user can set the formats to be used when displaying numerical values in the user interface and paths to external programs to be used for displaying the contents of the selected file (see the View menu). In the `basics` section of the configuration file there are the `theme file` option, which contains the path to the YAML file containing the colour tuning of the program, and the `log file` option with the path to the output log file.

Warning: *By installing and using this SW, the user confirms that he/she agrees unconditionally to the license terms of this SW* (i.e. the terms of the GNU General Public License v3.0).

Note: The installation package does not include data files with which it would be possible to test the software.

4 User interface

DISKMODtools is a program with a graphical user interface. The basic inputs of the program are the input and output files of the transport calculation of the Flow123d simulator, specifically version 3.0.5 or 3.9. Flow123d allows to output data in two basic formats, namely GMSH (file extension *.msh) and VTK (file extensions pvd, vtu, vtk). Basic information about the formats used is given in the Flow123d user manual (Březina et al. 2022). More detailed information can be found in the documentation of the programs GMSH (<https://gmsh.info/>), (Geuzaine C., Remacle J. F. 2022) and ParaView (<https://www.paraview.org/about/>), (Paraview). From these formats, DISKMODtools allows you to load files in the GMSH format, which was exclusively used during the project realisation.

After starting, the main window is displayed. It which consists of:

- Main menu at the top of the window.
- Toolbar for quick selection of main (frequently performed) actions.
- Workspace.
- Status bar with basic information about memory usage.

The main part of the window is occupied by the work area, which is divided into two parts horizontally or vertically according to the current settings. In the first part of the workspace, a record of activities performed by the program (i.e. `protocol`) is displayed. The second part of the desktop displays information that is gradually saved in a log file. While record management is controlled by the user, logging occurs continuously without user intervention.

