

DHI-WASY Software

FEFLOW[®] 6.2

Finite Element Subsurface Flow
& Transport Simulation System

User Manual

DHI-WASY GmbH



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1

Introduction

1.1 Welcome to FEFLOW

Thank you for choosing FEFLOW! You have selected one of the most comprehensive, well-tested and reliable programs for the simulation of flow, groundwater age, mass- and heat-transport processes in porous media.

This manual explains FEFLOW's extensive modeling capabilities so that the easy-to-use intuitive graphical user interface can be used to its full potential.

Please take your time to familiarize yourself with the software to ensure maximum productivity and efficiency in your projects.

1.2 The FEFLOW Package

The FEFLOW user interface supports the entire workflow from preprocessing via the simulation run to postprocessing. In addition, there are a number of supporting applications for specific purposes:

FePEST

A convenient graphical user interface for using PEST by John Doherty with your FEFLOW models for parameter estimation, uncertainty analysis and much more. FePEST runs with a FEFLOW license.

FEFLOW Viewer

Free visualization and postprocessing tool for FEFLOW files.

Command-Line Mode

In command-line mode, FEFLOW runs without any graphical user interface. This is especially useful for batch runs or integration into other simulation environments.

WGEO

WGEO is a geo-imaging software. Its most important fields of application in connection with FEFLOW modeling are georeferencing of raster maps and coordinate transformation.

FEPLOT

As FEFLOW itself does not provide printing capabilities, FEPLLOT can be used to create plot layouts and

1. Introduction

print maps composed of vector maps, graphical elements, and text.

FE-LM2

This tool provides functionality for curve fitting, e.g., for obtaining the parameters for parametric relationships in unsaturated flow or for sorption isotherms.

1.3 FEFLOW Documentation

The FEFLOW documentation provides an introduction to the practical application of the software as well as a detailed description of the underlying concepts and methods. While you obtained the Installation Guide in print, the User Manual is available in pdf format on the installation disk or on our web site.

The comprehensive book “FEFLOW – Finite Element Modeling of Flow, Mass and Heat Transport in Porous and Fractured Media” written by H.J. G. Diersch represents a theoretical textbook and covers a wide range of physical and computational issues in the field of porous/fractured-media modeling. The book is general and will be useful for both students and practitioners in engineering and geosciences as well as in other fields where porous-media flow dynamics and computational methods are of specific concern.

The book starts with a more general theory for all relevant flow and transport phenomena on the basis of the continuum approach, systematically develops the basic framework for important classes of problems (e.g., multiphase/multispecies nonisothermal flow and transport phenomena, discrete features, aquifer-averaged equations, geothermal processes), introduces finite-element techniques for solving the basic balance equations, in detail discusses advanced numerical algorithms for the resulting nonlinear and linear problems

and completes with a number of benchmarks, applications and exercises to illustrate the different types of problems and ways to tackle them successfully (e.g., flow and seepage problems, unsaturated-saturated flow, advective-diffusion transport, saltwater intrusion, geothermal and thermohaline flow).

The book is available for sale online and is included with every FEFLOW 6.2 license.

This User Manual and the step-by-step Tutorial contained in the DVD booklet complement the documentation on the more practical side.

A full reference of the user interface elements along with a detailed description of the handling is available in the help system of the graphical interface.

Screen casts for the exercises described in the tutorial sections as well as for the demonstration exercise are available online at www.feflow.com.

1.4 Scope and Structure

This User Manual is intended as a practical guide to groundwater modeling with FEFLOW. It aims to explain the essential work steps of model setup, simulation and postprocessing, and to present alternative options and settings with their specific advantages and disadvantages for specific applications. Thus the User Manual can serve both as an introduction for FEFLOW ‘newbies’, and as a reference for more experienced users. Its position within the complete set of documentation is between the theoretical basis in the FEFLOW book and the detailed description of the user-interface elements and work flows in the help system.

The manual follows a typical modeling workflow—starting from basic maps and finishing with postprocessing and extending FEFLOW’s capabilities. Each chapter starts with an introduction to the topic, presents

the relevant FEFLOW tools, describes the concepts and workflows, and ends with a tutorial.

1.5 Notation

Most of the tutorials are based on prepared files, thus they require installation of the FEFLOW demo data package. <FEFLOW demo> in a file path refers to the folder of the demo data installation. The default installation location may differ between operating systems. On Microsoft Windows, the typical installation locations are:

- Windows Vista, 7 and 8:
C:\Users\Public\Documents\WASY FEFLOW 6.2
\demo

1. Introduction

2

What's New in FEFLOW 6.2?

New features and improvements

FEFLOW 6.2 features a substantially extended range of functionality.

This chapter presents the highlights of the new version in an overview of the most important new features and improvements.

2.1 FePEST

FePEST that is now included with every FEFLOW license is a graphical user interface for using PEST by John Doherty with FEFLOW for, e.g., model calibration, sensitivity and uncertainty analysis as well as predictive analysis. Its advantages include graphical support during the setup process and immediate graphical feedback on the simulation progress.

Chapter 15 provides an extensive introduction to FePEST, the available functionality and supported PEST methods.

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2.2 New Problem Class: Groundwater Age

Groundwater Age is available as a new kind of problem class – similar to mass or heat transport. For age simulations, the parameters *groundwater age*, *lifetime expectancy* and *exit probability* can be calculated and provide the means to analyze flow dynamics and mixing processes, estimate risk vulnerability or evaluate outlet capture zones and the origin of water.

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2.3 Subdomain and Storage Budget

Storage Capture/Release is a new component in the *Rate-Budget* and *Period-Budget* panels for flow and transport. With this, storage change and solution error (*Imbalance*) can be clearly separated in transient models.

Flow across a model-internal subdomain boundary can be calculated exactly in new *Subdomain Boundary Rate* and *Subdomain Boundary Period* panels for flow and transport. Combined with the options of the

2. What's New in FEFLOW 6.2?

already existing *Rate-Budget* and *Period-Budget* panels, complete and exact water balances for arbitrary subdomains within a model can be easily obtained.

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2.4 Temporal Element Deactivation

With the new parameter *In-/active Elements*, mesh elements can be de- and reactivated. Elements can be made inactive for an entire simulation or only during specific periods during a simulation.

With this new feature, time-varying model geometry as encountered in open-pit or long-term simulations with morphological changes can be simulated as well as permanently impermeable structures.

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2.5 Temporary Boundary Condition Deactivation

Time series describing transient boundary conditions or boundary constraints can now contain gaps during which a boundary condition or constraint will be completely deactivated.

This new feature allows to turn any kind of boundary condition off and on during a simulation without the need for inefficient constraints or additional plugins.

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2.6 Random-Walk Particle Tracking

FEFLOW 6.2 provides extended options for streamline and pathline analysis: *Random-Walk Particle Tracks* incorporate diffusion and dispersion, bringing field-line analysis a large step closer to the capabilities of a full advection-dispersion solution. As this option does not require the setup of a transport problem, pre-processing effort and computational cost remain comparably low.

➡ [Page 115](#)

2.7 New Solvers

PARDISO (developed by O. Schenk and K. Gärtner) is a parallelized direct solver. As a direct solver, it provides a noniterative exact solution of the equation system, at an often affordable computational cost thanks to parallelization. PARDISO is the new default direct equation system solver.

FEFLOW 6.2 provides a new version of the algebraic multigrid solver, SAMG 2.7. Additionally, the FEFLOW-specific settings for SAMG have been adapted to better match the typical FEFLOW models. With this, FEFLOW reaches a new level of solution performance, robustness and stability.

➡ [Page 54](#)

2.8 Modulation Functions

In transient models, boundary conditions can be modified by applying a time series as a *modulation function*. With this new feature a large number of boundary conditions can very efficiently be turned off

at specific time stages if the modulation function contains gaps, or boundary-condition values can be modified, e.g., for calibration purposes or to incorporate seasonal changes, etc.

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2.9 Scene Library

Settings for *Slice*, *3D*, *Supermesh* and *Cross-section* views can be stored in the new *Scene Library* panel and organized in a user-defined folder structure.

With this new option, even large numbers of view settings (including animation settings) can be easily stored without the overhead of always recreating the respective view windows when loading the model, thereby reducing the required memory demand significantly.

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2.10 Databases and Map Files

Tabular data from Microsoft Excel workbooks and Microsoft Access databases as well as geometries and tabular data in ESRI Geodatabases, PostgreSQL and Oracle databases can now be used for map display, data import and export, without the need for re-formatting. With additional joining and selection options, project data, including geographical data, can now be easily stored without redundancies and in one single place.

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2.11 Interactive 1D Linear Interpolation

1D linear interpolation along lines can be performed interactively without the need for maps containing boundary-condition or boundary-constraint values and line geometry. The input of constant values, time-series IDs or usage of user-defined expressions is supported.

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2.12 Measure Tool

The FEFLOW 6.2 interface provides a new tool to measure distances and areas in *Supermesh* and *Slice* views and distances in *3D* views.

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2.13 Additional Functionality

2.13.1 Results Evaluation and Visualization

FEFLOW 6.2 provides an extended set of tools and features for improved results evaluation and visualization.

- 3D spheres and cylinders available as starting locations for field-line analysis
- **Péclet Number** available in *Auxiliary Data*
- Predefined user distributions for error norms for flow, mass, age and heat
- Export of georeferenced snapshots from *Slice* views
- Export of process-variable results for multiple or all stored time steps in *.dac files

2. What's New in FEFLOW 6.2?

- Field lines: Consideration of retardation due to Henry-type sorption

- Import/export of multiple location sets and selections

2.13.2 Map Data Handling

- User-defined folder structure in *Maps* panel with maps of arbitrary type in each folder
- Search option for folder and map names in *Maps* panel
- **Quick Parameter Import** option for previously exported maps from FEFLOW without the need for parameter links
- Import/export of relative map locations and all map settings from/to map reference files (*.fmr)
- Import/export of map layers from/into *.fml file
- Import/export of layer styles from/into *.fms file
- Automatic loading of exported maps to *Maps* panel
- List of maps in *View Components* panel reflects *Maps* panel structure

2.13.4 Further Improvements

- Isolines with in-line labels in **3D** views (*p. 71*)
- Labelling of line and polygon maps
- Optional display of solver residuals and solver CPU usage in *Log* panel
- Handling of **Discrete Features**: Scaling of conductivity values depending on the saturation within the feature

2.13.3 Workflow and GUI Improvements

- Auxiliary *Spatial Units* panel(s)
- Conversion of stored selections into various geometry types
- Copy/paste functionality for chart plots
- **Expression Editor** with units
- **Inspection** panel: Separate sections for parameters and map attributes, search/filter options available
- Export option for **Discrete Features** and Reimport via **Quick Import**
- Multi-selection option in *Maps*, *Data* and *View Components* panel for visualization and data export

The User Interface

How to use the basic user interface components

3.1 Philosophy

The user interface of FEFLOW 6.2 is designed to provide as many tools as possible without the need to open nested dialogs or menus. While allowing an efficient workflow for experienced FEFLOW modelers, the interface might look complex to first-time users.

Therefore only the interface components that are relevant at the current stage of model setup or for the current model class are shown. The five main interface components—menus, toolbars, views, panels and

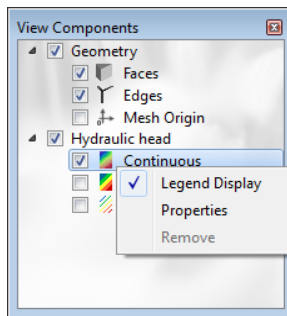


Figure 3.1 Context menu in the View Components panel.

charts—all adapt automatically to the current context.

To provide often-needed functionality as quickly as possible, many controls are also accessible via context menus that are available for most user-interface elements, for example, parameters in the *Data* panel or legends in a view window.

3.2 Graphics Driver

The FEFLOW user interface makes use of OpenGL (Open Graphics Library) for visualization. OpenGL is a well-proven standard that gives access to the capabilities of the graphics hardware for accelerated display. To efficiently use OpenGL, a graphics driver provided by the graphics-card or chipset manufacturer should be installed. The standard drivers included with an operating system might not support OpenGL to a sufficient extent. Especially on laptop computers, drivers provided at purchase have been found to contain OpenGL bugs in several cases. We recommend to download the most recent drivers from the graphics-card or chipset manufacturer's web site before using FEFLOW or when problems in the graphical display are observed.

3. The User Interface

3.3 Customizing the Interface

The interface is completely customizable, i.e., the location and visibility of all components except the main menu can be chosen arbitrarily. Components can be docked to a certain main-window location, or they can be floating as separate windows.

To switch between docked and floating status, double-click the header of a panel or move a component to another location by dragging it while pressing the left mouse button. To avoid docking, the <Ctrl> key can be pressed before and while moving a panel or chart window.

Panels and charts can also be tabbed so that two or more of these elements are placed above each other. Clicking on one of the tabs brings the corresponding panel or chart to the front.

Floating toolbars, panels and charts can be moved outside the main application window. This is especially helpful to enlarge view windows on one screen while arranging toolbars and panels on another screen.

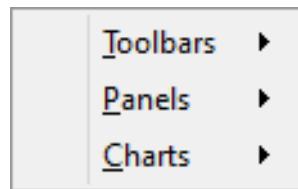


Figure 3.2 Context menu.

View windows can also be set floating with <Ctrl> + <F11> and then moved outside the main window (e.g., to a second screen). Full-screen mode is available for all view windows via <F11>.

Toolbars, panels and charts can be turned on and off

by using the context menu on 'empty' parts of the user interface, i.e., parts where no other context menu comes up (Figure 3.2). Panels and charts can also be closed by clicking on the closing icon in the upper right corner of the element.

While exploring the new interface you may come to a situation where most panels and toolbars are hidden, and the remaining ones are not where you want them to be. In such a case, just switch on **Reset Toolbar and Dock-Window Layout** in the **View** menu, and FEFLOW will come up with the default layout when starting it the next time.

3.4 View Windows

View windows contain different views of the model, possibly along with maps and other visualization features. Limited only by the available memory, any number of windows can be displayed simultaneously to show different model components (listed in the **View Components** panel for the active view). Each view has its own settings and components handling.

3.4.1 Types of View Windows

FEFLOW has six types of view windows:

- **Supermesh** view
- **Slice** view
- **3D** view
- **Cross-Section** view
- **Slice Data-Trace** view
- **Data-Trace** view

New view windows can be opened via the **Window** menu. For opening **Cross-Section** and **Slice Data-Trace** views, a 2D surface line has to be selected in the **Spatial Units** panel. Opening a **Data-Trace** view

requires creating and selecting a 3D line first.




3.4.2 Navigation

Navigation in view windows is most straightforward by using the left and right mouse buttons and the mouse wheel. By default, the left mouse button is used to pan in *Slice* views and to rotate in *3D* views. Besides invoking the context menu on a view, the right mouse button also allows zooming when a navigation tool is active. In *Slice* views, the mouse wheel has zooming functionality, while in *3D* views it is used for rotation. <Shift> on the keyboard in combination with the mouse wheel changes the directional exaggeration (in y direction in *Slice* views and z direction in *3D* views).

Keyboard shortcuts allow to quickly return to the full view (<Home>), to reset the rotation (<Ctrl>-<Home>), and to reset the scaling (<Shift>-<Home>).

Additional tools in the *View* toolbar can also be used to return to full view, to return to a preferred view defined via *Positioning* in the *View* menu, and to undo/redo view changes.


3.5 Tutorial

When FEFLOW is started it opens with an empty project by default. To create a new model, we click on  **New** which opens the *New FEM Problem* dialog. Here, we need to define the initial work area for mesh design. This can either be done via a manual input of the initial domain bounds or with the use of maps that are loaded in a subsequent step. For a quick start, for example to set up a simple test model in local coordinates, select  **Manual input of the initial domain bounds** and accept the default domain bounds with a click on  **Finish**. The following components are

now visible in the workspace:

- the active view window—the *Supermesh* view
- the main menu on top
- a number of panels and toolbars

By default, not all panels and toolbars are displayed. To get familiar with the graphical user interface we now add a further panel to our workspace.

Go to  **View > Panels** in the main menu and click on the entry **Plug-ins Panel**. The panel now appears at the bottom right corner of the FEFLOW window.

Change the panel position by dragging it to a different location while holding the left mouse button. Leave the panel as a separate floating window or dock it at a certain location.

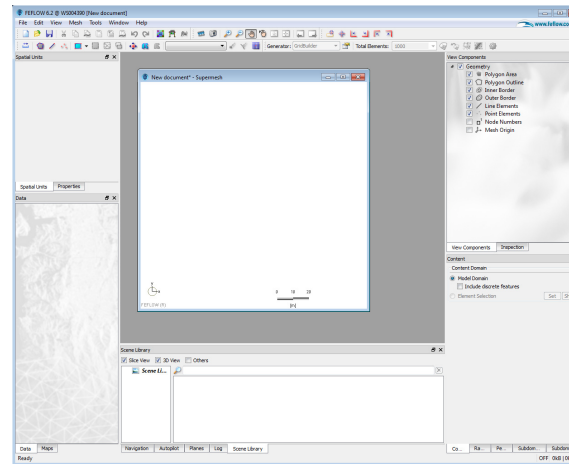





Figure 3.3 The FEFLOW standard layout.

Add another panel using a different method. Right-click on an empty part of the user interface, e.g., in the grey part above the  **Inspection** panel. A context menu with the entries  **Toolbars**, **Panels**, **Charts** opens up. Go to  **Panels** and click on **Map Proper-**

3. The User Interface

ties Panel. The panel now appears in our workspace as a separate floating item. Dock the panel with a double-click on its header. The **Spatial Units** and the **Properties** panel are tabbed so that only one is visible at a time. Click on the tab **Properties** to bring this panel to the front. Remove the two panels by clicking on the closing icon in the upper right corner of the respective panel.

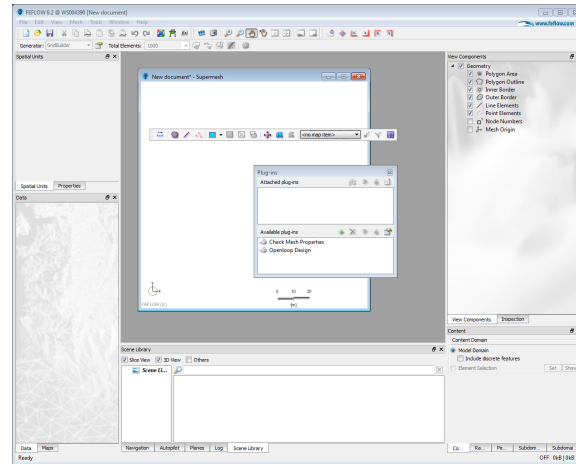


Figure 3.4 A floating panel and toolbar in the workspace.

Only toolbars relevant to the currently active view can be shown. Aside from this restriction, toolbar visibility and position are user-controlled. As an exercise, click on the left border of the **Mesh-Editor** toolbar and drag it to a different location, e.g., into the **Supermesh** view.

To restore the default settings for the graphical user interface go to **View** and select **Reset Toolbar and Dock-Window Layout**. When FEFLOW is started the next time, toolbars and panels will be arranged accord-

ing to the default layout.

To move the **Supermesh** view outside of the main window, open its context menu with a click on the right mouse button and select **Floating Window**. The view window can now be moved to an arbitrary position on the screen.

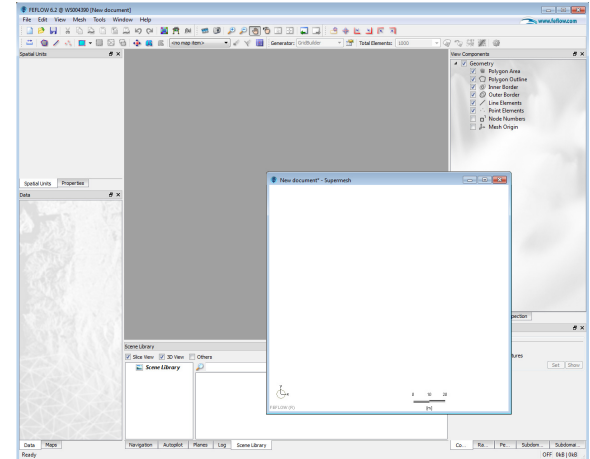


Figure 3.5 The supermesh view as floating window.

To see the **Supermesh** view in full-screen mode, hit <F11>. The full-screen mode is turned off by hitting <F11> once again.

4

Working with Maps

Loading and managing different kinds of maps

4.1 Maps—What For?

Maps are an integral part of all but very simple modeling projects. Their most obvious role is to provide a basis for convenient orientation in the model area. FEFLOW, however, makes much wider use of maps in the modeling workflow. Map geometries can be used to influence the mesh generation process, they can serve to geometrically define the target nodes, elements, edges or faces for parameter assignment, and attributed maps can even provide the input data themselves.

4.1.1 Raster Maps/Maps Containing Data

We have to distinguish between raster maps and maps which contain data. Data can be provided in the form of tables or as vector maps if they contain geometry information.

Pixel-based raster maps in formats such as tiff, jpeg, png, or bmp can only provide visual information. Vector maps contain discrete geometries (points, lines, and

polygons). Formats supported by FEFLOW include ESRI Shape Files, AutoCAD Exchange Files, DBase Tables, and several ASCII (text) file formats. In addition to geometrical information these file formats also encompass attribute data, i.e., numerical and/or textual information related to certain geometrical features. While some formats like shp support an unlimited number of user-defined attributes, others like dxf only allow drawing attributes such as color or line style, and very simple formats such as trp (ASCII triplet format—XYF) only support one single attribute value.

4.1.2 Microsoft Excel Worksheets and Access Tables

Tabular data from Microsoft Excel worksheets and Microsoft Access databases can be imported into FEFLOW as maps. Export of parameter values and chart data into Excel and Access is supported as well. Supported import and export formats include *.xls, *.xlsx, *.mdb and *.accdb.

Each Excel worksheet needs to be imported as a separate map. For workbooks containing multiple worksheets, the worksheet to be imported is selected

4. Working with Maps

via an import dialog (see Figure 4.1).

The import of tables from MS Access databases works similarly. After selecting a database, each table needs to be imported as a separate map via a selection dialog.

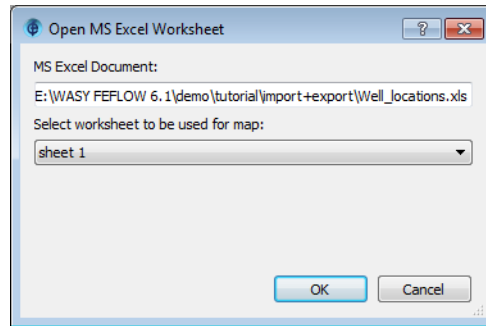


Figure 4.1 Selecting worksheets for import from a MS Excel workbook.

Exported data can either be added as new worksheets or tables to an existing Excel workbook or Access database or they can replace an existing worksheet or table.

4.1.3 Geodatabases

Besides the possibility to load separate maps of various file formats, FEFLOW also provides the option to connect to different types of geographical databases for data import via the **Maps** panel and export via the **Data** and **View Components** panels.

The following database systems are supported:

- PostGIS
- Oracle
- ESRI Geodatabase



Export into an existing table/feature class erases all previous content of the table/feature class. The export option cannot be used to append information to existing tables!

Connecting to ESRI Geodatabases is only possible with the 32-bit version of FEFLOW and with an adequate ESRI license.

4.1.3.1 Database Connection

The connection to a Geodatabase is managed through a **FEFLOW Database Connection File** (*.fedb). The connection file contains all settings for the connection to a specific geographic database, i.e., information on the host, port name of the database, user name and password.

An existing connection file can be opened via **Add Map(s)...** in the context menu of the **Maps** panel or by clicking on the search icon in the panel. Creating a new connection file or editing an existing one is possible via the file-selection dialog evoked via **Add Map** or the search option in the **Maps** panel. Make sure that the displayed file types in the file-selection dialog include the format *.fedb.

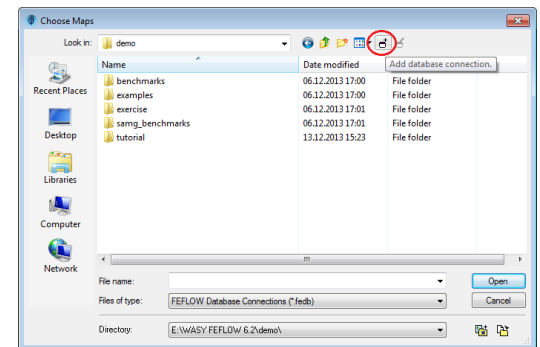


Figure 4.2 Adding a database connection.

As an example, the dialog for creating a connection

to a PostGIS database is shown in Figure 4.3.

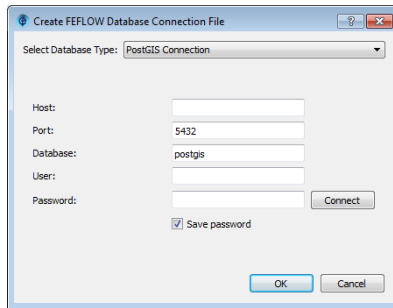


Figure 4.3 Creating a *.fedb file for PostGIS.

Depending on the database type, different options are available when creating a new connection file. For all details on the available settings, please refer to the FEFLOW help system.

After the connection to a database, the procedure differs depending on the type of database.

PostGIS and Oracle

For PostGIS and Oracle databases, the *Open PostGIS Table* and *Open Oracle Table* dialogs are opened, respectively. The upper part of the dialog provides a summary of the *Connection Properties* while the lower part gives access to the data: Existing tables can be opened or user-defined SQL queries can be used to derive database data. To obtain geometries from the database when using SQL queries, a geometry column needs to be specified in addition. Clicking on *Verify* in the dialog checks the SQL syntax and displays the available columns so that the one containing the geometry information can be selected.

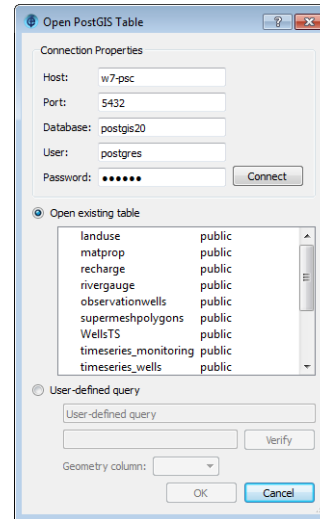


Figure 4.4 Open PostGIS Table dialog.

ESRI Geodatabases

For ESRI Geodatabases, the standard *OpenARC-GIS Table or Feature Class* dialog is brought up after opening a *FEFLOW Database Connection File*. Here, it is possible to select a feature class from the database.

4.1.4 2D/3D Maps

ESRI Shape Files, AutoCAD Exchange Files and tabular files (dbf, dat) may contain three-dimensional map information. FEFLOW supports 3D map display in 3D view windows (Figure 4.5).

4. Working with Maps

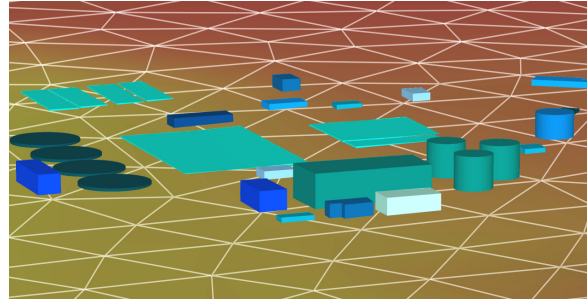


Figure 4.5 3D map in 3D view window.

4.2 Coordinate Systems

Dealing with spatial data requires the definition of a unique coordinate system as a reference. FEFLOW can use data in any metric cartesian system, i.e., any system with orthogonal x and y axes and coordinates in meters. The most popular of these systems is the UTM coordinate system.

To achieve better precision in the calculations, FEFLOW always uses a local and a global coordinate system at the same time. The axes in both systems have the same orientation, only the origin of the local system has an offset in global coordinates.

Locations in the local system can be expressed in cartesian or polar coordinates. The coordinate system used in a particular view window can be defined in the **View** menu. The offset of global and local coordinate system is defined automatically via map extents or manually when starting a new model, but can be edited later on in the **Coordinate-System Origin** dialog which is accessed with a click on the **Edit Origin** button in the **Origin** toolbar. In practical cases, it is usually sufficient

to deal with the global coordinate system.

In 2D cross-sectional and axisymmetric models the y coordinate refers to the elevation. In these cases an offset between local and global coordinates in y should be avoided so that there is no doubt about the elevation reference. Internally, FEFLOW uses the local y coordinate as the reference for elevation-dependent parameters, e.g., when converting hydraulic head to pressure head and vice versa.

4.3 Georeferencing Maps

The WGeo software provided with FEFLOW can add a geographical reference to raster images such as scanned maps in tiff, jpeg, png or bmp format for use as maps in FEFLOW. WGeo can also perform coordinate transformation for raster and vector maps applying a 7-parameter Helmert transformation routine.

In Plus mode (separate licensing required), WGeo also provides functionality for georeferencing of ESRI Shape Files (shp) and AutoCAD Exchange Files (dxf). Additional coordinate transformation routines are also available on demand.

Please refer to the WGeo manual and its help system for a detailed description of the respective work flows.

4.4 Handling Maps

The *Maps* panel is used to load and manage raster and vector maps as well as database connections. Available formats are tif, jpg and png, bmp for raster maps, and shp, lin, ply, pnt, trp, ano, dxf, smh, dbf, dat, pow, xml, *.xls, *.xlsx, *.mdb, *.acdb. To open a connection to a geographical database, an *.fedb file needs to be loaded. In case of tabular data, the columns containing coordinate values have to be chosen at the time of import, unless they correspond to some defaults like X, Y and Z. The available supermesh (polygons, lines and points) of the current model is also displayed as map data in the panel.

By default, maps are sorted according to their format in the *Maps* panel. For more convenience especially in large projects, the tree structure can be customized according to the user's needs: The order of folders and maps within a folder can be changed by

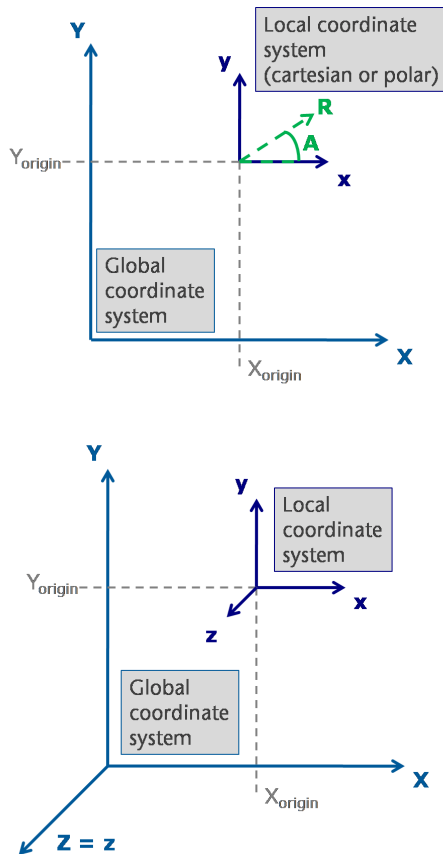


Figure 4.6 Global and local coordinates (2D/3D).

4. Working with Maps

drag and drop and maps can be moved to different folders. Existing folders can be renamed by pressing <F2> or via their context menu and new folders can be created via the context menu of the **Maps** panel or by clicking on the search icon at the top of the panel.

The search bar at the top of the Maps panel allows to filter map and folder names by a full-text search.

The relative map locations and all map settings can be exported to *.mre (FEFLOW map reference) files and thus easily be transferred between different FEFLOW models. Export is available for folders and maps, while the import option is limited to folders.

Map Layers

While raster maps already contain information about the display color for each pixel, this is typically not the case for features in vector maps. The display information for these kinds of maps is contained in so-called layers. When loading a map, FEFLOW creates a layer named **Default** with just one single style (color, line style, etc.) applied to all features in the map. The properties of the default layer can be edited, and additional layers can be added by using the functions in the context menu of the layer and the map. All layers of a specific map can be exported into an *.fml (FEFLOW map layer) file via the map's context menu. The map layer file can then be used to import all layers to the same or a different map in the same or a different FEFLOW model.

Map Properties

The properties of a map layer can be edited in the **Map Properties** panel which is opened via the context menu of the layer. Basic settings such as opacity, lighting options and 3D drawing options can be applied to all features of the map. The map can be classified based

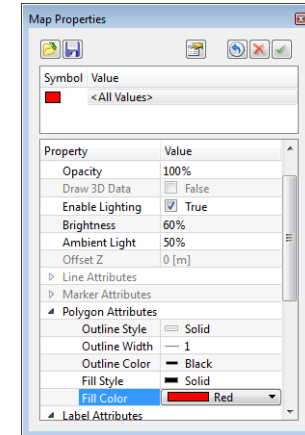


Figure 4.7 Map Properties panel.

on one of the attribute fields of the map either by applying a different style to each unique attribute value, or by partitioning the overall range of values of a numeric attribute into a number of classes. Predefined color palettes are readily available to be applied to the classes or unique values.

Color and other styles can also be edited manually for any individual class or for a selection of multiple classes.


Via the context menu of a map layer, all styles can be exported into an *.fms (FEFLOW map style) file and imported again for a specific map layer.

4.5 Map Data


Vector maps or databases can be applied as a basis for data assignment or data regionalization, deriving the basic data directly from the map file. For details on

the assignment of map data, please refer to chapter 10 of this User Manual.

Map Table

The attribute data of vector maps or database files can be shown via  **Show Map Table...** in the context menu of a map. The **Map Table** dialog will display the different records and attribute data contained in the map in tabular format.

Map Data Selection/Map Joining



Besides using the entire data range provided in a map, it is possible to use only selected map data. To limit the data range of a map, SQL selection statements on attribute data can be used via  **Join/Select Map(s) Data...** in the context menu of a map.

The option **Join/Select Map(s) Data...** also provides the possibility to join additional data tables to a map, using a common identifier in both tables.


For tables imported from a geographical database, the context menu of the table header in the **Join Maps** dialog can be used to display the defined relationships with other tables of the database. Selecting a defined relationship automatically imports the corresponding table and relation.

4.6 Map Export

All the model properties and results can be exported to different kinds of map files, retaining the geographical reference of the model.

Export of parameters is invoked via the context menu of the parameter in the  **Data** panel, or via the context menu of the parameter in the  **View Components** panel. Both export for the entire model domain and for the selected geometries or the values in the cur-

rent slice/layer only are supported. In a results (*.dac) file, process-variable results can be exported for the current time step or for all or a selection of time steps.


Visualization options such as isolines or fringes can be exported to a map file via the context menu of the visualization style in the  **View Components** panel.

Exported maps can automatically be loaded to the **Exported Maps** section within the **Maps** panel of the current FEFLOW model.



Quick Parameter Import

The **Quick Import** option can be used to assign data of a previously exported map to several parameters at once without the need for defining parameter links via the **Parameter Association** dialog first. The import can be limited to specific model parameters and/or to the current slice/layer or the current selection. To match the input data to the mesh elements or nodes, different selection methods are available. A detailed description of this import option and a tutorial are provided in chapter 10.

4.7 Tutorial


In the following exercises we want to get familiar with the handling of maps in the FEFLOW workspace. The most important tool in this context is the  **Maps** panel which is used to load and manage maps.

As a first exercise, we load a number of maps of different formats that could be used to set up a supermesh.

Start with an empty FEFLOW project. In the **New FEM Problem** dialog choose the second option and click on  **Finish**. In the import + export folder, select the file **SimulationArea.jpg** that is used as a background map for orientation. The map now appears as Geo-JPEG in the  **Maps** panel. Double-click on

4. Working with Maps

this entry to add the map to the active view.

Next, load some further maps that contain information on the model site. Click on the  search icon in the **Maps** panel and choose **Add Map(s)...** Select the files

- **demo_wells.pnt**
- **model_area.shp**
- **rivers.shp**
- **sewage_treatment.shp**
- **waste_disposal.shp**

We can either load the maps one by one or import them all at once by pressing the <Ctrl> key while we select the maps.

Depending on the respective file formats, the maps now appear in different tree branches in the **Maps** panel, together with a **Default** (layer) entry that FEFLOW creates automatically. Add all maps to the active view with a double-click on their **Default** entry.

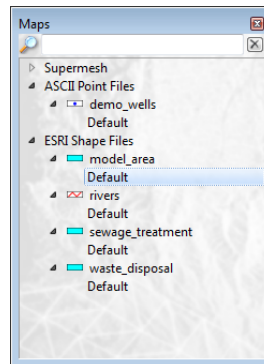


Figure 4.8 Maps panel.

Maps that have been added to the active view also appear in the **View Components** panel. Here, maps can be switched on and off temporarily via the check boxes. Their drawing order follows the tree structure of

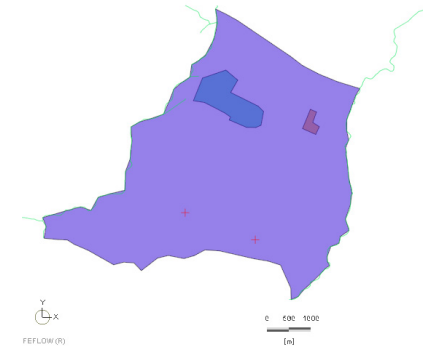









Figure 4.9 Maps displayed in the active view.



the **Maps** panel but it can be changed by dragging maps with the mouse cursor to another position within the folder or by dragging entire folders to a different position within the tree. If not all of the loaded maps are visible in the **Supermesh** view change their order in the **View Components** panel to bring maps covered by others to the surface.

We change the sorting within the **Maps** panel by creating new folders and moving several maps to a different folder location.




Click on the  search icon at the top of the **Maps** panel and select **Create Folder**. Enter **Contamination sources** as a new name and hit **Enter**. The new folder now appears as the first entry after the **Supermesh** maps. Select both the **sewage_treatment** and **waste_disposal** maps while keeping the <Ctrl> key pressed and move the maps to the new folder via drag and drop. Next, click on **ESRI Shape Files**, press <F2> and rename the folder to **Model geometry**. Move the map **demo_wells** to this renamed folder and then delete the now empty folder **ACII Point Files** by clicking on it and hitting



. Confirm the deletion with **Yes**.

To store all settings of the  **Maps** panel in a map-reference file, click on the  search icon and select  **Export Map Reference(s)...** Enter `maps` as name for the *.mre file and confirm with <Enter>. Now delete all loaded maps via  **Remove All Maps** in the context menu of the panel. After confirming with Yes, the maps are removed from the **Supermesh** view and the  **Maps** and  **View Components** panels.



The maps and all settings can now easily be imported again via the previously exported map-reference file. Select  **Import Map Reference(s)...** from the context menu of the  **Maps** panel and load the file **maps.mre**. The maps and our user-defined folder structure are now automatically reimported. Double-click on each of the default entries again to display the vector maps in the active view.


4.7.1 Map Layers

The map *model_area* defines the outer boundary of the model area. To change the style of the **Default** layer of this map make a right-click on **Default** in the  **Maps** panel and select  **Edit Properties** from the context menu. In the upper part of the  **Map Properties** panel that now opens click on <All Values> and go to **Polygon Attributes**. Change the fill color of the polygon and also the outline style. Confirm the new settings with the **Apply Changes** button and close the panel.

For the next map *sewage_treatment* we create a new layer besides the already existing default layer. Open the context menu of this map with a right-click and select  **Create Layer**. A new entry **Layer 1** is now added to the tree of this map. Open the  **Map Properties** panel for this layer as previously described

and click again on <All Values>. Change the fill color and the outline style of the polygon and also the opacity and confirm the settings with a click on **Apply Changes** before closing the panel.



Double-click on **Layer 1** in the  **Maps** panel to add this layer to the active view. You can switch between different layers of a map using the check boxes in front of these layers in the  **View Components** panel. The last one activated is always the uppermost layer. Figure Figure 4.9 gives an example for a certain style of the imported maps.

The remaining maps that we have loaded contain spatial information on rivers and wells, i.e., line and point structures. To enhance the appearance of the rivers in the active view we change width and color of the line, again using the  **Map Properties** panel for the **Default** layer of the map *rivers*.

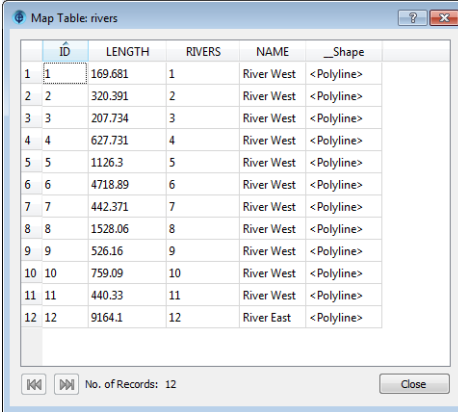
For the map *demo_wells* the style settings of the markers and for the labels can be edited separately.

4.7.2 Map Data

Instead of showing both rivers contained in the map *rivers*, we only want to plot the eastern one. To do so, we use a SQL selection statement on the attribute field **NAME** of the map to create a data selection that is limited to the river in the east.

Open the context menu of the map *rivers* with a right-click on the map and select  **Show Map Table...** to display the attribute data of the map in tabular format (see Figure 4.10). For the attribute field **NAME** two different data sets exist, **River West** and **River East**. Close the **Map Table** dialog and now choose  **Join/Select Map(s) Data...** to open the **Join Maps** dialog. In the input field of **Select record where** enter `NAME="River East"` as SQL selection statement

4. Working with Maps



ID	LENGTH	RIVERS	NAME	_Shape
1	169.681	1	River West	<Polyline>
2	320.391	2	River West	<Polyline>
3	207.734	3	River West	<Polyline>
4	627.731	4	River West	<Polyline>
5	1126.3	5	River West	<Polyline>
6	4718.89	6	River West	<Polyline>
7	442.371	7	River West	<Polyline>
8	1528.06	8	River West	<Polyline>
9	526.16	9	River West	<Polyline>
10	759.09	10	River West	<Polyline>
11	440.33	11	River West	<Polyline>
12	9164.1	12	River East	<Polyline>

Figure 4.10 Map Table dialog for the map rivers.

to select the map data for the eastern river only. Make sure to enter the name with a capital R and E as the SQL syntax is case sensitive.