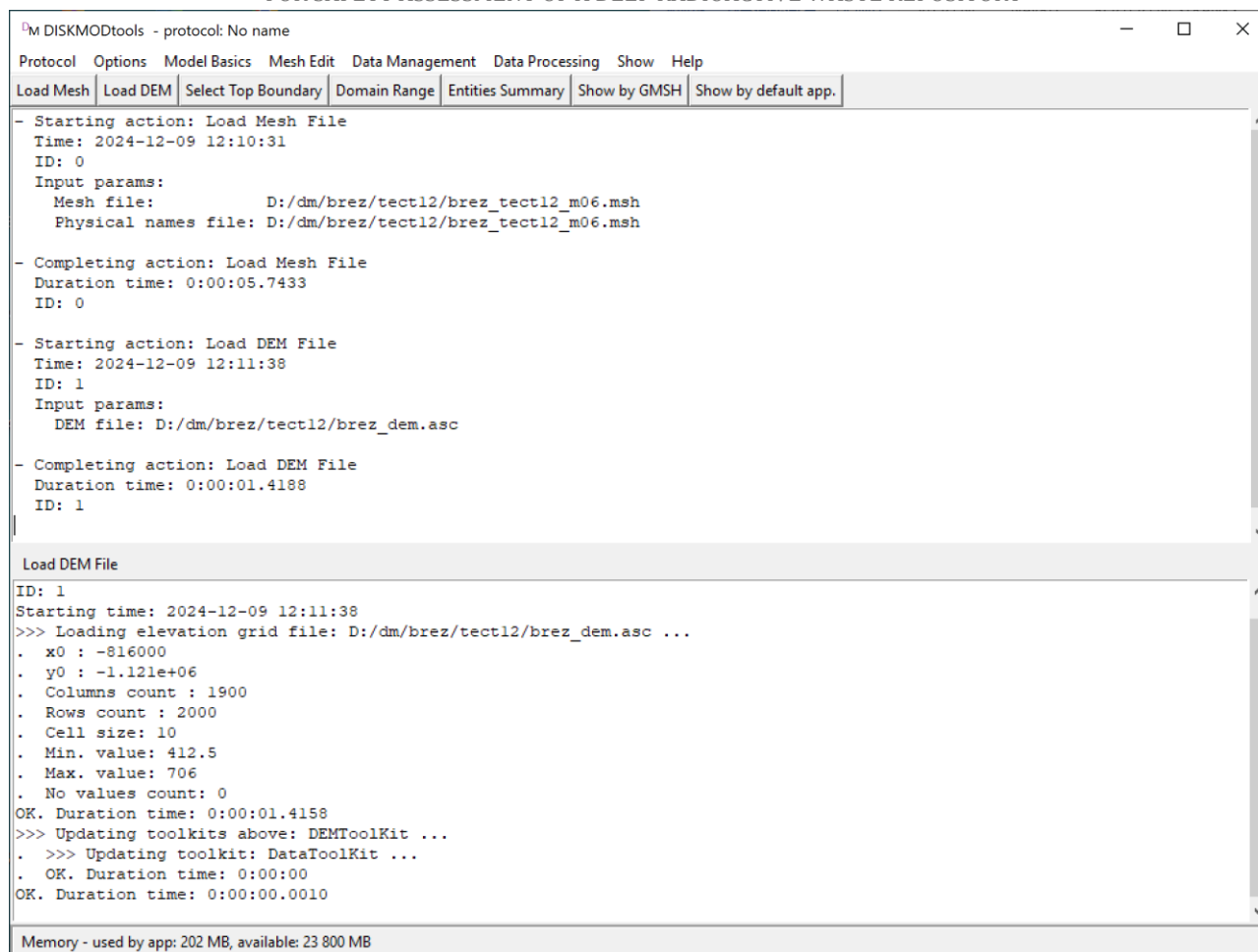


Fig. 1 Main window

4.1 Menu Protocol

The menu contains options for working with the protocol and for ending the program. These are the following items:

- *New* – After selecting the option, the content of the part of the work area with the protocol is deleted. In the case of a not yet saved, modified protocol, the user is prompted to confirm the action.
- *Open and Execute* – Allows the user to open a previously saved protocol, with execution the individual actions recorded. Work in DISKMODtools will thus get to the state where the opened protocol was saved.
- *Save* – Allows to user to save the log to a disk file. Repeated execution means saving to the same file.
- *Save As* – Allows to user to select a disk file to which the log should be saved. It is then written to the file.
- *Exit* – Ending the program. The user is prompted to confirm the action.

4.2 Menu Options

The menu contains several options that can be used to change the program settings (user environment settings):

- *Menu Style* – The option allows to user to change the appearance of the program's main menu. It is possible to choose either the display of all main menu items in the upper part of the window (option *Menu Bar*), or the drop-down menu available via the button in the upper left corner of the window area (option *Popup Menu*). By default, the *Menu Bar* option is set.

- *Log Position* – The option allows to user to influence the relative position of the area allocated to the protocol and the logged information. Logged information can be displayed either in the bottom (option *Bottom*) or in the right (option *Right*) part of the desktop.
- *Show Log File* – The option allows to user to hide or display the log file. By default, the log is displayed in the lower part of the desktop of the main program window.

4.3 Menu *Model Basics*

The menu contains a few options, execution of which is necessary for the functionality provided through items in other parts of the main menu.

The basic purpose of the program is to provide certain manipulations with meshes that are available in the MSH format and with the data associated on the mesh. At the same time, there is an intention to support such functionalities that are needed in certain phases of the processing of the model of groundwater flow and transport of dissolved substances in Flow123d. The model is generally defined in a three-dimensional space, the model domain is usually divided into sub-entities (physical entities, model subdomains), and another entities are formed as a sets of boundary surfaces to assign the boundary conditions of the calculation. When processing some functionalities, it is possible to work with a depth that can be derived from a certain set of boundary entities or from an explicitly (not within the mesh) entered surface representing information about the terrain/relief elevation (DMR) in the area of the model.

The above imply the basic actions of the program that are: loading of a mesh file, entry of entities of the upper boundary surface, loading of the file defining the terrain elevation in the model domain. Other options then refer to the implicit setting of the next dimension of the discrete elements in the network and the position of the reference point to which some of the analyses relate.