To ensure that the syntax is correct click on **Bu Preview**. The map table now only shows one record for the **River East** and reflects a reduced data selection according to the SQL statement. Leave the **Map Table** dialog with **Bu Close** and the **Join Maps** dialog with **Bu OK**. The active view now also reflects the reduced map data set by only displaying the eastern river.

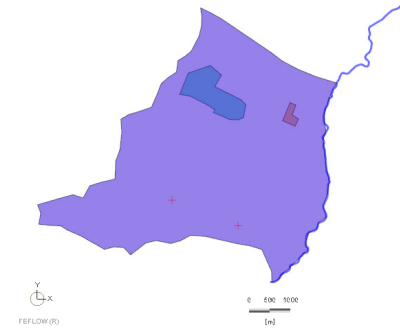


Figure 4.11 Map Rivers after Select Map(s)

5

Supermesh Design

Setting up the framework for mesh generation

5.1 What is a Supermesh?

The so-called *Supermesh* in FEFLOW forms the framework for the generation of a finite-element mesh. It contains all the basic geometrical information the mesh generation algorithm needs.

While in the very simplest case the *Supermesh* only defines the outline of the model area, i.e., consists of one single polygon, the concept offers many more possibilities: *Supermeshes* can be composed of an arbitrary number of polygons, lines and points. Their respective features and purposes are described in the following sections.

5.1.1 Supermesh Polygons

A subdivision of the model area into a number of separate polygons can be useful for a number of reasons:

- Finite-Element edges will honor the polygon boundaries, allowing for example an exact zoning of parameters and setting of boundary conditions in exact locations later.

- The required density of the finite-element mesh can be specified for each polygon.
- The polygons can be used for parameter assignment and results evaluation later.

5.1.2 Supermesh Lines

Lines in the *Supermesh* are applied to represent linear structures in the finite-element mesh to be created. Their advantages include:

- Finite-element edges will honor the line, providing for example the basis for later applying the boundary condition for a river exactly along the river axis.
- The mesh may be automatically refined during mesh generation along the line.
- The lines can be used for parameter assignment and results evaluation later.

5.1.3 Supermesh Points

Points in the *Supermesh* are typically placed in the locations of production or injection wells or in observation locations. They make sure that a finite-element node is set at exactly this location during mesh genera-

5. Supermesh Design

tion, they allow a local mesh refinement around the point, and they can be used for parameter assignment, e.g., to set the boundary condition for a pumping well.

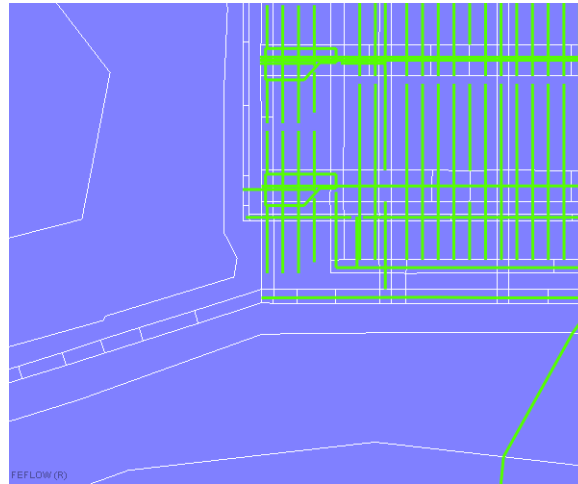


Figure 5.1 Example for a Supermesh detail.

5.2 Editing Supermesh Features

Sets of polygons have to fulfil some requirements:

- No overlapping polygons are allowed.
- No polygons can be entirely contained by another polygon.

The user-interface tools ensure that these requirements are met at any time. Internal holes in the supermesh are possible. They are indicated by another color for the internal boundary (Figure 5.2).

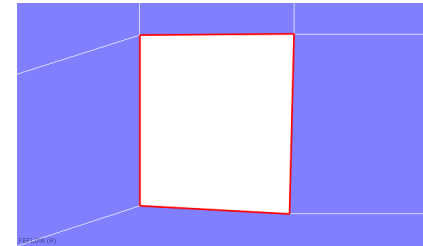


Figure 5.2 Inner Supermesh border.

The *Mesh-Editor* toolbar provides the tools to digitize and edit *Supermesh* polygons, lines, and points.

In *Move Node* mode, both the originally digitized nodes and smaller nodes in between can be moved. Moving the small nodes results in curved polygon edges (parabolic or circular shape) that are typically applied to curved structures such as borehole edges or pipe walls in small-scale models.

When digitizing a polygon next to an existing one, the editor will automatically follow the existing polygon boundary to close the new polygon (Figure 5.3).

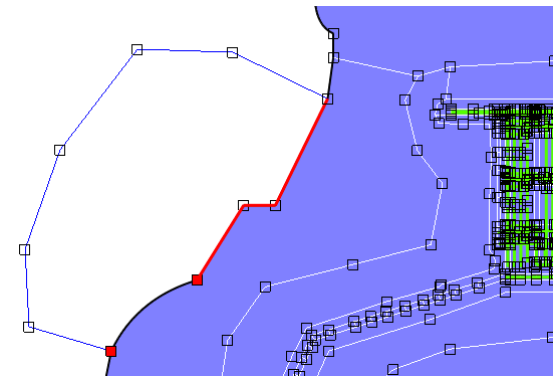


Figure 5.3 Follow existing boundaries.

5.3 Converting Map to Supermesh Features

Instead of digitizing *Supermesh* features on screen, they can be imported from background maps. This is done via the **Convert to Supermesh** entry in the context menu on the name of the map file in the *Maps* panel.

All features of the map (or all selected features when applying an SQL selection query on the map) are converted to supermesh features using this approach. Polygons that would overlap with already existing polygons are not converted.

5.4 Export of Supermesh Features

Once a finite-element mesh has been generated, all *Supermesh* features (points, lines, polygons) are displayed in the *Maps* panel. The export of *Supermesh* features as maps is available via the context menu of the *Supermesh* entry or of the respective *Supermesh* features in the *Maps* panel.

5.5 Tutorial

5.5.1 Tools





All of the tools that are used in this exercise are located in the  **Mesh-Editor** toolbar.





Figure 5.4 Mesh-Editor toolbar.

5.5.2 Polygons, Lines and Points

To get some hands-on training in supermesh design we design a first supermesh that consists of a single polygon.

Open an empty FEFLOW project with a click on  **New** and specify the initial mesh extent to define the initial area for mesh design. In the **New FEM Problem** dialog choose  **Manual input of the initial domain bounds** and accept the default extent with  **Finish**. The domain bounds have now been set to 100 m x 100 m.

Now, click on  **Add Polygons** in the  **Mesh-Editor** toolbar in the upper left of the window. Set polygon nodes with a left-click in the *Supermesh* view window and finish by clicking on the first node of the polygon again. The finished polygon appears shaded in grey.

Now, add a second polygon that adjoins the first one. Pay attention to how the mouse cursor symbol changes depending on its position in the *Supermesh* view: The cross-hairs cursor indicating that polygon nodes can be set only appears outside the existing polygon. This makes sure that only non-overlapping polygons are created. Clicking inside the polygon FEFLOW does not create a new node. Place the first node of the new polygon on the edge of the existing polygon, continue with some more nodes and set a last node on the polygon edge again. To finish the polygon, use the autoclose function by double-clicking on the last node. FEFLOW now automatically closes the polygon along the existing polygon edge.

5. Supermesh Design

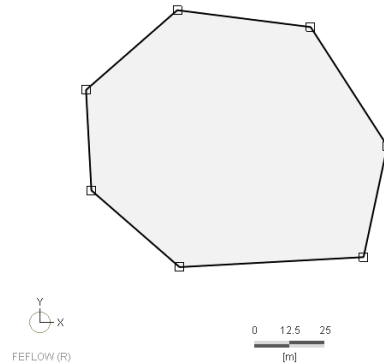


Figure 5.5 A finished polygon in the Supermesh view.

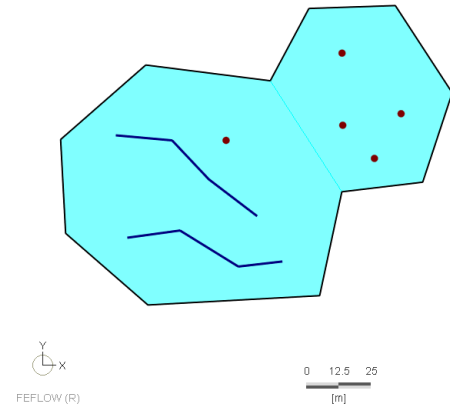











Figure 5.6 Polygons selected for joining.



Also, add some line and point features to the supermesh, using the  **Add Lines** and  **Add Points** tool. Finish a line with a double-click on the last node.

The polygons that we have created can be merged with the  **Join Polygons** option. First, both polygons need to be selected. Activate the  **Select in Rectangular Region** tool in the  **Mesh-Editor** toolbar and click into both polygons while holding <Ctrl>. The selected polygons are now highlighted in turquoise. Now the  **Join Polygons** button in the  **Mesh-Editor** toolbar is activated. Click this button to merge the two polygons.

Polygons, lines and points that have been misplaced can also be deleted. Activate one of the selection tools available in the drop-down list that opens with a click on the small arrow next to  **Select in Rectangular Region**. Click on the merged polygon (if it is not still selected). Then simply press the key to remove the polygon. You may try the same with one or several of the lines or points.

 Unlike other toolbars, the **Pin Coordinates** toolbar cannot be opened via the **View** menu or a context menu. It is called by pressing <F2> whenever the chosen tool supports direct coordinate input.

5.5.3 The Pin Coordinates Toolbar

Polygon nodes can also be positioned exactly. In the next step, we design a square polygon with the dimensions of **100 m x 100 m**. First, select all remaining polygons, lines and points and press to delete them. Next, click  **Add Polygons** and press <F2>. The  **Pin Coordinates** toolbar appears. Insert 12^3 **0,0** to set the first node and press <Enter>. In the same way, enter the coordinates of the remaining three nodes of the polygon. To finish the polygon, enter the coordinates of the first node again or simply click on it.

If one or several nodes are misplaced while a line or a polygon is drawn, the last node(s) can be deleted by clicking on a previous node of the same line or polygon.

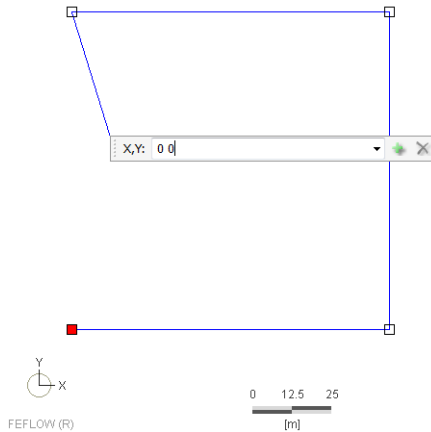


Figure 5.7 Using the Pin Coordinates toolbar.

5.5.4 Supermesh Import via Maps

In the next step we do not design a supermesh manually on screen but import the supermesh features from a map. Start an empty FEFLOW project and in the *New FEM Problem* dialog, select the second option to define the initial work area via imported maps. Click on **Bu** *Finish* and in the file selection box select the files

- **demo_wells.shp**
- **model_area.shp**
- **sewage_treatment.shp**
- **waste_disposal.shp.**

These maps are now displayed under ESRI Shape Files in the **Maps** panel. Double-click on the entry

Default of each map to make all of them visible in the *Supermesh* view. Figure 5.8 shows the loaded maps in the *Supermesh* view.

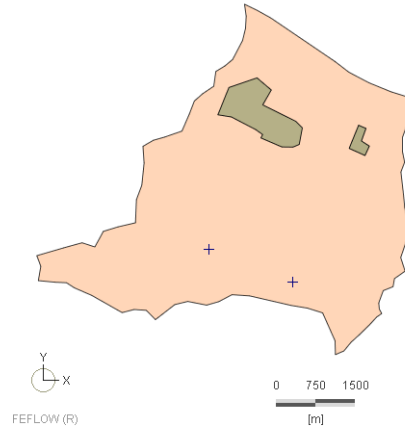






Figure 5.8 Maps displayed in the Supermesh view.

First we want to create a polygon that describes the total model area. We import this polygon from the map *model_area*. Open the context menu of this map with a right-click and select **Convert to > Supermesh Polygons**. When we click on the **Add Polygons** button in the **Mesh-Editor** toolbar, the imported polygon becomes visible.

In addition to this polygon we want to include two well locations as points in our supermesh. The workflow to import these points is completely analogous to the polygon import. The map *demo_wells* contains the well locations. Right-click on this map to open its context menu and select **Convert to > Supermesh Points**. The two well locations are now visible as red points in the *Supermesh* view.

As a last step we want to include the two contami-

5. Supermesh Design

nation sites in the supermesh. These cannot be imported from a map via the  **Convert to** option as this would lead to overlapping polygons. Instead, we will split the existing polygon and cut out the contamination sources. Start with the eastern source of contamination. Click on  **Split Polygons** and select the map **waste_disposal** from the dropdown list in the  **Mesh-Editor** toolbar. To digitize the contamination source accurately we can use a tool that snaps to the fixed points of this map. To activate the snapping click on  **Snap to Points** right next to the dropdown list.

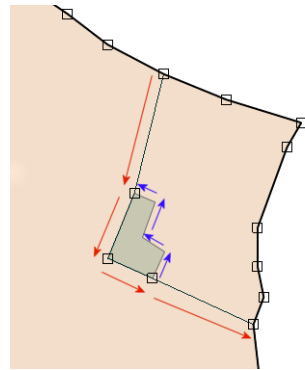



Figure 5.9 Polygon splitting along contamination site.

Polygon splitting must start and end at an already existing polygon border. As the contamination sources are located completely inside the model area two cuts are necessary. Start on an arbitrary point on the model boundary and go halfway around the contamination source. To complete the first cut, return to the model boundary on the other side (see figure 5.9). Complete the polygon with a second cut along the missing parts of the contamination source polygon.

Complete the supermesh by creating the polygon for the second contamination source in the same way, this time selecting **sewage_treatment** from the dropdown list in the  **Mesh-Editor** toolbar.

An exemplary finished supermesh setup is shown in figure 5.10.

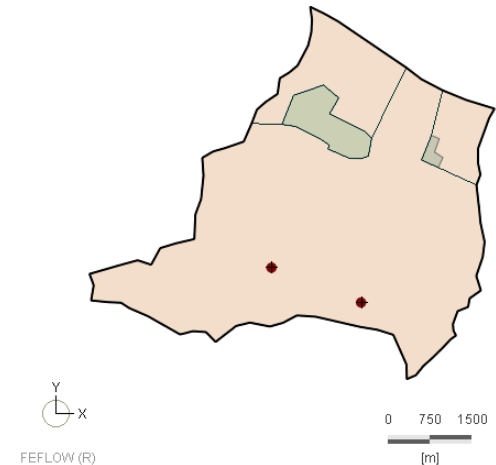


Figure 5.10 Completed supermesh.

Finite-Element Mesh

Obtaining a suitable spatial discretization of the model domain

6.1 Spatial Discretization

This section describes the generation of finite-element meshes. During the simulation, results are computed on each active node of the finite-element mesh and interpolated within the finite elements. The denser the mesh the better the numerical accuracy, and the higher the computational effort. Numerical difficulties can arise during the simulation if the mesh contains too many highly distorted elements. Thus some attention should be given to the proper design of the finite-element mesh. For transport simulations, the Péclet criterion can be useful for determining the required mesh density. The *Péclet Number* is available as elemental distribution in *Auxiliary Data* in the *Spatial Units* panel. To assist in creating a well-shaped mesh, FEFLOW offers various tools, including local refinement and derefinement of the mesh and (selective) mesh smoothing. Local refinement during mesh generation will typically lead to a better mesh quality than later subdivision of elements.

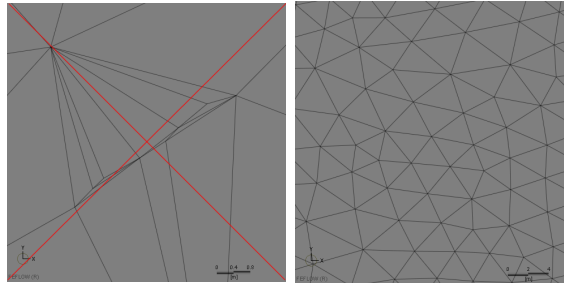


Figure 6.1 Examples for bad and good mesh geometry.

6.2 Mesh Generation Process

FEFLOW supports either triangular or quadrangular finite-element meshes. A separate toolbar is available to support the mesh generation process. The generation is generally based on the input of an approximate number of finite elements to be generated. The desired mesh density of each supermesh polygon can be edited separately.

Different algorithms for the mesh generation are

6. Finite-Element Mesh

provided, all of them with their specific options and properties. Some algorithms can consider also lines and points in the supermesh and allow a local mesh refinement at polygon edges, lines and points.

Mesh generation is typically a trial-and-error process. The user hereby iteratively optimizes element numbers, generator property settings and—if necessary—the supermesh until a satisfactory mesh is obtained.

Significant effort can be involved in mesh generation, especially in cases with a large number of geometrical constraints (many polygons, lines and points). In typical cases, however, the effort required for generating a good finite-element mesh saves time at later stages of the modeling process due to reduced risk of instabilities.

6.3 Mesh Generation Algorithms

There are many different strategies for the discretization of complex domains into triangles or quad elements. As each has its specific advantages and disadvantages, FEFLOW supports three different algorithms for triangulation and one for quad meshing.

6.3.1 Advancing Front

Advancing Front is a relatively simple triangular meshing algorithm that does not support any lines or points in the supermesh. If present, they are simply ignored in the generation process. Its main advantages are its speed and its ability to produce very regularly shaped elements.

6.3.2 GridBuilder

GridBuilder—developed by Rob McLaren at the University of Waterloo, Canada—is a flexible triangulation algorithm. *GridBuilder* supports polygons, lines and points in the supermesh as well as mesh refinement at points, lines, or supermesh polygon edges.

6.3.3 Triangle

Triangle is a triangulation code developed by Jonathan Shewchuk at UC Berkeley, USA. It is extremely fast, supports very complex combinations of polygons, lines and points in the supermesh, allows a minimum angle to be specified for all finite elements to be created, and provides the means for local mesh refinement with a maximum element size at lines or points of the supermesh.

FEFLOW provides a convenient interface to *Triangle*, which can be freely downloaded from the developer's website. Please refer to the FEFLOW help system for a detailed description of the process to enable *Triangle* in FEFLOW. Free use of *Triangle* is based on conditions defined in a usage agreement available in the FEFLOW help system and from the *Triangle* website.

6.3.4 Transport Mapping

Transport Mapping is the algorithm used in FEFLOW for generating meshes of quadrilateral elements. This option requires that the quad meshing option in the *Mesh* menu is selected and that all supermesh polygons have exactly four nodes.

Lines and points in the supermesh are ignored when generating quadrilateral meshes.

6.4 Mesh Import from Maps

The finite-element mesh geometry cannot only be generated from scratch, but it can also be imported from maps via **Import Mesh...** in the **File** menu. This is especially useful if the area of an existing model has to be extended and the user does not wish to start over with a completely new model.

It is possible to import an arbitrary number of maps and to combine them to a new 2D finite-element mesh. All maps have to contain either triangular or quadrilateral elements, a mixed geometry is not possible. Furthermore, polygons in the imported maps must not overlap, and nodes at common boundaries have to be identical in number and location.

6.5 Mesh Editing

Some specific modifications of the finite-element mesh are possible at any time after mesh generation, even after model parameterization:

- Mesh refinement by element subdivision
- Mesh derefinement (after previous refinement)
- Splitting of quad elements into triangles
- Smoothing of the mesh at selected node locations or of the entire mesh
- Flipping element edges
- Moving nodes within the area of the surrounding elements

All the mesh-editing functionality is contained in the **Mesh-Geometry** toolbar.

6.6 Mesh-Property Check

FEFLOW provides some basic tools to check the properties of a finite-element mesh, which are accessi-

ble via **Auxiliary Data** in the **Data** panel. The following parameter distributions can be shown in the currently active view:

- Max. interior angle of triangles
- Delaunay criterion violations

For 3D models, two additional distributions are available:

- Slice distance
- Layer thickness.

For transport models, FEFLOW provides an additional distribution which is calculated and updated at each time step during the simulation:

- Péclet Number.

Distances and areas in **Slice** and **Supermesh** views and distances in **3D** views can be measured using the **Measure** tool. If the **Supermesh** is the active view, the **Measure** tool is located in the **Mesh-Editor** toolbar. For active **Slice** views, the tool is accessible via the **Inspection** toolbar.

6.7 Mesh-Element Deactivation

By default all mesh elements are active and results are computed at each mesh node. Using the **In-/active Elements** parameter in the **Geometry** section of the **Data** panel, elements can be deactivated for the entire simulation period or only for specific time steps during a simulation run. In case that all elements surrounding a mesh node are inactive, FEFLOW does not compute results at these specific node locations.

With this option, time-varying geometries as well as impermeable structures can easily be simulated.

In 3D models, the parameter **In/outflow on top/bottom** is applied to the first set of active elements if elements within the top layer are set to inactive. This

6. Finite-Element Mesh

ensures that assigned recharge or evapotranspiration values are passed on to deeper locations of the model domain correctly.

6.8 3D Discretization

For 3D models, FEFLOW applies a layer-based approach. The triangular or quadrangular mesh is extended to the third dimension by extruding the 2D mesh, resulting in prismatic 3D elements. In FEFLOW terminology, all (typically) horizontally adjacent 3D elements comprise one layer, while a slice is either the interface between two (typically) vertically adjacent layers or the top or bottom of the model domain. All mesh nodes are located on slices.

The extension of a 2D model to a 3D model is facilitated by the **3D Layer Configuration** dialog that is accessed via the **Edit** menu. Initially defined layers are plane. Real elevations are assigned like a process variable for each node as discussed in chapter 10.

All the layers in 3D models have to be continuous over the entire model domain. Thus model layers representing lenses or pinching-out stratigraphic layers have to be continued to the model boundary. Typically, they are then assigned a small thickness and the properties of the layer immediately above or below.

3D model setup is in most cases based on a vertical extension of a horizontal mesh. For applications such as modeling of dams where a high level of detail is needed vertically, but less along the horizontal axis, the mesh can be generated in vertical projection and extended horizontally. In the latter case, the y axis in FEFLOW points in the direction opposite to gravity,

similar to a 2D cross-sectional model.

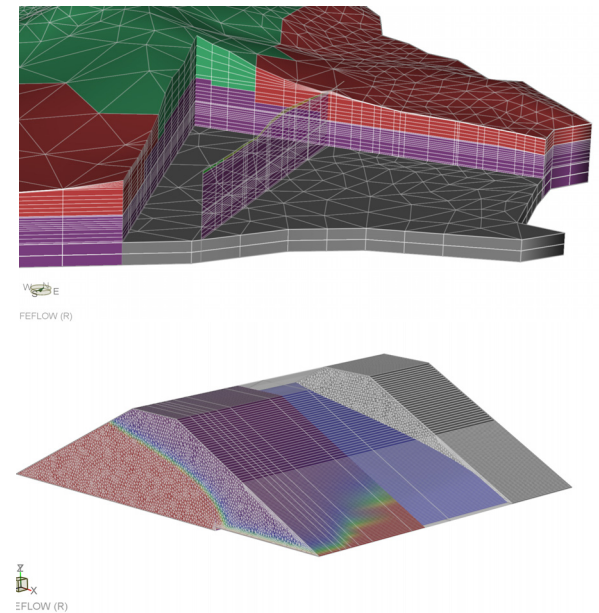


Figure 6.2 Horizontal and vertical layering approaches.

The **3D Layer Configuration** dialog also provides tools to add or remove layers from existing models, and to change layer thicknesses globally. The **Validate** option allows to verify slice elevations with respect to a certain minimum slice distance. Model properties of new layers can be conveniently inherited from already existing layers.

6.9 Geotransformation


FEFLOW expects all attached maps and the model itself to share the same coordinate system. Maps using differing coordinate systems can be transformed in

advance using the external software WGEO, which is part of the FEFLOW software package.

In case that a geotransformation of the model itself is necessary, the *Geographic Transformation* option in the *Mesh-Geometry* toolbar can be used.

6.10 Tutorial

6.10.1 Tools

All of the tools used in these exercises are located in the  *Mesh-Generator* toolbar

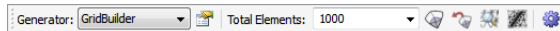


Figure 6.3 Mesh-Generator toolbar.

and in the  *Mesh-Geometry* toolbar.



Figure 6.4 Mesh-Geometry toolbar.


Some mesh-editing options also require the tools of the  *Selection* toolbar.




Figure 6.5 Selection toolbar.

The first drop-down list in the toolbar gives access to the available selection tools. The third drop-down list allows to switch between different target geometries (nodes, elements, edges, faces) for selections.

6.10.2 Mesh Generation

6.10.2.1 Triangulation

To get some hands-on experience in how the available mesh-generator algorithms work we apply the three different mesh generators on the same supermesh and study the resulting finite-element meshes.

First, click on  *Open* to load the supermesh file **mesh.smh** from the supermsh folder. This supermesh consists of two polygons, one line and three point features.

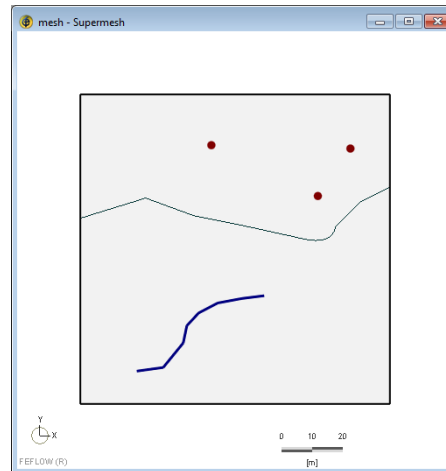





Figure 6.6 Supermesh.

Start with the *Advancing Front* algorithm which can be selected from the generator list of the  *Mesh-Generator* toolbar.

Enter a *Total Number* of  2000 elements in the input field and click on  *Generate Mesh* to start the mesh-generation process. A new window, the *Slice*

6. Finite-Element Mesh

view, opens with the resulting finite-element mesh.

As figure 6.7 shows, *Advancing Front* ignores the line and point features which are included in the super-mesh.

Now, use the same supermesh to generate a finite-element mesh with the *GridBuilder* algorithm. Click in the *Supermesh* view to make the **Mesh-Generator** toolbar visible again and select *GridBuilder*. Without any further changes simply click on **Generate Mesh**.

The resulting finite-element mesh looks similar to the one created with the *Advancing Front* algorithm, except that polygon edges, lines and points are now honored by the mesh.

As a next step, we will refine the mesh around the point and line features. First, activate the *Supermesh* view with a click. The refinement settings are located in the **Generator Properties** dialog in the **Mesh-Generator** toolbar.

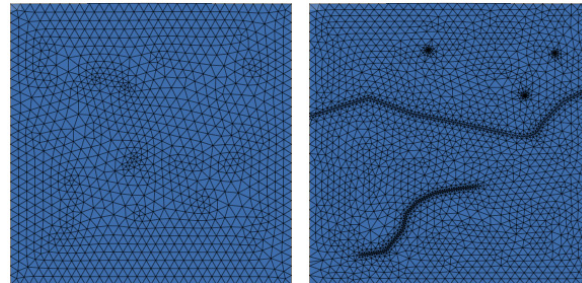


Figure 6.7 Advancing Front and GridBuilder.

Open the dialog and activate a refinement for all three geometrical features. For polygon edges, choose a refinement level of **5**, for lines a level of **8**, and for points a gradation of **10**. Make sure that the option *Apply to SELECTED polygon edges or line segments*

is activated before you leave the dialog.

To select the elements to be refined go back to the *Supermesh* view and click on **Refinement Selection**. Click on all segments of the line and of the edge that separates the two polygons. The selected edges are shown in green. Then click on **Generate Mesh** again. The resulting finite-element mesh with local refinement is shown in figure 6.7.

Next, we will apply the *Triangle* algorithm to generate a finite-element mesh.

Choose *Triangle* from the generator list in the **Mesh-Generator** toolbar. Open the **Generator Properties** dialog and activate refinement for polygon edges, line and point elements with the following settings:

Refinement around **SELECTED** polygon edges

- Polygons: gradation: 5, target element size: 1.0 m
- Lines: gradation: 3, target element size: 0.5 m
- Points: gradation: 3, target element size: 0.5 m
- Leave the dialog and use the **Refinement Selection** tool to select the edge between the two polygons in the *Supermesh* view. Clicking on



Generate Mesh should now produce a finite-element mesh that looks similar to the one on the left in figure 6.8.

Separate Editing of Polygons

For every supermesh polygon the mesh density can be defined separately while the total number of elements remains constant. Go to the *Supermesh* view and activate the tool **Edit Meshing Density** in the **Mesh-Generator** toolbar. FEFLOW now automatically selects a polygon for which a meshing-density factor can be specified. Start with the proposed polygon and enter a factor of 1^{23} **10**. After hitting <Enter> the number in the input field turns red, indicating that



The *Triangle* mesh generator engine is not provided with FEFLOW! For details about how to obtain the *Triangle* mesh generator, see the FEFLOW help system.

the meshing density for this polygon has been modified. Proceed with the second polygon. Select it with a single click and enter a density factor of $10^3 \cdot 2$ in the input field. Hit <Enter> again and start the mesh generation with a click on  **Generate Mesh**. The right mesh in figure 6.8 shows the resulting finite-element mesh. To reset the meshing density factors to the default value of 1, click on  **Reset Meshing Density**.

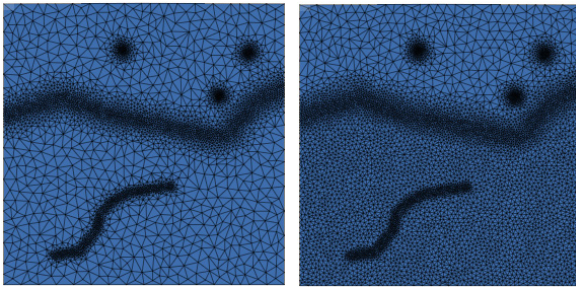





Figure 6.8 Meshes generated with the Triangle algorithm.

6.10.2.2 Quad Meshing

A finite-element mesh with quadrilateral elements can be generated using the **Transport Mapping** algorithm.

We load a new file which is similar to the one used for the triangulation exercises, except this supermesh consists of only one polygon that has exactly four nodes. Click on  **Open** and load the file **quad-mesh.smh**. **Transport Mapping** requires supermesh polygons with exactly four nodes. Lines and points are ignored in the mesh-generation process.

To enable the quad meshing option go to  **Mesh** and activate  **Quadrilateral Mode**. Select **Transport**

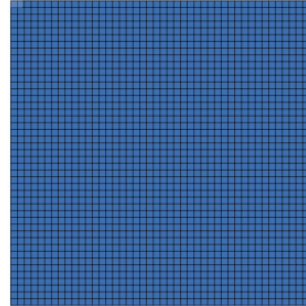


Figure 6.9 Quad mesh.


Mapping in the  **Mesh-Generator** toolbar, enter a **Total Number** of $10^3 \cdot 2000$ elements and click on  **Generate Mesh** to start the meshing process.

The resulting finite-element mesh is shown in figure 6.9.

6.10.3 Editing the Mesh Geometry

6.10.3.1 Triangular Meshes




For this exercise load the file **triangle.fem**.



The geometry of the finite-element mesh can be edited after the mesh-generation process has been finished. All the necessary tools are located in the  **Mesh-Geometry** toolbar.

It is possible to refine the mesh globally (entire mesh) or locally (only selected parts). A derefinement option for previously refined parts of the mesh is also available.


If we want to apply local mesh refinement we have to select a target area first. Make sure that the **Slice** view is the active view. All necessary selection tools

6. Finite-Element Mesh

can be found in the  **Selection** toolbar. To create an element-based selection choose  **Select Elements** from the drop-down list of target geometries. Then, activate  **Select in Rectangular Region** tool from the drop-down list of selection tools to draw a rectangle around the line feature.

Now click on  **Refine Elements** in the  **Mesh-Geometry** toolbar. Each selected element is subdivided into four elements. The result is shown in figure 6.10.

The derefinement tool is used similarly; however, only those parts that were previously refined can be derefined.

Elements can also be deleted from the finite-element mesh. Select a couple of elements and click on  **Delete Elements** to cut out these elements. On the right hand side of figure 6.10 a (purely illustrative) example for a mesh with deleted elements is shown.

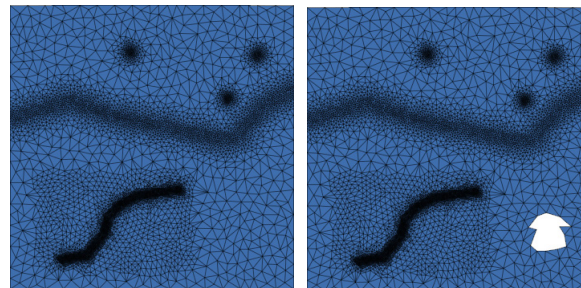







Figure 6.10 Refinement and deleted elements.

 If elements are set to active or inactive via map assignment, the active or inactive status needs to be expressed by numeric values: 1 for active and 0 for inactive.

To deactivate elements during the simulation we use the parameter **In-/active Elements** in the **Geometry** section of the  **Data** panel. Double click on **In-/active Elements** to set this parameter active and use the tool  **Select in Rectangular Region** to create an element selection. Make sure that the input field of the

 **Editor** toolbar shows the setting *inactive* and click on  **Assign** to set the selected elements to inactive. The result is shown in figure 6.11.

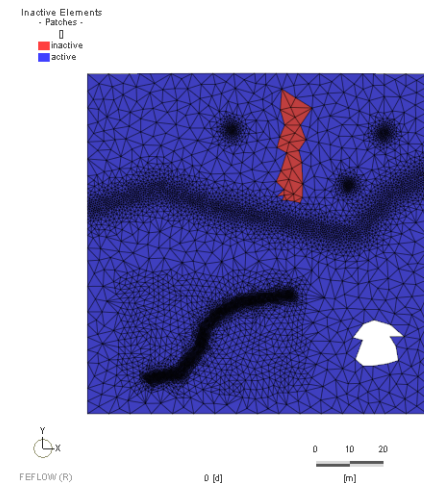








Figure 6.11 Active and inactive mesh elements.

Mesh smoothing can produce more regularly shaped elements and reduce the number of obtuse-angled triangles. To use the  **Smooth Mesh** tool in the  **Mesh-Geometry** toolbar, the nodes which are allowed to be moved during the smoothing process have to be selected first. Activate  **Select Nodes** in the  **Selection** toolbar and draw again a rectangle around the line feature. Click on the  **Smooth Mesh** tool that is now active and clear the selection with a click on  **Clear Selection**. Figure 6.12 shows the selected mesh location before and after the smoothing.

6.10.3.2 Quad Meshes

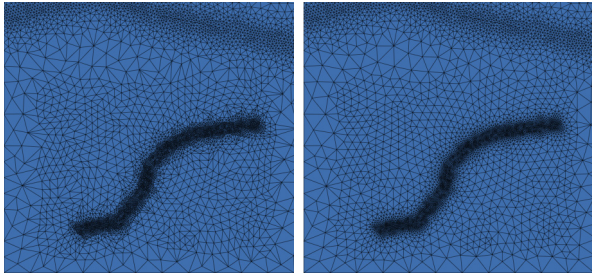


Figure 6.12 Mesh before and after smoothing.

To check for obtuse angles and triangles violating the Delaunay criterion, we use the tools provided in *Auxiliary Data* in the **Data** panel. First, double-click on *Max. interior angle of triangles* to show obtuse-angled triangles in the active view. Pay attention to how the angle distribution changes when we click on **Undo** in the **Standard** toolbar to return to the unsmoothed mesh. Next, double-click on *Delaunay criterion violations* and then click on **Redo** in the **Standard** toolbar to return to the smoothed mesh again. Both distributions indicate that the mesh smoothing has significantly improved the mesh quality.

Use the **Move Node** tool in the **Mesh-Geometry** toolbar and drag a mesh node to change its position within the mesh. Also, use **Flip Edge** and click on an element edge to change the subdivision of two adjacent triangles. Edge flipping will freeze the mesh so that derefinement of previously refined areas will no longer be possible.

Click on **Open** to load the file **quadmesh.fem** for this exercise.

Except for the derefinement and the flip edge tool all editing options are also available for quad meshes.

As an additional option, quad meshes can be transformed into triangular meshes. Four different triangularization methods are available of which we will use one. Select the method **Four Triangles around Center** from the drop-down list in the **Mesh-Geometry** toolbar to subdivide every quad element into four triangular elements. The resulting finite-element mesh is shown in figure 6.13.

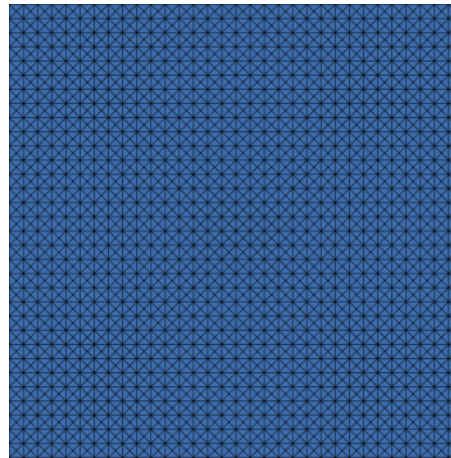




Figure 6.13 Refined quadmesh.

6. Finite-Element Mesh

6.10.4 Extending a Model to 3D

After the model has been discretized in 2D we now extend it to a 3D model. Click on  **Open** and load the file **triangle.fem** for this exercise.

To perform the extension to a 3D model, go to the  **Edit** menu and open the **3D Layer Configuration** dialog. The table on the left displays the number of slices and layers, and also the elevation of each slice.

The 3D model shall consist of 3 slices and 2 layers and the top slice shall be located at an elevation of **5 m**.

To set the elevation of the top slice, enter **5** in the **Elevation** input field and hit <Enter>. Increase the number of slices to **3** and hit <Enter>.

The table now shows 3 slices with elevations of **5 m**, **4 m** and **3 m** (see Figure 6.14).

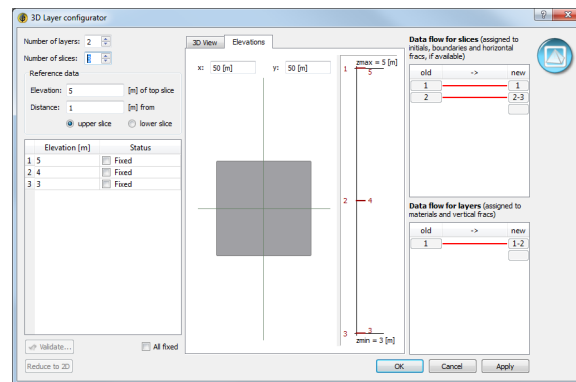


Figure 6.14 3D Layer Configurator.

Click on **OK** to apply the settings and to leave the dialog.

A new view window, the **3D** view, now automatically opens, displaying the model in 3D. The in-slice spatial discretization in plan view remains the same but

the previously 2D finite elements have now been extended to 3D prismatic elements.

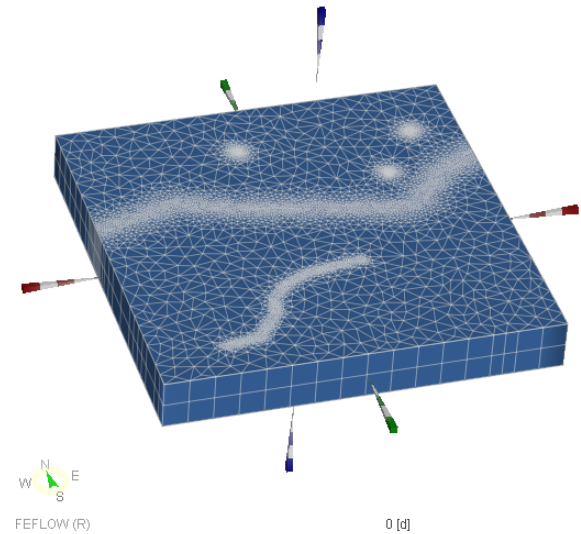


Figure 6.15 The model in 3D view.

7

Problem Settings

Defining the modeling approach

7.1 Problem Class

7.1.1 Physical Processes

FEFLOW allows the simulation of flow, groundwater age, mass- and heat-transport processes in either saturated, or in variably saturated media. The basic settings defining the simulated processes are done in the **Problem Settings** dialog that is accessed via the **Edit** menu.

Saturated / Unsaturated

Saturated groundwater flow is described by the equation of continuity with a Darcy flux law. Different options for handling a phreatic surface are described in chapter 7.1.5.

For unsaturated/variably saturated flow, FEFLOW solves Richards' equation that assumes a stagnant air phase that is at atmospheric pressure everywhere. Substantial computational effort can result from the typically nonlinear relationships between capillary pressure and saturation and between saturation and hydraulic conductivity.

FEFLOW provides two different options to define these relationships:

- **Spline Models**
- **Empirical Models.**

Spline Models are used to derive the parametric relationships from tabular data using one of several different spline interpolation techniques.

Alternatively, the following six **Empirical Models** are available:

- **Van Genuchten**
- **Modified Van Genuchten**
- **Brooks & Corey**
- **Haverkamp**
- **Exponential**
- **Linear.**

As the FEFLOW implementation of Richards' equation also includes the proper terms for saturated flow, it is generally applicable to variably saturated conditions.

7. Problem Settings

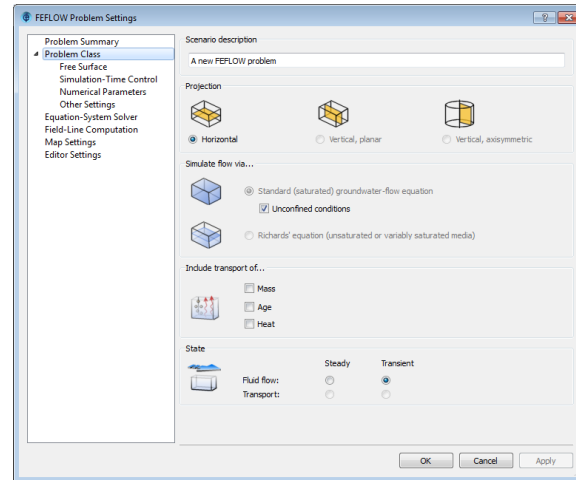


Figure 7.1 Problem Settings dialog.

Flow / Transport

A transport simulation is always performed in conjunction with a flow simulation. FEFLOW provides capabilities for single-species and multispecies solute-transport simulation, groundwater-age simulation with the possible species age, lifetime expectancy and exit probability as well as heat-transport simulation. A combined mass-and-heat (“thermohaline”) transport problem can be simulated, also together with groundwater age.

A detailed discussion of the application and available settings for groundwater-age simulations, can be found in chapter 14.

Steady State / Transient

Transient simulations proceed from an initial condition and cover a specified time period. In contrast, a

steady-state solution can be obtained directly and represents the state of a system having been subject to fixed boundary conditions and material properties for an infinitely long time. It is possible to combine a steady-state flow with a transient transport simulation. In such a case, the flow system is solved once at the beginning with all storage terms set to zero to obtain a steady-state solution as the basis for the transient transport calculation.

7.1.2 Dimension and Projections

FEFLOW supports 2D and 3D models. Finite elements of a lower dimension (1D in 2D models, 1D/2D in 3D models), so-called discrete features can be added, representing for example fractures or boreholes.

2D Models

A newly generated finite-element mesh always represents a 2D model. Two-dimensional models can be of horizontal, vertical, or axisymmetric projection.

A typical application for horizontal 2D models are regional water-management models without significant vertical flow components. Vertical models are used, for example, for the simulation of unsaturated flow and saltwater intrusion. Axisymmetric models have a radial symmetry such as the cone of a pumping or injection well. Essential for the suitability of an axisymmetric model are material properties and outer boundary conditions that are homogeneous along the circumference of the well cone or mound.

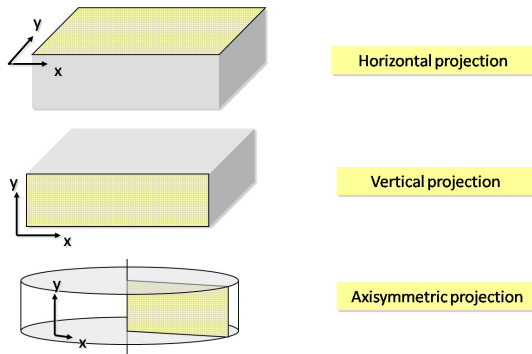


Figure 7.2 2D model projections.

3D Models

3D models can be created by expanding the mesh in the third direction into layers via the **3D Layer Configuration** dialog which is accessed via the **Edit** menu or via <Ctrl>+<L>. As all layers have an identical 2D discretization, the 3D mesh consists of prismatic or cuboid elements and each layer extends over the entire model domain.

In 3D models, the direction of gravity can be set to match any of the major coordinate directions (see chapter 6.8).

7.1.3 Temporal Settings

Corresponding to the discretization in space a discretization in time has to be specified for transient simulations.

FEFLOW supports three different options:

- Constant time steps
- Varying time steps

- Automatic time-step control

As constant time steps have the disadvantage that the most dynamic moment expected during the simulation controls the time-step length for the entire simulation, the definition of varying time steps offers some more flexibility. However, this option requires the specification of the length of each single time step in advance. Thus in most cases FEFLOW simulations use an automatic time-step control scheme, where an appropriate length of the time step is determined based on the change in the primary variables (head, mass concentration, groundwater age, temperature) between the time steps.

First Versus Second Order Accuracy

The automatic time-stepping procedure in FEFLOW is based on a predictor-corrector scheme.

The second-order accurate, semi-implicit Forward Adams-Bashforth/backward trapezoid rule (AB/TR) is the default for standard flow and combined flow and transport simulations. While the second-order approach applied for the prediction in this method in many cases provides a more accurate estimation of the predicted result for the next time step and thus a faster solution, it also may more easily lead to instabilities under highly nonlinear conditions in unsaturated or density-dependent models. Thus for unsaturated model types the first-order accurate, fully implicit Forward Euler/backward Euler (FE/BE) method is used by default and should be applied for density-dependent flow simulations manually.

7.1.4 Error Tolerance

The dimensionless error tolerance is used for two purposes in FEFLOW:

7. Problem Settings



Convergence is determined by a comparison of the input error tolerance, and the absolute error normalized by the maximum head (typically input in m ASL). Thus the accepted absolute error depends on the elevation of the model. Higher elevations require a lower error tolerance to obtain the same accuracy!

- The determination of convergence in iterative processes based on the change of results between iterations, e.g., the 'outer' iteration within a time step or in a steady-state solution to take care of nonlinearities in the basic equations.
- The determination of an appropriate time-step length in automatic time-stepping procedures based on the deviation of calculated from predicted solutions.

The absolute error (e.g., head difference) is normalized by the maximum value of the corresponding primary variable in initial or boundary conditions (maximum hydraulic head, maximum concentration, etc.).

7.1.5 Free Surface

By default, a newly created FEFLOW model reflects a confined aquifer. Saturated simulations of unconfined conditions require specific treatment of the phreatic groundwater table.

7.1.5.1 2D Model

In unconfined two-dimensional models with a horizontal projection the saturated thickness is iteratively adapted to the resulting hydraulic head. For this purpose, material-property input includes the aquifer top and bottom elevations.

When the hydraulic head exceeds the aquifer top elevation, the model calculations presume confined conditions in the respective area, i.e., the saturated thickness is limited to the difference between top and bottom elevation. Aquifers with partly confined conditions are thus easily simulated.

Two-dimensional vertical cross-sectional and axisymmetric models are always assumed to be completely confined. Modeling of unconfined conditions in these cases strictly requires a simulation in unsaturated/variably saturated mode, hereby applying Richards' equation.

7.1.5.2 3D Model

In three-dimensional models with gravity in the direction of the negative z axis (default 'top view' models) two different strategies can be applied in FEFLOW for handling the phreatic surface besides simulating in unsaturated mode. It is important to note that these methods were originally designed for regional water-management models. They are clearly limited (with very few exceptions) to cases with a single phreatic surface. Simulations where partial desaturation of the model is expected below saturated parts, e.g., due to drainage in a lower aquifer, have to be simulated in unsaturated/variably saturated mode. In contrast to an often-heard opinion, despite the nonlinearity of Richards' equation unsaturated models can be as computationally efficient or even more efficient than saturated models with phreatic-surface handling if appropriate simplifications are applied to the unsaturated material properties.

As both options for phreatic-surface handling have their specific advantages and disadvantages, the methods applied in FEFLOW will be explained in detail:

Free & Movable

This mode takes care of the phreatic surface by vertically moving the calculation mesh in a way that the top of the model is exactly at the water-table elevation

at any time. For this purpose, layer elevations are changed at each time step (transient simulation) or for each iteration (steady-state simulation). The movement is done by using the so-called BASD technique which places layer interfaces (slices) at elevations of slices in the original stratigraphy whenever possible.

Material (elemental) properties are mapped from the original stratigraphy to the actual stratigraphy, whereas nodal properties such as boundary conditions and slice-based observation points are moved with the slices.

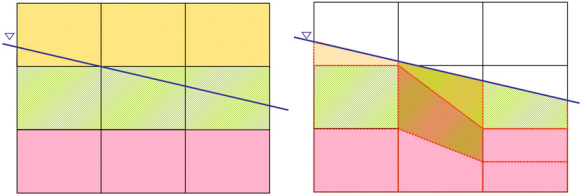


Figure 7.3 Schematical views of mesh movement and parameter interpolation in free&movable mode.

The most important advantage of this method is its ability to exclude all partially saturated or unsaturated parts of the initial stratigraphy from the model so that only saturated parts are simulated at all times. The main disadvantage is a consequence of the layer movement: In cases where the actual water table cuts through slices of the initial stratigraphy, model elements may occur that are located in multiple layers (and material zones) of the original stratigraphy. In these cases, a volume-weighted averaging for the material properties is applied, giving rise to material properties that differ from the original input. When interpolating between aquifer and aquitard properties, this approximation might not be acceptable (Figure

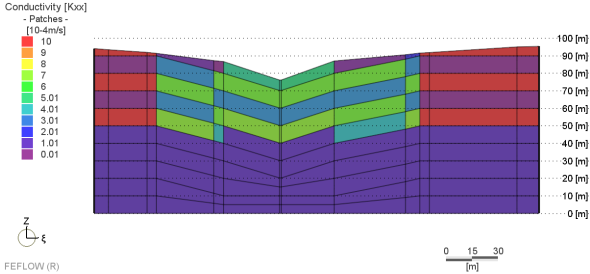


Figure 7.4 Unintended conductivity interpolation in free&movable mode in a schematized layered aquifer (cross-section view).

7.4).

As a rule of thumb, the free&movable method is particularly suitable for cases where the water table varies within one model layer. It is less applicable to models where steeply dipping phreatic surfaces are expected.

Phreatic

In phreatic mode, the model stratigraphy is fixed and, as a consequence, elements may become dry or partially saturated. In contrast to unsaturated mode, the calculation of the unsaturated zone is highly simplified and (with rarely occurring exceptions) only one phreatic surface is possible.

For each partially saturated element, the partial saturation is calculated by dividing the saturated thickness of the element by the total thickness of the element. Conductivity values in all directions are then linearly reduced by multiplying them with the partial saturation of the element.

For entirely dry elements (hydraulic head below the element bottom), a residual water depth is applied for

7. Problem Settings

the calculation of the partial saturation and reduced conductivity. This residual water depth can be defined on the **Free Surface** page in **Problem Class**.

Groundwater recharge is applied on the top of the model in phreatic mode and therefore has to pass the partially saturated/dry elements before reaching the water table.

The phreatic mode avoids all slice movement and related parameter interpolation and is therefore applicable to water tables with steep gradients that extend over multiple layers. On the other hand, dry elements with low conductivity values can lead to strong contrasts in the model, making the solution more difficult. The default low residual water depth might cause difficulties for the infiltration of recharge into dry soil, especially in cases with time-varying groundwater recharge.

In phreatic mode, the unconfined storage term is always only applied to the slice set to 'phreatic', i.e., usually to the top slice. The values for drain-/fillable porosity, however, are correctly derived from the layer where the water table is located at a given time. While this simplification has no negative consequences for typical regional models with significant horizontal flow components, it makes the phreatic mode less suitable for problems in which vertical flow is important, such as simulations of drainage of a soil column from the bottom.

Source and sink parameters assigned within phreatic layers can be scaled by the local pseudosaturation if the option **Scale sources/sinks by pseudosaturation** is set active. This will result in reduced source/sink values wherever the hydraulic head falls below the element top elevation (elements are not fully saturated). By default, the scaling of source/sink values is enabled to maintain compatibility with older FEFLOW ver-

sions not providing the two options.

Free Surface Settings

To allow combining of different methods of phreatic-surface handling, the method is set for each slice separately.

Typically, the first slice is set to either phreatic or free, while all the slices below are set to dependent except for the bottom slice which is always set to fixed. Dependent slices are defined by the first slice above that is non-dependent, e.g., dependent slices below a free slice can move if necessary.

Layers whose top slice is set to confined are treated as fully saturated, no matter whether the hydraulic head is above or below the layer. In models using the free&movable approach, fixed is especially useful to avoid slice movement (and possible material-property interpolation) in layers that are known to be saturated during the entire simulation.

7.1.5.3 Head Limits for Unconfined Conditions

In models with a phreatic surface, two particular cases may occur:

- All layers can be dry in a certain location.
- The water level can exceed the top of the model.

FEFLOW provides two options for dealing with a dry model bottom:

- Unconstrained head (default):
Hydraulic-head values lower than the model bottom are tolerated. The saturated thickness is considered equal to the residual water depth at these locations.



In models with thick dry layers the residual water depth should be increased for more numerical stability.

- **Constrained head:**
FEFLOW will prevent hydraulic-head values below the model bottom. For this purpose, first kind boundary conditions are internally applied at all bottom nodes that would otherwise fall dry, with a fixed head that equals the bottom elevation plus the residual water depth as defined on the **Free Surface** page.

For the top of the model domain, similar options are available:

- **Unconstrained head (default):**
Hydraulic-head values exceeding the model top elevation are tolerated, and the parts above the top are treated as part of the first layer, i.e., calculation is done with the properties of the first layer (3D models). For 3D models using the phreatic mode for the free surface, alternatively the aquifer can be treated as confined as soon as it gets fully saturated. In 2D horizontal unconfined models, the model is treated as confined if the water level exceeds the top elevation, which is a material property in this model type and therefore can be set higher if this behavior is not desired.
- **Constrained head:**
FEFLOW will prevent water levels higher than the model surface. If hydraulic-head values higher than the top elevation would occur, FEFLOW sets fixed-head boundary conditions with a value of the top elevation at these locations.

Optionally, the setting **Prevent inflow** can be enabled for the top head limit. With this setting, the fixed-head boundary conditions act as seepage faces, i.e., FEFLOW applies an additional constraint condition that only allows outflow. This causes an iterative setting of the head limits per time step. Only up to 30 iterations are performed. If there are still changes in the

location of these additional head boundary conditions after 30 iterations, FEFLOW proceeds to the next time step.

If the **Prevent inflow** option is disabled (default), the checking for nodes with a water level higher than the top is only done once per time step. The **Prevent inflow** option is more accurate, but requires more computational effort as up to 30 iterations per time step might be performed.



Constraining the water table on top or bottom changes the overall water balance of the model. Especially adding water on the model bottom might not be acceptable.

7.1.6 Anisotropy of Hydraulic Conductivity

7.1.6.1 2D Model

In a 2D model, the anisotropy of the hydraulic conductivity is defined through a set of material properties and not via the **Problem Settings** dialog. **Conductivity [max]** (**Transmissivity [max]** for confined models) defines the maximum conductivity. The direction of the maximum hydraulic conductivity is defined as **Anisotropy angle** (defining the angle between the x-axis and the max hydraulic conductivity). The ratio between the maximum and minimum hydraulic conductivity is finally defined as **Anisotropy of conductivity**.

7.1.6.2 3D Model

In a 3D model, the **Anisotropy Settings** page of the **Problem Settings** dialog offers different approaches for the definition of anisotropy of hydraulic conductivity.

The following settings are available:

- **Axis-Parallel Anisotropy** (default):

The three different conductivities (K_{xx} , K_{yy} ,

7. Problem Settings

K_{zz}) are directed along the x, y and z axes of the model.

- **General Anisotropy with Computed Angles:**

The principle directions for the main conductivities K_{1m} , K_{2m} , K_{3m} coincide with the layer inclination. The inclination is determined separately for each element.

- **General Anisotropy with User-Defined Angles:**

The principle directions for the three main conductivities and the three Euler angles needed for the rotation of the coordinate axes are defined as material properties for each element.

7.2 Equation-System Solvers

FEFLOW offers multiple iterative and two direct equation solvers. As the computational demand of the built-in, Crout-based method direct solver increases with the third power of the number of mesh nodes, the applicability of this solver has a practical limit of about 100,000 nodes. Storage and computational demand of the parallel sparse direct solver PARDISO are directly linked to the numbering of the finite-element mesh (and consequently the bandwidth of the global finite element matrix) and the number of degrees of freedom. As a consequence, PARDISO is particularly well-suited to solve matrices originating from 2D models even up to some millions of nodes (depending on hardware availability). For 3D problems with more than 1 million nodes, the use of PARDISO can still be considered but storage demand and solving time are problem and hardware dependent. Below the practical limit of 1,000,000 nodes, it is recommended to use PARDISO because the solution error then theoretically is at the level of machine precision.



By default, FEFLOW uses iterative solvers because




they are suited for problems of arbitrary size. In advanced selection mode, separate iterative solver types can be selected for the symmetric (flow) and unsymmetric (transport) equation systems. The default options are a preconditioned conjugate-gradient (PCG) solver for flow and a BICGSTABP-type solver for transport. Alternatively, for either type of equation systems an algebraic multigrid solver can be chosen (SAMG). The main advantages of SAMG are its parallelization on multicore or multiprocessor systems, and its more efficient solution algorithm, in particular for steady-state simulations and simulations with large ranges of element sizes in the mesh. As the algebraic multigrid technique is not always the most efficient one, the SAMG solver automatically selects between a CG-type or AMG-type solution strategy according to the current conditions.

7.3 Tutorial

In this exercise we load a number of models with different problem types to get familiar with the available problem settings.

7.3.1 Confined/Unconfined Models

We start with a very basic 2D flow model. Start FEFLOW and click  **Open** to load the file **quad-mesh.fem**. To check the basic settings of the model, open the **Problem Settings** dialog via the  **Edit** menu.

On the **Problem Class** page we can see that the standard (saturated) groundwater-flow equation is used for the flow simulation and that confined conditions are assumed. Switch from a  **Horizontal** projection to  **Vertical, planar** and click  **Apply**. The option

Unconfined conditions is now disabled as **Vertical, planar** models are always assumed to be confined. Additionally, the **Gravity Direction** page is displayed under **Problem Class**.

Switch back to a **Horizontal** projection and choose **Unconfined conditions**. Once we confirm the changes with **Apply**, the **Free Surface** page is added in **Problem Class**. In the **Data** panel, the material-properties list automatically adapts to the changed settings. **Transmissivity** is replaced by the parameter **Conductivity [max]**, and **Top** and **Bottom elevation** now need to be defined.

Additionally, for unconfined (phreatic) models **head limits for unconfined conditions** can be set to define the model behavior when the water table touches the top surface, or the model falls dry at the bottom.

Leave the **Problem Settings** dialog with **Cancel** and close the model without saving the changes.

We proceed by studying a 3D flow model. Click **Open** and load the file **free3d.fem**. Again, open the **Problem Settings** dialog via the **Edit** menu. The **Problem Class** page shows that a saturated model type is set.

In contrast to 2D models the projection is fixed for 3D models, but the gravity direction can be changed from the default negative z-axis to a different direction.

On the **Free Surface** page, a **Fully confined system** or the setting **Unconfined aquifer(s)** can be chosen where two different options are available for the latter. Currently, a **Free & Movable** approach is chosen. When we change the status of slice 1 to **Phreatic**, we can also define whether the top slice will be treated as confined or unconfined when the water level reaches the top surface.

Leave the dialog with **Cancel**, activate the **3D**

view and click **Start** in the **Simulation** toolbar to start the simulation. We can see the mesh moving in such a way that the top of the model is always at the water level elevation.

When the simulation has stopped, leave the simulator with a click on **Stop**. Reload the same file via **File** > **Recent FEM Problem files**.

Go back to **Edit** > **Problem Settings** and switch to **Fully confined system** on the **Free Surface** page. Click **Apply** and leave the dialog with **OK**. Start the simulation run for the changed conditions with a click on **Start**. The mesh geometry is now fixed and the resulting hydraulic head distribution differs from the **free & movable** model run.

Terminate the simulation with a click on **Stop** and close the model without saving the changes.

7.3.2 Unsaturated Models


We continue with a 2D unsaturated flow model. Click on **Open** and load the file **dam_seepage.fem**.

Start with the **Problem Settings** dialog located in the **Edit** menu. The **Problem Class** page shows that flow is simulated via Richards' equation and that the state is set to **Steady**.

The page list on the left-hand side now contains a new entry for **Unsaturated Flow**. Here, the basic settings for unsaturated models such as the form of the Richards' flow equation, iteration schemes and hysteresis settings can be changed. Do not do any changes here and switch to the **Problem Class** page again. As we can see, only **Vertical, planar** and **Vertical, axisymmetric** projections are available for 2D unsaturated models. Leave the dialog with **Cancel**.

In unsaturated models additional parameters are

7. Problem Settings

available in the  **Data** panel. **Saturation** and **Moisture content** are added to the list of **Process Variables** and the **Material Properties** list now contains unsaturated-flow parameters. Double-click on **Unsaturated-flow model type**. The **Slice** view now shows that a **Van Genuchten modified** model has been chosen to describe the capillary pressure vs. saturation and saturation vs. hydraulic conductivity relationships.

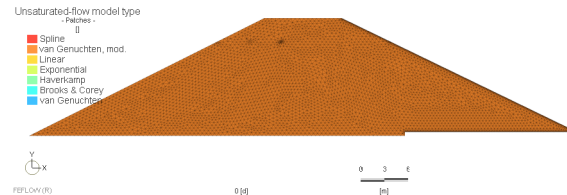





Figure 7.5 Unsaturated-flow model type.


7.3.3 Transport Models


To get familiar with the settings for transport simulations load the model **simulation.fem**.

Open the **Problem Settings** dialog via the  **Edit** menu and start on the **Problem Class** page. Saturated conditions are assumed and transport of **Mass** is included. The state for both flow and transport is set to **Transient**.

In mass-transport simulations, the **Problem Settings** dialog contains two additional pages: In **General settings** on the **Transport Settings** page, we can choose between the **Convective** and the **Divergence form** of the transport equation and change the settings for the calculation of fluid viscosity and density. Additionally, the **Reference concentration** for the mass-transport calculation, and the **Reference temperature** for heat-transport problems are specified here.

Switch to the **Chemical Species** page. Here, additional species that are associated with the fluid or the solid phase can be defined if the model requires more than one species. To add or remove species from the list, the  **Add species** or  **Delete current species** tools can be used.

Proceed to the **Numerical Parameters** page. On this page, the settings for the **Error tolerance** and for the computation of mass matrices are located. Additionally, different upwinding techniques, e.g., **Full upwinding** or **Shock capturing** can be selected to stabilize the transport calculation. As we can see, for the current model the default option **No upwinding (Galerkin-FEM)** is set. Click  **Cancel** to leave the dialog without any changes.

Notice how the  **Data** panel has changed compared to a flow simulation: The **Process Variables**, **Boundary Conditions** and **Material Properties** trees now each contain an additional branch for mass transport (see Figure 7.6).

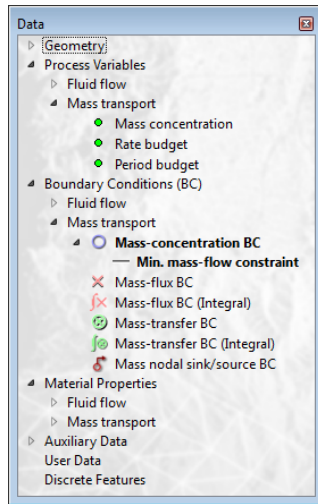


Figure 7.6 Data panel with mass-transport parameters.

In models with multiple chemical species, a separate branch is created for each species so that initial concentrations, boundary conditions and material properties can be defined separately for each species.

Start the simulation with a click on **Start** in the **Simulation** toolbar. The **Rate-Budget** and the **Period-Budget** panels now have two tabs, one for **Fluid** and one for **Mass**. To monitor the mass budget during the simulation, click on the tab **Mass** in both panels and set the check mark in front of **Active**. If a model contains multiple species, the panels contain a separate tab for each species.

The **Content** panel also contains additional entries for transport. To evaluate the amount of dissolved mass in the model, start the content calculation by checking **Dissolved Species Mass**. In a multi-

species model, the **Content** panel contains a separate tab for each species.

Terminate the simulation with a click on **Stop**.

7.3.4 Steady / Transient Models

To study the available settings for simulations in steady and transient state, load the file **enclosed_valley_3.fem**.

Access the **Problem Settings** dialog via the **Edit** menu and go to the **Problem Class** page. Flow is simulated via the **Standard (saturated) groundwater-flow equation** and the state is set to **Steady**.

Leave the dialog with **Cancel** and start the simulation with a click on **Start** in the **Simulation** toolbar. After a brief computation the steady-state solution is reached. In addition to the **Hydraulic-Head** chart the **Error-Norm History** is shown which plots the remaining dimensionless error for every iteration (see Figure 7.7).

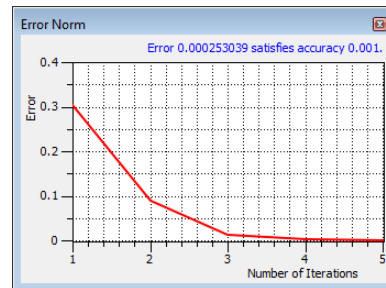


Figure 7.7 Error-Norm History.

Terminate the simulation with a click on **Stop** and reload the same file via **File > Recent FEM Problem files** without saving the changes. Open the **Problem Settings** dialog again, select **Transient** on

7. Problem Settings

the **Problem Class** page and click **Apply** to confirm the changes. To specify the time discretization for the transient simulation, go to the **Simulation-Time Control** page that now appears in the list on the left-hand side. The available time-stepping options are **Constant time steps**, **Varying time steps** and **Automatic time-step control**. By default, an **Automatic time-step control** based on a **Predictor-corrector scheme** with a **Second-order accurate (FA/BT)** integration scheme is assumed. For the automatic time stepping, an **Initial time-step length** and a **Final simulation time** need to be specified. Change the **Final simulation time** to **3650** days and click **OK** to apply the changes and to leave the dialog.

Start the transient simulation by clicking **Start**. The current simulation time is displayed in the **Simulation** toolbar and, optionally, also at the bottom of each view window. All process variables such as hydraulic head can be monitored during the simulation. Instead of the **Error-Norm** chart that is displayed for steady-state simulations, the **Time-Steps** chart appears and shows the elapsed simulation time versus the time-step length (see Figure 7.8).

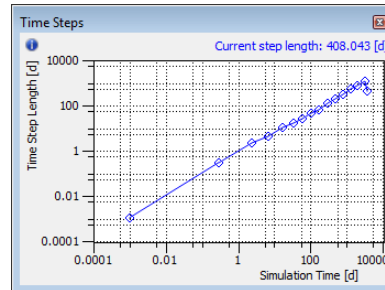


Figure 7.8 Time-Step History.

Working with Selections

Use selections efficiently for parameter assignment and results evaluation

8.1 Introduction

Selections of nodes, elements, edges and faces are among the fundamental concepts in FEFLOW. They are the basis for parameter input, visualization and postprocessing.

Selections can be stored with the model for repeated use—for example, to apply flow and mass-transport boundary conditions at the same nodes, or to start pathlines from nodes with well boundary conditions.

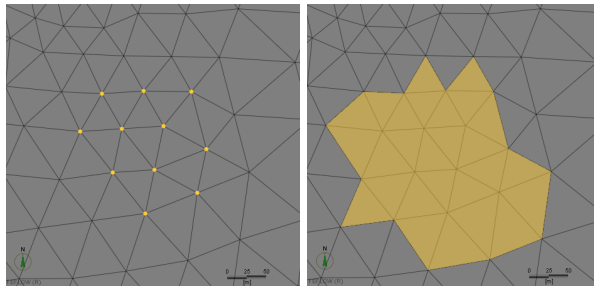


Figure 8.1 Nodal and elemental selections (Slice view).

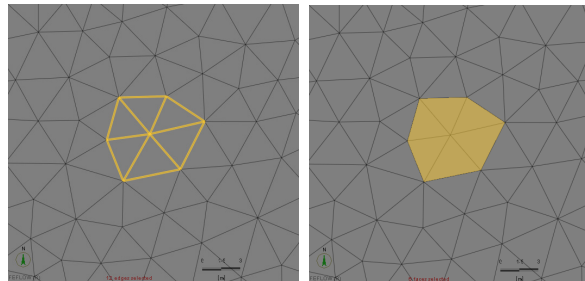


Figure 8.2 Edge and face selections (Slice view).

8.2 Selection Tools

Selections can be created by applying one, or a combination, of the available manual or map-based selection tools. The selection tools work on a node, element, edge or face basis, depending on the nature of the parameter that is currently active in the **Data** panel or on the target geometry that is set in the **Selection** toolbar.

8. Working with Selections

The manual selection tools are:

- **Select Individual Mesh Items**
- **Select Complete Layer/Slice (3D view)**
- **Select in Rectangular Region (Slice view)**
- **Select Using a Lasso (Slice view)**
- **Select in Polygonal Region (Slice view)**
- **Select by Map Point**
- **Select by Map Line**
- **Select by Map Polygon**
- **Select Nodes along a Border (Slice view)**
- **Select Arbitrary Node Path**



To avoid that unintentionally previous selections are kept as part of a new selection, it is recommended to clear selections after using them.

Map-based selection requires that the desired map is active in the **Maps** panel. An active map is indicated by a map name in bold letters. Selection based on both 2D and 3D maps is supported.

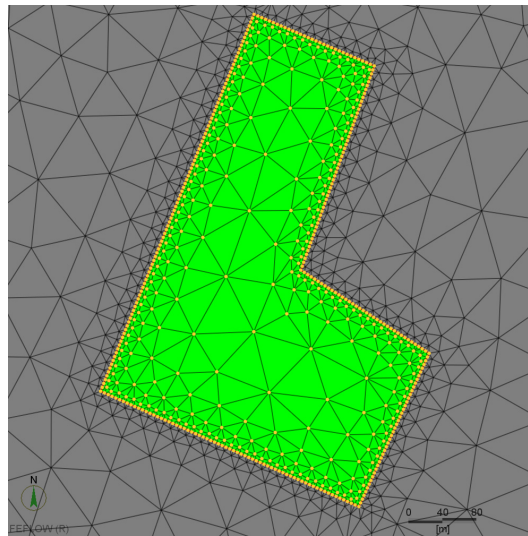


Figure 8.3 Nodal selection based on a map polygon (Slice view).

Interactive selection for a map includes selection based on points, lines, and polygons. The availability of certain selection modes depends on the map type: While for polygon maps polygon, line (edge) and point (node) selection is possible, for point files only point selection is available. In the **Slice** view, clicking on a map element triggers the selection of all nodes, elements, edges or faces within the snap distance as defined in the **Snap-Distance** toolbar (Figure 8.3). For selections based on 3D map geometries in the **3D** view the snap distance is ignored but the chosen map settings in the **Problem Settings** dialog determine how a selection is created.

A selection can also be performed for all map elements without user interaction.

For nodes and elements a further selection option exists: FEFLOW's **Expression Editor** can be used to create a selection based on a user-defined expression. The expression can contain process variables, boundary conditions, material properties, mesh data such as node/element numbers or coordinates and also temporal data like time series.

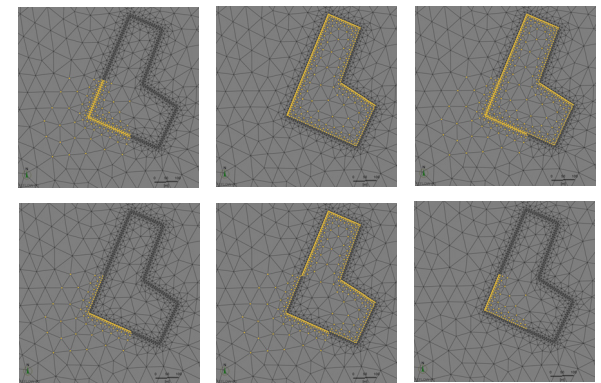


Figure 8.4 Selection modes: start selection, new, add, remove, toggle, intersect (upper left to lower right).

By default, applying a selection tool to a group of nodes or elements toggles the selection state of these nodes, elements, edges or faces, i.e., previously unselected mesh items become selected, and already selected ones are deselected. Alternative selection modes are available via the **Selection** toolbar: Create a new selection every time, always add to the current selection, remove from the selection, or intersect with the current selection (Figure 8.4).

8.3 Storing Selections

Using the context menu of either the active view or a **Spatial Units** panel, selections can be stored with the model for later use in parameter assignment, visualization or postprocessing.

Stored selections appear in the **Spatial Units** panel and can be renamed via their respective context menu or set as the current selection. Moreover, the nodes/elements/edges or faces of the stored selection can be added to, removed from, or intersected with the current selection.

Any stored selection can be applied as navigation reference in the active view to redefine the settings for full view and the center of rotation according to the selection.

Stored node selections can also be used as domain of interest for the **Rate-** and **Period-Budget** panels. Additionally, the budget history can be displayed as a time series in the **Rate-Budget** and **Period-Budget** charts.

Stored element selections are available as budget or transfer-budget domain for the **Rate-** and **Period-Budget** and **Subdomain Boundary Rate** and **Subdomain Boundary Period Budget** panels, as well as content or flux-integration domain for the **Content** panel and the

Flow-Rate and **Flow-Volume** panels.

The current or any stored selection can be converted into a selection of a different geometry type via the context menu of the selection in the **Spatial Units** panel. If a **Slice** view is the active view, the user can choose between converting a selection into a new selection on the current slice/layer (option 2D) or into a 3D selection.

One or multiple selections (keeping the <Ctrl> key pressed while selecting) which can be of different geometry types can be exported as **Location Set Collection** via their context menu in the **Spatial Units** panel. A re-import option for the **Location Set Collection** is also accessible via the context menu of the **Spatial Units** panel. This allows for a convenient transfer of stored selections between different model scenarios.

8.4 Tutorial

8.4.1 Tools



Figure 8.5 Selection toolbar.

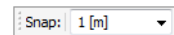



Figure 8.6 Snap-Distance toolbar.

8.4.2 General Remarks


Whether nodes, elements, edges or faces are selected depends on the target geometry chosen in the  **Selection** toolbar.

In the following exercises all selections are created for nodes. Selections on an elemental basis or edge/


8. Working with Selections





face selections can be created following the same principle, though.

8.4.3 Manual Selection

As a first exercise, we create a number of selections manually. First, click on  **Open** and load the model **selections.fem**. Two views are displayed, a *Slice* view (2D) and a *3D* view window.

8.4.3.1 Selections in 2D

Click in the *Slice* view to make it the active view and then browse to slice 1 in the slice list of the  **Spatial Units** panel.

Choose the tool  **Select Individual Mesh Items** from the  **Selection** toolbar, choose  **Select Nodes** as target geometry and click on an arbitrary number of nodes on slice 1. The selected nodes are highlighted in yellow. Delete this selection again with a click on  **Clear Selection**.

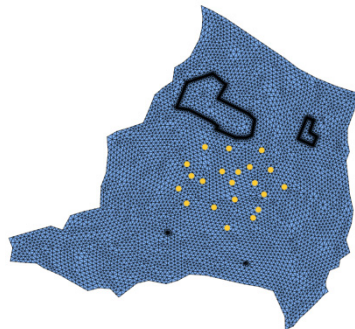









Figure 8.7 Node selection in Slice view.

Instead of selecting individual nodes, we can use  **Select All** to create a selection that contains all nodes if a *3D* view is active, or all nodes on the current slice in an active *Slice* view.

After a click on  **Clear Selection**, choose the tool  **Select in Rectangular Region** and draw a rectangle to create a new selection. Draw a second rectangle that partially overlaps the first one. As we can see, the selection is toggled: The already selected nodes are removed and newly selected nodes are added to the selection. This default selection mode can be changed by clicking  **Toggle in Selection** which exposes all available modes. Click on  **Undo Last Selection Step** to reverse the selection created with the second rectangle. Now, activate the  **Set New Selection** mode and draw a rectangle similar to the one we just removed. The result is quite different: The nodes in the first rectangle are now deselected and a new selection is set instead. Once again, click  **Undo Last Selection Step** and try the other modes available for setting selections.

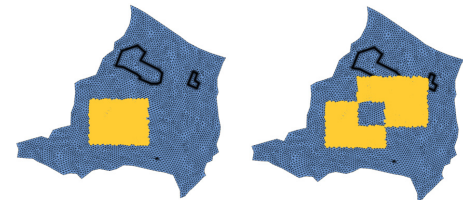







Figure 8.8 Toggled Selection.

A tool that is only available for node selections in the *Slice* view is  **Select Nodes along a Border**. Clear the current selection and switch back to the  **Toggle in Selection** mode. Click and hold the left mouse button on the western most node of the southern border. Move the cursor further along and release it at

the last node of that border. The selected nodes are now highlighted in yellow.

To also select the corresponding nodes on the slices below, we use the  **Copy Selection to Slices/Layers** tool in the  **Selection** toolbar. Choose all slices as the target slices. Confirm with  **OK**. In the **3D** view we can see that the nodes of the southern border have been selected on all slices.

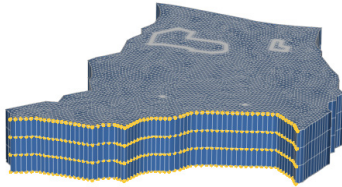








Figure 8.9 Selected nodes at southern border.


8.4.3.2 Selections in 3D


Six selection tools are available in a **3D** view:

-  **Select All**
-  **Select Individual Mesh Items**
-  **Select Complete Layer/Slice**
-  **Select by Map Point**
-  **Select by Map Line**
-  **Select by Map Polygon**


For node selections an additional seventh tool for the assignment of 1D arbitrary **Discrete Features** is available:

-  **Select Arbitrary Node Path**








We now create a selection that contains all nodes of the top slice. Make sure that the **3D** view is the active view window. Choose the  **Select Complete Layer/**




Slice tool from the drop-down menu of the  **Selection** toolbar. Placing the mouse cursor over any node in the top slice highlights all its nodes. Create the selection with a single click. The selected nodes are displayed as yellow disks.

8.4.4 Map-based Selections



A further option to create selections is to use maps. The points, lines and polygons contained in the **Supermesh** are available in the  **Maps** panel and selections can be set based on these features.


For this exercise, we use the same FEFLOW model as in the previous exercises. This model contains a number of maps and also its **Supermesh**. Selections based on 2D maps are only possible in the **Slice** view, so we first have to make sure that this is the active view.

In the first exercise we select the nodes of the well locations contained in the map **demo_wells**. These locations have also been included in the **Supermesh** and correspond to the refined areas in the southern part of the model area. Browse to slice 4 in the  **Spatial Units** panel, then switch to the  **Maps** panel and activate **demo_wells** (not the **Default** entry) with a double-click. Enter  **1 m** in the  **Snap-Distance** toolbar, activate the tool  **Select by Map Point** and click on  **Select by All Map Geometries** to create the selection. The selected nodes are now highlighted in yellow. Before we proceed, clear the selection with a click on  **Clear Selection**.

In the next step, we create a selection for the polygon that is defined in the map **sewage_treatment**, the refined area on the left side of the model. Activate this map in the  **Maps** panel with a double-click, click on  **Select by Map Polygon** and then click  **Select**


8. Working with Selections


by **All Map Geometries** again. Alternatively, it is possible to select this polygon by clicking on it in the **Slice** view while  **Select by Map Polygon** is the active selection tool. Again, finish with a click on  **Clear Selection**.


The **Supermesh** can be used to create selections in the same way. Activate **Supermesh > Polygons** in the  **Maps** panel. When the mouse cursor is moved over a polygon it is highlighted. Set the selection with a single click.

8.4.5 Expression-based Selection

The **Expression Editor** can be used to create selections based on a user-defined expression.

Click on  **Clear Selection** to make sure that no selection is active and switch to the **3D** view.

To open the **Expression Editor**, click on the tool  **Select by Expression**. We want to create a node selection that contains all nodes with a hydraulic-head value of less than 65 m.

First, click into the working window and delete the **true** statement. The table on the right-hand side of the editor contains all input parameters in FEFLOW and also some temporal data and mesh properties that can be used within an expression. Open **Process Variables > Fluid Flow** in the table and double-click on **Head**. Hydraulic head is now added to our expression. To finish the expression that will be evaluated for the selection, click on the  **less-than** operator symbol and then type 1^{23} 65 without a unit. The current user unit for each parameter is displayed in the table on the right-hand side or in the tooltip of the parameter in the work area. User units can be changed via the context menu of a parameter in the **Expression Editor**. The final expression should look like the one shown in figure 8.10.

ure 8.10.

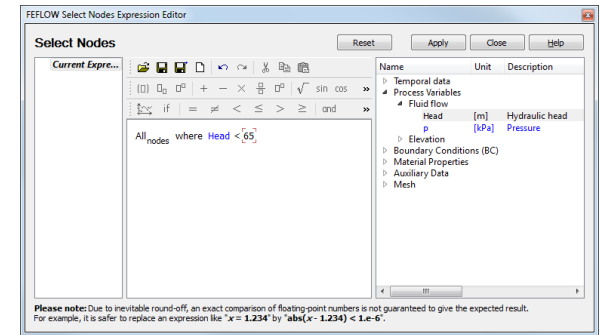









Figure 8.10 Expression Editor for node selection.

To create the selection based on the defined expression click on  **Apply**. Leave the dialog again with  **Close** or by activating a different tool.

8.4.6 Storing Selections

Selections can be stored for later use in parameter assignment, visualization or postprocessing actions.

To store the current selection, invoke the context menu by right-clicking in the active view or on an empty part in the  **Spatial Units** panel. Choose the option  **Store Current Selection** in the context menu and either enter a new name or accept the suggested default name for the node selection and confirm with \langle Enter \rangle . The stored selection appears in the **Node Selections** branch in the  **Spatial Units** panel.

Clear the selection with  **Clear Selection**. To set the selection active again, double-click on it in the  **Spatial Units** panel.

8.4.7 Converting Selection Types

Make sure that the *Slice* view is the active view and use the *Slice* entries in the *Spatial Units* panel to switch to slice 1. Activate the stored node selection *Navigation Selection* with a double click. We now convert this node selection into an element selection: Right click on *Navigation Selection* and select *Convert to > Element Selection 2D*. FEFLOW now automatically selects all elements adjacent to the nodes of the stored selection. The result is shown in figure 8.11.

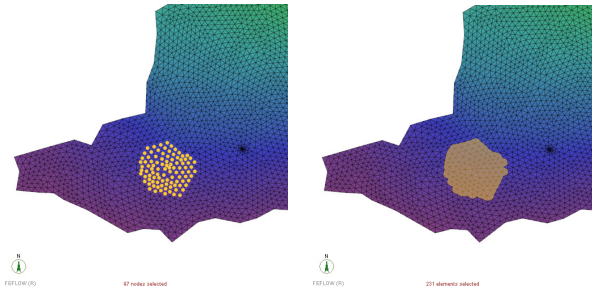


Figure 8.11 Node selection converted into element selection.

8.4.8 Exporting and Reimporting Selections

Selections can be exported and reimported, e.g., for use in alternative model scenarios.

Click on *Navigation Selection* in *Node Selections* in the *Spatial Units* panel, press the <Ctrl> key and click on the name of the node selection which we have stored in chapter 8.4.6. Next, right click on one of the highlighted selections, select *Export Location Set Collection* from the context menu and specify a name

for the file to be exported. Confirm with **⌘ Save**.