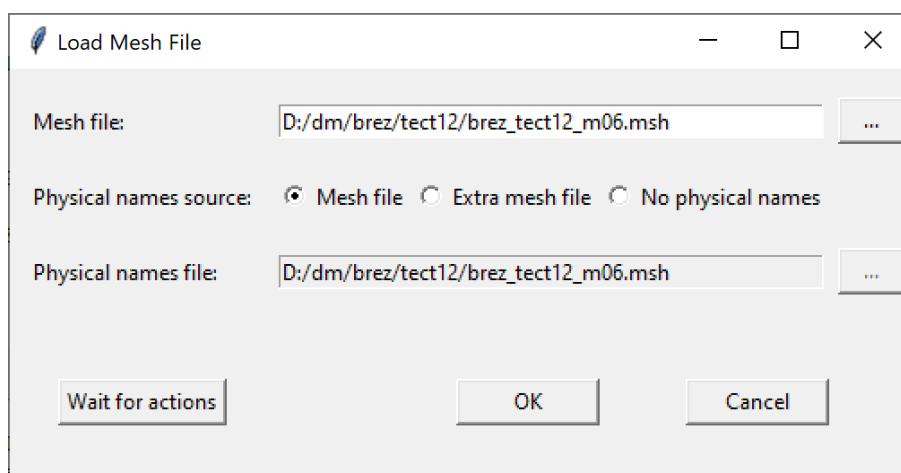


Fig. 2 Load Mesh File dialog box

- *Load Mesh File* – Allows to use to select a file with a mesh. The file must be in MSH format. The dialog box displayed after selecting an option also allows you to select a file from which the list of entities that are present in the mesh should be loaded. For each entity it is a number, dimension and name. As a rule, the list of entities can be read directly from the network file, but in some cases they may not be included or it may be advantageous to have different names assigned to the corresponding numerical identifiers.
- *Load DEM File* – Allows you to select a raster file with terrain elevation. The file must be in ASC (ASCII Grid Format).
- *Top Boundary Entity* – Allows to user to specify which of the network entities represent boundary entities at the top edge of the network.

- *Set Entity Cross Section* – Allows to user to enter another dimension for individual entities of discrete elements (fractures, fracture/tectonic zones).
- *Set Reference XY Position* – Allows to user to enter a reference point in the horizontal plane.

4.4 Menu Mesh Edit

The menu offers options that provide basic information about the loaded network, and options that allow certain changes to an existing loaded network and its subsequent saving to a disk file. These are functionalities that can be used in the mesh preparation phase.

- *Model Domain Range Summary* – It displays information about the ranges of individual coordinates of the currently loaded mesh to the user. If the user selects "*Write to protocol*", the displayed information is written to the protocol when the information dialog is closed.
- *Model Entities Summary* – A dialog box is displayed to the user. There the user can select a set of mesh entities. Basic information about coordinate ranges and total volume or total area is displayed for the selected set of entities. By pressing the "*Write to protocol*" button, the currently displayed information is written into the protocol.
- *Change of Z-coordinates on Top Boundary Only* – It allows the z-coordinates of the mesh to be adjusted so that the upper boundary corresponds to the desired elevation of the terrain. To perform this action, it is necessary to have the computational mesh, the DMR file, and the defined boundary entities that form the upper boundary of the network loaded. The option will then ensure that the z-coordinates of the grid points are modified only in the upper boundary surface. This will change the geometry of the elements in the subsurface part. The option is suitable only in cases where the modifications require only small changes in the z-coordinate (up to 25% of the dimension of the elements in the sub-surface parts).
- *Change of Z-coordinates from the Specified Level* – Similar to the previous option, it allows adjusting the z-coordinates of the grid so that the upper boundary corresponds to the desired elevation of the terrain. Unlike the previous option, the z-coordinates of all elements from the specified z-level up to the upper border are adjusted. It modifies the geometry of elements above the selected z-level. To perform this action, it is necessary to have a computational network, a DMR file, and defined edge entities that form the upper boundary of the network loaded.
- *Remove Entities* – Enables to remove the selected entity(ies) from the mesh.
- *Merge Entities* – Enables to merge several entities to a one.
- *Change Entities Name/Number* – Enables to change the naming or numbers of individual mesh entities.
- *Save Modified Mesh* – Enables to save the mesh in its current form to disk file.

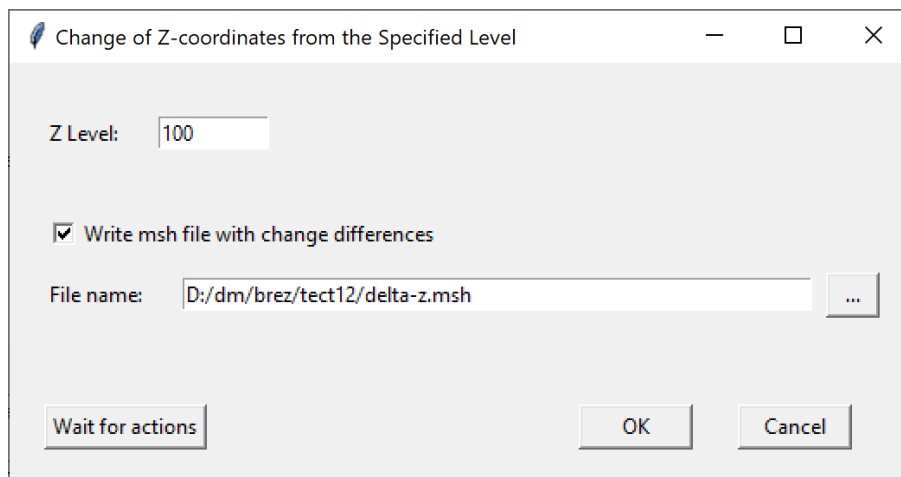


Fig. 3 Change of Z-coordinates from the Specified Level dialog box

4.5 Menu Data Management

The menu contains options that enables to user to create data arrays from data stored in disk files.

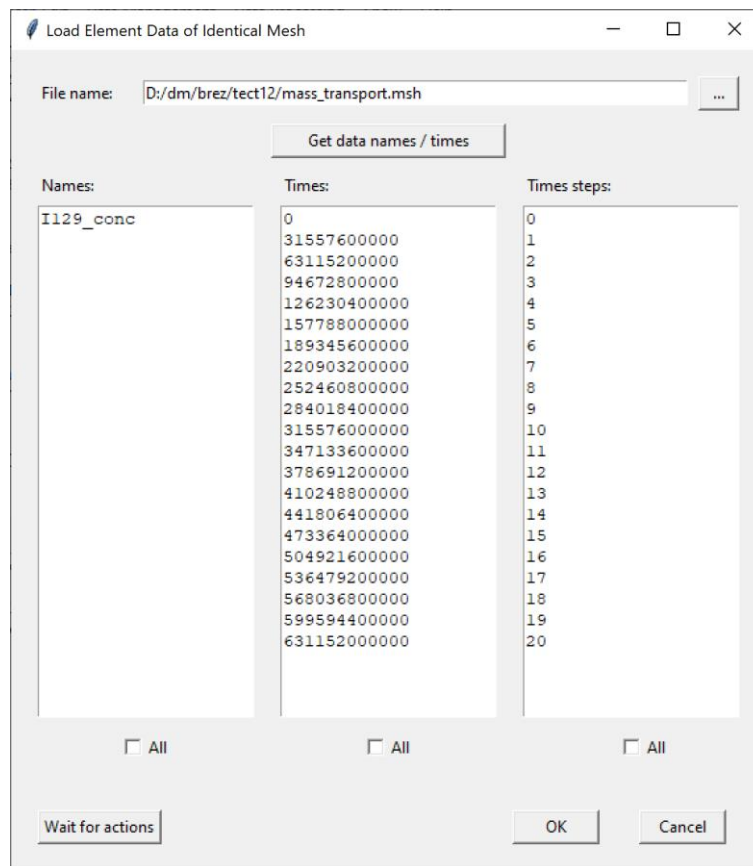


Fig. 4 Load Element Data dialog box

- *Load Element Data of Identical Mesh* – A dialog box for selecting a data file on the mesh is displayed. The file must be in MSH format. In this case, the data on the network must be identical to the currently loaded mesh. In the dialog box, after entering the file, you can select which part of the data should be loaded from the file – only some data fields, or some simulation times or time steps can be selected. The amount of retrieved data can be limited after retrieving the basic information from the file, which can be done by pressing "Get data names/times", and then removing unwanted items from the appropriate list. Alternatively, the user can request the loading of all data fields or times by selecting the "All" option under the relevant column.
- *Load Element Data of Any Mesh* – A dialog box for selecting a data file on the mesh is displayed. The file must be in MSH format. In this case, the data can be on any network. This is assumed to be data in the domain defined by the currently loaded mesh. In the dialog box, after entering the file, you can select which part of the data should be loaded from the file – only some data fields, or some simulation times or time steps can be selected. The amount of retrieved data can be limited after retrieving the basic information from the file, which can be done by pressing "Get data names/times", and then removing unwanted items from the appropriate list. Alternatively, the user can request the loading of all data fields or times by selecting the "All" option under the relevant column.
- *Assign Data to Boudary Elements* – When loading data by „Load Element Data“, the values of the relevant data field are assigned to the „bulk“ elements. This option ensures the subsequent calculation of values for elements of the boundary entities. Subsequently, it is then possible to analyze, for example, concentration values on boundary entities.
- *Loaded Element Data Summary* – An overview of all loaded/created data fields is displayed to the user..