Before reimporting the exported selections, we delete the currently stored node selections. Again, select both selections simultaneously using the <Ctrl> key and then press the key twice to remove both selections from the *Spatial Units* panel at once. Now, right click either on *Node Selections* or in an empty part of the *Spatial Units* panel, select *Import Location Set > Location Set Collection* and choose the file that we have just exported. The previously exported selections now reappear under *Node Selections* in the *Spatial Units* panel.

8.4.9 Using Selections as Navigation Reference

Make sure that the *3D* view is the active view and double-click on the stored node selection *Navigation Selection* in the *Spatial Units* panel to set it active. Next, open the context menu of the selection with a right click and select *Set as Navigation Reference in Active View*. The settings for full view and the center of rotation are now adapted according to this selection.

8. Working with Selections

9

Parameter Visualization

Plotting input parameters and results

9.1 Introduction

Visualization of the model parameters is not only essential during model parameterization but for checking the assigned model properties, for evaluating the model results, and for the presentation of model properties and simulation results.

9.2 View Windows

All visualization options refer to a specific view window (see chapter 3.4). Depending on the type of the view window, different options for visualization are available. Each view window manages its own list of visualized parameters and visualization styles and settings. The panels controlling visualization always reflect the active view window.

9.3 Model Geometry and Data Plots

In the *Spatial Units* panel, the visualization target geometry is chosen. For example, in a *3D* view, a

parameter may be plotted on the outer boundary of the model domain, but also on a single slice or the boundary of a parameter zone.

For *Slice* views, the target geometry is a layer or slice, depending on whether nodal or elemental parameters are shown. The *Spatial Units* panel (or the <Pg Up> and <Pg Down> keys) can be used to switch between different layers/slices. *Cross-sectional*, *Slice Data-* and *Data-Trace* views are not affected by the *Spatial Units* panel. In case the active view is a *3D* view, the geometry of any spatial unit can be added to the view by a double-click on the unit, or via the context menu.

To provide more convenience for working with models with a large number of layers/slices and spatial units such as stored selections, it is possible to open more than one *Spatial Units* panel at a time via the context menu of the panel. This allows to use one panel for switching between different slices/layers while stored selections or surface and domain locations can easily be accessed via a second panel.

A parameter or parameter group (e.g., the group of all flow boundary conditions) is added to the view by double-click on the parameter in the *Data* panel, or by using the context menu of one or several selected

9. Parameter Visualization

parameters. The parameter will be plotted on the geometry that is active in the *Spatial Units* panel. Parameters can be plotted on more than one geometry at the same time, e.g., on the bottom slice and the vertical hull.

9.4 Visualization Options

All geometry (3D view) and parameter information currently available in the active view are listed in a tree in the *View Components* panel. As the tree always reflects the active view, it automatically changes when switching between the view windows. By changing the check box in front of the leaf and branch items in the tree, visibility of the corresponding view components can be toggled.

For parameters, different visualization styles may be available, one of which is active by default. For example, hydraulic head can be shown as continuous plot, fringes, isolines, or isosurfaces in a *3D* view.

The parameters and visualization styles have properties that can be edited in a *Properties* panel. The panel is opened by double-clicking on the parameter or style in the *View Components* panel, or by using the context menu of the parameter or style. The contents of the *Properties* panel depend on the parameter or style, and are described in detail in the FEFLOW help system.

Whenever a new parameter is added to a view, by default the previously shown parameter is removed. While this is a convenient behavior for quickly editing different parameters one at a time, in many cases it is preferable to visualize multiple parameters simultaneously. For this purpose, parameters can be locked via their context menu in the *View Components* panel. Locked parameters are not removed when adding a new component.

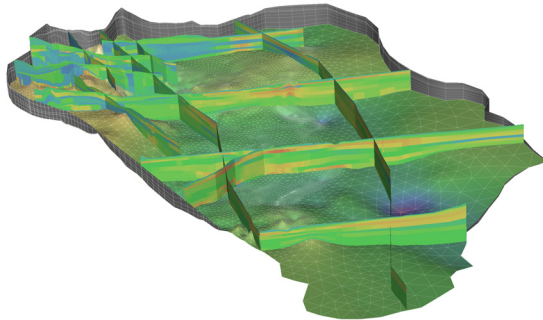
9.5 Clipping and Carving

Up to six planes can be arbitrarily defined and combined in each *3D* view window to expose data otherwise hidden within the model domain. Each of the six planes of the active view can be accessed via the *Planes* panel. For each plane, the panel provides controls to activate the respective plane and to specify whether the plane is to be considered as part of a cutout combination or as a simple clipping plane. A simple clipping plane clips all parts of the object located on its back side. When using a cutout combination, only those object parts are clipped that are on the back side of all clipping planes of the cutout combination.

Simple clipping planes can be applied in addition to a cutout combination.

The location of each clipping plane can be changed in the *Plane definition* dialog that is opened by clicking on the respective model view icon in the *Planes* panel. While modifying the plane equation, the plane is shown in the active view window.

Whether a visualization item is clipped or not is controlled via its context menu in the *View Components* panel.



FEFLOW (R)

Figure 9.1 Cross-section visualization in 3D.

9.6 Inspection

The active parameters in the current view and the attributes of maps shown in the view can be inspected, using the **Inspection** tool which is invoked via the **Inspection** toolbar. The properties of the target location are shown as constant values or curves for transient properties in the **Inspection** panel.

Parameters and map attributes can be displayed in the same list or the panel can be split into two separate parts, the upper one listing the parameters and the lower one displaying the map attributes.

The panel content can be filtered by a full-text search which is accessible via the search bar on top of the panel or in the split-panel sections.

9.7 Scene Library

View settings for **Supermesh**, **Slice**, **3D** and **Cross-section** views can be stored in a **Scene Library**. For models with a large number of views, this bears the benefit of reducing the required memory or CPU load significantly compared to keeping all views open all the time. With the provided export and import functions a large number of identical views can easily be created in different model scenarios.

View settings can be stored as scenes via the context menu of a view or with <Ctrl>-<Shift>-<S>. The stored scenes appear as tiles in the **Scene Library** panel and can be renamed by pressing <F2>. Placing the mouse cursor on a stored scene shows a large preview of the scene as a tooltip.

Scenes can easily be restored in existing or new view windows via their context menu. Double-clicking on a scene icon applies the scene to an existing view of the same type or opens a new view window in case that no other view of the same type already exists.

Scenes can be organized in a user-defined folder structure and also be filtered using the check boxes for **Slice View**, **3D View** and **Others** in the **Scene Library** panel or via a full-text search. The entire **Scene Library**, selected scene(s) or folders can be exported into an *.xml file via the context menu of a specific entry in the **Scene Library** panel.

Additional **Scene Library** settings are accessible via the menu **Tools** and **Global Settings > Tool Properties**.

9. Parameter Visualization

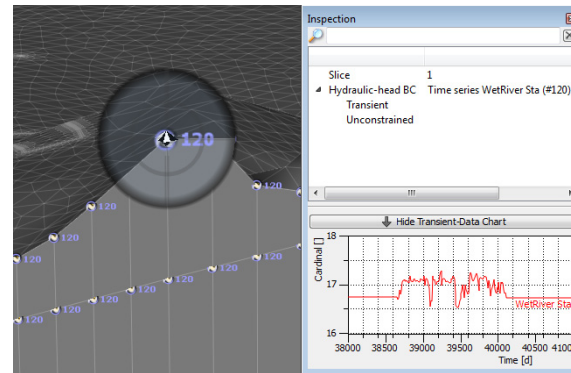


Figure 9.2 Checking boundary conditions with the Inspection tool.

9.8 Stereoscopic Visualization

FEFLOW 6.2 supports 3D stereoscopic display of model geometries and data. Especially for 3D models with complex geometries, stereoscopic visualization of the model helps to highlight 3D structures due to the enhanced depth perception. Prerequisite for stereoscopic visualization are computer displays, TVs or projectors that support 3D stereoscopic display and adequate glasses.

The export of stereoscopic images in JPS or PNS format and animations in AVIS format is supported. FEFLOW is compatible with common 3D interface standards (shutter and polarizer technology).

Different view settings for stereoscopic visualization and snapshot or movie export are available. FEFLOW supports the following visualization modi:


- Row-interleaved
- Active 3D (Quad-buffered)
- Horizontal Side-by-Side
- Vertical Side-by-Side





These settings can be accessed via *Extended View Settings* in the context menu of a **3D** view window or in the export dialogs for movie or snapshot export. The choice of a modus depends on the capabilities of the available 3D hardware.

9.9 Tutorial

The visualization options described in the following exercises are available during model setup, simulation run and also in postprocessing.

9.9.1 View Windows

Start FEFLOW, click on  *Open* and load the file **visualization.fem**. A **3D** and a *Slice* view are displayed. For the **3D** view, *Conductivity K_{xx}* is the active parameter. *Hydraulic head* is the active parameter in the *Slice* view.

Pay attention to the changes when we switch between different views: Click in the *Slice* view to set it as the active window. *Hydraulic head* then becomes the active parameter in the  *View Components* and in the  *Data* panel and *Conductivity K_{xx}* is removed from the  *View Components* panel. Additionally, the  *Spatial Units* panel now shows that we are currently working on slice 1.

9.9.2 Add Model Geometry and Parameters

Click in the **3D** view to set it as the active view. Double-click on **Hydraulic head** in the **Data** panel to plot this parameter. Note that the previously displayed parameter disappears from both the active view and the **View Components** panel when a new parameter is plotted.

It is also possible to display different parameters at the same time: Open the context menu of the entry **Hydraulic head** in the **View Components** panel and select **Lock Data View**. The **lock** icon now appears in front of **Hydraulic head**. In the **Data** panel double-click on **In/outflow on top/bottom** to add this parameter to the active view. Both parameters are now displayed at the same time.

In the **3D** view not only parameters but also additional geometry can be added to the active view. Go to the **Spatial Units** panel and double-click on the entries **Slice 1** and **Slice 4**. These slices are now added to the active view. A new item for each slice appears in the **Faces** and **Edges** branches of the **Geometry** tree in the **View Components** panel. To plot only slices 1 and 4 and not the entire domain uncheck the entries **Faces > Domain** and **Edges > Domain** and also **Hydraulic head > Continuous > Domain** and **In/outflow on top/bottom** in the **View Components** panel. We now want to plot a different parameter on each of the two slices. Start with slice 1. In the **Spatial Units** panel click on **Slice 1** to set it as target geometry for the plot. Then, double-click on **Hydraulic head** in the **Data** panel. Now click on **Slice 4** in the **Spatial Units** panel and double-click **Drain-/fillable porosity**. Not only parameters but also maps can be plotted to selected geometries. In the **Spatial**

Units panel, set **Slice 1** as target geometry. Uncheck **Hydraulic head** in the **View Components** panel and double-click on **topography_rectified** in the **Maps** panel. The map is now visible on slice 1 in the **3D** view. The resulting plot in the **3D** view is shown in figure 9.3.

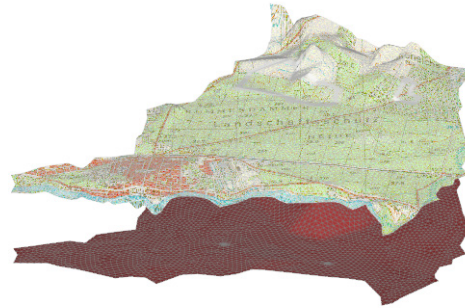


Figure 9.3 Plotting on selected geometries in 3D.

9.9.3 Visualization Options

We now select different visualization styles for the parameter **Hydraulic head**. Set the **Slice** view as active view. In the **View Components** panel, three styles are available for this parameter: **Continuous**, **Fringes** and **Isolines**. Display the different styles by checking the check box in front of the respective entry.

The properties of each style can be edited in the respective **Properties** panel. Open the context menu of **Hydraulic head > Isolines** in the **View Components** panel with a right-click and select **Properties**. Several editing options are available: In the **Iso** tab, the isolines settings can be changed. Use a **Prescribed**

9. Parameter Visualization

interval for isolines, deactivate the **Automatic** option and enter 10^{23} **0.25** as constant isoline interval. Switch to a **Fixed** color source for the labels on the tab **Color** and click **Apply** to confirm the changes.

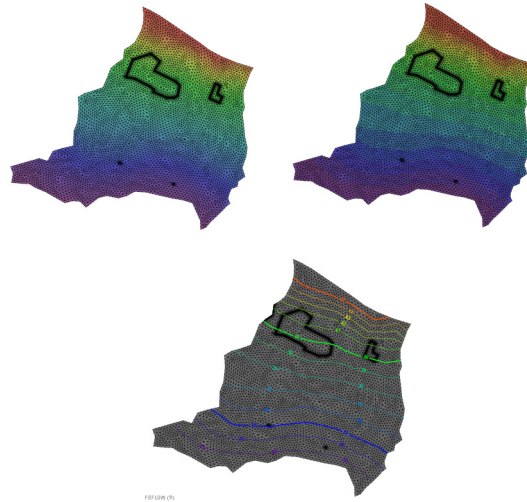


Figure 9.4 Hydraulic head values displayed as continuous, fringes and isolines plot.

To hide the legend of a particular parameter style open the context menu of the style entry in the **View Components** panel and uncheck **Legend Display**.

To edit the number format of the displayed parameter legend select **Number Format** in the context menu of **Hydraulic head** in the **View Components** panel. Here, switch to **Fixed floating-point** and change the number of significant digits to 10^{23} **2**. Clicking **OK** confirms the changes and the legend is now displayed with the new settings.

The data range of the parameter plot and also the

color scheme are edited in the **Properties** panel of the parameter. To open the panel right-click on **Hydraulic head** in the **View Components** panel and select **Properties**. Uncheck the box in front of **Auto-update range** and set a new minimum value of 10^{23} **34 m** and a maximum value of 10^{23} **42 m** for the data range. The changes are confirmed with a click on **Apply**. Uncheck **Hydraulic head > Fringes** in the **View Components** panel. At the grey parts of the model the hydraulic-head values exceed the defined minimum and maximum values for the hydraulic-head display. To plot these zones of the model with the same color as the minimum and maximum values, check the option **Tolerate Outliers** in the **Properties** panel and click on **Apply**. Both the parameter plot and the legend in the active view reflect the now tolerated outliers.

To change the color style of the parameter plot right-click in the colored sidebar and switch to one of the available presets, e.g., the FEFLOW Classic style. The changes are immediately applied and displayed in the active view.

9.9.4 Clipping and Carving

Go to **Window > New > 3D View** to open a new window. In the **Navigation** panel click on the **Projection** tab on the right-hand side of the panel and move the **Scaling** slider bar upwards to stretch the model and to add some vertical exaggeration for better visibility of the different layers.

In the **Planes** panel six different planes available for clipping and carving are displayed. Activate the plane in the second box by setting the check mark in front of **Active**. All parts located on the yellow (front) side of the plane are now clipped away. To

change the position of the plane open the *Plane definition* dialog by clicking into its view in the **Planes** panel. Use the slider bars to change the offset or the normal vector. Confirm the settings with **Bu Apply** and leave the dialog with **Bu Close**.

Now activate plane number 4 and select the option **Carving** for both planes. Now, only the features on the yellow sides of *both* planes are cut away.

Visualization examples with carved models are shown in Figures 9.5 and 9.6.

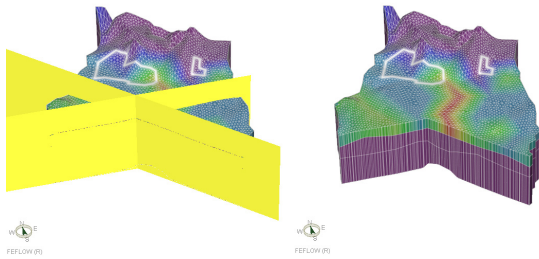


Figure 9.5 Carving planes and carved model domain in 3D view.

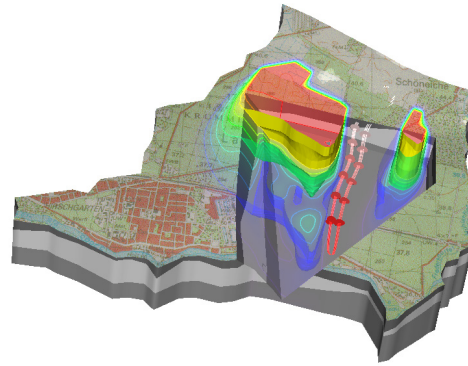


Figure 9.6 3D visualization example.


9.9.5 Scene Library

We use the **Scene Library** panel to store the settings of some of the views that we have just created. Right-click into the current **3D** view and select **Create Scene from Window**. The stored scene now appears as a tile in the **Scene Library**. To show a large preview of the scene, place the mouse cursor on the icon. A large preview, the name of the scene and the creation date and time are now displayed.

To rename the scene, click on its icon and press <F2>. For better identification of the scene, we also add a comment in addition to the name. Right-click onto the scene's icon and select **Edit Scene Properties**. Add a comment to the scene and confirm with **Bu OK**.


We now create a new folder in the **Scene Library**. Right-click into an empty part of the panel and select **Create Folder**. To rename the folder, click on it and

9. Parameter Visualization

press <F2>. In order to view the folder structure within the **Scene Library**, select  **Show Folders** from the context menu of the panel.

To store a scene in this specific folder, double-click on it before creating a scene. Next, switch to the **Slice** view and use the context menu of the view to create a scene of this view as well. The scene now appears in the subfolder and not in the main level of the **Scene Library**.

To move the stored scene to the main level, click on the scene and move it to the entry **Scene Library** while keeping the <Shift> key pressed. Dragging and dropping a scene to a different location in the library without pressing the <Shift> key creates a copy of the scene instead of moving it.

Close the currently open **Slice** view. To create a new view from the stored slice-view scene, double-click on its icon in the **Scene Library** or use  **Create View from Scene** in the scene context menu.

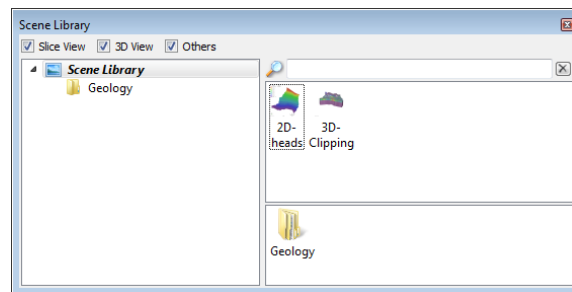


Figure 9.7 Scene Library panel.

Parameter Assignment

Input of initial and boundary conditions, material properties, user data and discrete features

10.1 Introduction

The task of assigning model parameters is in many cases repeatedly performed during model setup and application. After the initial parameterization, model properties may have to be changed during calibration, or parameters need to reflect different scenarios. Thus the work flows for parameter assignment are crucial for the efficient handling of a groundwater model.

Typical assignment procedures are based on the activation of a property to be assigned and the selection of the target nodes or elements. The tools for selecting nodes or elements are described in detail in chapter 8.

There are some exceptions from this standard workflow: When working with map data, FEFLOW provides the means to automatically activate a parameter and/or select the target geometry based on information in the map or linked to the map.

10.2 Input Parameters

FEFLOW distinguishes between seven groups of parameters, all of them visible on the first level of the

tree view in the *Data* panel (Figure 10.1):

- *Geometry*
- *Process Variables*
- *Boundary Conditions*
- *Material Properties*
- *Auxiliary Data*
- *User Data*
- *Discrete Features*

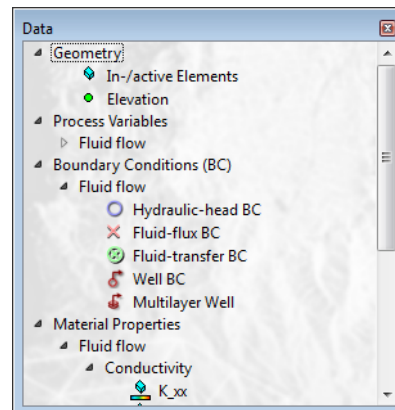


Figure 10.1 Data panel.

10. Parameter Assignment

The **Geometry** section of the **Data** panel contains the option to set mesh elements active or inactive for a simulation and the node elevation values in 3D models. While process variables (including initial conditions and with the exception of elemental Darcy fluxes) and boundary conditions are defined on the mesh nodes, material properties representing the characteristics of the medium are assigned on an elemental basis. Auxiliary data cannot be edited or assigned but can be used to check some properties of the finite-element mesh or to visualize stream functions in 2D models. User data are additional nodal or elemental distributions that can also be based on user-defined expressions. Assignment and usage are discussed in section 10.5.2. Discrete features can be added along element edges or faces to represent high-conductivity features or they can connect two arbitrary nodes.



The process variables are used for both providing initial conditions and storing the results. After a simulation has started, they do no longer reflect initial conditions!

10.2.1 Geometry

With the elemental parameter **In-/active Elements** mesh elements can be activated or deactivated during the entire simulation or only at specific time stages. By default, all mesh elements are active after mesh generation. More information on the handling of inactive elements can be found in chapter 6.7.

In 3D models, the elevation is included in the geometry section as a nodal parameter. In models with a fixed mesh, the elevation does not change during the simulation. In models representing a phreatic surface with the free & movable approach (see 7.1.5), the actual nodal elevation changes during the course of the simulation. The parameter **Reference Elevation** preserves the original node elevations.

10.2.2 Process Variables

Process variables include the primary variables hydraulic head, mass concentration, mean age, mean lifetime expectancy, exit probability and temperature (as applicable). When setting up the model, they describe the initial conditions. During and after the simulation these process variables reflect the then-current conditions.

Other process variables contain values derived from the original primary variables. For example, pressure is not stored separately in FEFLOW, but calculated from hydraulic head and elevation ‘on the fly’. When these secondary parameters are used as input variables, the input is converted into the original primary variable based on current conditions.

The third type of process variables are auxiliary variables supporting results evaluation and visualization, such as Darcy flux, rate and period budget and streamlines or pathlines. They cannot be used as input parameters.

10.2.3 Boundary Conditions

By default, all model boundaries in FEFLOW are impervious. To allow flows into or out of the model, boundary conditions have to be defined. FEFLOW supports four basic types of boundary conditions for flow, mass, groundwater age and heat transport which can be defined as constant over time or time-varying values. For flow and heat transport, additional fifth boundary condition types are available:

- **Dirichlet-type BCs:**
Hydraulic-head BC / Mass-concentration BC / Temperature BC

- **Neumann-type BCs:**
Fluid-flux BC / Fluid-flux BC (Gradient) / Mass-flux BC / Heat-flux BC
- **Cauchy-type BCs:**
Fluid-transfer BC / Mass-transfer BC / Heat-transfer BC
- **Nodal source/sink type BCs:**
Well BC / Mass nodal sink/source BC / Heat nodal sink/source BC
- **Multilayer Well (flow)**
- **Borehole Heat Exchanger (heat transport)**

For groundwater age, only the first boundary condition type is displayed by default and additional types have to be added via the respective context menu in the **Data** panel.

Except for Borehole Heat Exchangers, the sign convention for boundary conditions in FEFLOW defines flows out of the model as positive (e.g., well abstraction), while inflows are negative (Figure 10.2). Notably, this convention differs from other parts of FEFLOW, such as the **Rate-** and **Period-Budget** or the **Subdomain Boundary Rate** and **Subdomain Boundary Period Budget** panels or the definition of constraints, where inflows are considered as positive, outflows as negative (Figure 10.4).

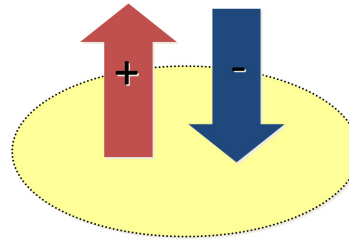


Figure 10.2 Algebraic signs for boundary conditions.

Dirichlet-type BCs

This boundary condition type - often also referred to as Dirichlet or 1st kind boundary condition - specifies a time-constant or time-varying value for the primary variable at a node, i.e. hydraulic head for flow, concentration for mass transport, groundwater age and lifetime expectancy, probability of exit and temperature for heat transport. The inflow or outflow to/from the model domain at the node can be calculated from the simulation result.

In certain model types, such as unsaturated or density-dependent simulations, it is possible to derive the primary variable hydraulic head from input such as:

- Pressure
- Saltwater Head
- Saturation
- Moisture Content

While converting input from a different quantity in these cases, and providing the possibility to visualize the boundary conditions in terms of another quantity, the actual boundary condition stored and used during the simulation is always a Hydraulic-head BC.

10. Parameter Assignment

Neumann-type BCs

The flux-type boundary condition describes an in- or outflow of water/mass/energy at element edges (2D) or element faces (3D). Though nodally defined, the condition must be applied for at least two adjacent nodes (2D) or all nodes of a vertical or horizontal element face (3D) to be effective. The given value in flow simulations is a Darcy flux perpendicular to the boundary. An optional alternative formulation for unsaturated models allows the definition of a hydraulic-head gradient instead of the Darcy flux.

The successful application of Mass-flux BCs and Heat-flux BCs is linked to the application of the convective or divergence form of the transport equation (7.3.3). The FEFLOW Book and the help system should be consulted for details.



The resulting hydraulic head at well nodes depends on the local spatial discretization. Quantitative comparisons should be made with care.

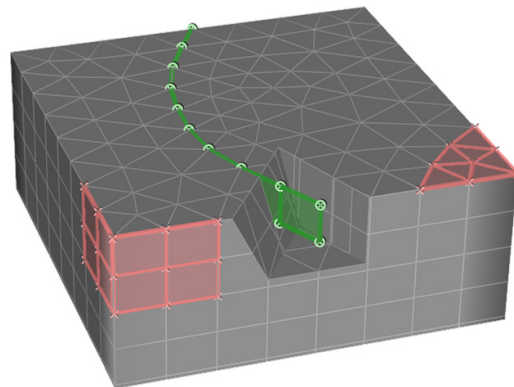


Figure 10.3 Flux and transfer boundary conditions in 3D model.

Cauchy-type BC

Fluid-transfer BCs can be used to describe rivers, lakes, and known hydraulic heads in a distance from the model boundary (sometimes called 'general head' boundaries). The condition is used to apply transfer properties between a reference value for the primary variable (hydraulic head, concentration, or temperature) and groundwater. Thus the value of the boundary condition is a reference hydraulic head (e.g., river water level), reference concentration, or reference temperature. The hydraulic conductance (e.g., properties of a clogging layer), mass-transport conductance or thermal conductance are defined as material properties on elements adjacent to the boundary condition. Similar to the **Neumann-type BC** the transfer boundary condition must be specified along a line (2D) or for an entire element face (3D—Figure 10.3).

Nodal source/sink-type BCs

Well BCs and their counterparts for mass and heat transport simulation are nodally applied and represent a time-constant or time-varying local injection or abstraction of water, mass or energy at a single node or at a group of nodes.

If it is intended to simulate a well screened in different layers it is recommended to use the multilayer-well boundary condition.

The successful application of **Mass nodal sink/source BC** and **Heat nodal sink/source BC** is linked to the application of the convective or divergence form of the transport equation (7.3.3). The FEFLOW Book and the help system should be consulted for details.

Multilayer Wells

In 3D models, multilayer-well boundary conditions can be used to simulate water injection/abstraction via a well screen. The screen can extend over one or multiple model layers.

The well radius and screen top and bottom together with the well capacity are used as input parameters for this boundary condition. Internally, the total injection/abstraction rate is assigned at the bottom-most node of the well and a highly conductive 1D discrete feature is placed along the well screen. Flow within the well along the screened interval is simulated via the Hagen-Poiseuille (cubic) law. The appropriate parameters of the discrete feature are derived from the specified well geometry.

The properties of a multilayer well are defined in the **Multilayer Well Editor** dialog. The dialog is invoked by activating the boundary condition in the **Data** panel and double-clicking on **Multilayer Well** in the **Editor** toolbar.

The partitioning of the injection/abstraction rate to the different model slices/layers that are part of the well screen depends on the surrounding material properties and hydraulic-head distribution and therefore is a result of the simulation. It is calculated from the model results and can be visualized as a property of the multilayer well during and after the simulation run.

Borehole Heat Exchangers

Borehole heat exchangers are used to simulate closed-loop geothermal installations. A refrigerant circulates within closed pipes and heat exchange with the surrounding aquifer system is solely driven by thermal conductivity.

Borehole heat exchangers are represented as embedded 1D elements and linked to the FEFLOW nodes along join edges in a 3D model.

To define the inflow boundary of a heat exchanger, a time-constant or time-varying flow rate of the circulating refrigerant and the inflow temperature are required. While the flow rate is always directly specified, FEFLOW provides the following four options for the definition of the inflow temperature, each of them possibly also being time-varying:

- Inlet Temperature
- Heat-input Rate
- Temperature Difference
- Power

Additionally, the properties of the refrigerant and the components of the borehole heat exchanger need to be specified in a so-called **Borehole Heat Exchanger Data Set** that can be used for a number of BHEs.

FEFLOW supports four different heat-exchanger geometries:

- Double U-shape
- Single U-shape
- Coaxial shape with annular inlet
- Coaxial shape with centered inlet

The processes within heat exchangers can be modeled via an analytical, quasi-stationary approach in which a local thermal equilibrium between all heat-exchanger components is assumed or via a numerical, fully-transient approach. The latter provides higher accuracy for short-term (time ranges of few hours) pre-



For a precise calculation of the ground temperature at the location of a borehole heat exchanger nodes adjacent to the heat exchanger need to be placed within a certain distance. Details are provided in the FEFLOW help system.

10. Parameter Assignment

dictions especially for conditions with quickly changing inflow temperatures. For long-term predictions with less frequent and only moderately changing inflow temperatures, the quasi-stationary method provides reasonably accurate results at much lower computational cost.

Borehole heat exchangers are defined in the **Borehole Heat Exchanger Editor** which is invoked by activating **Borehole Heat Exchanger** in the **Data** panel and double-clicking on the same entry in the **Editor** toolbar.

For the simulation of arrays of borehole heat exchangers, FEFLOW provides the possibility to connect BHEs serially or parallelly.

Boundary Constraints

In FEFLOW, all boundary conditions can be physically constrained. For example, a fixed hydraulic-head condition at a certain node can be limited by a maximum or minimum flow. Technically, these constraints are realized by temporarily changing the respective boundary condition. If the flow at a fixed head boundary condition would exceed the maximum flow set as a constraint condition, the corresponding boundary condition is internally transformed into a well boundary condition with the value of the maximum flow, and the time step is repeated. Because this test is performed for all affected nodes at every time step, considerable computational effort can be associated with the use of boundary constraints.

Constraints are typically complimentary to the respective boundary condition, i.e., head-type boundary conditions are constrained by minimum/maximum flow, while flux-type conditions are constrained by minimum/maximum head. Exceptions from this rule include additional constraints for transfer boundary

conditions (to limit the infiltration at disconnected rivers) and for all transport boundary conditions (to limit their application to a certain range of hydraulic head).

Boundary constraints are not shown in the **Data** panel by default. They can be added to the tree by using the context menu of the corresponding boundary condition.

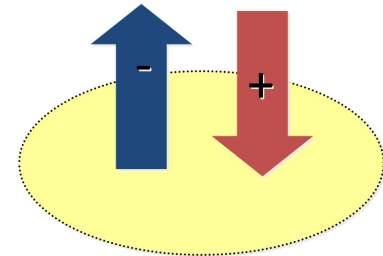


Figure 10.4 Algebraic signs for boundary constraints and budget.

Modulation Functions

In transient models, boundary conditions can be modified by applying a time series (see section 10.4 for more information on time series) as a modulation function. The modification is realized by multiplying the time-series values of the modulation function with the boundary condition value at each time step during the simulation.

This functionality can be used, e.g., to modify boundary condition values for calibration purposes or to distribute a total value onto a number of nodes and also to turn boundary conditions off temporarily if modulation functions contain gaps: Time-series gaps are defined as ‘NAN’ (not a number) values and the

multiplication of NAN values with boundary condition values again leads to the result 'NAN' which deactivates the boundary condition. The same modulation function can be applied to an arbitrary number of boundary conditions with different values or time series at the same time. This reduces the effort for turning a large number of boundary conditions off at the same time significantly compared to defining gaps for each boundary condition separately.

As for boundary constraints, modulation functions are not displayed in the **Data** panel by default but have to be added to the list of available parameters using the context menu of the respective boundary condition(s).

10.2.4 Material Properties

The material properties describe the relevant characteristics of the porous medium for the considered flow and transport processes to be simulated. They are defined on an elemental basis.

For the flow simulation, material properties encompass quantities such as hydraulic conductivity in different directions according to the selected anisotropy model, drain-/fillable porosity (specific yield) and specific storage (compressibility), and transfer rates (e.g., to represent river-bed conductance). Parameters such as source/sink or in/outflow on top/bottom (often used for groundwater recharge) are mathematically close to boundary conditions; however, their typically distributed spatial reference justifies their placement in material properties.

10.2.5 Auxiliary Data

In Auxiliary data, nodal and elemental distributions are available that provide information on different

properties of the finite-element mesh. For 2D models, the flow field can also be visualized using stream functions. Auxiliary data cannot be edited by the user, but the distributions are automatically updated according to changes in the mesh geometry.

In 2D models, the two elemental distributions **Max. interior angle of triangles** and **Delaunay criterion violations** exist which can be used to check the mesh quality. In 3D models, the additional distributions **Slice distance** and **Layer thickness** are provided which can also be used as parameters in the **Expression Editor**. For 2D models, a nodal distribution for the **Vorticity stream function** is available. In transport models, the elemental distribution **et Number** is available which can be used to check whether the spatial discretization is sufficiently fine for a specific transport problem. As the calculation of the **et Number** is based on velocities, parameter values are only available during a simulation.

10.2.6 User Data

Arbitrary nodal or elemental distributions of user data can be created via the **Data**-panel context menu. They can be assigned and visualized like the 'regular' FEFLOW parameters, but the distributions are currently limited to time constant data.

User data can provide input for the FEFLOW **Expression Editor** (e.g., for defining kinetic reactions in multispecies transport), they can be used for storing the data needed by FEFLOW plug-ins (see 16), or for comparing the model results to certain reference conditions.

User data can also be expression-based parameter distributions. In this case, the values of a distribution are calculated on the fly based on the user-defined

10. Parameter Assignment

expression. Expression-based distributions can be used, for example, to dynamically plot the water table draw-down at different simulation times.

FEFLOW offers a set of predefined distributions to display the error norms (normalized predictor-corrector errors) for flow, mass, groundwater age and heat. In transport models with multiple chemical or age species, a separate distribution for each species is available.

10.2.7 Discrete Features

Discrete features can be added to models to represent highly conductive one- or two-dimensional features, such as tunnels, pipes, drains, faults or fractures.

They are finite-elements of a lower dimension than the basic finite-element mesh, i.e., onedimensional discrete features can be added in both 2D and 3D models, while two-dimensional discrete features are only available in 3D models.

Discrete features are assigned along element edges (1D) or faces (2D) or they can connect two arbitrary nodes within the mesh. In the latter case, interaction between the arbitrary discrete feature and the finite-element mesh is only possible at connected mesh nodes.

Discrete features can be added via the context menu in the **Data** panel at locations where an edge or face selection is active or where an arbitrary node path has been defined.

For each discrete feature, geometry and flow and possibly also mass-, age- and heat-transport properties need to be defined. For the simulation within discrete features, the user can choose between three different flow laws:

- Darcy
- Hagen-Poiseuille
- Manning-Strickler

By default, the entire feature is turned off if the pressure of all nodes belonging to a discrete feature drops below zero. In case that at least one, but not all discrete-feature nodes are located in an area with negative pressure, the conductivity of the discrete feature is scaled by a smoothing function.

10.3 Assignment of Constant Values

The most basic approach for data assignment is the input of time-constant parameter values at the currently selected mesh items (see 8). Precondition for the assignment is that a single target parameter has been activated in the **Data** panel by a double-click or via the context menu. An active parameter is indicated by bold letters.

The assignment of a constant value for the parameter to the target selection is executed by typing the value into the input box in the **Editor** toolbar and clicking the green check mark button immediately to the right of the input box (or hitting <Enter> on the keyboard). If the units of the current input value differ from the current parameter units, the unit can be typed in with the parameter. Units recognized by FEFLOW are accepted and automatically converted.

10.4 Assignment of Time Series Data

10.4.1 Time Series

The input of time-varying boundary-condition data is based on time series. Once defined, a time series can be used for multiple boundary conditions. Time series



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can also be used for the assignment of time-varying material properties, boundary constraints or modulation functions.

Time series can be imported from files (*.pow format) or directly be defined and edited in the **Time-Series** dialog that is opened via the **Edit** menu. A third option is to paste tabular data copied from, e.g., Microsoft Excel/Access or simple text editor files, directly into a time series in the editor from the clipboard.

A time series consists of a unique ID and an arbitrary number of (time, value) data pairs. Optionally, a name can be specified for each time series. The time intervals do not have to be equal. When defining time series, it should be considered that automatic time-stepping procedures make sure to meet each time value with a time step, so that short-interval time series may lead to higher numbers of calculation time steps. Interpolation between the data pairs can be defined as linear, constant (step function) or Akima/Akima2.

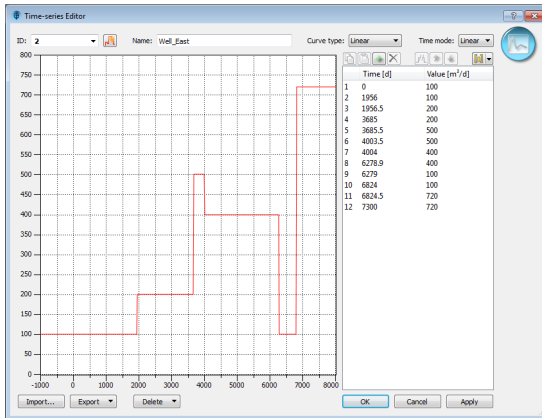


Figure 10.5 Time-series editor.

Time series can be applied to the model cyclically, i.e., a time series defined for part of the simulation time

is applied repeatedly until the end of the simulation, or they can be used in linear mode. If the time series only covers a part of the simulation time in linear mode, the first value is used from the simulation start to the beginning of the time-series definition, and the last value in the series is applied until the end of the simulation.

Time series can also contain gaps to turn a boundary condition off during specific time intervals or to limit the application of a boundary condition to a certain time period. Gaps at the beginning and end of a time series can be used to make sure that the time-series values are not applied before the first and after the last defined time-series step as described above for the linear time mode. As time-varying material properties need to be defined for the entire simulation time, FEFLOW does not allow to use time series which contain gaps for material-property assignment.

Units for Time Series

By default, time series do not contain any information on the units of the time/value pairs and FEFLOW will use the internal unit of a specific parameter for the assignment of the time-series data, e.g., [m³/d] for well boundary conditions and [m] for a hydraulic-head boundary condition. It is however possible to define the unit class and user unit for editing the data of a time series. While the unit class for the **Time** data is always time, a time series may contain values of pumping rates, hydraulic head or concentration. Selecting a user unit for **Value** therefore requires prior definition of the appropriate unit class (e.g., pumping rate, length, concentration).

10. Parameter Assignment

10.4.2 Assignment

Time-series data are assigned similarly to time-constant values. Elevation in 3D models cannot be varied in time (except by using the programming interface). Precondition for the time-series assignment is that the corresponding parameter has been activated in the **Data** panel, and that a selection of target nodes or elements has been made. The input box in the **Editor** toolbar has to be switched to time-series mode. The assignment is executed by choosing the ID of the time series to be applied at the selected nodes or elements in the input box in the **Editor** toolbar and clicking the green check mark button besides the input box (or hitting the <Enter> key on the keyboard).

10.5 Assignment of Map Data

Map information can be used in different ways for parameter assignment, ranging from using the map geometry to define targets for interactive data input to regionalization based on map-attribute data.

The input options for attribute data depend on the map and target (node/element/face/edge) geometries as shown in Figure 10.6 and Figure 10.7.

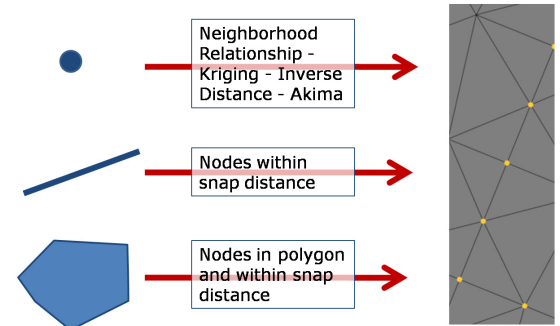


Figure 10.6 Map data input for nodal properties.

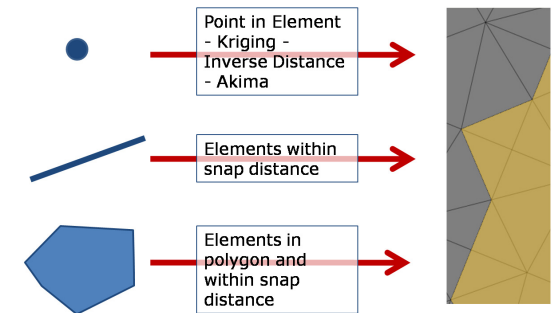


Figure 10.7 Map data input for elemental properties.

10.5.1 Interactive Data Input

Interactive data input is chosen in cases where the map geometry (points, lines, polygons) serves as target geometry for data input, but the actual values to be assigned are unrelated to the map.

This mode can be used in conjunction with the input

modes for constant data, time series, or lookup tables in the *Editor* toolbar. After hitting the button for point, line, or polygon input the target geometry in the model is chosen by clicking the corresponding geometry. All mesh items within the distance defined in the *Snap-Distance* toolbar are assigned the value. Existing selections are hereby ignored.

10.5.2 Automatic Data Input

Many of the map formats compatible with FEFLOW can contain attribute values, e.g., simple triplet-text or ESRI-Shape files. These attributes can be used as the data source for parameter assignment.

Depending on the type of map data (point, line, polygon), the properties may be applied to the target geometries either directly, or via a regionalization algorithm.

Parameter Association

For all automatic data input, it is necessary to link the desired map attribute to a target FEFLOW parameter. As this link is stored permanently with the model, the import can be quickly repeated when the map data have changed. The link is defined in the *Parameter Association* dialog that can be accessed via the context menu of the respective map in the *Maps* panel.