- *Select and Save Element Data* – Enables to select a part of a mesh and a data field and save that data to a new file, with only the part of the mesh specified by the selection being saved to the file.
- *Select and Save Element Data With Complete Mesh* – Enables to select a part of the network and a data field and save this data to a new file, with the entire initially loaded mesh to the file.
- *Load Water Flow Raw* – Lets to user load a flow results file in `raw_flow_output` format. The file contains the results of the flow simulation after the mixed hybrid finite element method (MH FEM) calculation. In addition to the calculated pressure (in the element centres and on the element edges), these data also include flow rates through the individual edges of mesh elements. Flux data are required to evaluate the flow balance between individual parts of the model domain, see the option “*Analyse Flux between Entities*”.

4.6 Menu Data Processsing

The menu contains options for manipulating with current data fields, performing analyses, saving outputs to disk files.

- *Analyse Flux Between Entities* – Calculating the flux between two sets of entities.
- *Analyse Element Data Statistics* – Analysis of the statistics of the selected data field in the selected part of the network. A part of the mesh can be defined by a set of entities, a range of coordinates and a range of depths. The result can be written to the protocol or/and to a disk file in CSV format.
- *Vector Element Data to Scalar Data* – Converting a vector data to a scalar data. Scalar fields can be created for individual coordinates, vector norm or vector angle in/to the XY surface.
- *Create New Element Data by Formula* – Creating a new data field by calculating from an existing one.
- *Save Z-level Raster* – Allows to create raster data from the selected data field at the specified z-level. The user selects the range of x- and y-coordinates, the corresponding z-level, the step of the raster, the parameters of the interpolation algorithm and the output disk file. The output to the file is in ASC or MSH format, according to the user's choice.
- *Save Depth Raster* – Allows to create raster data from the selected data field at the specified depth. The user selects the range of x- and y-coordinates, the corresponding depth, the raster step, the parameters of the interpolation algorithm and the output disk file. The output to the file is in ASC or MSH format, according to the user's choice.
- *Save Point Data* – Allows to user to save the data of the selected data field in the specified points to the CSV file. Points are entered by coordinates. The IDW algorithm is used for interpolation to the specified points.
- *Save Point Data of Depth* – Allows to user to save the data of the selected data field in the specified points to the CSV file. Points are entered by x and y coordinates and a depth. The IDW algorithm is used for interpolation to the specified points.

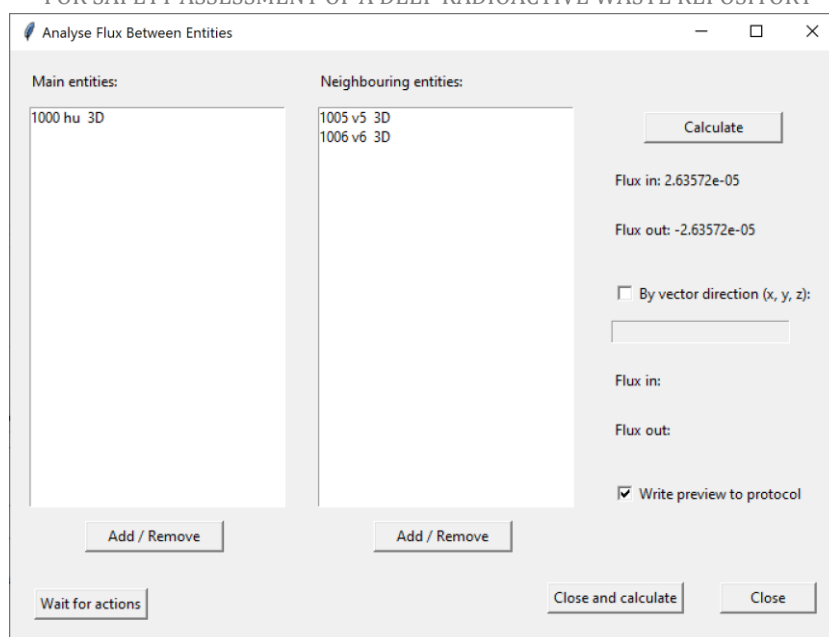


Fig. 5 Analyse Flux Between Entities dialog box

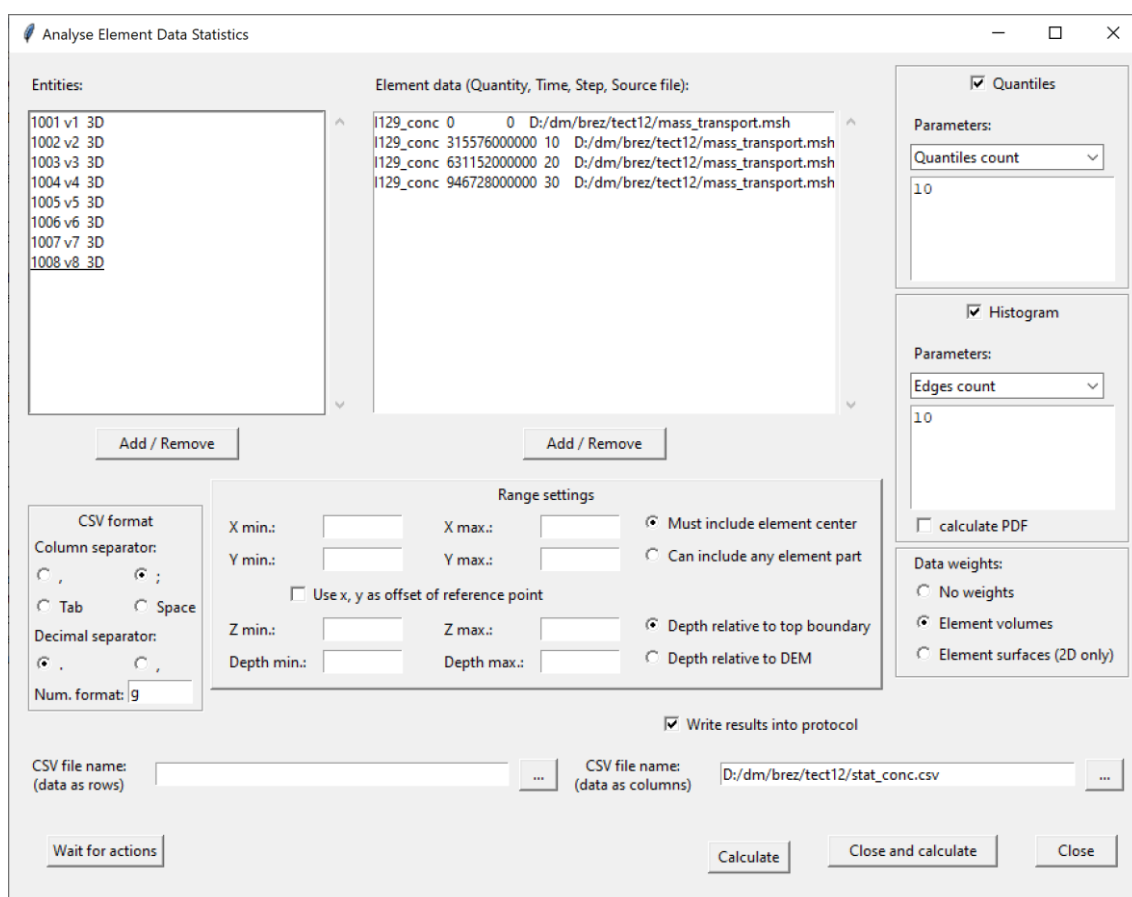


Fig. 6 Analyse Element Data Statistics dialog box

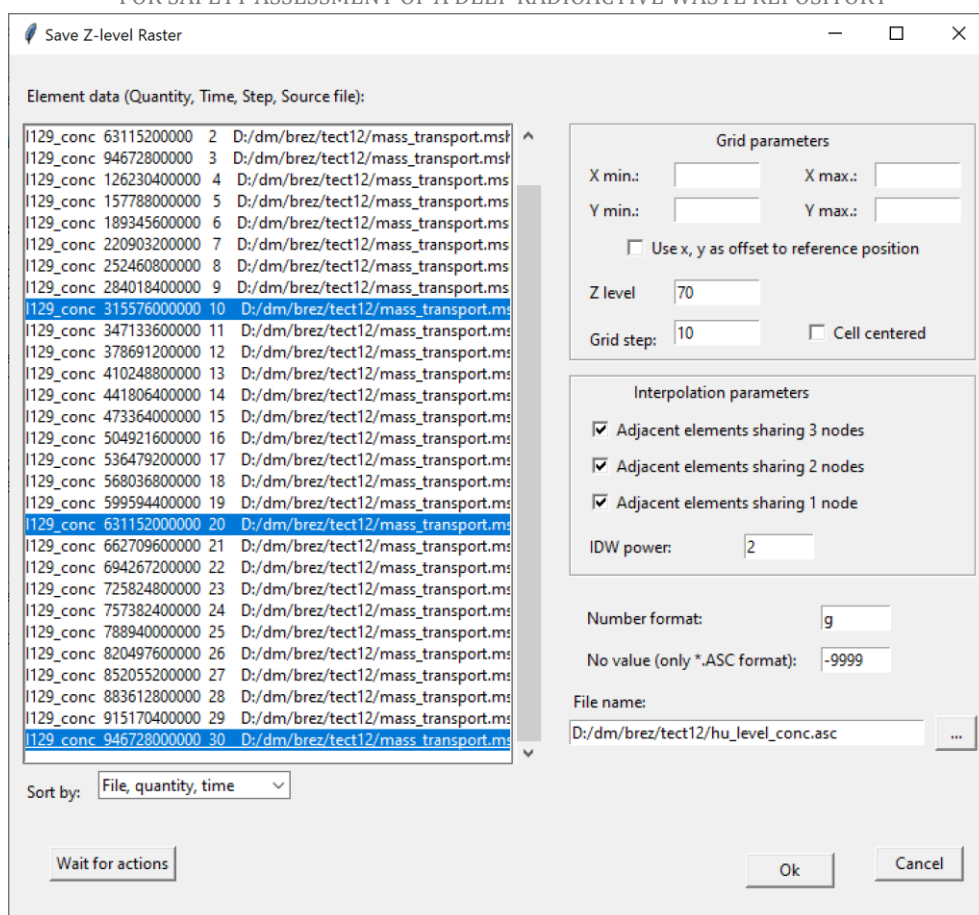


Fig. 7 Save Z-level Raster dialog box

4.7 Menu Show

In the part of the desktop with the displayed log, you can select a part of the text by dragging the mouse. If the selected/highlighted part of the text contains a path to a disk file, then one of the items in this menu can be used to display the relevant file in an external program. The file format must be compatible with the external program in question. The external program must be installed on the computer. Then the display can be performed by one of the following external programs, depending on the options:

- *Show Selected Filepath by GMSH*
- *Show Selected Filepath by Notepad (Windows)*
- *Show Selected Filepath by Microsoft Excel*
- *Show Selected Filepath by Libre Calc*

4.8 Menu Help

- *Documentation* – Shows this documentation file.
- *About Program* – Displays basic information about the program..

5 Source files structure

In the main directory of the program there are several basic source files, from which `DISKMOD.py` is used to start the program. The file `main_app.py` there performs the creation of basic elements of the user interface. Other source files of the program are then divided into three subdirectories:

- Subdirectory `dialogs` contains the source codes of individual dialog boxes used in the graphical user interface.

- In the `diskmod_tools` subdirectory there are files containing algorithms for manipulation (analysis, conversion, etc.) with the program data..
- The `workflow_GUI` subdirectory contains a library providing basic application handling related to logging, logging and parallelization of the execution of partial program activities.

The configuration files `options_default.yaml` and `mwt_dark_theme.yaml` are then in the main directory of the program. The first contains the program's default settings. The second of the listed files contains settings for a "dark-tuned" user interface.

6 Reference

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