Detailed settings for the data transfer can be defined in the properties of the link in the *Parameter Association* dialog. Here, it is defined whether the attribute data are interpreted as distribution of time-constant parameter values or as the ID of a time series for boundary conditions or constraints or whether time-varying material properties are assigned. For time-constant data and for time-varying material properties, the source data unit can be specified, and, for point data

sources, the regionalization method and its properties are set. Furthermore, it is possible to relate data to a certain slice or layer if the slice or layer number is contained in the attribute data of the map. If another map is defined as the selection map, that map defines the target geometry. Thus for example an interpolation from point geometries can be limited to the nodes within a polygon or along a line obtained from another map. Either a selection map or a selection can be stored to easily repeat the data import.

Regionalization

The regionalization settings are edited in the *Parameter Association* dialog as part of the link properties for point maps. For classic two-dimensional data interpolation, FEFLOW contains three interpolation methods with their respective property settings:

- *Inverse Distance*
- *Kriging*
- *Akima*

The *Neighborhood Relationship* regionalization assigns a property to the nearest node, or to a number of nodes close to a map point. One typical example is the import of pumping wells in cases where the well locations have not been considered in the design of the *Supermesh*. The wells are then applied at the node closest to the original well location (*Single Target*), and if more than one well is mapped to the same node, the pumping rates will be summed up (*Aggregation: Sum*).

Corresponding to the *Neighborhood Relationship*, the *Point in Element* regionalization method for elemental properties assigns a value to those elements that contain a source data point. If more than one point is located within the same element, the point attribute values can be either summed or averaged.

10. Parameter Assignment

A *1-dimensional linear interpolation* method along lines is available if a line map has been chosen as the link selection. Intended mainly for river water levels, this regionalization provides the means for interpolation between time-constant or time-varying water levels, e.g., for considering the translation of a flood wave along the river. Extrapolation from the last data point in direction or opposite to the line direction as well as in both directions is also supported.

Assignment

After defining the parameter association link, the actual data assignment is invoked by clicking the green check mark in the *Editor* toolbar presuming the following conditions are met: The input field in the toolbar is in map input mode, the correct map has been selected, the corresponding parameter is active, and if no selection map has been chosen as a link property, the target nodes or elements are selected. All requirements except the selection can be fulfilled at once by double-clicking on the entry for the link in the *Maps* panel, or, including the selection, by double-clicking on a previously stored node/element selection or selection map entry for the link in the *Maps* panel.

10.5.3 Assignment via Quick Import

The *Quick Import* option can be used to assign multiple attributes of a previously exported map to several parameters at once without the need for defining parameter links via the *Parameter Association* dialog first. This option is accessible in the context menu of a map in the *Maps* panel. Prerequisites for successful assignment via this option are:

- The map data has been exported from FEFLOW,

- The export and import model are equal or similar so that slice and layer numbers match for both models,
- The parameter units in both models match,
- Additional required information, e.g., time series, Borehole Heat Exchanger datasets are loaded before performing the quick import.

The import can be limited to specific model parameters and/or to the current slice/layer or the current selection. To match the input data to the mesh elements, one of the selection methods *Select by element number* or *Select by nearest element center(s)* needs to be applied in the *Quick Import* dialog.

10.6 Assignment via Expression

Values for the currently active parameter can be assigned based on user-defined expressions which are specified in FEFLOW's *Expression Editor*. A double-click in the input field of the *Editor* toolbar opens the *Expression Editor* for editing the current expression or any of the stored expressions if the *Editor* toolbar is in *Expression* mode.

10.7 Assignment of Lookup Table Values

10.6.1 Assignment

Values for the active parameter are assigned at nodes or elements by selecting the currently defined or one of the previously stored expressions from the drop-down list of the *Editor* toolbar and by clicking the green check mark symbol next to the input field.

10.7 Assignment of Lookup Table Values

10.7.1 Lookup Tables

Parameter lookup tables allow the definition of named properties, e.g., material types, each representing a set of parameters, such as conductivity, drain-/fillable porosity, etc. When assigning a parameter, the property name can then be used instead of assigning a value. The definition of the lookup table is located in *Global Settings*, accessed via the *Tools* menu.

The lookup table is independent of the current model, so that the properties can be used in different projects.

10.7.2 Assignment

The assignment of parameters from a lookup table is similar to the input of constant or time-series data. The input box in the *Editor* toolbar, however, has to be in lookup-table mode. The properties in the lookup table that contain a value for the current input parameter can be selected from a drop-down list.

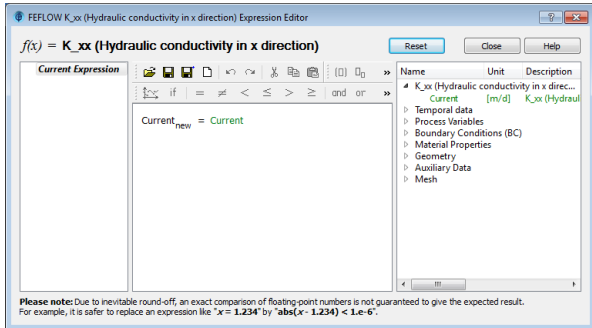


Figure 10.8 Expression Editor.

Arbitrary user-defined expressions are set up in the work area in the center of the dialog. The available model parameters that can be used within an expression are listed on the right-hand side of the dialog. Several toolbars provide access to loading/saving expressions and to mathematical operators and templates that can be used for composing equations.

All parameters and time series as well as the left-hand side of the equation carry units which can be inspected via the tooltip of each parameter in the work area or the list on the right-hand side of the dialog. By default, the editor uses the user-defined unit which has been set via the context menu of a parameter in the *Data* panel. Changing the unit is possible via the context menu of the respective parameter in the work area or in the parameter list in the dialog.

Expressions can be stored or renamed using the context menu of an entry in the list on the left-hand side of the editor.

10. Parameter Assignment

10.8 Copying of Data Values

Parameter values in the current selection can be copied to the clipboard and pasted either to the same nodes/elements of another parameter of the same type (e.g., **Conductivity K_{xx}** to **Conductivity K_{yy}**), or to another slice or layer. For time-varying material properties, the entire time-dependent material data can be copied and pasted to another parameter of the same type. Pasting of parameter values to multiple material times of a time-varying parameter is also possible.

The Copy and Paste functions are available in the context menus of the parameters, in the *Edit* menu, and in the *Standard* toolbar.

10.9 Assignment of Multiple Parameters

Besides assigning values to different input parameters one after the other, it is also possible to edit multiple parameters simultaneously. This option can be accessed via *Assign Multiple...* in the context menu of parameters in the *Data* panel.

The dialog displays different parameters depending on the entry via which the dialog was opened. Homogeneous values and input units can be changed, the checkmark in front of a parameter determines whether a new value will be assigned or not.

The assignment of new values can be applied to the *entire model domain*, to the *current slice/layer* if the *Slice* view is the active view or to the *current selection*

only.

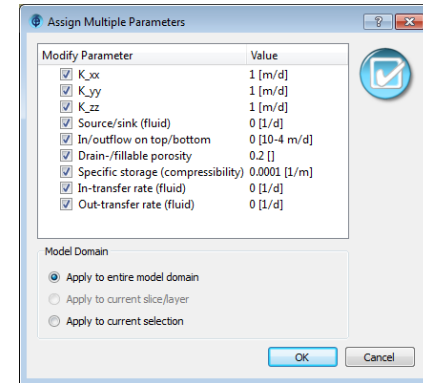


Figure 10.9 Assign Multiple Parameters dialog.

10.10 Time-Varying Material Properties

For the definition of time-varying material properties, FEFLOW provides a number of different settings and assignment options. As for time-series, *Linear* and *Akima interpolation* are available for interpolation between given material times. The defined time-varying data can be applied to the model cyclically, or it can be used in linear mode. If the defined time stages only cover part of the simulation time in linear mode, the first material-time value is used from the simulation start until the first defined time stage is reached, and the last material-time value is used until the end of the simulation. Time stages can be added and deleted and a parameter can also be made stationary again, selecting the material time for obtaining a stationary distribution for the parameter. All settings are located in *Edit Time Dependency* in the context menu of a time-varying material property in the *Data* panel. Time-varying

10.10 Time-Varying Material Properties

material properties are indicated by a blue wave symbol in front of the parameter's name in the **Data** panel.

Time-varying material data can be inspected using the **Inspection** tool. The **Inspection** panel displays the current material time and value and also the time-dependency settings (cyclic/linear, Akima/Linear interpolation). The **Transient-Data** chart in the **Inspection** panel shows a preview of the time-series curve for a time-varying parameter.

10.10.1 Manual Assignment

To assign time-varying values to a material property manually, the parameter has to be made transient via its context menu in the **Data** panel first. In the **Material Data Time Stages** dialog, a list with material times can be edited manually or imported from a time-series (POW) file (Figure 10.10).

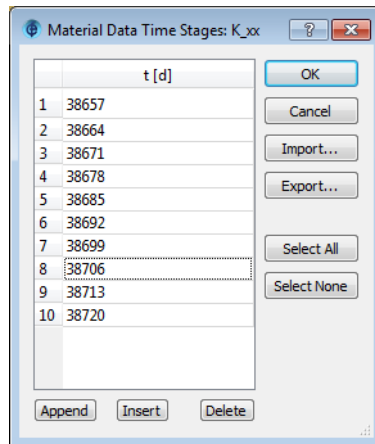


Figure 10.10 Material Data Time Stages dialog.

To assign values to a certain material time, the

parameter needs to be active, the material time has to be selected via **Material Time** in the context menu of the parameter in the **View Components** panel. The currently selected material time is always displayed in the parameter legend in the active view and shown in the parameter entry in the **View Components** panel. The assignment to the target element selection is executed by typing the value for the selected material time into the input field in the **Editor** toolbar and by clicking the green checkmark to the right of the input field (or by hitting <Enter>).

10.10.2 Manual Assignment from Time Series

The assignment of time-varying material properties via time series is completely analogous to using time series for boundary-condition assignment (see chapter 10.4.2). As time-varying material properties need to be defined for the entire simulation period, time series containing gaps are not supported for material properties.

It is only possible to use those time series for material-property assignment which carry the same unit class as the parameter or cardinal units. FEFLOW hides all time series carrying a different unit class and does not display them in the input field of the **Editor** toolbar.

10.10.3 Assignment of Map Data

For the automatic assignment of time-varying material properties via input maps, it is necessary to create a link between the desired map attribute and the FEFLOW target parameter in the **Parameter Associa-**

10. Parameter Assignment

tion dialog that is invoked via the context menu of the input map in the **Maps** panel. To access the different options for time-varying material-data assignment in the **Parameter Association** dialog, the context menu of the material property to be edited has to be used. By default, material properties are assumed to be time-constant.

The available settings for the link definition and for regionalization methods are introduced in chapter 10.5.2.

After defining the link in the **Parameter Association** dialog, the actual data assignment is invoked by clicking the green checkmark in the **Editor** toolbar presuming the following conditions are met: The input field in the toolbar is in map input mode, the correct map has been selected, the corresponding parameter is active, and if no selection map has been chosen as a link property, the target elements are selected. All requirements except the selection can be fulfilled at once by double-clicking on the entry for the link in the **Maps** panel, or, including the selection, by double-clicking on a previously stored element selection or selection map entry for the link in the **Maps** panel.

Assign Material Data to Current Time

Prerequisite for this assignment is that the parameter to be edited has already been made transient before accessing the **Parameter Association** dialog. Additionally, the parameter needs to be set active with a double-click on the parameter's name in the **Data** panel, and the time stage to be edited needs to be selected via **Material Time...** in the context menu of the parameter in the **View Components** panel.

In the **Parameter Association** dialog, the option **Assign material data to current time** needs to be selected from the context menu of the respective mate-

rial property. The map attribute that contains the data for the current time stage can then be linked to the FEFLOW parameter. The **Source data unit** can be changed and depending on the format of the input map, further link properties can be defined. The remaining necessary steps to complete the data assignment based on maps are listed in chapter 10.5.2.

Assign Material Data to Time Stages

For this assignment option, the input map needs to contain an attribute field for each material time. Selecting **Assign material data to time stages** in the context menu of a material property in the **Parameter Association** dialog invokes the **Material Data Time Stages** dialog in case that the parameter is still time-constant. Material times can be edited manually or imported from a POW file. The time stages are displayed as a list underneath the now time-varying material property. Each attribute field that contains the values for a specific time stage needs to be linked to the corresponding material time. To create multiple links at the same time, all or several attribute fields that contain time-varying data can be selected using the <Ctrl> or <Shift> keys and double-clicking on the first time stage. The selection order defines which data set will be assigned to which time stage. It is sufficient to define the link properties in one of the created links, the settings will automatically be transferred to all remaining links.

Assign Time Series to Material Data

For this assignment method, no time-series files are used but the input map contains one attribute field with all the time stages and a second attribute field with the parameter values for each time stage. Choosing **Assign time series to material data** from the context menu of a material property in the **Parameter Association** dialog

adds the entries *Time* and *Value* underneath the material property. A link between the map attribute that contains the time stages and the field *Time* and a second link between the attribute with the parameter values and the field *Value* are required. For both links, the *Source data unit* can be changed.

Time-Series Joining to Maps

If a map only contains an attribute field with time-series IDs to be used as input for time-varying material properties but not the data directly, the required time series (POW file) can be joined to a map in the *Parameter Association* dialog. Time series can be joined via *Join/Select Map(s) Data* in the context menu in the input map: The field *TimeSeriesID* in the time-series file is linked to the attribute field with the time-series IDs in the input map. Time stages and corresponding values specified in the time-series file are now available as attribute fields that can be linked to a material property. The link is completed following the same steps as described in the previous section *Assign Time Series to Material Data*.

10.10.4 Assignment via Expression

Time-varying material properties can also be assigned via user-defined expressions set up in the *Expression Editor*. All time series loaded to a model and also the simulation time can be used as parameters within an expression. The necessary steps to complete the assignment based on a user-defined expression are explained in section 10.6.1.

10.11 Use Parameter Expression

Instead of being defined by time-constant or time-varying values, the FEFLOW parameters *Source/sink* and *In/outflow on top/bottom* can also be linked to a user-defined expression to account for dependencies on other parameters. The defined expressions are evaluated iteratively during the simulation run and the parameter values are updated according to the specified dependencies.

Source/sink and *In/outflow on top/bottom* are linked to an expression by selecting *Use Parameter Expression* in the respective context menu in the *Data* panel. A link to an expression is indicated by a sigma symbol in front of the parameter in the *Data* panel.

10.12 Interactive 1D Linear Interpolation

An alternative option to using maps for the interpolation between boundary conditions or constraints along a line is the *Interactive Linear 1D Interpolation*. This assignment tool can be activated in the *Editor* toolbar if a boundary condition or constraint is the active parameter in a *Slice* view. The interpolation between time constant values, time series and also values calculated via the *Expression Editor* is supported.

The line path along which values are interpolated is drawn manually with the tool being active. By pressing <Ctrl> while placing a new vertex, a boundary-condition or -constraint value can be set together with the vertex, applying the constant value, time series or user-defined expression currently entered in the input box of the *Editor* toolbar.

10. Parameter Assignment

Additional settings for, e.g., the interpolation of time-varying values or the consideration of already existing data along the interpolation path are accessible via the main menu **Tools > Global Settings > Tool Properties**.


10.13 Units

FEFLOW uses a standard unit for each parameter that is listed in the parameter description in the help system. For parameter input and display, other units can be applied in one of the following ways:

- The standard unit for a physical unit (such as velocity, time, etc.) can be changed globally for the user interface via **Units** in the **Tools** menu. One of three predefined systems or a user-defined unit set can be applied.
- For each parameter, the unit for the active model can be chosen via the context menu of the parameter in the **Data** panel. This unit is then the output and default input unit. This setting is stored within the *.fem file and applied whenever a specific model is loaded.
- The unit of the input values can be defined at the time of input: For manual input, the unit of the input value can be typed in with the value. When assigning the value, the unit is automatically converted. For map-based data input, a unit conversion can be specified as part of the **Parameter Association** link.
- For assignment via user-defined expressions, the user unit of each parameter within the expression and of the parameter to be assigned can be changed in the **Expression Editor**.

10.14 Tutorial

In the following exercises we use different methods to assign process variables, boundary conditions, material properties and discrete features.

Click  **Open** and load the file **parameters.fem**. This model is a 3D transient flow and transient mass-transport model.

10.14.1 Tools



Figure 10.11 Selection toolbar.

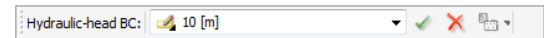




Figure 10.12 Editor toolbar.

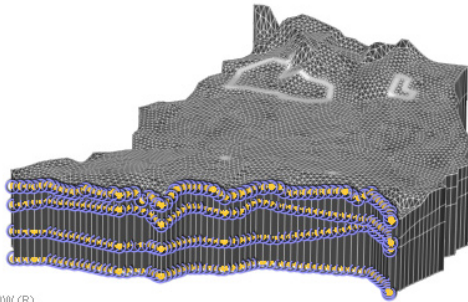


Figure 10.13 Snap-Distance toolbar.

10.14.2 Assignment of Constant Values

In the first exercise we assign constant values manually. We start with the assignment of boundary conditions for flow and mass transport.

Set the **3D** view active, go to the  **Data** panel and activate **Boundary Conditions (BC) > Fluid flow > Hydraulic-head BC** with a double-click. Next, select the nodes to which the boundary condition is to be assigned. We use the node selections displayed in the  **Spatial Units** panel to set a selection. Double-click



FEFLOW (R)

Figure 10.14 Boundary conditions at southern border.

on **Southern Border** to set the selection active. The selected nodes of the southern border now appear as yellow spheres.

Now, enter a value of 10^3 32.1 m in the input box of the **Editor** toolbar and click **Assign**. The selected nodes are now surrounded by blue circles, the symbol for a 1st kind boundary condition (see figure 10.14). Clear the selection with a click on **✕** and proceed with the northern border.

Double-click on **Northern Border** in the **Spatial Units** panel to set this node selection active. Enter 10^3 46 m in the **Editor** toolbar and click the green check mark to assign the value.

We proceed with the assignment of mass-transport boundary conditions for the two borders. Go to the **Spatial Units** panel and click on **Domain**. In the **Data** panel, activate the parameter **Mass transport** > **Mass-concentration BC**. In the **Spatial Units** panel open the context menu of **Southern Border**. This time, select the option **Add to Current Selection** to select both the southern and the northern border. Type a value of 10^3 0 mg/l in the **Editor** input box and click **Assign**.

To ensure a free outflow of mass at these borders we add a constraint. First, click on **Domain** in the **Spatial Units** panel again. In the **Data** panel, open the context menu of **Mass-concentration BC** and select **Add Parameter** > **Min. mass-flow constraint**. Double-click on **Min. mass-flow constraint**, enter 10^3 0 g/d in the input box of the **Editor** toolbar and assign the value with a click on the green check mark. The constraint will limit the applicability of the 0 mg/l fixed-concentration BC to flow entering the model domain (here treated as positive). At BC nodes with outgoing (here negative) flow, the fixed-concentration BC will be replaced by the constraint. The minimum constraints are displayed as white bars below the boundary-condition symbols in the model. Make sure to clear any selection before proceeding to the next assignment.

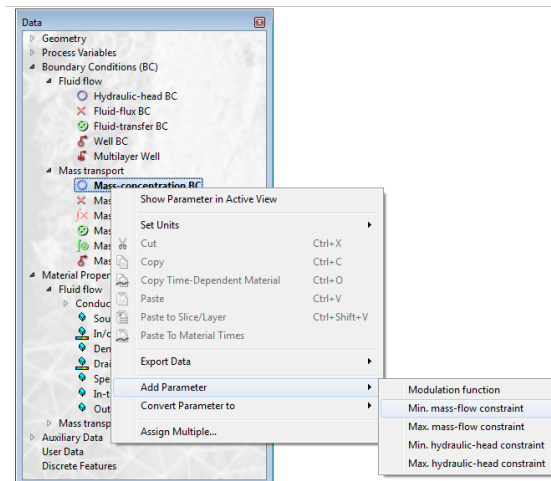


Figure 10.15 Adding boundary constraints.

10. Parameter Assignment

10.14.3 Assignment of Time Series Data

We assume a mass source that is defined as time-varying mass-flux boundary condition in our model. We therefore use a time series to assign time-varying boundary condition values.

Open the *Time-Series Editor* via **Edit > Time Series**. The ID list on the top left of the dialog is still empty and shows that the model does not contain any time series yet. To load the time series click on **Bu Import** and choose the file **massflux.pow**.

This file contains one times series with the ID 10 that is now added to the time-series list. Before the time series can be assigned, we need to include a gap in the series in order to turn the boundary condition off during a specific time period. Additionally, we need to define the unit class of the time-series values. The time-series graph currently shows a linear increase of the mass flux between days 60 and 90. In order to deactivate the boundary condition between these two time stages, we include a gap after day 60. To do so, click into the line for day 60 in the time/value list on the right-hand side of the editor and then click on **Insert Gap**.

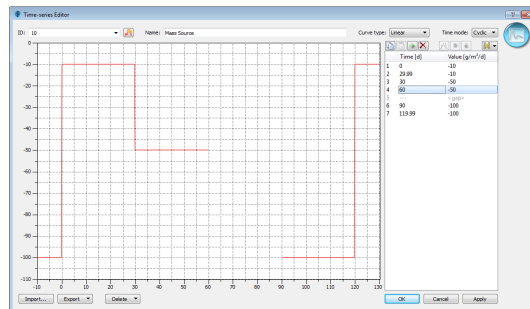


Figure 10.16 Time series including a gap.

Both the time/value list and the time-series graph now reflect that the boundary condition will be turned off between days 60 and 90 (see Figure 10.16.).

To change the unit class of the time-series values, right-click on *Value*, select **Change Unit Class** and then click on **Integrated mass rate**. The displayed user unit now switches from cardinal to [g/m²/d].

Click on **Bu Apply** and **Bu OK** to confirm the changes and to leave the dialog.

Make sure that the *Slice* view is the active view and that *Slice 1* in the **Spatial Units** panel is selected. Double-click on **Mass transport > Mass-flux BC** in the **Data** panel and also on the stored node selection **Mass Source** to set the selection active. To assign the time-varying mass flux, click on the symbol in the input box of the **Editor** toolbar until it switches to **Time Series** input mode and the time series for the mass-flux boundary condition is displayed. Complete the assignment with a click on **Assign**. The time-varying character of the boundary condition is indicated by a white wave symbol on top of the boundary condition in the active view. The time-series ID is also

displayed next to the BC symbol (Figure 10.17).

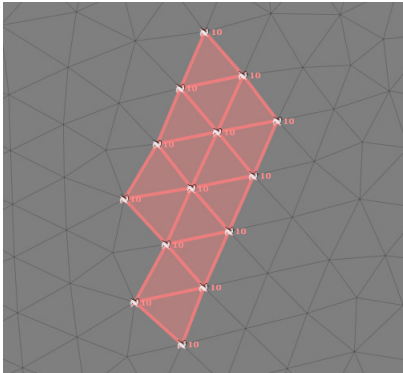


Figure 10.17 Time-varying mass-flux BCs.


10.14.4 Assignment of Map Data

10.14.4.1 Interactive Data Input

To complete the boundary conditions we assign a fixed concentration (1st kind Mass BC) to the nodes of the two contamination sites.

Instead of creating a selection prior to the parameter assignment, we perform the assignment using the map geometry as target geometry.

First, click on **Slice 1** in the **Spatial Units** panel when the **Slice** view is the active view. Activate the parameter **Mass-concentration BC** in the **Data** panel. Double-click **Supermesh > Polygons** in the **Maps** panel. Enter a concentration of 10^3 500 mg/l and switch to the now active tool **Assign Data by Map Polygon** located in the map-assignment tools next to the input field of the **Editor** toolbar. Reduce the **Snap distance** to 10^3 1 m in the **Snap-Distance**

toolbar to limit the selection to the nodes within the contamination sites. Clear any active node selection with a click on . Move the mouse cursor over the contamination sites until they are highlighted. Assign the concentration with a single click into each of these areas. The boundary conditions now appear as blue circles around the nodes.

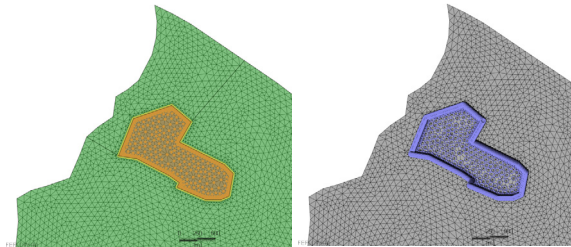


Figure 10.18 Highlighted contamination site (left) and assigned boundary conditions (right).

10.14.4.2 Automatic Data Input

Parameter Association, Regionalization and Assignment

Having the boundary-condition assignment completed we proceed with the assignment of material properties. To assign values for hydraulic conductivity and recharge we use some of the maps that are included with the model. These contain attribute values which have to be linked to the respective FEFLOW parameters.

Start with assigning hydraulic-conductivity values to the top layer of the model. Go to the **Maps** panel and open the context menu of the map **conduc2d** with a right-click. Select the entry **Link to Parameter** to

10. Parameter Assignment

open the *Parameter Association* dialog.

The list on the left hand side contains the attribute data which are stored in the map. Click on **CONDUCT**. To link these data to the FEFLOW parameter now double-click on *Material Properties > Fluid flow > Conductivity K_{xx}* in the list on the right hand side. A black line shows the created link. The link properties are edited in the table below.

Leave the *Link Type* as *Time constant data* and set [10^{-4} m/s] as source data unit for the conductivity values. Do not change the fields *Element/Layer Selection* and *Default Link Selection*.

As the map contains point data, we need to define a regionalization method for data assignment.

From the list of available methods select the *Akima* method. Set a *Linear Interpolation Type* and choose **3 Neighbors** and **0 Over-/Under Shooting**. Confirm the link settings and leave the dialog with **OK**.

To assign the linked conductivity data, make sure that the *Slice* view is the active view and double-click on the entry for the link in the *Maps* panel. *Conductivity K_{xx}* now becomes the active parameter in the *Data* panel, the assignment mode is changed to *Maps* and the correct map for assignment is automatically set in the input field of the *Editor* toolbar.

Browse to slice 1 in the *Spatial Units* panel. Now, select all elements of the top layer with a click on *Select All*. To assign the data click the green check mark in the *Editor* toolbar.

10.14.4.3 Assignment via Quick Import

To demonstrate how all or multiple exported model parameters can conveniently be reimported into the

same model or an alternative scenario of the same model we export all boundary conditions and then reassign them using the *Quick Import* option.

To export all flow and mass-transport boundary conditions into one file, right-click on *Boundary Conditions (BC)* and select *Export Data > All Nodes* and save the file as **boundary_conditions.shp**. Confirm the automatic import of the map into the current model with **Yes**. The map *boundary_conditions.shp* now appears under *Exported Maps* in the *Maps* panel.

To illustrate that all boundary conditions are assigned correctly via the *Quick Import*, we delete all boundary conditions first. The fastest option to do this is again to right-click on *Boundary Conditions (BC)* in the *Data* panel and to select *Assign Multiple*. Make sure that the setting *Apply to entire model domain* is active and confirm the deletion with **OK**.

Now, go to the *Maps* panel, right-click on the map **boundary_conditions** and select *Quick Import...* from the context menu. Make sure that all the boundary-condition types that we want to reimport are checked. Choose the option *Select by node number* as *Node Selection Mode* and *Apply to entire model domain* as *Model Domain* (see Figure 10.19). After clicking on **OK** all fluid-flow and mass-transport

boundary conditions are reimported.

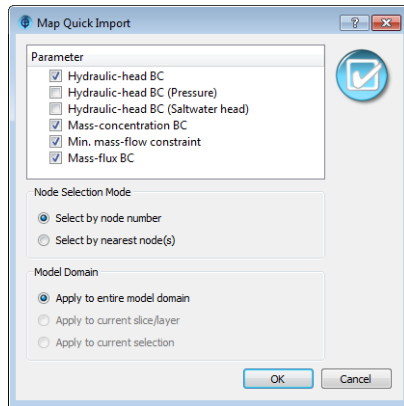


Figure 10.19 Assignment via Quick Import.

10.14.5 Assignment via Expression

The hydraulic conductivity in z-direction is assumed to be smaller by a factor of ten than the conductivity in x-direction. To assign the conductivity values in z-direction, a user-defined expression is applied.

In the **Data** panel, double-click on **Conductivity K_{zz}** . Right-click on the symbol in the input box of the **Editor** toolbar and switch to **Expression** assignment mode. Open the **Expression Editor** with a double-click on **Current Expression** in the **Editor** toolbar. Delete **Current** in the working window and open **Material Properties > Fluid flow > Conductivity** in the list of model parameters on the right-hand side of the dialog. Double-click on **CONDx** and then click on the **Insert a fraction template** symbol. To complete the expression, click into the blue input box and

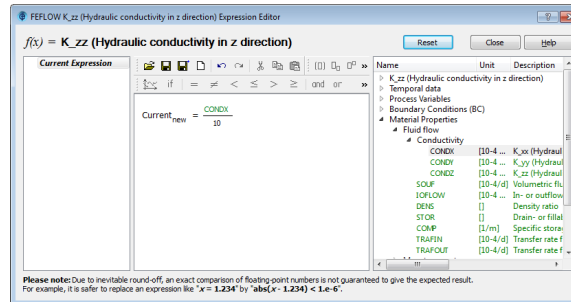


Figure 10.20 Expression-based assignment.

enter **CONDx / 10**. Hydraulic conductivity in z-direction is now linked to conductivity in x-direction.

Leave the dialog with **Close**. Select all elements of the top layer with a click on **Select All** in the **Slice** view and execute the assignment with a click on **Assign**. The completed expression is shown in Figure 10.20.

10.14.6 Assignment via Copy and Paste

For the conductivity in y-direction the same values as for the x-direction shall be applied. To assign the values we copy the **K_{xx}** values to the parameter **K_{yy}** .

First, we have to create a selection from which we want to copy. Again, select all elements of the top layer with **Select All**. In the **Data** panel, open the context menu of **Conductivity K_{xx}** and click on **Copy**. Then, right-click on the parameter **Conductivity K_{yy}** and select **Paste**.

Values cannot only be copied to other parameters but also to the same parameter on a different slice or layer. Make sure to click **Clear Selection** before proceeding. Browse to layer 3 in the **Spatial Units**

10. Parameter Assignment

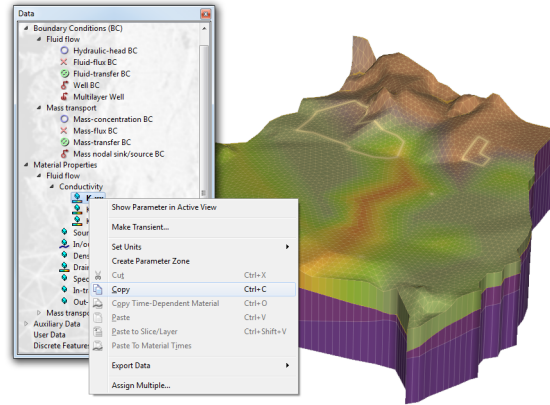


Figure 10.21 Parameter assignment using Copy/Paste.

panel and select all elements of this layer with a click on **Select All**.

Now double-click on **Drain-/fillable porosity** in the **Data** panel and select the option **Copy** from the context menu of the parameter. Open the context menu once more, click on **Paste to Slice/Layer** and select layer 1 as target layer. The values for **Drain-/fillable porosity** are now copied from layer 3 to layer 1.

10.14.7 Assign Multiple Parameters

The material properties for mass transport are assumed to be homogeneous throughout the entire model domain. Except for the parameters **Longitudinal** and **Transverse dispersivity** the already assigned values are accepted.

To edit these two parameters simultaneously, open the context menu of **Material Properties > Mass transport** in the **Data** panel, with a right-click and select

Assign Multiple... Uncheck all parameters except for the two dispersivities. Double-click into the **Value** field for **Longitudinal dispersivity** and enter a value of 10^3 **70 m**. Press the <Tab> key on the keyboard and enter 10^3 **7 m** as **Transverse dispersivity** value. Make sure that the option **Apply to entire model domain** is selected and confirm the assignment with **OK**.

10.14.8 Time-Varying Material Property Assignment

Continue with assigning recharge which in FEFLOW is treated as a material property. Go to the **Maps** panel and select **Link to Parameter** in the context menu of the map **year_rec** to open the **Parameter Association** dialog.

The map contains five different data sets which we will assign as cyclic transient recharge data. To define time-varying recharge values, open the context menu of **In/outflow on top/bottom** in the list on the right hand side and select the option **Assign material data to time stages**. In the **Material Data Time Stages** dialog, click on **Import...** and select the file **material_times.pow** to load the time stages for which the input map contains recharge data. Confirm the import with **OK**. The loaded time stages are now listed below **In/outflow on top bottom**. Click on the entry **ULTRAWET_Y**, hold the <Shift> key and click on **ULTRADRY_Y**. To set all links between the map attributes and the corresponding material times at once, double-click on **0 [d]** on the right-hand side. Black lines indicate that five links have been defined. Click on one of the links to display the link settings.

As source data unit for the recharge values keep the default unit of **[10⁻⁴ m/d]**. Do not modify the fields **Element/Layer Selection** and **Default Link Selection**.

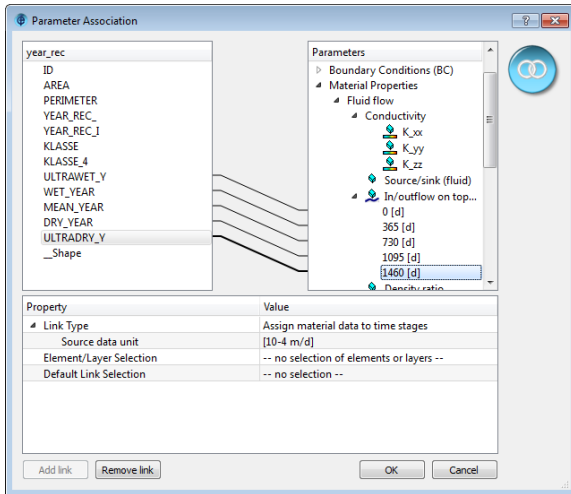


Figure 10.22 Parameter Association dialog for time-varying recharge data.

As this map is a polygon shape file no regionalization is necessary to import the data. All necessary settings are shown in figure 10.22.

Click on **OK** to confirm the settings and to leave the dialog. The link between the map data and the FEFLOW parameter is now shown in the **Maps** panel in the tree **year_rec > Linked attributes**.

To assign the linked recharge data, reduce the snap distance to 10^3 **0 m** and follow the same steps as for the assignment of hydraulic conductivity in section 10.14.4.2

The legend of **In/outflow on top/bottom** in the **Slice** view displays the time stage that the plotted parameter distribution belongs to.

To use the defined recharge values in cyclic mode, open the context menu of **In/outflow on top/bottom** in the **Data** panel and select **Edit Time Depen-**

ency > Cyclic.

10.14.9 Assignment via Interactive 1D Interpolation

In the next step we assign a time constant boundary condition via **Interactive 1D Linear Interpolation**. The boundary condition is assigned along the outer model boundary but the interpolation at locations within the model domain works completely analogously.

Make sure that the **Slice** view is the active view and navigate to the top slice via the **Spatial Units** panel. Activate the boundary condition **Hydraulic-head BC** with a double click on the parameter in the **Data** panel. Once the boundary condition is activated for assignment, the tool **Linear 1D Interpolation** becomes available in the drop-down list of tools located at the far right in the **Editor** toolbar. To use the tool, simply click on it.

We will define both the geometry and the values to be used for the interpolation interactively. In the input field of the **Editor** toolbar, enter a value of 10^3 **40 m** and click on a node along the model boundary in the East while you keep the <Ctrl> key pressed. Pressing <Ctrl> assigns the value, time series or expression currently entered in the **Editor** toolbar at the selected node location while a simple click only adds a vertex along the interpolation path without a value. The assigned head value of 40 m is automatically displayed next to the first vertex.

Place additional vertices along the outer model boundary by clicking the left mouse button: A green line indicates the element edges along which the line geometry will be placed. As the snap distance is used for the selection of vertices, make sure that it is large enough for a convenient use of the interpolation tool.

10. Parameter Assignment

In case that you would like to remove the last vertex of a line, place the mouse cursor on top of it and then hit .

To finish the line and to start the interpolation between the defined values and locations, enter 10^3 **38 m** in the **Editor** toolbar, hit <Ctrl> and then double-click on a node at the outer model boundary which represents the end of the line. To display the interpolated boundary-conditions values, check the entry **Value Label** in **Hydraulic-head BC** in the **View Components** panel. An example for interpolated boundary conditions is shown in Figure 10.23.

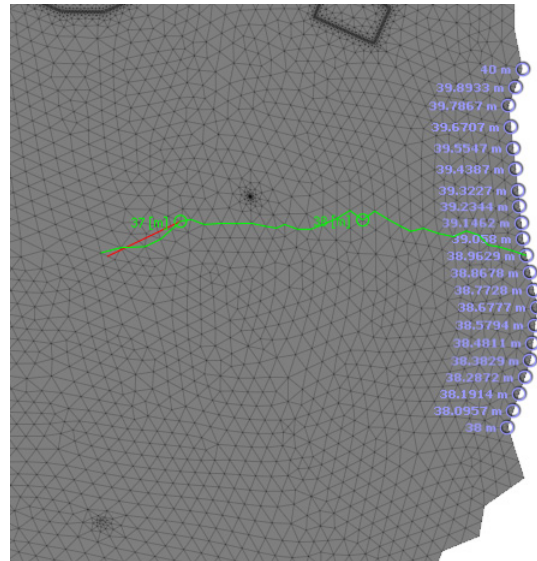


Figure 10.23 Interpolated boundary conditions.

Additional options to ignore boundary-condition values already assigned along the line geometry during the interpolation process, options for the interpolation of time-varying data or extrapolation are accessible via

Tools > **Global Settings** > **Tool Properties** > **Linear 1D Interpolation**.

10.14.10 Multilayer-Well Assignment

For the wells, we assume that the pumping rate is time-constant and that the wells are screened over the entire model depth.

After switching to the **Slice** view activate **Boundary Conditions (BC)** > **Fluid flow** > **Multilayer Well** in the **Data** panel. In the **Spatial Units** panel, set the join-edge selection **Well West** active with a double-click.

The currently active assignment mode is **Multilayer Well** which is shown by the **Multilayer Well** symbol in the input box of the **Editor** toolbar. Double-click into the input box to open the **Multilayer Well Editor** dialog (see figure 10.24).

The preview on the right-hand side of the dialog shows the well coordinates and the currently selected join-edges along which the well screen will be placed.

As **Capacity**, enter a value of 10^3 **1000 m³/d**. For all other parameters we accept the default values. Set the **Multilayer Well** with a click on **Assign** and leave the dialog with **Close**. A red **Multilayer Well** symbol now indicates the position of the specified boundary condition. Use the **Attributes** tree in the **View Components** panel to display the different attribute values of the **Multilayer Well**.

Proceed with the remaining well. In the **Spatial Units** panel, double-click on the stored join-edge selection **Well East** and open the **Multilayer Well Editor** dialog again with a click into the input box of the **Editor** toolbar.

Change the capacity of the well to 10^3 **500 m³/d** and follow the same assignment steps as described for the

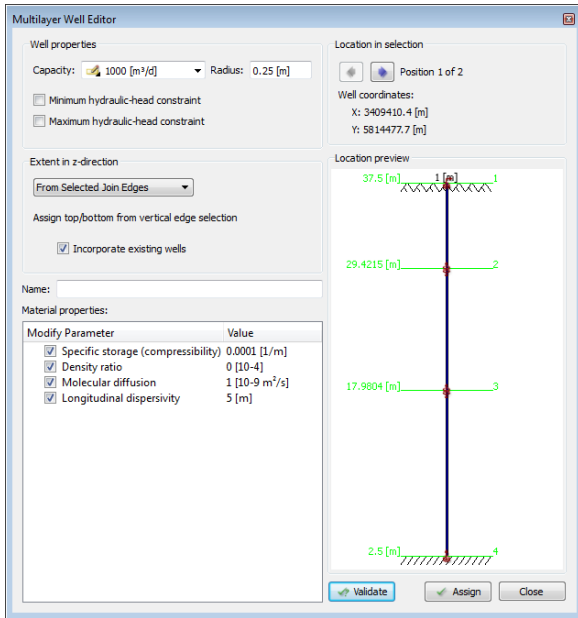


Figure 10.24 Multilayer Well Editor.

western well.

10.14.11 Assignment of Borehole Heat Exchangers

Reload the model **parameters.fem** to add a **Borehole Heat Exchanger** (BHE) to the model.

First, open the **Problem Settings** dialog via **Edit** > **Problem Settings** and switch to **Include transport of...** **Heat** on the **Problem Class** page. Confirm the changes with **Bu** **Apply** and leave the dialog with **Bu** **OK**.

In the **Data** panel, activate **Boundary Conditions (BC)** > **Heat transport** > **Borehole Heat**

Exchanger with a double-click. In the **Spatial Units** panel, double-click on the stored join-edge selection **BHE** to set the edges active along which the BHE will be placed.

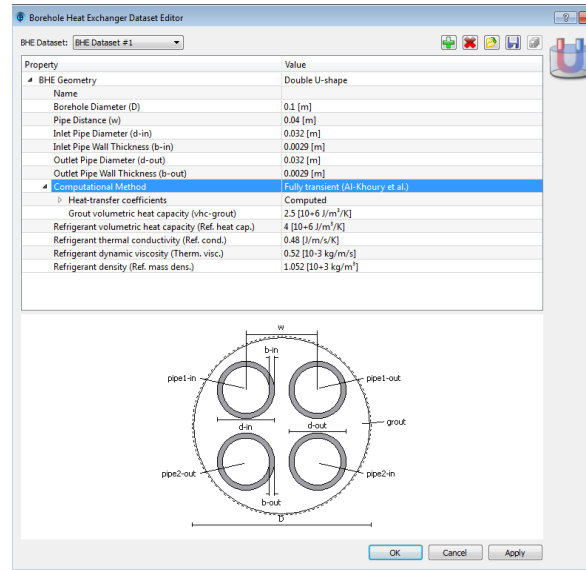


Figure 10.25 Borehole Heat Exchanger Dataset Editor.

As a first step, a BHE dataset has to be created that defines the geometric characteristics of the heat exchanger and also contains the information on the properties of the refrigerant and exchanger components. Double-click on **Borehole Heat Exchanger** in the input box of the **Editor** toolbar to enter the **Borehole Heat Exchanger Editor**. To add a new dataset, click on **Edit borehole heat exchanger datasets** and then on **Add new borehole heat exchanger dataset**. This creates the new **BHE Dataset #1**. Alternatively, the **BHE Dataset Editor** can be accessed via

10. Parameter Assignment

Click **Edit BHE Datasets** in the **Borehole Heat Exchanger** toolbar if the *Slice* view is the active view.

Leave the *Double U-shape* geometry and only reduce the *Borehole Diameter* to 10^{-3} **0.1 m**. The geometry change is automatically reflected in the borehole sketch at the bottom of the dialog window. For the *Heat-transfer coefficients* switch from *User-defined* to *Computed* mode. Confirm the settings and return to the *Borehole Heat Exchanger Editor* with a click on **Bu OK**.

The BHE data set is now available for assignment and the geometric properties are displayed in the dialog. Two remaining properties need to be defined, the flow rate of the refrigerant within the borehole pipes and also the inlet temperature. Instead of applying a constant inlet temperature, we assign a temperature difference between the inlet and the outlet of the BHE. Switch from *Inlet Temperature* to *Temperature Difference* and enter a value of 10^3 **3° C**. Next, enter a *Flow Rate* of 10^3 **30 m³/d**. For the extent in z-direction leave the setting *From Selected Join Edges*. The dialog with all settings is shown in figure 10.26. Assign the *Borehole Heat Exchanger* with a click on **Bu Assign** and leave the Editor with **Bu OK**.

Use the **Attributes** tree in the **View Components** panel to display the different attribute values of the heat exchanger.

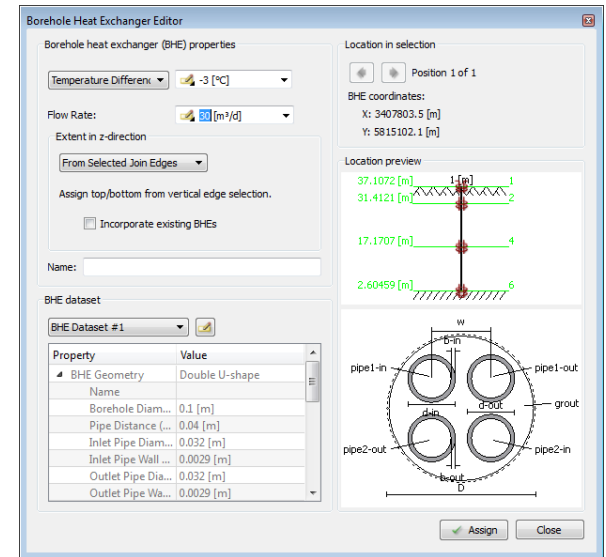


Figure 10.26 Borehole Heat Exchanger Editor.

10.14.12 Discrete-Feature Assignment

Reload the model **parameters.fem**.

On slice 3 we assign some onedimensional discrete features that represent highly conductive fractures. In the **Spatial Units** panel, double-click on the stored slice-edge selection *Fractures*. Use the slice list in the **Spatial Units** panel to switch to slice 3.

To add discrete features at the selected locations, go to the **Data** panel and open the context menu of *Discrete Features*. Select **Add Slice-Edge Feature Element > Hagen-Poiseuille** (see Figure 10.27).

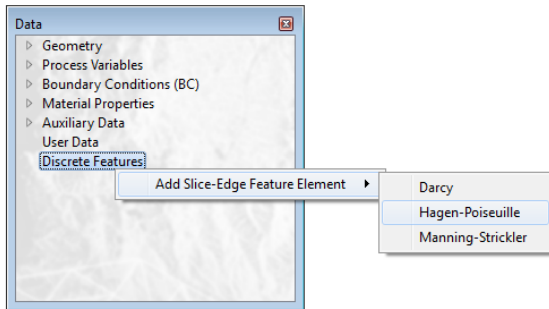


Figure 10.27 Adding Discrete Features.

The discrete feature is now added to the **Data** panel as *Feature 1*. The chosen flow law and geometry type are displayed behind the feature's name. Change the name of the feature to *Fractures* by selecting **Rename...** in the context menu of *Feature 1*.

To show the discrete feature in the active view, click on *Slice 3* in the **Spatial Units** panel and then double-click on one of the discrete-feature parameters in the **Data** panel.

We want to edit the parameter *Hydraulic aperture* at all slice-edges belonging to the discrete feature. Double-click on *Hydraulic aperture* and also on *Fractures* in the **Data** panel to set the edge selection active again in case that you have already cleared the selection. Enter a value of 10^{-3} **1 m** in the input box of the **Editor** toolbar and click on the green checkmark button to assign the value.

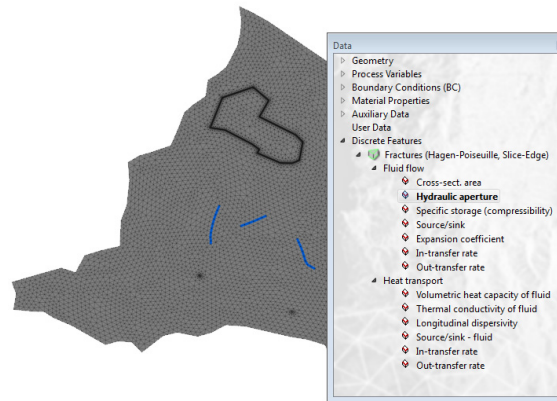


Figure 10.28 Discrete Features in the view and Data panel.

10. Parameter Assignment

Simulation

Running a FEFLOW model

11.1 Introduction

The FEFLOW user interface keeps all visualization options available during the simulation. The simulation progress can thus be conveniently monitored and problems can be detected early.

FEFLOW does not separately store initial conditions of hydraulic head or concentration/age/temperature during the simulation. So the hydraulic-head process variable contains the initial head values before the simulation, the current hydraulic head results at each time step of a transient simulation, and the final hydraulic head after the simulation. These final results are also retained when leaving the simulation mode by clicking **Stop** in the **Simulation** toolbar.

11.2 Model Check

Before running the model, all input parameters and other model properties should be thoroughly checked. A basic overview of the model characteristics is provided in the **Problem Summary** page in the **Problem Settings** dialog. The icon preceding each material prop-

erty in the **Data** panel indicates whether the respective parameter is homogeneous or heterogeneous (see chapter 11.6.2).

11.3 Results Output

Simulation results can be stored in two different formats: a reduced results file (*.dar) and a full simulation record (*.dac). Both results files can be recorded at the same time.

The reduced format contains text output for the observation points and well locations only. It is especially useful for automatic output processing with user-programmed scripts or optimization software such as PEST. Reduced results files always contain values for all the time steps.

In contrast, the full simulation record contains all nodal values of the primary variables (hydraulic head, concentration, temperature) and of the flow velocities. By default, results at all time steps are stored. It is possible, however, to skip a number of time steps between each output, or to specify the simulation moments for which output is desired. In the latter case, the automatic time-stepping scheme ensures that results are calculated exactly at the prescribed output moments.



After the simulation the process variables contain the final results. To restart the simulation using the original initial conditions for head, concentration, age and temperature, the model has to be loaded again from the original file.



If a given simulation record does not contain all the time steps, postprocessing methods that cover multiple time steps, such as transient pathline analysis or time-integrated budgets, can only give approximate answers.

11. Simulation

It is also possible to record a results file that only contains the final time step.

11.4 Running the Simulation

The handling of the interface is as easy as starting a tape or video recorder: The **Start** button in the **Simulation** toolbar starts the simulation, the **Pause** button pauses it, the **Stop** button exits the simulation mode, and when the **Record** button is pressed before starting the simulation, the results are recorded in a file while the simulation runs.

All visualization and also some results-evaluation features (**Rate-** and **Period-Budget** panels, Subdomain Boundary Rate and Subdomain Boundary Period panels, **Content** panel) can be used during the simulation. It should be considered, however, that some of these features might slow down the simulation. Especially more elaborate visualization options such as isosurfaces or budgeting may require significant calculation effort.

After the simulation finishes, FEFLOW remains in paused simulator mode. Thus simulation results such as flow velocities and the solution of the last time step remain available for postprocessing. Only when exiting the simulation mode via **Stop** these data are removed from memory, and streamline/pathline calculation or budget analysis are no longer possible. Any postprocessing then requires loading of the full simulation-record file.

11.5 Convergence

When solving non-linear problems for steady state, or for transient conditions with constant or varying time steps, an **Error-Norm** chart is shown. Once the

change in results between two subsequent iterations is below a certain error tolerance (see chapter 7.1.4), the simulation is terminated. FEFLOW brings up an alert box and shows a message in the **Log** panel if no convergence was achieved within the defined maximum number of iterations.

In transient simulations with an automatic time-stepping procedure, the time step is shortened if necessary to achieve convergence. Only if repeated time-step reductions do not improve the situation, a log message is shown indicating that time-step reduction failed. The simulation is continued with the results of the last calculation for the time step. In general, models that show convergence problems even after greatly reducing the time-step length should be checked for errors in the input data or for insufficient mesh resolution.

11.6 Tutorial

11.6.1 Tools

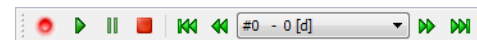




Figure 11.1 Simulation toolbar.

11.6.2 Model Check

Load the file **simulation.fem** via  **Open**. Before we start the simulation we want to make sure that all necessary parameters have been properly assigned, that the problem settings have been set correctly and that all necessary settings for later postprocessing have been made.

Start with the problem settings. Go to  **Edit** > **Problem Settings** and open the **Problem Summary**

page in the dialog. Here, an overview of key simulation control and model parameters is presented. The problem class settings, information on the mesh quality and boundary condition types and numbers are displayed (see Figure 11.2).

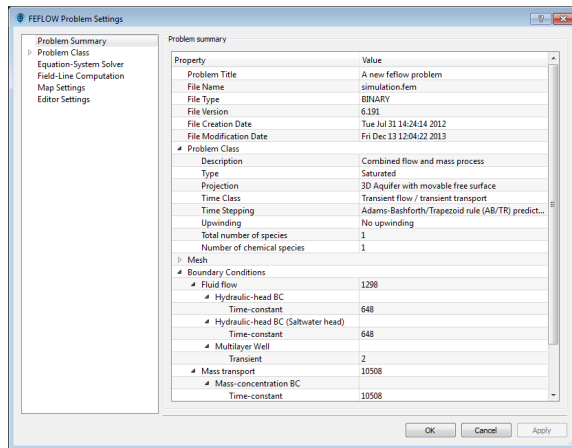


Figure 11.2 Problem Summary.

Leave the **Problem Settings** dialog with **Cancel**.

To check values at specific nodes or elements we can use the **Inspection** tool. Double-click on **Boundary Conditions (BC) > Fluid flow** in the **Data** panel. All fluid-flow BCs are now displayed in the **Inspection** panel. After clicking on **Inspection** move the mouse cursor over the nodes where boundary conditions are set to check the values that have been assigned there. The value for the respective boundary condition, the node and the slice number are shown in the **Inspection** panel.

Both constant values and time series can be checked with the **Inspection** tool. Set the **Slice** view as active

view and move the mouse cursor over the nodes where a multilayer well is set. The assigned time series for the capacity is then shown in the **Transient-Data** chart in the **Inspection** panel. The well geometry and further well properties are also displayed in the **Inspection** panel (see Figure 11.3).

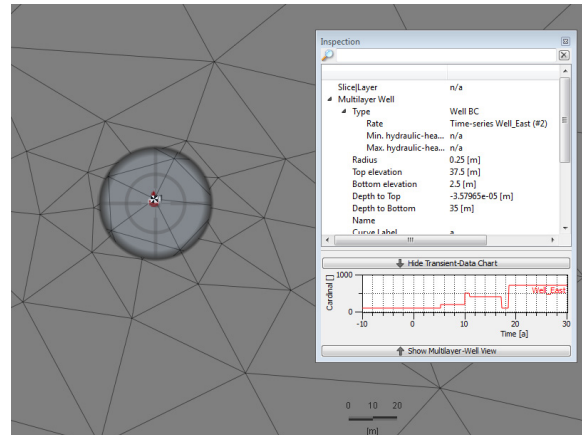






Figure 11.3 Checking boundary conditions with the Inspection tool.

The distribution type of a material property can be quickly checked in the **Data** panel. Homogeneous values are indicated by a  symbol, heterogeneous values by a  symbol in front of the parameter.

11.6.3 Results Output



Before we start the simulation we define how and where the results should be recorded. Click on **Record** in the **Simulation** toolbar to open the **Record Properties** dialog. Check the check box for **Save complete results (DAC file)** to create an out-

11. Simulation

put file. Click on  **Browse** to choose the location for the results file. As we intend to calculate the accumulated mass that leaves the model via the southern border, we cannot skip any time steps. Leave the dialog with  **OK**.



11.6.3.1 Budget Groups

If time series for the fluid- and mass-rate and period budget at selected node locations are to be calculated and recorded, these locations need to be selected and activated for this kind of budgeting before a simulation is started.





In the  **Spatial Units** panel, open the context menu of the stored node selection **Wells** and select  **Budget-History Charting** > **BCs** to calculate fluid and mass quantities related to the specified multilayer well BC that leave the model at these locations. Repeat the same steps for the node selection **Southern Border**. For both selections, a time series will be shown in the **Fluid-** and **Mass-Rate Budget** and **Fluid-** and **Mass-Period Budget** charts.

11.6.3.2 Observation Points

We also import observation points to monitor and compare the obtained hydraulic-head results at certain locations against measured water levels.

Set the **Slice** view active. In the  **Maps** panel, open the context menu of the shape file **obs_points** and select  **Convert to** > **Observation Points**.

In the **Observation Points - Column Bindings** dialog, select the field  as **Slice number** and the field  as **Label**. For the reference data,

set  **Hydraulic head** as **Parameter ID** (see Figure 11.4). As the flow equations are solved for transient conditions, the reference data that the results will be compared to are loaded from time series and not as time-constant values. Choose the field  as **Time series ID**. The time series that contain the reference data have already been loaded to the model. As **Confidence interval**, choose  and confirm the observation-point import with  **OK**.

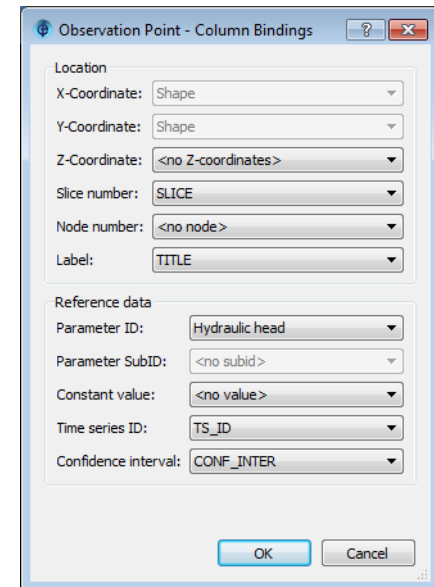




Figure 11.4 Observation Points import.

To check the properties of the observation points, click on  **Edit Observation Point Properties** in the  **Observation-Point** toolbar. The reference values and confidence interval for each observation point are then displayed in the dialog (see Figure 11.5).

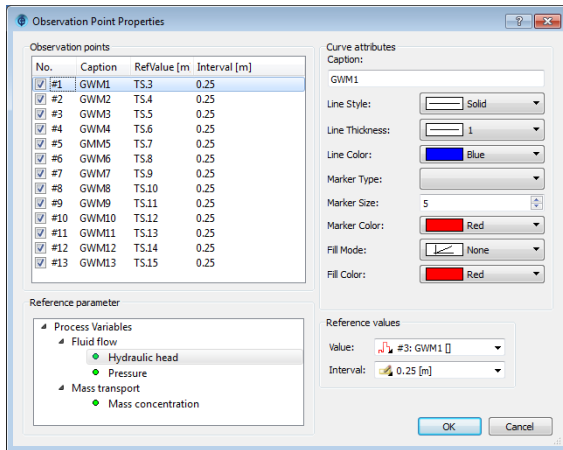


Figure 11.5 Observation Point Properties.

Open the **Rate-Budget** panel via **View > Panels** and set the check mark in front of **Active** to monitor the fluid-rate budget while the simulation is running. After a short computation time the rate budget for each boundary condition type, for source/sink terms, storage capture and release and the imbalance are displayed.

Now click **Stop** to terminate the simulation. Once the simulation has stopped, notice that the rate budget is no longer displayed in the **Rate-Budget** panel due to the now lacking fluid-flux vector field. Evaluation of flux-based results is still possible by loading the simulation record.

11.6.4 Running the Simulation

After checking the model properties and defining the record location we start the simulation by clicking **Start** in the **Simulation** toolbar.

Five different charts appear: **Hydraulic Head**, **Pressure**, and since we are simulating transient flow and transport, also the **Time-Steps** and **Local- and Average-Concentration** charts. Graphs for the well locations and also for the observation points are displayed.

The elapsed simulation time is shown at the bottom of every view window.

During the simulation we can display different parameters in the active view. Go to the **Data** panel and double-click on **Process Variables > Mass transport > Mass concentration** to see how the mass distribution changes with time.

11. Simulation

Results Evaluation

Analyzing the simulation results

12.1 Introduction

As the evaluation of modeling results takes place both during and after the simulation, the content of this chapter applies to monitoring the simulation results at runtime, after finishing the simulation, and after loading a simulation record (postprocessing).

Results evaluation also involves all visualization and animation options described in chapter 9 and chapter 13. This section focuses on the tools specifically designed for output interpretation.

12.2 Observation Points

Observation points are used to monitor simulation results at specific locations in the model domain via chart windows. Using the tools in the **Observation Point** toolbar, observation points can be defined either manually in a **Slice** view, or by converting the current node selection into observation points. Features of point maps can be directly converted into observation points using the context menu of the map in the **Maps** panel. The import also allows to obtain a label and slice

or node number for the point from the attribute data of the map, as well as reference information, typically from measured field data. Observation points can be placed on a slice or at an arbitrary xyz position.

During the simulation, charts are automatically shown for the results of the primary variables (hydraulic head, concentration, and temperature) at the observation points. Additional charts, e.g., for pressure, can be added via the **View** menu.

By selecting **Observation Points** as plotting target (in the **Spatial Units** panel) for a process variable, the deviation between computed and measured values can be displayed in the current view. This includes graphical comparison of the deviation using error bars and the confidence intervals, as well as labels showing the absolute deviation.

Observation points can be added before the start of a simulation or when a results file is loaded.

12.2.1 Scatter Plot

The deviation between observed data and computed results can also be shown in **Scatter plots**. **Scatter plots** are invoked via the context menu of the charts for the primary and process variables. FEFLOW automatically

12. Results Evaluation

uses the loaded observation data to calculate the deviation. Additionally, the absolute error, the root mean square (RMS) and the standard deviation are displayed.

In a results file, the plot always reflects the currently displayed simulation time.

12.3 Budget Analysis

12.3.1 General Budgeting

The **Rate-Budget** panel can show the current fluid-, heat-, or mass rate balance for a selected domain of interest (DOI) at the current simulation time. A budget can be calculated for the entire model domain, a selection of nodes or an arbitrary subdomain consisting of elements. Any stored nodal or elemental selection can be used as a DOI either via context menu in the **Spatial Units** panel, or by pressing the green 'plus-sign' button in the upper left corner of the budget panel after selecting one or more stored selections in the **Spatial Units** panel. All budgets set active will be computed and dynamically updated whenever FEFLOW is in simulator mode, i.e., when the simulation is running, is paused, or has completed.



Calculated storage values represent a lumped result of both confined storage (related to specific storage) and unconfined storage (related to drain-/fillable porosity or unsaturated-flow porosity).

The **Period-Budget** panel shows the accumulated, i.e., time-integrated budget for the simulation period specified in the panel. The period-budget calculation can only be activated before a simulation is started, or when postprocessing a simulation-record (*.dac) file. Activating a period budget will implicitly activate the corresponding rate budget as well.

The respective fluid, heat, or mass balance is subdivided into flows related to the various boundary-condition types, contributions from distributed sources/sinks (e.g., groundwater recharge), storage capture (negative) and release (positive), and a remaining imbalance term

arising from solver residual error and errors due to the spatial and temporal discretization. When using an element selection (i.e., a subdomain) as DOI, the additional - **Internal Transfer** - category appears in the **Rate-** and **Period-Budget** panels. This category represents the transfer across those parts of the DOI boundary that are *inside* the model domain. Model-internal flows crossing the subdomain-boundary into and out of the DOI are considered as positive and negative, respectively.

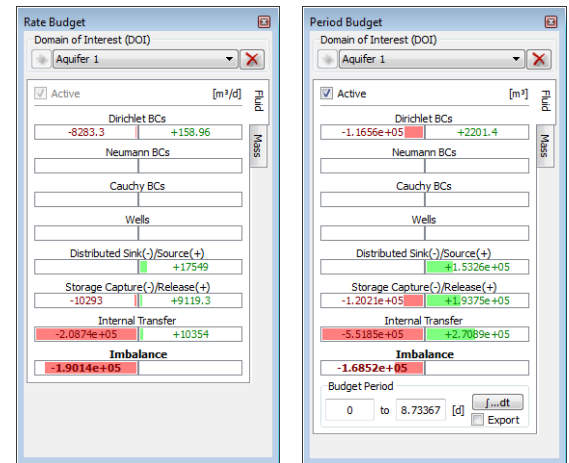


Figure 12.1 Rate-Budget and Period-Budget panels.

By activating the export option in the **Period-Budget** panel before starting the budget calculation, the associated rate- and period-budget values for the specified simulation period can be exported to a (*.txt) file.

The budget results of the currently selected time step can also be exported via **Export Current Values...** in the context menu of the **Rate-** and **Period-Budget** panels after the budget calculation.

12.3.2 Subdomain-Boundary Budget

To calculate the fluid, heat, or mass flow across the boundary of a specific subdomain within a model, the *Subdomain Boundary Rate* and *Subdomain Boundary Period Budget* panels can be used. While the concept and sign convention of these two panels correspond to those of the general *Rate-Budget* and *Period-Budget* panels, there are some key distinctions:

- Subdomains are always defined as an *element selection*, so only element selections can be used as DOI for subdomain-boundary budgeting.
- Only the *boundary* of the subdomain will be considered in the budgeting.
- Values shown in the *BCs* category will only include budget values for those BC-assigned nodes that are located (1) on the subdomain boundary and (2) not shared with any part of the model domain adjacent to the DOI.
- A *masking domain* can be defined to limit the extent of the subdomain boundary that is considered in the budgeting.

If no masking domain is applied, the values shown in the *Internal Transfer* category will correspond to those in the same category of the general budget panel for a given subdomain, i.e., element selection.

In many cases though, it may be of particular interest to compute the flow through only a part of the boundary of a subdomain. This is accomplished by using a second elemental selection as a *Masking Domain (MD)*. Any stored or the current elemental selection can be applied as a MD by selecting it in the *Spatial Units* panel and pressing the green check mark button in the *Masking Domain (MD)* section of the *Subdomain Boundary Rate* panel.

By default, the masking will constrain the budget

evaluation to those parts of the subdomain (DOI) boundary that also belong to the MD. The *MD* panel section also provides an option to invert the masking so that only those parts of the DOI boundary are considered that do *not* belong to the MD.

Subdomain-boundary budgets supersede the now-deprecated *Flow-Rate* and *Flow-Volume* panels whose results are based on approximated Darcy-flux values and which are kept for compatibility and comparison purposes only. As subdomain-boundary budgets are obtained by using the primary solution together with the respective terms of the Continuity Equation, they can be generally expected to be more accurate.

12.3.3 Budget Groups

Any stored node selection in the *Spatial Units* panel can be used as a separate *budget group* for which the summed calculated rate and period budget can be displayed as time series in the *Rate-Budget* and *Period-Budget* charts, e.g., to calculate the flow balance along a river or to determine drained water volumes in dewatering scenarios, etc.

To invoke this budgeting option and to display time series for a node selection in the budget charts, *Budget-History Charting* and one of the following four budget-evaluation options need to be selected in the context menu of a stored node selection in the *Spatial Units* panel:

- BCs: Flows related to boundary conditions,
- Distributed Sink(-)/Source(+),
- Storage Capture(-)/Release(+),
- Imbalance: Sum of flows related to boundary conditions, distributed sinks/sources and storage capture/release.

As an additional fifth option, '*Total Balance*' is

12. Results Evaluation

available as a legacy mode which includes flows related to distributed sources/sinks + boundary conditions, but no budgeting of storage changes.

The budget time series for a stored node selection can only be displayed in the budget charts if the budgeting option for a node selection was activated before the simulation was started. Adding budget groups to an existing simulation record is not yet supported.

The calculated summed rate and period budgets can be exported via the context menu of the *Rate-* and *Period-Budget* charts.

12.4 Multilayer Wells: Flow per Layer

For multilayer wells, the total capacity is internally associated with the lower-most node that belongs to the well screen. Therefore, the *Rate-* and *Period-Budget* panels only display the total pumping/injection rate or volume and not the rates or volumes associated with each layer.

To check the flow for each layer that belongs to a multilayer-well screen, *Multilayer well* needs to be plotted in the active view. The entry *Flow per Layer* in the list of multilayer-well attributes in the *View Components* panel can then be activated to display the flow for each layer.

12.5 Content Analysis

The *Content* panel provides access to the values for various spatially integrated quantities, always at the current simulation time. Depending on the FEFLOW problem class of a given model, the panel contains separate tabs for *Fluid*, *Mass*, *Groundwater Age* and *Heat*. In case of multiple chemical or age species, a

separate tab is created for each species. Depending again on problem class and type, content integration can provide quantities such as domain size, pore space, fluid volume, dissolved mass, absorbed mass, heat energy in fluid and solid phases, etc.

If the entire model domain is considered, discrete features can be included in the calculation as well. Alternatively, the current element selection or any stored element selection (i.e., subdomain) can be used for content evaluation via the context menu in the *Spatial Units* panel.

12.6 Streamlines and Pathlines

Streamlines and pathlines can be very helpful in visualizing steady-state and transient flow fields. While a streamline represents the trajectory of a particle in a flow field assumed to be constant in time, a pathline follows a particle in a transient flow field. Pathline computation therefore requires loading a simulation record of a transient model. Pathlines and streamlines are coincident in a steady flow field.

Streamlines and pathlines can be calculated forwards or backwards from the starting point. The starting points (seeds) can be set at points, circles around points, at the surface of a cylinder or sphere or distributed along lines. Distributed seeds can either be equally spaced along the starting line, or spaced such that the distance between adjacent seeds is inversely proportional to the local flux magnitude.

Streamlines can also be shown during a transient simulation. In this case, the computed trajectory will change with the flow field after each time step.

To visualize travel times of the particles along streamlines and pathlines, isochrone markers or period

sections can be used.

The correct calculation of travel times requires the definition of an effective porosity. For this, one of the available porosities for the given model type (specific yield, porosity for unsaturated flow, mass or heat transport porosity) or an arbitrary reference distribution can be applied.

For mass-transport models FEFLOW additionally provides the option to account for retardation due to Henry-type sorption.

To display streamlines or pathlines, a selection of an appropriate source geometry in the *Spatial Units* panel (node selection, 3D point set, 3D polyline, 3D loop, cylinder or sphere) is required. Node selections can be created by storing the current selection, tools for generating the other 3D geometries are available in the *Drawing* toolbar.

The second important component for streamline/pathline generation is the *Pathlines* or *Streamlines* entry in the *Process Variables* section of the *Data* panel. Following a double click on either *Forward* or *Backward* the pathlines/streamlines are calculated and added to the active view. Pathline properties are found in two different locations: While the effective porosity for isochrone calculation is selected in the *Problem Settings* dialog, view-specific visualization options such as number of seeds along a line, line width or time periods for period sections are controlled via the *Properties* of the pathlines or period sections entry in the *View Components* panel.

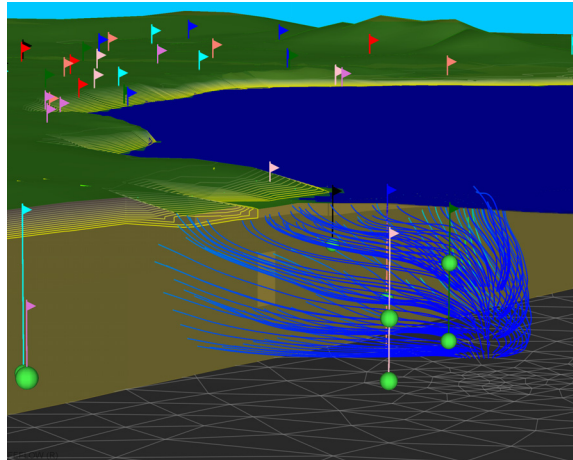


Figure 12.2 Pathline analysis.

12.6.1 Random-Walk Particle-Tracking

Random-Walk Particle-Tracking (RWPT) solutions can be obtained by proceeding as with standard advective streamlines and pathlines, and by distributing the required additional dispersive parameters: molecular diffusion and coefficients of dispersivity. RWPT solutions are theoretically consistent with advection - dispersion equation solutions - provided that a sufficiently large number of particles is used.

12.7 Export

The FEFLOW export options can roughly be grouped into export of raster images (movies and snap-

12. Results Evaluation


shots of a view), and export of vector data (data and plots).

Snapshots of the active view are exported by using the camera button in the **View** toolbar. A resolution enhancement can be applied to the image and texts (e.g., legend text) to obtain high-resolution output suitable for poster printing. Snapshots of a **Slice** view can also be exported as georeferenced images. Additional 3D export settings are used when exporting stereoscopic images. Chapter 13 describes how movies are created from a view animation.

Data and plot export encompasses a variety of different file formats, ranging from simple column-based text files to GIS and CAD files. Data of process variables, boundary conditions, material properties and reference distributions are exported via the context menus of one or several selected parameters in the **Data** or **View Components** panel. If a full simulation results file is loaded, data can be exported for the current time step, a user-defined selection or for all recorded time steps.

Visualization features such as isolines or fringes are exported by using their context menu in the **View Components** panel. If supported by the output format (e.g., ESRI Shape file, AutoCAD Exchange file), plot files are exported in 3D from 3D models.

12.8 Tutorial

In the following exercises we use a simulation record to evaluate the modeling results after the simulation. Start FEFLOW and click  **Open** to load the file **results.dac**. The file contains the complete results for every calculated time step of a transient flow and mass transport simulation.


12.8.1 Tools



Figure 12.3 Simulation toolbar.

12.8.2 Observation Points

For the loaded simulation record, nine different charts can be displayed: **Time Steps**, **Hydraulic Head**, **Pressure**, **Local** and **Average Concentration**, **Fluid-Rate** and **Fluid-Period Budget**, and **Mass-Rate** and **Mass-Period Budget**.

To open a chart, right-click in an empty part of the FEFLOW workspace, select  **Charts** and then the chart that is to be displayed. For each observation point a curve is plotted so that the hydraulic head, concentration and pressure changes at these locations can be monitored during and after the simulation.

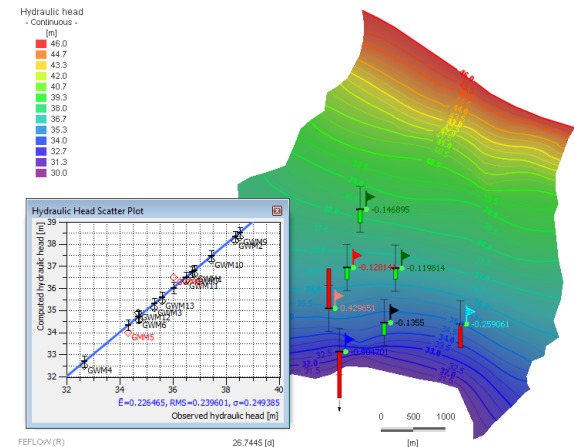


Figure 12.4 Observation points with error bars and labels and hydraulic-head scatter plot.

To compare the field data for *Hydraulic head* to the calculated head results at observation-point locations, activate the *Slice* view first, switch to slice 2 and select *Model Locations > Observation Points* in the *Spatial Units* panel. Next, double-click on *Process Variables > Fluid flow > Hydraulic head* in the *Data* panel. The deviations between measured and computed water levels are now shown as colored bars and as labels next to the observation-point locations (see Figure 12.4). The error bars and labels always refer to the currently selected simulation time. Use the tools in the *Simulation* toolbar to switch to different simulation steps to check how the deviations change. Green bars indicate deviations within the confidence interval, red bars indicate that the deviations exceed the confidence interval. The position of an error bar indicates whether the deviation is positive or negative.

In addition to displaying the water-level deviations in the active view, we open a scatter plot to compare measured and computed data. Open the context menu of the *Hydraulic-head* chart and select *Scatter plot*. The plot always reflects the results at the currently selected simulation time, displayed in both the *Simulation* toolbar and the view windows.

12.8.3 Budget Analysis

We can use the *Rate-Budget* panel to monitor the fluid and mass flows that enter and leave the model domain, or only specific areas.

For mass-transport simulations, the *Rate-* and *Period-Budget* panels contain two tabs, one for fluid and one for mass (see Figure 12.1). To start the budget calculation for the entire model domain set the check mark for *Active* in the respective tab for fluid

and mass. After a brief computation, the *Rate-Budget* panel shows the flow rate for each boundary condition type, for sources and sinks, storage capture and release and the imbalance term representing the remaining residual error. Flows that leave the model have a negative algebraic sign while flows that enter the model have a positive algebraic sign.

Use the *Period-Budget* panel to calculate the time-integrated budget the first 1000 days of the simulation: Switch to day 1000 via the drop-down list of stored time steps in the *Simulation* toolbar and then click on *f...dt* in the panel to start the calculation.

We now calculate the fluid budget for the border in the south instead of taking the entire model as budget domain. Go to the *Spatial Units* panel, open the context menu of *Southern Border* and select *Use Selection as Budget Domain*. The domain of interest is automatically switched from *Domain* to *Southern Border* in both the *Rate* and the *Period-Budget* panels. Start the rate-budget calculation with *Active*. The rate budget is now calculated for the selected nodes only. The budget shows that water is leaving the model domain through the border in the south.

12. Results Evaluation

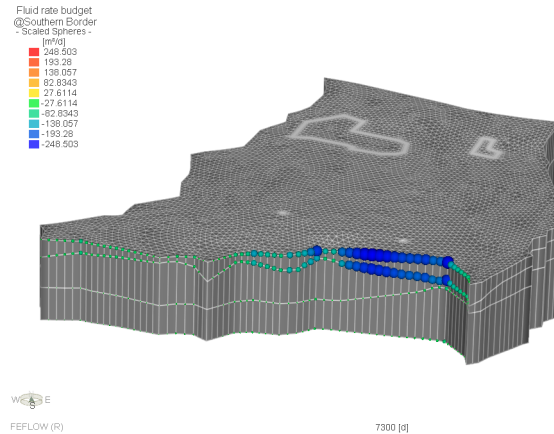


Figure 12.5 Scaled budget spheres along the southern border.

Additionally, the in- and outgoing flows can be visualized as scaled spheres. Set the **3D** view as active view and click on **Southern Border** in the **Spatial Units** panel.

Now, double-click on **Fluid flow > Rate Budget** in the **Data** panel. Blue and green spheres of different sizes are plotted at nodes along the southern border where water leaves the model. We now increase the relative size of the spheres in order to make smaller spheres visible. Open the context menu of **Fluid rate budget > Scaled Spheres** in the **View Components** panel and select **Properties**. In the **Size** tab increase the relative size to 10^{23} **3.0** and click **Apply**. Figure 12.5 shows the resulting plot in the **3D** view.

To check how much mass has left the model via the border in the south over time, we use the **Mass-Period Budget** chart. Open the chart via **View > Charts > Mass-Period Budget History** and check the curve **Southern Border**.

12.8.4 Subdomain-Boundary Budget

To evaluate how much mass enters the lower aquifer via the two contamination sources, we apply the **Subdomain Boundary Budget** panels.

First, we need to define layer 5 as domain of interest for the budget calculation. In a subsequent step, we create a second element selection which we will apply as masking domain. This step is required as we would like to compute the mass flow through only those boundary parts of layer 5 which are in direct contact with the contamination sites.

Activate the **Slice** view and switch to slice 6 in the **Spatial Units** panel. Make sure that the geometry type is set to **Select Elements** in the **Selection** toolbar and select the entire bottom layer with a click on **Select All**. Right-click into the **Slice** view and select **Store Current Selection**. Rename the selection to 10^{23} **Lower Aquifer** and finish with <Enter>. The stored selection now appears in the **Spatial Units** panel. To use this selection as domain of interest in the **Subdomain Boundary Budget** panels, right-click on **Lower Aquifer** and select **Use Selection as Boundary-Budget Domain**. The selection is now available as domain of interest in both the **Subdomain Boundary Rate** and **Period Budget** panels. In the **Subdomain Boundary Rate Budget** panel, switch to the **Mass** tab and start the budget calculation with the **Active** check box. The panel now displays the mass rate entering and leaving this subdomain at the currently selected simulation time.

As we are only interested in the amount of mass entering the lower aquifer via the bottom sections of the two contamination sites, we now apply a second selection as masking domain. First, clear the current selection with a click on **Clear Selection**. Now

switch to slice 5 in the **Spatial Units** panel and activate the **Supremesh Polygons** map for selection via a double-click on this entry in the **Maps** panel. Then, reduce the **Snap distance** to 10^3 **1 m** in the **Snap-Distance** toolbar and switch to the **Select by Map Polygon** tool in the drop-down list in the **Selection** toolbar. Move the mouse cursor over the model domain and create the two selections with a single click into the two contamination sites. Use the context menu of the **Slice** view to store the selection as **12³ Contaminations**. To apply this second selection as masking domain, click on **Contaminations** in the **Spatial Units** panel and then click on the green check-mark symbol in the **Masking Domain** section in the **Subdomain Boundary Rate Budget** panel. The mass-flow calculation is now limited to these element faces which are shared by both selections (see Figure 12.6).

The settings of the **Subdomain Boundary Period Budget** panel follow those of the **Rate** panel. To invoke the time-integrated budget calculation, set the check mark in front of **Active**, enter the starting time for the budget calculation and click on **f...dt**. After a brief computation time, the mass entering and leaving the domain of interest via the selected boundaries is displayed (Figure 12.6).

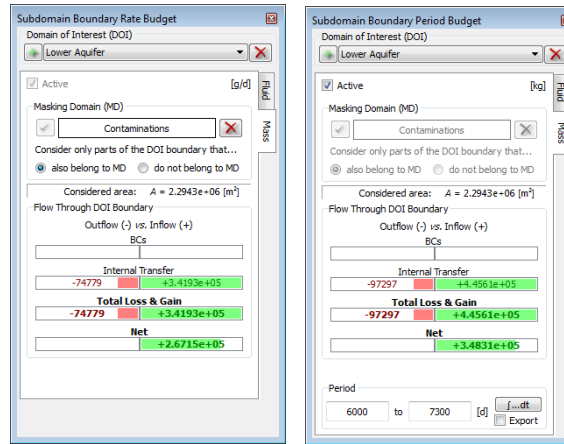


Figure 12.6 Subdomain Boundary Rate and Period Budget panels with results for the selected DOI.

12.8.5 Content Analysis

To check how much mass the model domain contains at different time steps we use the **Content** panel. Switch to the tab **Mass** and activate the content calculation for **Dissolved Species Mass**. The currently contained amount of mass is now displayed in grams. Browse the time-step list in the **Simulation** toolbar to check how the mass content changes with time.

12.8.6 Streamlines, Pathlines

To visualize the steady and transient flow field we plot both streamlines and pathlines. Start with a 3D plot of streamlines that start at the two well locations.

First, set the **3D** view as active view and deactivate

12. Results Evaluation

Geometry > Faces in the **View Components** panel as otherwise the streamlines located below slice 1 would be concealed.

Now, click on **Node Selection > Wells** in the **Spatial Units** panel and double-click on **Streamlines > Backward** in the **Data** panel. Start the plot by setting **Traces** in the **View Components** panel active. After a brief computation the streamlines are shown in the **3D** view.

To visualize the flow field in the vicinity of the wells we increase the radius for the streamline seeds around the wells. To change the radius and other streamline properties, open the context menu of **Travel time, backward streamlines seeded@Wells** in the **View Components** panel and select **Properties**. In the upcoming **Properties** panel type 12^3 30 m as radius, hit <Enter> and click **Apply**. Several streamlines are now plotted around the two wells. Figure 12.7 shows a 3D plot of streamlines around the wells.

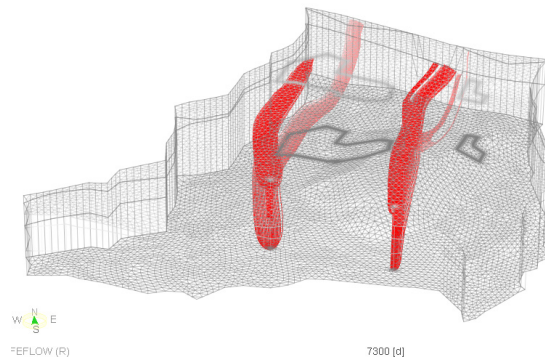


Figure 12.7 3D Streamlines around the wells.

To visualize the transient flow field with pathlines,

go back to the **Data** panel and double-click on **Pathlines > Backward**. To start the plot, repeat the same steps as previously described for the streamlines. Furthermore, select time step **#66** in the **Simulation** toolbar.

We also add **Period Sections** to visualize particle travel times. In the **View Components** panel, deactivate **Traces** and activate **Travel time, backward pathlines seeded@Wells > Period Sections** and then double-click on this entry to edit the period-sections settings in the **Properties** panel. On the **Iso** tab, deactivate the **Automatic** option, enter an interval of 12^3 365 d and confirm the changes with **Apply**.

To plot each period section in a different color, open the **Properties** panel of **Travel time, backward pathlines seeded@Wells** via its context menu in the **View Components** panel. Right-click into the color bar on the left-hand side of the panel and select **Presets > Rainbow**. Figure 12.8 shows the resulting plot.

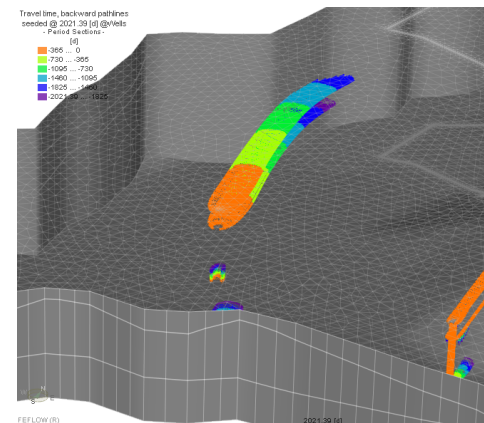


Figure 12.8 Period sections.

Streamlines or pathlines can also start from poly-

lines. To draw a polyline for streamline plotting, open the context menu of **Streamlines** > **Forward** and select **Draw seed line/points** > **Draw a 3D Line**. Start an arbitrary line on the top slice of the model with a single click. Extend the line by adding points and finish with a double-click.

The line is now displayed in the active view and is shown as **Domain Locations** > **3D Polyline #1** in the **Spatial Units** panel.

Now, click on **3D Polyline #1** in the **Spatial Units** panel and start the streamline plot with a double-click on **Streamlines** > **Forward** in the **Data** panel. Figure 12.9 shows an example for a streamline plot from a polyline.

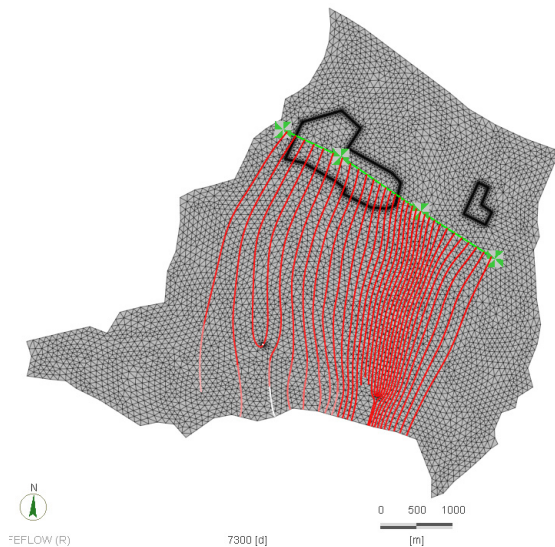


Figure 12.9 Streamlines starting at a polyline.

12.8.7 Random-Walk Particle-Tracking (RWPT)

To illustrate a RWPT event we select **Backward Random-Walk Tracks** in the **Data** panel, for the same seeded wells as in the previous section.

Go to **Edit** > **Problem Settings** > **Field-Line Computation** > **Random-walk tracks** and use the default, homogeneous dispersive parameters for molecular diffusion and the coefficients of dispersivity.

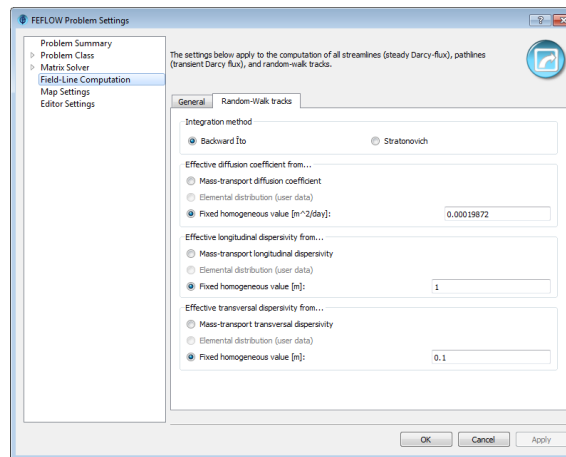


Figure 12.10 Defining RWPT parameters.

Note that dispersivity values are small. As opposed to standard advection-dispersion solution techniques, the RWPT does not suffer from numerical dispersion effects and stability constraints. Thus, there is no need to distribute dispersive coefficients according to mesh size. In other words, RWPT can be solved even if the mesh is very coarse with arbitrary dispersive coefficients, in preference close to their physical values.

12. Results Evaluation

In order for RWPT solutions to be consistent with advection-dispersion solutions, a sufficiently large number of input particles must be used. The greater the amount of used particles the more the RWPT and advection-dispersion solutions will be comparable. However, RWPT solutions can be very memory-demanding when many particles are used so it is recommended to (i) start with a relatively small amount of particles (e.g. 100), (ii) analyze the runtime and memory occupation, and (iii) subsequently increase the number of used particles if possible. Most problems will require a minimum number of about 10.000 particles for RWPT solution to be able to explore all possible advective-diffusive/dispersive paths and thus be consistent with advection-dispersion solutions. Note that there is a control during the RWPT solution phase on memory usage such that memory overflow situation should not occur.

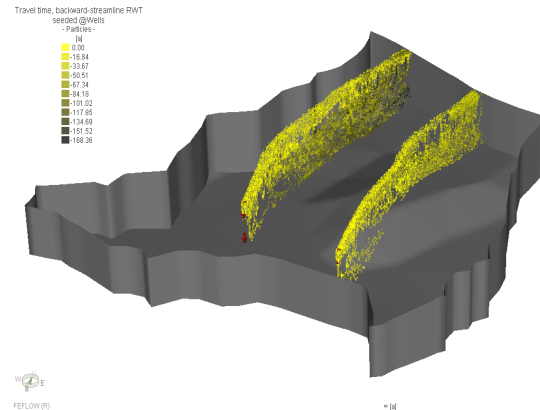


Figure 12.11 Backward RWPT solution from the wells.

12.8.8 Export of Results

To export the mass distribution obtained at the end of the simulation browse to the last time step in the **Simulation** toolbar and double-click on **Mass concentration** in the **Data** panel. Open the context menu of **Mass concentration** in the **View Components** panel and select **Export Data > Current Time #116 7300 d > All Nodes**. Select a file name and choose the ESRI Shape File 3D format (.shp). The exported data can be loaded again as a map and assigned as initial mass distribution in subsequent simulations.

Plots can be exported in the same way as data. To export the isolines plot open the context menu of **Mass concentration > Isolines** in the **View Components** panel and select **Export Plot**. Choose a file name and format for the exported isolines and finish the export with **Save**.

A further option to export simulation results is to take snapshots of the active view window. Click **Snapshot of the Active View** in the **View** toolbar and choose a resolution enhancement factor for the exported snapshot. After clicking **OK**, choose a name and file format for the snapshot.

Animation and Video Export

13.1 Introduction

Dynamic visualization is essential when presenting model results to clients, authorities and the public, and facilitates understanding of complex processes.

13.2 Creating a Presentation

A dynamic presentation can be set up for each view window using its autopilot. The autopilot of the active view window is accessible via the *Autopilot* panel where up to four separate categories, *Simulation Time*, *Position*, *Clipping*, and *Visibility* can be set up along a common presentation-time line. Presentation time is real time as observed on a wrist watch during presentation play-back. The available categories depend on the type of the respective view window. Each category has an *Engage* checkbox that acts similarly to a clutch. When engaged, the autopilot completely controls the respective category. For example, engaging the autopilot *Position* category will disable user-controlled navigation via the *Navigation* panel or mouse tools and all object positioning becomes autopilot-controlled.

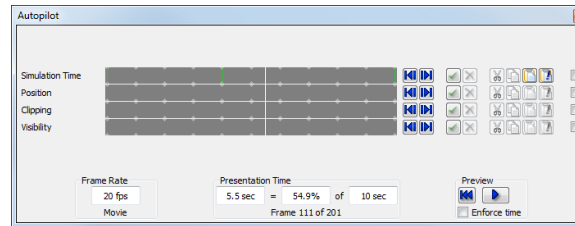


Figure 13.1 Autopilot panel.

The total length of the presentation (in seconds) can be entered in the *Autopilot* panel. The displayed percentage value corresponds to the position of the timeline slider. It can be edited to explicitly set a timeline position.

A play-back function is provided to preview the autopilot animation sequence.

A simple movement is produced by defining two object-position keys, one at the beginning and one at the end of the presentation-time line. Whenever the autopilot *Position* category is engaged (e.g., during autopilot play-back and movie export), all intermediate object positions are automatically interpolated between

13. Animation and Video Export

the bracketing keys, resulting in a continuous object movement. To produce more complex paths, additional keys can be freely placed along the presentation-time line.

When visualizing FEFLOW simulation records (*.dac files) for transient problems, the simulation-time axis (often covering days, months, or years) has to be mapped to the presentation-time axis (typically, seconds or minutes long). The autopilot performs this mapping simultaneously with the dynamic object positioning.

While the autopilot *Simulation Time* category is engaged, the candidate time step shown in the *Simulation* toolbar is obtained by interpolating the user-defined simulation-time keys on the presentation timeline. By default, beginning and end of the simulation period are mapped to beginning and end of the presentation timeline, respectively. Thus, in the simplest case, no additional simulation-time keys have to be specified at all.

To obtain animation effects such as a gradually extending cut-out section progressively exposing internal isosurfaces, the autopilot of a 3D view window can dynamically interpolate between predefined (key) clip settings.

While the autopilot *Clipping* category is engaged, the settings for clipping and cutout planes are obtained by interpreting the user-defined clipping keys on the presentation timeline. At a given presentation moment, the status of each plane ('Disabled', 'Clipping', or 'Cutout') will be given by the respective previous clipping key on the presentation timeline while position and orientation of all planes are continuously interpolated between the respective bracketing clipping keys.

The autopilot can dynamically apply predefined feature-visibility settings to control the display of mul-

iple data sources in sequence or to display features such as the finite-element mesh or a surface map during only a portion of the entire presentation.

While the autopilot *Visibility* category is engaged, the feature-visibility settings are obtained from the user-defined visibility keys on the presentation timeline. At a given presentation moment, the visibility status of each feature will be given by the respective previous visibility key on the presentation timeline.

13.3 Movie Export

Export of the autopilot presentation of the active view to a movie is evoked via *Export AVI from Active View* in the *File* menu or the *View* toolbar. Any of the video compression codecs available on the operating system can be chosen for the export. As formats, the standard AVI format can be selected or the animation can be exported as 3D stereoscopic movie in AVIS format.

13.4 Tutorial

13.4.1 Tools

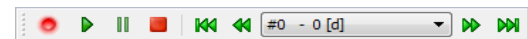



Figure 13.2 Simulation toolbar.


13.4.2 Creating a Presentation

In this exercise we create a presentation from a results file of a transient free & movable simulation and export the presentation as a movie. First, click  **Open** and load the file **animation.dac**.


We start with a very simple presentation in the **3D**







Movie Export is currently only possible on Microsoft Windows operating systems.


view in which we show how the mesh stratigraphy changes during the simulation. Switch to the  **Autopilot** panel located below the view windows and make sure that the **3D** view is the active view.

By default, beginning and end of the simulation are mapped to beginning and end of the presentation timeline, respectively. The two green bars at beginning and end of the **Simulation Time** line show that time keys are set at these positions.

For showing the mesh movement during the simulation no additional settings are necessary. Simply click  **Preview** to preview the first presentation.

In the next step we extend the animation to 20 seconds and add further time line-keys to slow down the animation at the stages where strong changes are visible.

First, enter  **20 sec** as total presentation time and hit <Enter>. In the upcoming **Expand presentation** dialog select the option **Rescale all existing key timings** and click  **Rescale**. Now, browse to time step **40** in the time step list in the  **Simulation** toolbar, type  **8.0 sec** in the left input field of presentation time and hit <Enter>. Alternatively, the white slider bar can be moved manually to **8.0** sec of presentation time. To set a key at this time step click the green checkmark in the **Simulation Time** line. A green bar appears indicating that a key has been set here.

Repeat the same steps to set the second time key for time step **65** at **16** seconds of presentation time. After this time key has been set, move the white slider bar to the beginning of the presentation and click  **Preview** again to see the presentation.



In addition to presenting the mesh movement during the simulation we want to change the model position in the active view during the presentation.

The model is to move from the upper left corner

towards the center of the active view during the presentation. An increasing zoom factor and some rotation are also desired.







First, press the middle mouse button and drag the model to the upper left corner of the view. Now, use the right mouse button to zoom out and then, with the left mouse button, slightly rotate the model backwards and to the left. To set the first key at this position move the white slider to the beginning of the presentation time and click the green checkmark in the **Position** line.

For the second key, position the model in the center of the view, zoom in and rotate the model to the right. Move the slider to the end of the presentation and click the green checkmark in the **Position** line again. The position of the model will now dynamically change between these two prescribed positions during the presentation.

We complete the presentation by removing the handles from the active view. Right-click in the view window and deselect  **Show > Handles**. Now click  **Preview** again to see the final presentation.

13.4.3 Movie Export


When all presentation keys are set we proceed with the export of the presentation as a movie.



In the  **Autopilot** panel, choose a **Frame Rate** of  **20 fps** and click  **Export AVI from Active View** in the  **View** toolbar. Choose a name for the movie and click  **Save**. Finally, select one of the available compression codecs and the desired quality and click  **OK** to start the movie export.

13.4.4 Export Settings

Presentations can also be exported and reloaded

13. Animation and Video Export

again. The presentation settings are exported together with the settings of the active view. After creating the presentation right-click in the active view window and select  **Export Settings** to save the presentation and view settings as xml-file.

Reloading the animation and view settings works in the same way: Go to  **Window > New** and select **3D View**. Right-click in the new **3D** view to invoke the context menu, select  **Import Settings** and load the file that we have just exported. The view and animation settings are now adopted from the xml-file.

Groundwater Age Calculation

Crucial information on flow dynamics and mixing, and for capture zone analysis and risk assessment

14.1 Introduction

FEFLOW provides the capabilities to conveniently calculate groundwater age, lifetime expectancy and exit probability. These three properties are rooted in the same theoretical framework of *component exposure time* and are obtained by solving standard mass-transport equations for which specific coefficients and boundary conditions must be defined. Transport of age therefore is available as a new problem class, similar to the transport of mass or heat. Solving for lifetime expectancy and exit probability in addition to groundwater age requires the definition of these additional **Age Species** in the **Problem Settings** dialog and the assignment of the corresponding transport parameters.

The solutions of groundwater age, lifetime expectancy and exit probability can be used to perform specific diagnoses on a flow field, such as the analysis of the flow dynamics and mixing processes, the estimation of outlet vulnerability, or the evaluation of outlet capture zones and the origin of water.

14.2 Groundwater Age

Mean age represents the elapsed average time spent in the aquifer since groundwater has entered the model domain, i.e., it indicates the travel time from the inflow boundary to the current location. Typically, it is assumed that groundwater ‘life’ starts at inflow into a model and FEFLOW therefore automatically assigns a Dirichlet boundary condition of 0 days at all inflow boundaries. If groundwater age is not assumed to be 0 at inflow boundaries, an age-concentration BC with the specific age value needs to be assigned at these locations manually.

Age solutions provide information on underground travel times and mixing processes and the results on mean groundwater age can be used for calibration purposes if age data are available.

14.3 Mean Lifetime Expectancy

Lifetime expectancy is defined as the average time for groundwater still needed before exiting the domain via an outlet. It therefore corresponds to the expected

14. Groundwater Age Calculation

travel time from the current location to an outflow boundary. As lifetime expectancy is 0 at outflow boundaries, FEFLOW automatically assigns a LTE-concentration BC with a value of 0 days at these locations.

Results for lifetime expectancy can be used for risk-vulnerability assessments and the analysis of groundwater dynamics: Zones with longer lifetime expectancy indicate groundwater divides whereas areas close to outflow boundaries show shorter travel times.

14.4 Exit Probability



To calculate exit probability for multiple outflow boundaries with overlapping capture zones simultaneously, multiple age species of type Exit Probability can be used.

The parameter exit probability can be used to calculate the probability of water exiting the model domain at specific locations. In contrast to age and lifetime expectancy simulations, boundary conditions for exit probability are not applied automatically. Instead, outflow locations for which the exit probability is to be calculated have to be selected manually. As the probability of exit is 100% at an outflow boundary, a probability BC with a value of 1 needs to be assigned there.

Assigning a probability boundary condition of 1 at a pumping-well location allows to delineate the capture zone of the well and also to determine the origin of the pumped water.

Evaluating exit probability via the *Content* panel provides information on the amounts of water related to the capture zone of the well. The proportions of water extracted can be calculated according to their origin of infiltration using the Rate- and Period-Budget tools.

14.5 Tutorial

In the following exercises we set up a groundwater-age simulation problem and solve for *Mean Age*, *Lifetime Expectancy* and *Exit Probability*. The results will be used to delineate the capture zone for a pumping well and to determine the contributions of the different sources to the total pumped water.

14.5.1 Tools



Figure 14.1 Selection toolbar.

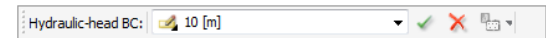


Figure 14.2 Editor toolbar.

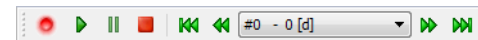






Figure 14.3 Simulation toolbar.

14.5.2 Setting up a Groundwater Age Simulation

Start FEFLOW and click  *Open* to load the file **age.fem**. To setup an age, lifetime expectancy and exit probability solution problem, open the *Problem Settings* dialog via the  *Edit* menu. On the *Problem Class* page activate the option *Include transport of...* *Age* and confirm with a click on  *Apply*. By doing so a new page named *Age Species* is created in the tree on the left-hand side of the dialog. Enter the *Age Species* page and click  *Add species* twice to

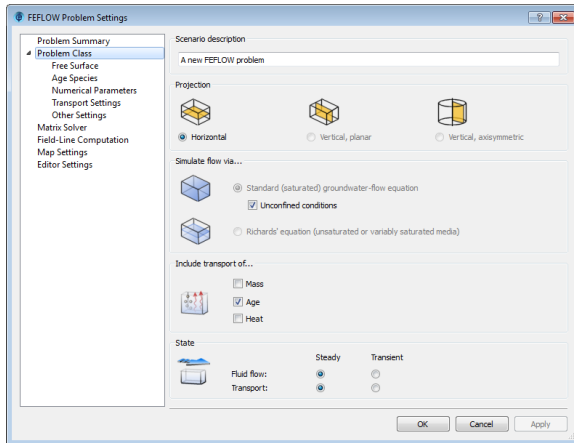


Figure 14.4 Activating groundwater age as problem class.

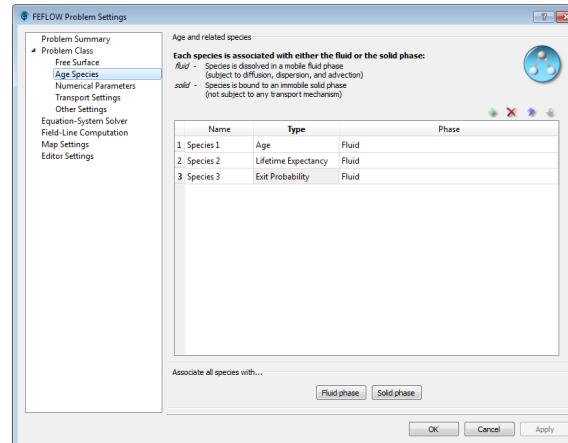


Figure 14.5 Defining age species in the Problem Settings

create three age species in total. Change the *Type* of the second species to **Lifetime Expectancy** and the third species to **Exit Probability** (Figure 14.5). Confirm the changes with **Apply** and leave the dialog with a click on **OK**.

Each declared age species is now defined as a transport property and transport parameters such as porosity, molecular diffusion and coefficients of dispersivity need to be defined accordingly. By default, FEFLOW only displays the Dirichlet-type boundary condition for each age species: **Age-concentration BC**, **LTE-concentration BC** and **Probability BC**. Additional boundary-condition types can be added via **Add Parameter** in the context menu of the specific boundary-condition section if needed.

The boundary conditions for fluid flow consist of a fluid-flux BC in the upper west model region, a fluid-transfer BC representing a river and two pumping wells. Additionally, water enters the domain via

recharge.

To determine the capture zone for the upper pumping well, we need to assign a **Probability BC** of unity at this node location. Double-click on **Probability BC** in the **Data** panel and then double-click on the stored node selection **Pumping well** to set the selection active. Enter a value of **1** in the input box of the **Editor** toolbar and hit <Enter> to complete the assignment. Boundary conditions for mean age and mean lifetime expectancy do not have to be assigned as these will be set automatically once the simulation starts.

The transport parameters for the different age species do not have to be changed as we will use the default parameters.

To start the simulation, click on **Start** in the **Simulation** toolbar.

14. Groundwater Age Calculation

14.5.3 Results Evaluation

14.5.3.1 Travel-Time Analysis

Mean Age and Mean Lifetime Expectancy

The results for mean age and mean lifetime expectancy are displayed in units of time. To plot these nodal distributions in the active view, go to the **Spatial Units** panel and click on **Domain**. Next, double-click on **Mean age** in the **Process Variables** section in the **Data** panel. Water enters the model domain with an age of zero and locations close to inflow boundaries therefore show short travel times. To identify the nodes at which water enters the model domain, double-click on **Mass transport - age#1 (f) > Age-concentration BC**. Inflow locations are now indicated by an age-concentration BC with a value of 0 days.

For better visibility we uncheck the **Edges** entry in the **View Components** panel. To plot the remaining travel time for water molecules to reach an outflow boundary, double-click on **Mean lifetime expectancy** in the **Data** panel. As we would like to combine this plot with the exit-probability distribution in a later step, lock this parameter in the view by right-clicking on **Mean lifetime expectancy - lte#1 (f)** in the **View Components** panel and selecting **Lock Data View**. Uncheck the **Continuous** plot and activate **Isolines** instead. To change the interval to be used for the isoline plot, double-click on **Isolines**. This opens the **Properties** panel and we remove the check mark in front of **Automatic**. Change the **Prescribed interval** to 1^{23} 2 [a] and confirm the changes with **Bu Apply**. The resulting plot is shown in Figure 14.6.

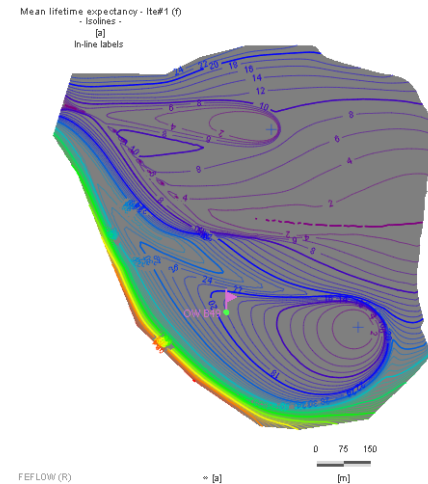


Figure 14.6 Distribution of mean lifetime expectancy.

Total Travel Time

To determine the total travel time from inlet to outlet, **Mean age** and **Mean lifetime expectancy** need to be summed up. The sum can be calculated and displayed using a nodal expression.

The model already contains a prestored nodal expression called **Total travel time** which can now be edited. Open the context menu of **Total travel time** in the **Data** panel with a right click and select **Edit Parameter Expression**. Delete the right side of the expression and double-click on the process variable **Mean age**, then enter 1^{23} + and double-click on **Mean lifetime expectancy** in the list on the right-hand side of the dialog. The expression should look like the one in Figure 14.7. Leave the dialog with **Bu OK**.

Double click on **Total travel time** to plot the total

travel time from model inlet to outlet.

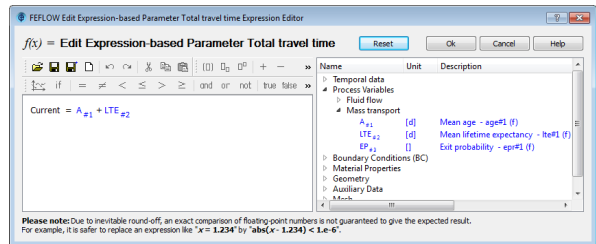


Figure 14.7 Nodal Expression for total travel time.

14.5.3.2 Capture Zone Delineation - Exit Probability

The distribution of exit probability represents the capture zone of the target which in our example is the pumping well. A typical limit for capture-zone delineation is the 0.5-probability contour.

To plot the capture zone for the well, double-click on **Exit probability** in the **Process Variables** section in the **Data** panel. To limit the plot to probability values between 0.5 and 1, double-click on **Exit probability - epr#1 (f)** in the **View Components** panel. In the **Properties** panel of this parameter, uncheck the option **Auto-update range**, enter **0.5** as the minimum value and confirm the changes with **Apply**. The colored area now represents the well-capture zone.

By examining exit probability in combination with the isolines for mean lifetime expectancy it is possible to determine the remaining travel time from a specific location within the capture zone to the outlet.

Figure 14.8 shows the capture zone of the well considering a probability of 0.5 together with the mean lifetime-expectancy contours.

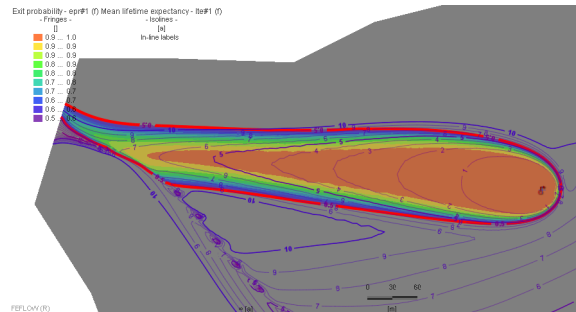


Figure 14.8 Well-capture zone and plot of remaining travel times.

Outflow nodes can be displayed by plotting the **Probability** boundary condition. FEFLOW automatically assigns a boundary condition with a probability value of 0 at these node locations.

14.5.3.3 Capture-Zone Content, Source Partitioning and Origin of Water

To calculate the capture-zone water content, activate **Exit Probability Domain Fluid Volume** in the **Content** panel. If the capture zone is limited to probability values between 0.5 and 1, it is necessary to create an element selection for this limited probability range and to calculate the content for this element selection only.

Budget calculations for exit probability can be used to determine the different sources of water at an outflow boundary, as well as the proportions of the respective sources.

In the **Rate-Budget** panel, switch to the tab **EP - epr#1 (f)** and start the mass-budget calculation for exit

14. Groundwater Age Calculation

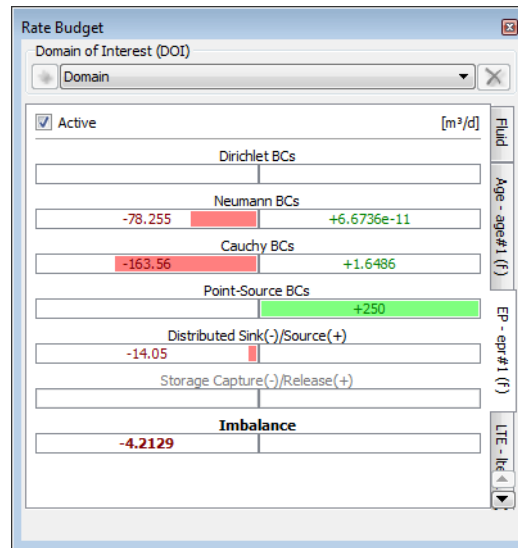


Figure 14.9 Mass budget returning the proportions of the pumping-well rate with respect to their origin of infiltration.

probability by checking the box in front of **Active**. As the flow field is inverted for the exit-probability solution, positive values indicate outflow and negative values indicate inflow boundaries.

The displayed budget indicates that the pumping well captures water which entered the model domain via fluid-flux and fluid-transfer boundary conditions and also via recharge.

The source locations can be displayed in the active view by double-clicking on **Mass transport - epr#1 (f)** > **Rate budget** in the **Data** panel (see Figure 14.10).

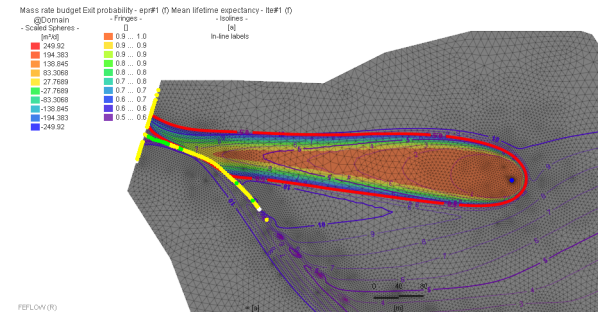


Figure 14.10 Budget spheres for exit probability representing source locations

The graphical user interface for running FEFLOW models with PEST

15.1 Introduction

This chapter aims at FEFLOW users that may or may not have prior experience with PEST. Various references to the PEST documentation and other texts are provided within the text for further reading.

The methods are described in their functional relation to the overall workflow and their relation to other methods. This initial orientation will help to understand how PEST works, and should motivate the user on the way of becoming proficient in uncertainty modeling.

The focus will be (with some exceptions) on those PEST methods that are actually supported by FePEST. It should be emphasized that PEST provides many more, exciting features, which will become available in future releases of FEFLOW. To use them already now, we encourage you to see the PEST manual for further information.

15.1.1 What Is PEST?

PEST is a software widely used in environmental modeling to calibrate models, to determine uncertainty

associated with parameters and predictions, and for related tasks. Today, PEST is probably the most commonly used software for the calibration of groundwater models.

However, PEST provides much more than calibration. Besides assisting the modeler in classical calibration tasks, it implements methods that address the fact that the outcome of a calibration is not unique, and that the prediction given by a calibrated model is only one out of many possibilities.

Instead of only providing one calibrated model, PEST aims to analyze the spectrum of possible solutions and consequently the uncertainty range associated with parameters and predictions. Of course, these methods (for both traditional calibration and uncertainty analysis) must be learned and understood before they can be successfully applied. Fortunately, good literature is available to do so. See the literature review (section 15.1.5) for more information.

PEST is model-independent. Any modeling software that reads input and writes output from a file—or can be adapted to do so—can be linked to PEST. The effort to do this depends on the complexity of the file format.

On a more technical level, PEST can be seen as a

15. FePEST

toolbox of different programs to setup, run, and evaluate the results of a specific task (e.g. calibration). These programs are all started from the command-line prompt, and are configured using command-line parameters and/or configuration files without a graphical user interface. FePEST has been developed to provide more convenient access to PEST functionality when using FEFLOW models—without limiting it.

15.1.2 Where to Get PEST?

PEST is free software. It is developed by John Doherty (Watermark Numerical Computing) and can be downloaded, including all documentation, from www.pesthomepage.org.

Please also see the FePEST installation instructions for further information.

15.1.3 What Is FePEST?

FePEST links PEST with a FEFLOW model through a convenient graphical user interface.

With FePEST it is possible to use a range of PEST functionality without the need to learn the syntax of its various command line tools and configuration files, and to manually adapt FEFLOW's model files for usage in PEST. Visual feedback on the optimization progress is provided during and after the model run. This will give the user major savings of time both in terms of learning and productive work.

The range of supported PEST features in this release of FePEST includes:

- Model calibration (including Regularization and pilot point parametrization)
- Subspace methods

- Parallelization (locally and/or using remote servers, incl. file transfer)
- Linear sensitivity analysis
- Predictive analysis (worst-/best case evaluation)

15.1.4 Where to Start...

15.1.4.1 If You Are New to PEST

Most PEST features required for model calibration using PEST are accessible through FePEST. The user is in many cases not required to make changes to the PEST files and therefore does not need to learn the syntax of the files and commands of PEST.

However: It is still essential that the methods of PEST are understood to be able to interpret the results of a PEST run correctly! It is suggested that the time saved on understanding PEST's file structure and command line tools is invested in understanding these methods.

15.1.4.2 If You Are an Experienced PEST User

PEST provides more functionality than FePEST can cover. We have chosen to implement those work flows that will be most relevant for most users (and more will be implemented in the future).

This does not pose a limitation to use FePEST for other methods at all. In fact, it is developed in an "open" way thus that the benefit of a rapid PEST file setup can be used even for unsupported methods. The following aspects will support experienced users to customize their setups:

- The user interface cites the original names of PEST variables and tools. Experienced users will therefore quickly recognise how the user interface relates to the respective PEST functionality.
- The file setup created by FePEST strictly follows the syntax specified in the PEST documentation and is fully accessible. The structure of these files - including several batch-files - are designed to allow adaptations for different purposes.
- Especially if the optimization involves the pilot-point method, experienced users will use FePEST for the otherwise elaborate fundamental work steps like the definition of observations and parameters, and then adapt the resulting PEST setup for the particular purpose.
- Users familiar with the FEFLOW IFM programming interface can use a respective feature in FePEST to allow IFM plug-ins to communicate with PEST directly. This extends the scope of FePEST beyond the predefined observation and parameter types.

15.1.5 Related Literature

The following list of literature should help users new to PEST to find a reasonably easy access to the science behind its tools. Initially, PEST might be sought as a tool to accelerate model calibration. PEST has a very high potential to accomplish this task if the underlying concepts are sufficiently understood. Later, more advanced methods might be applied to understand the uncertainties associated with calibrated models and predictions made by them.

- The document **Use of PEST and Some of its Utilities in Model Calibration and Predictive**

Error Variance Analysis: A Roadmap provides a first overview.

- For a more in-depth understanding, the PEST tutorial **Methodologies and Software for PEST-Based Model Predictive Uncertainty Analysis** is recommended. It provides a comprehensive introduction to basic and advanced methods, and conveys important knowledge of the concepts behind them.
- The **PEST Users Manual** and the **Addendum to the PEST manual** are the primary and most complete reference to all PEST features and tools. This manual will refer to these documents regularly for further reading.
- Another useful document **Getting the Most out of PEST** describes some general settings and procedures that avoids a major part of typical problems. FePEST uses a major part of these recommendations by default.

See www.pesthomepage.org for additional documentation on PEST.

15.1.6 Overall Workflow

The structure of this document follows the work flows to perform the supported tasks in FePEST.

After a brief introduction to some of PESTs methods and algorithms (section 15.2), the following tasks are explained:

- **Fundamental Problem Setup** (section 15.3)
The fundamental problem setup prepares the model to be processed by PEST. These configurations form the basis for all basic and advanced

PEST methods. It includes the definition of adjustable parameters, observation and prior knowledge, the choice for subspace regularization methods and the setup of remote servers for parallel computing.

- Parameter Estimation/History Matching/Calibration (section 15.4)

The history matching process targets the estimation of a parameter set that satisfies both the historical observations and the prior knowledge. After doing the required settings and starting PEST, the feedback of PEST is reviewed and the resulting model is opened in FEFLOW.

- Predictive Analysis (section 15.5)

For most environmental models it is possible to find more than one calibrated model, with predictions varying at different levels. Finding maximum or minimum possible key predictions among these models is a simplistic approach to identify worst-case or best-case scenarios of well-posed problems that are compatible with the calibration data set.

- Sensitivity Analysis (section 15.6.1)

FePEST allows to export the sensitivities of the parameters. These can be used to create sensitivity maps in FEFLOW, or be processed with other software or PEST tools.

- Customized PEST Setups (section 15.7)

Experienced PEST users may want to use PEST methods that go beyond the functionality of FePEST.

15.1.7 Acknowledgements

The author likes to thank John Doherty of Watermark Numerical computing for his ongoing support of

the development of FePEST and its documentation.

John Doherty is the author of PEST and as such provides regular training courses in calibration and predictive uncertainty analysis of numerical models. His documentation of PEST, as well as various papers and tutorial exercises on this topic are a valuable source of information learning-stage and on-going work with this software.

Parts of the text and several illustrations used in this manual have been derived from his work.

The FEFLOW model shown in Figures 15.6, 15.9 and 15.12 is based on work by J. Doherty and C. Moore.

15.2 Methods and Concepts

The fundamental methods applied by PEST during the calibration process are briefly described in the following. As already mentioned in section 15.1, this description allows the reader to quickly understand their respective role in the overall workflow. The PEST documentation, to which specific references are provided, describes the methods in full detail.

15.2.1 GLMA Search Algorithm

The central feature of the PEST engine is the GLMA search algorithm, that iteratively optimizes the model parameters to improve its fit to observed data and other objectives.

The fit to the observations is hereby expressed through the **Measurement Objective Function**. In the simplest case, this will be the weighted sum of squares of the residuals between measurement and simulation results

Def.	Observation type	Obs. point	X	Y	Z
mas	Mass concentration	TravelTime	250.00	0.00	0.00
hea	Hydraulic head	well01	65.00	615.00	0.00
hea	Hydraulic head	well02	245.00	615.00	0.00
hea	Hydraulic head	well03	425.00	615.00	0.00
hea	Hydraulic head	well04	65.00	435.00	0.00

Figure 15.1 The objective function is defined through the observation definition in FePEST.

$$\Phi = \sum_i w_i (h_i^{obs} - h_i^{sim})^2$$

where (h^{obs} denotes an observation (typically from a field measurement), h^{sim} its related simulation result, and w the weight that has been applied to the measurement (observation weights will be discussed in section 15.2.1.2).

The equation shown is also the formulation FePEST uses to define the measurement objective function. The observations hi are loaded from the FEFLOW model and the weights wi can be changed by the user within the user interface (Figure 15.1).

The search algorithm used in PEST is the **Gauss-Levenberg-Marquardt algorithm (GLMA)**. The GLMA changes the model parameters until a minimum objective function value is found. Running PEST, the user will observe two working steps per iteration:

- Derivative calculation: The parameters are changed incrementally. By repeating the model run for each parameter, and observing the resulting changes of observation values, the partial

derivative for each pair of parameter and observation can be calculated by finite-difference approximation. These derivatives form the elements of the **Jacobian matrix**. The numerical effort to calculate the Jacobian matrix usually dominates the iteration.

- The parameter values are adjusted aiming to reduce the objective function. The direction and magnitude of the adjustment is expressed by the **parameter upgrade vector**. To identify the optimal direction of this vector, the GLMA uses a combination of two strategies:

- While the objective function shows a predominantly linear behavior, the method of gradient descent is applied. This method determines the parameter upgrade vector from the direction of steepest descent of the objective function. This can often be observed during the initial phase of the optimization.
- Objective-function nonlinearity is addressed via the Gauss-Newton method. This method computes a parameter upgrade vector based on the presumption of a quadratic behavior of the objective function.

The two methods are not mutually exclusive: The GLM algorithm interpolates between them, controlled by a scaling parameter (the **Marquardt-Lambda**).

PEST dynamically updates lambda depending on the progress in reducing the objective function. The current lambda as displayed by FePEST during the PEST run is a good indicator for the current nonlinearity of the objective func-

15. FePEST

tion.

- high lambda values (e.g., > 10) indicate linear behavior (and predominant use of the gradient descent method).
- small lambda values (e.g., < 2) indicate nonlinear behavior (and predominant use of the Gauss-Newton method).

Figure 15.2 and Figure 15.3 illustrate the development of the objective function and the Marquardt lambda during a typical PEST optimization. Gradient descent is used in the first iterations, indicated by higher lambda values. When the objective function approaches its (local) minimum, Lambda falls to near zero indicating almost exclusive use of the Gauss-Newton method.

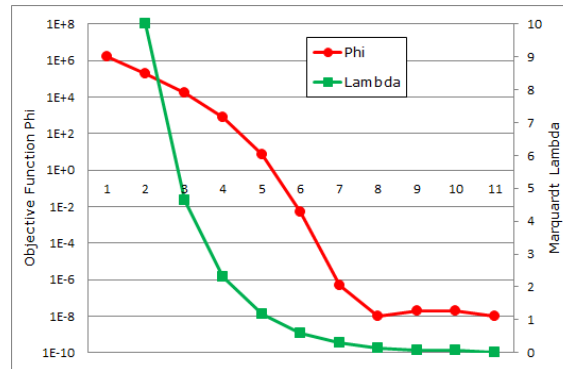


Figure 15.2 Development of the objective function and the Marquardt lambda during a PEST run.

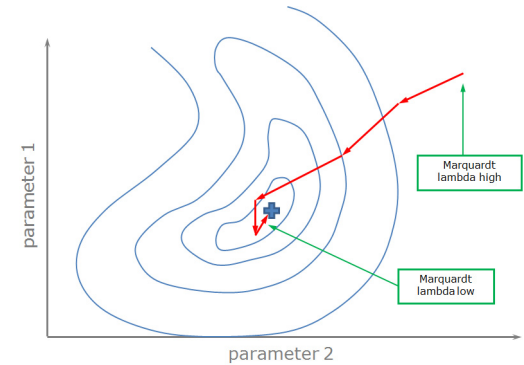


Figure 15.3 Schematic illustration of contours of the objective function and the path of the parameter upgrades vectors, after Doherty.

If successful, the GLMA will find a parameter set that constitutes a **local minimum** of the defined objective function. This is an important restriction because multiple local minima might be present, and it is not guaranteed that the one found is also the global minimum.

It is therefore possible that different PEST runs result in different parameter sets if the iteration starts at different initial parameter values. These should therefore be chosen as close as possible to those values that are expected.

The modeler should also critically review the resulting parameter set and the model-to-measurement-misfit (see Figure 15.4). Strong, but also very low (see section 15.2.4) departures indicate potential problems with the optimization.

Further reading: PEST Manual (5th Ed.), Ch. 2.1: The Mathematics of PEST.

15.2.1.1 Derivative Calculation

The calculation of derivatives is a fundamental element of the GLM algorithm.

The derivatives are calculated through numerical differentiation. Each parameter is incrementally changed, and the model is run each time to calculate and record the resulting change of the model observations. The derivative of each parameter \hat{a} observation relationship is then calculated through finite-difference techniques.

Correct calculation of derivatives is of critical importance to the optimization, as failure to it will lead to an unstable optimization procedure and PEST will not be able to lower the objective function.

Model instabilities are a frequent cause of PEST failures!

Instabilities introduce noise to the observation,

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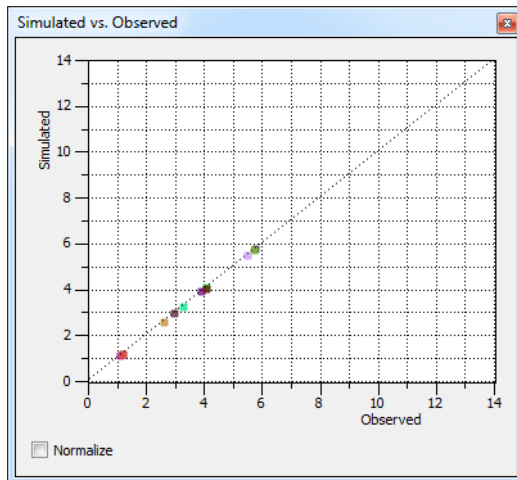
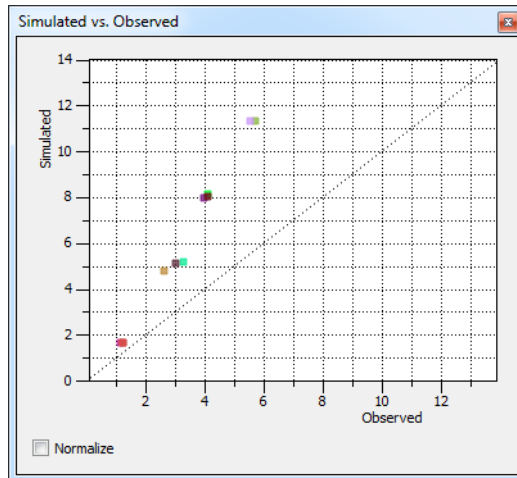


Figure 15.4 Scatter plot of simulated vs. observed data before (top) and after (bottom) optimization.

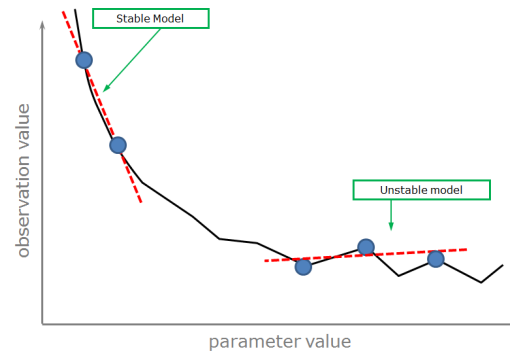


Figure 15.5 Calculation of derivatives during stable (left) and unstable (right) model behavior. If the model is unstable, random noise dominates the physical change of the observation value. PEST tries to compensate with higher-order finite-difference methods.

which is random and not related to the physical-based simulation result. Figure 15.5 illustrates this effect. If this noise - and not the incremental parameter change - dominates the observation response, the direction of the upgrade vector becomes random itself and the optimization will fail.

Even though certain countermeasures are available (see section 15.3.2.2), the modeler should always aim at maintaining maximum stability of the FEFLOW model. With **JACTEST** (section 15.6.2) PEST provides a tool to check the integrity of the derivatives calculation for specified parameters.

Further reading: PEST Manual (5th Ed.), Ch. 2.3: The Calculation of Derivatives.

15.2.1.2 Observation Weights

The weight of an observation controls how strong its residual (the deviation between computed and measured result) contributes to the measurement objective function. A reasonable choice of weights can positively influence the convergence behavior and result of the GLM algorithm.

Different weighting strategies can be applied (alone or in combination), some examples are given in the following.

- **Weighting by Measurement Noise**
A common strategy of adjusting observation weights is applying the inverse of its expected measurement noise as a weight factor. The contribution of less trustworthy observation values to the measurement objective function is reduced, limiting the risk of inaccurate measurements having a negative impact on the optimization and leading to the estimation of parameter

values which are thereby in error.

- **Weighting by Absolute Measurement Value**
The absolute values of observations in a PEST optimization can encompass several orders of magnitudes, especially (but not limited to) if observations of different types are involved (e.g., Hydraulic head [m] and Mass-concentrations [mg/l]).
Observations with small values are therefore under-represented in the measurement objective function. Normalizing the values by assigning a weight equal to the inverse of the absolute compensates for this effect and makes sure that the information contained in these values finds appropriate representation in the optimization.
- **Equalizing Observation-Group Contributions**
Observations of different types are assigned to different observation groups. One may also decide to manually assign observations of the same type to different observation groups. Using a spreadsheet or the PEST tool PWTADJ1 observation weights can be adjusted to equalize the total contribution of each observation group to the total objective function at the start of the optimization process. This helps to ensure that the information that is contained in each of these observation groups is used in estimation of model parameters, and not undervalued or overvalued because of too low or too high a contribution to the initial objective function.
- **Declustering**
Observations can be correlated. Water level measurements at observation wells close to each other are often not independent. It is likely that values and changes at these wells are similar,

and the worth of information contributed by one well is diminished because it was already contributed by a different well in its vicinity. The worth of the information provided by each of the wells is therefore lower than a separate measurement at a larger distance. In this case, the weight of correlated observations should be reduced.

Time series are good examples of this principle as well. Daily measurements of the groundwater level might carry the same worth of information as a measurement taken on a monthly basis does. Because the daily measurement has more measurement points, it would be overrepresented if the weights of each of these measurement points are not compensated for. This makes it advisable to normalize the weights of observations of time series by the sampling rate of the measurement.

Further reading: PEST Manual (5th Ed.), Ch. 2.1.2: Observation Weights.

15.2.2 Pilot-Point Method

The pilot-point method defines parameters as a spatially variable distribution.

In the classical calibration approach, it is a common assumption that geologic formations have spatially constant parameter values. In reality, this is rarely true.

Therefore, instead of applying a homogeneous parameter value across a zone, varying values for the parameter are assigned at particular locations (the **pilot points**). Each pilot point represents an adjustable parameter in PEST. An interpolation method then creates a continuous distribution of this parameter. Figure 15.6 illustrates the method.

The resulting large number of parameters adds to the degrees of freedom in the inversion process. This

will generally lead to a better fit to the measurement data. At the same time, it will increase the level of non-uniqueness and therefore better reproduce the uncertainty associated with the model predictions.

Pilot points often lead to lower objective functions and better fits to measured data. However, the modeler should be aware of the risk of **overfitting** the parameter field and should always check that the solution is plausible in a geological sense, and regularize it if necessary (see section 15.2.4.2).

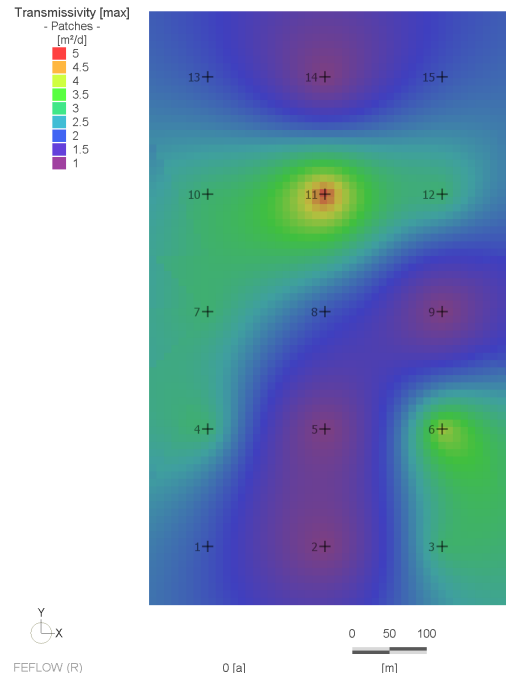


Figure 15.6 Distribution of hydraulic transmissivity, interpolated from a set of 15 pilot points.

Further reading: PEST Groundwater Data Utilities, Part A, ch. 5: Model Parameterization based on pilot-points.

15.2.3 Parameter Nonuniqueness

A typical challenge when history-matching (calibrating) an environmental model is the inherent **nonuniqueness** associated to the inverse solution. Usually many different parameter sets exist which are all compatible with the historical observation data.

Observation data is usually sparse and usually not sufficient to uniquely identify more than just a few of the large number of model parameters that can be made adjustable.

This has two consequences:

- Different calibrated parameter sets lead to different predictions. This makes it difficult to use a single model alone for decision-making.
- Some or many of the parameters will be insensitive to observations. The GLMA-based optimization process can become unstable under this condition, leading to long optimization run-times or even failure to optimize.

Regularization techniques can provide a defence against these issues. They restrict the parameter search to identifiable parameters, either by adding additional constraints to the parameters (Structural Regularization, **Tikhonov Regularization**) or separating identifiable parameters from non-identifiable parameters (**Subspace Regularization**).

This manual restricts itself to Tikhonov regularization (discussed in section 15.2.4.2) and Subspace regularization (discussed in section 15.2.5).

See the PEST tutorial Methodologies and Software

for PEST-Based Model Predictive Uncertainty Analysis, pp. 46 (see the literature review, section 15.1.5), for a very good discussion on different regularization techniques.

15.2.4 Prior Knowledge

Prior knowledge is introduced in the optimization if some knowledge about the estimated range of parameters values exists. (This is also referred to as pre-calibration parameter probability.)

The general procedure can be explained in comparison to the history matching process: In history matching, the departure of computed observations from their measured values is expressed as a function (the **measurement objective function**). Minimizing this function leads to a parameter set that reproduces the historical measurements, hence a calibrated model is found.

When using prior knowledge, the departure of the applied parameter values from parameter values preferred by the modeler is expressed as a second function (the **regularization objective function**). This kind of regularization is therefore a method that introduces knowledge about the plausibility of parameter values into the calibration process. This knowledge is often subjective, but nevertheless valuable.

PEST implements two principal methods to perform a concurrent optimization on measurement and regularization objective function: Prior Information and Tikhonov Regularization.

15.2.4.1 Prior Information

Prior information is the simplest way to implement

preference for parameter values or to preferred relationships between them (e.g., a preferred ratio between horizontal and vertical hydraulic conductivity). The sum of squares of departures from these equations contribute to the regularization objective function.

Minimization of the total of regularization and measurement objective function leads to a parameter set that reproduces the historical measurements and shows a plausible parameter distribution at the same time.

Further reading: PEST Groundwater Data Utilities (5th Ed.), ch. 2.1.3: The Use of Prior Information in the Parameter Estimation Process.

15.2.4.2 Tikhonov Regularization

The Tikhonov regularization method as implemented in PEST automatically generates a number of “information” equations, which defines the initial value of each parameter as the preferred value (see Figure 15.7). The user can also make changes to these equations, or set up his/her own additional equations.

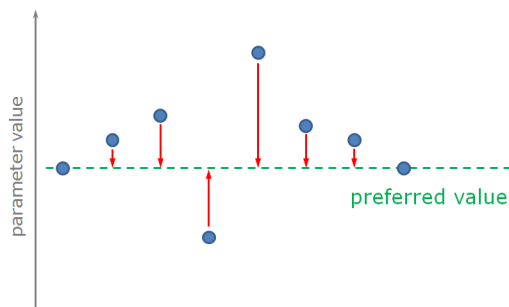


Figure 15.7 Regularization of parameters: departures (red) from preferred parameter values (green) are penalized.

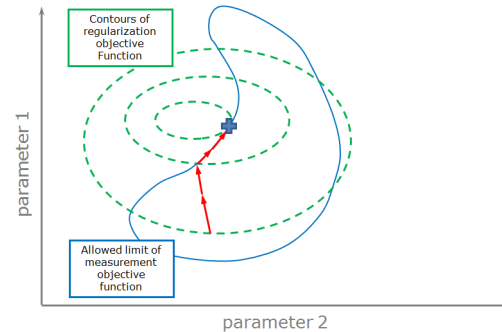


Figure 15.8 Constraint optimization: the regularization objective function (green contours) is minimized while staying within the defined limits (red contour) of the measurement objective function.

When using Tikhonov regularization the calibration process is formulated as a constrained minimization process as follows “minimize the regularization objective function while ensuring that the measurement objective function is set at the user-specified target”. Figure 15.8 illustrates this approach. If this user-specified target is not met, then PEST minimizes the measurement objective function. In the meantime it adjusts weights applied to prior information such that they act as Lagrange multipliers in the constrained optimization process. PEST thus determines the appropriate relative weighting between measurements and respect for prior information in accordance with a user’s choice of target measurement objective function.

As a result, Tikhonov-Regularization reduces the number of possible parameter sets that constitute a calibrated model by rejecting calibrated models with unrealistic parameter values.

Further reading: Methodologies and Software for

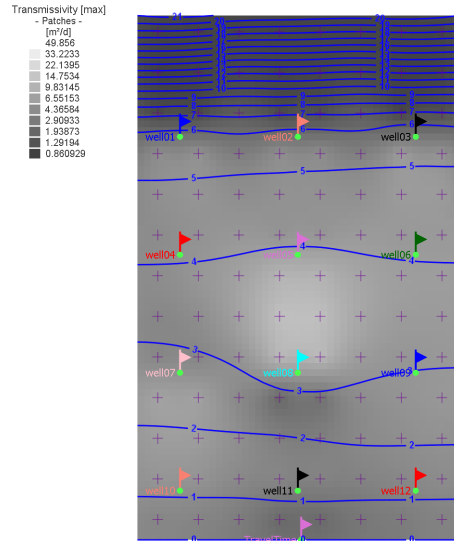


Figure 15.9 An overfitted parameter field.

PEST-Based Model Predictive Uncertainty Analysis: Regularization (p. 46).

15.2.4.3 Regularization of Pilot-Point Parameters

If parameter fields are defined as a varying distribution using the pilot point method, this will allow a better fit to the observation data during history matching compared to a result obtained using constant parameters. While this is favorable to some extent, the resulting parameter field might look implausible, especially when pilot points are placed at a high density.

Figure 15.9 provides an example. Because there are more pilot points (104, purple crosses) than observa-

tions (12, flags), a perfect match between observed and simulated results is obtained.

The transmissivity field however reveals that this result is flawed nonetheless: The distribution looks somewhat "bumpy", especially around the observations. Even more severe, the transmissivity above the northernmost row of observation points is totally different (lower) from the one in the remaining area.

A parameter distribution like this is unlikely, and accordingly a prediction made with this model has a high potential of wrongness even though it is perfectly aligned with its calibration data. This state is called **overfitting**.

To prevent overfitting, a second objective (next to the measurement objective function) is required, through that plausibility is preferred.

A common approach is to prefer homogeneous distributions of parameters over heterogeneous distributions. If different values are assigned to neighboring pilot points to lower the measurement objective function, this difference will be penalized and will give rise to the regularization objective function (See figure Figure 15.10). As a consequence, the optimization will yield a balanced compromise between calibration fit and homogeneity. Finding the right distance within these penalties are applied is important. Differences between closely located points needs to be penalized stronger as the likeliness of parameter differences becomes smaller. Pilot points located far apart (above a certain distance, the **correlation length**) do not need to be penalized at all.

This distance and the strength of correlation are defined through a variogram (Figure 15.11)

Further reading: *PEST Groundwater Data Utilities*,
 ch. 5.6: Regularization (of pilot points).

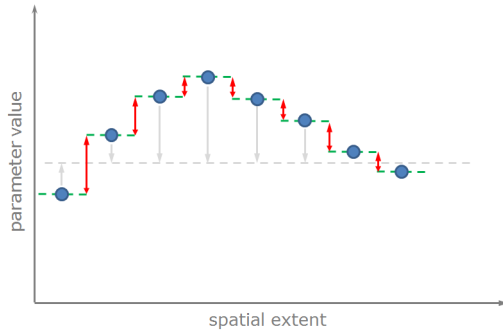


Figure 15.10 Regularization of pilot point parameters: by penalizing differences between pilot points (red), a homogeneous (smooth) distribution is preferred. Initial parameter values are still preferred through prior information (grey).

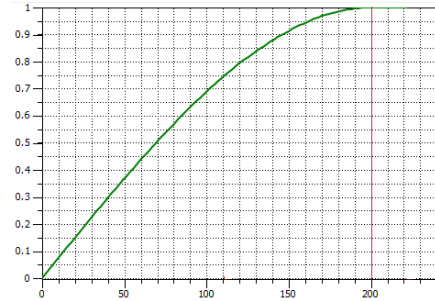


Figure 15.11 A spherical-type variogram with a correlation length (Range) of 200 m.

Thus, within the range of correlation, implausible heterogeneities are suppressed unless they are necessary to meet the targeted value of the objective function. PEST calculates the expected correlation between each two pilot points and creates a **covariance matrix** which is used to impose the correct weights. In summary, the correlation length allows to define a preferred variability of a model property, in addition to the preferred mean value that is provided through the initial parameter value.

Figure 15.12 shows the same model, regularized with a correlation length of 200 m. The transmissivity field is smoother, but still reflects general trends suggested by the observation data. Even though it yields a stronger model-to-measurement misfit, predictions made using this model will have higher confidence.

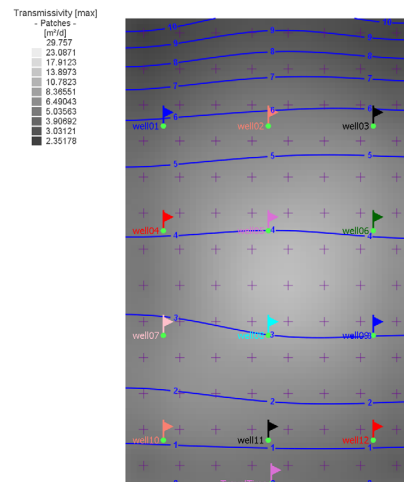


Figure 15.12 Regularization of pilot points parameters leads to a smoother parameter field (compare with Figure 15.9)

15.2.5 Subspace Regularization

Subspace regularization follows a different approach than Tikhonov regularization.

The fundamental idea of subspace regularization is to separate identifiable parameter components from non-identifiable parameter components in order to exclude the latter one from the parameter search.

The identifiability of a parameter is related to the way and extent it influences existing observation data (if a parameter does not influence any of the existing observations, it cannot be identified).

Parameters (called **base parameters** in the following) are usually neither completely identifiable or non-identifiable. It is however possible to create linear combinations of base parameters for which this is the case. These are called **super parameters**.

The transformed (super-)parameter space is separated into two subspaces: One subspace is comprised of combinations of parameters that have an influence on observations. These combinations of parameters can be uniquely estimated through the history matching process.

The remaining parameter combinations occupy the so-called **null subspace**. These combinations of parameters have no or very small influence on model outputs corresponding to observations; hence estimation of these parameters through history matching is not possible.

The groups are also denoted as sub-spaces of the **parameter space** (the parameter space is the combination of these two orthogonal subspaces, and contains all parameters):

- The group of identifiable parameters is called solution subspace (or often just **solution space**)

- The group of non-identifiable parameters is called null subspace (or often just **null space**)

15.2.5.1 Truncated Singular Value Decomposition

Singular Value Decomposition (SVD) is the name of the method through which the parameter space is partitioned into the two orthogonal solution and null subspaces.

In most groundwater modeling contexts the solution space is smaller than the null space. The earth is complex, and the information content of most calibration data sets is insufficient to provide unique estimation of the parameters which describe this complexity.

SVD analyzes the **Eigenvectors** of the covariance matrix to identify the super parameters. The **Eigenvalues** - a measure for the post-calibration variability of their associated Eigenvectors - are the criterion to decide if a parameter is associated with the solution space and therefore included in the optimization or not. The ratio of highest to lowest eigenvalue is a measure of the extent to which the inverse problem approaches ill-posedness. If this ratio is more than about $5e-7$ then the problem can be considered to be ill-posed (in which case PEST would fail to optimize).

The **truncated SVD** separates the parameter space into solution and null subspace using this ratio as a criterion, and therefore omits any super parameters that are too insensitive to be uniquely estimated. As a consequence, the inversion of the solution space is always well-posed and a stable optimization is guaranteed (unless flawed by other sources of error, e.g. bad derivative calculation, section 15.2.1.1).

FePEST applies truncated SVD with a threshold of

5e-7 by default in any PEST setup.

Further reading: *PEST Manual (5th Ed.)*, Ch. 8.4: *Truncated Singular Value Decomposition*.

15.2.5.2 SVD-Assist

The SVD-A method uses the concept of the SVD to reformulate the inversion problem in a way that it can be solved with much less numerical effort.

The SVD first identifies those combinations of parameters which are uniquely estimable on the basis of the current calibration data set and defines them as super parameters. SVD-A creates and run a new PEST setup based on super parameters instead of base parameters.

When calculating finite-difference derivatives of model outputs with respect to parameters, it actually calculates these derivatives with respect to the super parameters rather than the native model parameters (base parameters). Hence only as many model runs are required per iteration as there are dimensions in the solution space (i.e. number of super parameters).

This method is of fundamental importance for the pilot point method, as it allows calibration and predictive error analysis of highly parametrized models (e.g., using 1000+ parameters) with reasonable effort.

Further reading: *PEST Manual (5th Ed.)*, Ch. 8.5 *SVD-Assist*

15.2.5.3 Least Squares (LSQR)

Least Squares (LSQR) is an alternative to the SVD method for highly-parametrized inversion problems. Experience has shown that its application is useful

when more than 2500 parameters are involved.

Further reading: C. C. Paige and M. A. Saunders, *LSQR: An algorithm for sparse linear equations and sparse least squares*, *TOMS* 8(1), 43-71 (1982). and C. C. Paige and M. A. Saunders, *Algorithm 583; LSQR: Sparse linear equations and least-squares problems*, *TOMS* 8(2), 195-209 (1982).

15.3 Fundamental Setup

The fundamental setup prepares the model to be processed by PEST. Its steps are common to most PEST methods.

The fundamental setup comprises the definition of parameters, observations and prior knowledge (if available). A decision on using subspace methods is to be made, and finally, parallel computing may be configured to distribute workload on different computers.

15.3.1 FEFLOW and FePEST

FePEST requires a FEFLOW model as a starting point for any PEST setup. FePEST asks for the file name of the FEFLOW model when a new optimization project is created.

When setting up a FEFLOW model that is planned to be subject to a PEST optimization, bear in mind that the run-times should be reasonably short and that the model must run stable. It is possible to exchange the FEFLOW model by another one, provided that the new model file contains the same observation points and parameter zone selections (usually a modified version of the original model).

It is also possible to open a model simultaneously in FEFLOW and FePEST. If changes are made and the model is saved within FEFLOW, a reload must be per-

formed within FePEST to inform it about the changes made.

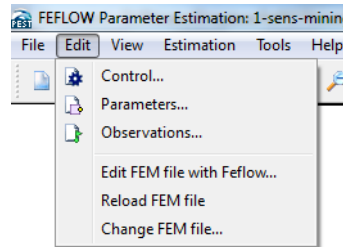


Figure 15.13 The Edit menu allows access to the problem settings dialog (Control / Parameters / Observations) and allows to open, reload and change the FEM file.

15.3.2 Adjustable Parameters

Choosing the model parameters that PEST can change to minimize the objective function is usually the first part of the setup.

An adjustable parameter can be described by its parameter type (e.g., hydraulic conductivity) and the zone of application (e.g., a certain geological formation).

- The **parameter type** can be any time-constant material property of the FEFLOW model.
- The **zone** can be any elemental selection that is stored in the FEFLOW model.

Note that the choice for the zones already constitutes a kind of regularization (called structural regularization), that has the power to significantly influence the calibration process (in a good or bad way).

If making changes to elemental selections in FEFLOW, remember that you must reload the model

after you have saved them in the FEFLOW file.

15.3.2.1 Definition of Parameters

An optimization problem commonly comprises many parameters sharing identical or similar settings.

To avoid that the user needs to setup these parameters one-by-one, similar parameters are defined through a **parameter definition**. A parameter definition allows central adjustment of default values of its dependent parameters which are created from it. This allows convenient management of large lists of parameters.

Usage of a parameter definition differs depending on the choice of the assignment method. Possible assignment methods are:

- **Zonally constant:**
The user specifies one or multiple zones in which the value of a parameter is to be estimated. A dependent parameter will be created for each of these zones (see Figure 15.14). During each model call of a PEST run, a constant value will be assigned to the chosen FEFLOW model property in each separate zone.



FEM file

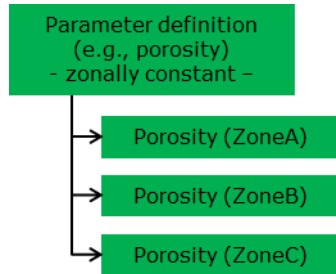


Figure 15.14 Zonal parameter distribution

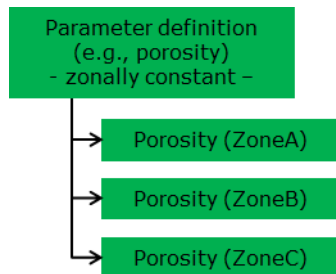


Figure 15.15 Pilot point based parameter definition

- Interpolate from pilot points:
The user chooses exactly one zone, which can be the model domain (a separate definition is required for each zone if pilot points are used). Within the limits of this zone, a cloud of pilot points is either imported from a file or is automatically generated by FePEST. Each of these points represents a single parameter of the PEST setup (see Figure 15.15)

The parameter definition of a pilot-point based parameter includes the settings of the interpolation method that is used to interpolate parameter values between pilot points. Available options are Kriging and Radial Basis functions.

Note that FePEST will apply the same settings to regularize the pilot-point parameters if the respective option for the Tikhonov Regularization is active.

The user can now define the settings that will be applied to the dependent parameters by default (individual changes can be done later). These include:

- Transformation of the parameter
 - **Logarithmic** transformation often allows faster and quicker reduction of the objective function by linearizing of the system).
 - A parameter can be **tied** to a different parameter, in this case its value will be changed according to the parent parameter, always maintaining the ratio of their initial values.
 - A parameter can be **fixed**, thereby removing it from the optimization.
- Change limit
This setting defines how to determine the maximum offset with that a parameter can be changed within a single iteration. Note that relative change limits are not allowed if the parameter is log-transformed.
- Initial value
The parameter value that is applied in the first iteration. The value assigned in the FEFLOW model will be used by default, assuming that this

15. FePEST

represents the preferred value of the expert modeler.

- **Bounds**
An upper and a lower limit can be defined for the parameters. A good approach is to use a very low and very high value initially that does not impose a restriction to the optimization.
- **Scale and offset**
Before a parameter value is assigned to the model, it is multiplied with Scale and then added to Offset. These settings usually do not need to be changed.

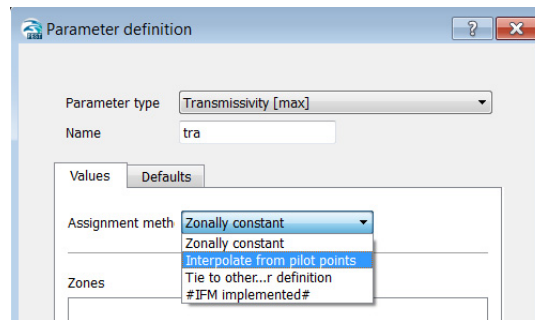


Figure 15.16 Creating a new parameter definition. Choose from Zonally constant or pilot point interpolated parameter distributions. The Defaults tab defines the standard settings for the dependent parameters.

Def.	Parameter type	Zone	Pilot point	Active	N.
tra	Transmissivity [max]		1	yes	tra-1
tra	Transmissivity [max]		2	yes	tra-2
tra	Transmissivity [max]		3	yes	tra-3
tra	Transmissivity [max]		4	yes	tra-4
tra	Transmissivity [max]		5	yes	tra-5
tra	Transmissivity [max]		6	yes	tra-6
tra	Transmissivity [max]		7	yes	tra-7
tra	Transmissivity [max]		8	yes	tra-8
tra	Transmissivity [max]		9	yes	tra-9
tra	Transmissivity [max]		10	yes	tra-1
tra	Transmissivity [max]		11	yes	tra-1

Figure 15.17 After a parameter definition has been created (top), its dependent parameters appear in the list below.

The OK button applies the new parameter definition. At the same time its dependent parameters are added to the parameter list.

These parameters inherit the default parameters of their parent definition (Figure 15.17). If required, changes to settings of individual parameters can be done (overriding the defaults), including the removal of parameters.

Working with large lists is easier with a spreadsheet program. The Copy/Paste buttons allow a quick transfer to and from other programs using the system clipboard.

Also see section 15.7.5 for information on how to implement parameters through IFM plug-ins.

15.3.2.2 Parameter Groups

The parameter groups allows the configuration of

the derivative calculation for the parameters (see section 15.2.1.1). FePEST applies default values that have been tested to work with most FEFLOW models, and often adjustments are not necessary when setting up a PEST model.

If the PEST optimization however fails due to bad derivatives calculations (which cannot be excluded as every model is different), a reconfiguration of these settings might be required. Detailed explanation and literature references to the different settings are given in the FePEST help system.

NOTE: The PEST utility tool JACTEST (section 15.6.2) is a utility to check for bad derivative calculation.

By default, FePEST defines one parameter group per FEFLOW parameter type and assigns the adjustable parameter to these groups accordingly:

- The Derivative method is chosen automatically (option "switch", starting with the more effective 2-point methods, switching to higher order methods if required)
- The Increment size (set to 1.5% by default) can be increased if minor model instability issues are observed. Do not increase this value unnecessarily, as high values would violate the linearity assumption of the derivative calculation.

15.3.3 Observations

The observations provide the primary (and only) measure that informs the optimization algorithm about the model-to-measurement misfit.

For each observation FePEST requires:

- its type (e.g., hydraulic head),

- its location (e.g. an observation data),
- the time at that it was recorded (in case of a transient model) and
- the value that was observed in reality.

Because the observation points set in FEFLOW already contain this information, it is possible to import them directly from the FEFLOW model.

By default, all observations are weighted with a weight of unity. These can be adapted by the user (compare section 15.2.1.2).

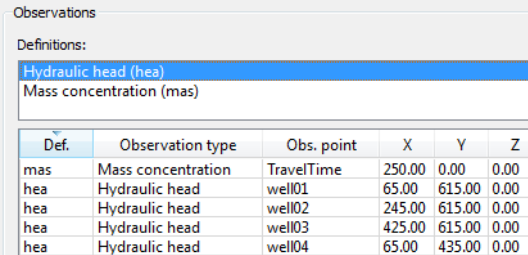
Supported observation types are all observations of system state (e.g., hydraulic head, saturation, mass concentration, temperature) depending on the models problem class. Reference values are constant values if the model is steady state. In a transient model, a time series contains the data of observations at different points in time.

Advanced users may also use IFM plug-ins or third party software for other types of observations.

15.3.3.1 Definition of Observations

Observations are defined in a similar way as parameters. If observations are of the same type (e.g., observations from the same well field), often similar or identical settings are required.

For convenience, and to avoid many repetitive adaptations of these setting when creating or making changes to observations, each observation depends on an **observation definition**. A definition allows central adjustment of the default values of its dependent observations (see Figure 15.18). This allows a better management of a large number of observations.



Observations

Definitions:

- Hydraulic head (hea)
- Mass concentration (mas)

Def.	Observation type	Obs. point	X	Y	Z
mas	Mass concentration	TravelTime	250.00	0.00	0.00
hea	Hydraulic head	well01	65.00	615.00	0.00
hea	Hydraulic head	well02	245.00	615.00	0.00
hea	Hydraulic head	well03	425.00	615.00	0.00
hea	Hydraulic head	well04	65.00	435.00	0.00

Figure 15.18 Observation definitions (top) and their dependent parameters (list below).

In the easiest case the definition of observations only requires the choice of the observation type (e.g., Hydraulic Head, Pressure, Mass concentration).

- FePEST can automatically import the observation points of the given type from the FEFLOW model. If the model is transient, it adds multiple observations per observation point, each representing a sample point of the respective time series. A weight of one is applied by default.
- Alternatively, an external file can provide the observation locations and data.
- Advanced users may choose to create additional observations in the PEST setup, that can be implemented using IFM plug-ins or third-party software (see also section section 15.7.5).

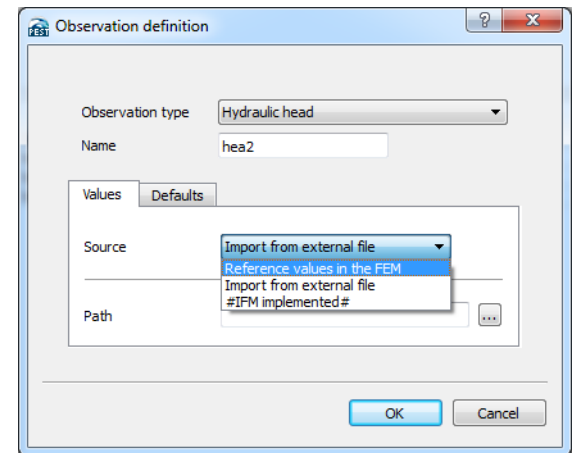


Figure 15.19 Creating a new observation definition

Observations created in this way now populate the observation list (this being the actual list of observations as PEST sees it).

It is possible to change settings of particular observations (overriding the defaults). This is required especially when adapting the observation weights to achieve better optimization behavior and results.

HINT: Working with large lists is easier using a spreadsheet program. The Copy/Paste buttons allow a quick transfer to and from other programs using the system clipboard.

15.3.3.2 Observation Groups

FePEST automatically assigns observations of different type to different observation groups. This allows PEST to distinguish how strong the different groups

contribute to the measurement objective function.

In the same way it is possible to allocate observations of the same type to different groups (e.g., to differentiate between hydraulic head measurements in different aquifers).

Advanced users may specify an observation covariance file to define the weights for these observations.

15.3.4 Prior Knowledge

Prior Knowledge - if available - can be described during this step of the PEST setup. In most cases the Tikhonov regularization option will be preferred over the manual setup of equations of prior information (see section 15.3.4 for details).

15.3.4.1 Prior Information

Equations of prior information allow to define preferred values for parameters, or preferred relations between parameters. Any deviation from this relationship will contribute to the regularization objective functions. As though there are certain similarities to observations:

- **Name**
A user-defined name to identify the equation.
- **Weight**
Each equation has a weight to allow to control the strength with that it contributes to the objective function (relative to other prior informations and field observations). Individual weights of prior information should reflect the trust that is associated with the underlying assumptions.

- **Group**
It is possible to associate different prior informations to different observation groups, hereby defining more multiple regularization groups. The principle is the same as for the observation groups.

The formula itself has to be written in a special syntax specified in the PEST manual. Note that FePEST will not check for correct syntax on its own, however the PESTCHECK feature can be performed from the Tools menu to do so (recommended after each change made to prior information).

A default formula is provided for convenience, which needs to be adapted for the specific purpose by the user.

15.3.4.2 Tikhonov Regularization

When activated, Tikhonov regularization can implement two different aspects of regularization in the PEST setup:

- **Regularization based on initial parameter values**
Assuming that the initial parameter value represent the expected values of the expert modeler, equations of prior information are created that will penalize departures of parameter values from initial values.
As a result, parameter values close to initial parameters will be preferred during the optimization.
- **Regularization of pilot point parameters using covariance matrices**
Pilot-point type parameter values for each defi-

dition are regularized taking into account the expected correlation (using a covariance matrix). Differences in parameter values of pilot-points closer than their correlation length will be penalized.

As a result, homogeneous (smooth) parameter definitions will be preferred over heterogeneous ones.

Objective Function Limits

As it is described in section 15.3.4, the Tikhonov regularization aims at finding a minimum of the regularization objective function, while maintaining user-defined limits for the measurement objective function (under which the model is still considered calibrated).

The following settings determine this limit:

- Target measurement objective function (PHIMLIM)

This is the limit for the measurement objective function below which the model is considered to be calibrated.

The value can be calculated by summing up the (weighted) measurement noise associated with the observations. If this is not possible, a value somewhat higher than the objective function that results from a calibration run without Tikhonov regularization can be chosen.

- Acceptable measurement objective function (PHIMACCEPT)

This additional threshold is usually set slightly (5% to 10%) above PHIMLIM. PHIMLIM and PHIMACCEPT define a buffer zone for the measurement objective function value for stability reasons. In this zone, an objective function value is tolerated even though it does not meet

the target value. This is necessary as the parameter upgrade vector will often "miss" the exact limit because it relies on a linearity assumption. Figure 15.20 illustrates how the iteration adapts to these limits.

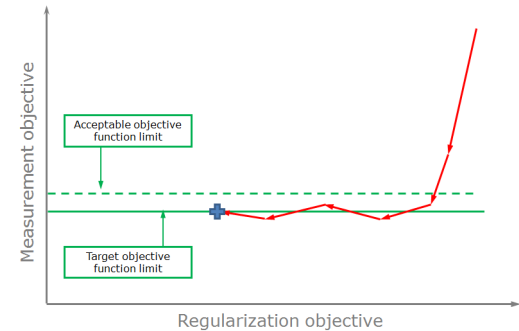


Figure 15.20 Development of the regularization and measurement objective function during Tikhonov-regularized parameter estimation.

- Successive reduction of the objective function Limit (FRACPHIM)
This option allows a different strategy to determine the target objective function limits. If set to a non-zero value (allowed values are between 0 and 1), PHIMLIM is determined by multiplying the last achieved value of the measurement objective function with FRACPHIM. In this way, PHIMLIM gets lower from iteration to iteration. It will however never be smaller than the value defined in PHIMLIM. Optimal values for FRACPHIM are normally in the range 0.1 to 0.3.

FePEST activates this option by default in combination with a very low objective function (these are the same defaults as applied by the PEST tool ADDREG1). This improves the well-posedness of the optimization and thereby leads to a more stable behavior of the GLMA optimization. The limits should however be adapted by the user as these settings might not yield the desired plausible parameter values.

See Section 7.3.3 of the PEST user manual for a full discussion of these variables.

Weight Factors and Adjustment

Settings to determine the weight factor can be used for fine tuning or trouble shootings. Their default values follow general recommendations that are suitable for most applications of PEST.

15.3.5 Subspace Regularization

As described in section 15.3.5, subspace regularization methods can greatly improve the stability and reduce the required modeling effort of an optimization.

15.3.5.1 Singular Value Decomposition

SVD is the recommended option for any PEST setup (unless LSQR has been chosen, which tends to be faster for PEST runs involving more than 2500 parameters). FePEST activates this option by default.

The particular settings determine how many singular values / super parameters are regarded during the optimization:

- The eigenvalue threshold, below which super

parameters will be truncated, is by default set to $5e-7$. At this value, the optimization is still regarded well-posed, which ensures stability of the optimization.

- In addition, it is possible to further limit the number of singular values / super parameters to maximum number.

See the PEST users manual (5th Edition), section 8.4.2: Implementation of SVD with PEST for a full discussion of these settings.

15.3.5.2 SVD-Assist

SVD-Assist (SVD-A) is useful to speed-up the calibration of highly parametrized models (often involving the pilot point method).

It can be chosen from two principle ways to determine the number of singular values:

- By default, PEST uses the SUPCALC tool to determine the optimal number automatically.
- Manual specification of the number of super parameters can be useful if the run is carried out on multiple CPUs in parallel:

Each iteration requires one model run per super parameter to calculate the Jacobian matrix. Optimal usage of computational resources is given of the number of super parameters equals a multiple of total amounts of slaves (See section section 15.3.6).

15.3.6 Parallelization

An inherent issue of calibration and uncertainty analysis, scenario runs and sensitivity analysis is the

15. FePEST

large number of required model calls and the often significant required run times.

Fortunately, many steps of a PEST run, especially the numerically expensive calculation of the Jacobian matrix, is very suitable for parallel computing. By involving a multitude of computers (whether this being a limited number of office PCs, a HPC cluster or cloud-based computers) computation times can be reduced to an acceptable level. But even if applied only locally on a single computer, parallelization can improve model run times significantly.

In case of highly-parametrized inversion processes, parallelization is often a requirement to finish a computation within typical project time frames.

FePEST deploys BeoPEST - a network capable version of PEST - for this task. FePEST also transfers the required model files to the slave computers.

The port denotes the network (IP) port of the local computer (Host) that FePEST uses for communication. If the default settings conflicts with a different application, choose a different port number. Make sure that no router, firewall or anti-virus software blocks the network connection even if no remote computers are involved (localhost only).

Slaves shows the list of servers that will be used to undertake model run jobs during the PEST run (initially empty). You can add and remove servers to the list, or edit the settings of existing entries.

See also installation instructions for parallel computing.

- **Host name**
The host name specifies the host name or IP-address of the server computer. Enter "localhost" to add the local computer to the list.
Note that FePEST has to be started in server mode on all remote servers (except the local

computer) before commencing the PEST run.

- **No. of Slaves**
The number of slaves is the number of models that will be run simultaneously on the computer. In most cases, this will be set to the number of available CPU cores on that computer.

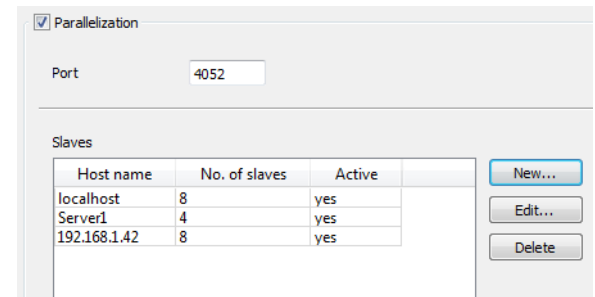


Figure 15.21 The parallelization page contains the slave machines running FePEST in server mode.

FePEST must be started and set to server mode (see Figure 15.22) on each of the slave servers.

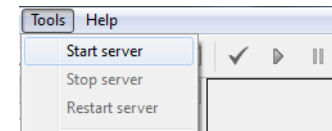


Figure 15.22 When running in server mode, the current computer acts as a slave server that can receive run jobs from another computer.

15.4 Parameter Estimation (History Matching/Calibration)

The terms parameter estimation, history matching and calibration are used synonymously in this document.

History matching of a model requires completion of the fundamental setup as explained in section 15.3.

After the fundamental setup has been completed, PEST can be advised to perform history matching. The history matching process targets the estimation of a parameter set that optimally satisfies both the historical observations and - if provided - the prior knowledge. The resulting parameter set is then regarded as a calibrated model.

This section explains the required settings, how the run is commenced and how to interpret the visual feedback during and after the run. Exporting a new FEFLOW model with optimized parameters is the final step.

15.4.1 Required Settings

15.4.1.1 Optimization Control

By default, FePEST assumes that history matching is to be performed and applies the respective PEST operation mode accordingly.

Note that the FePEST operation mode is slightly different than the PEST operation mode: If "Estimation" is set, FePEST chooses automatically from "regularization" mode (if the calibration involves Tikhonov regularization) and "estimation" mode (if not).

A second important option is the NOPTMAX set-

ting found in the termination criteria setting. For calibration purposes, this option must be set to "Number of iterations" and a sufficiently high value (e.g., 30 iterations, which is the default setting).

15.4.1.2 Other Settings

The default settings represent recommendations that are meant to be suitable for a range of optimization processes. Changes might be advised for fine-tuning and trouble shooting. The individual settings will not be explained in detail here, but detailed information is provided in the FePEST help system and the PEST documentation.

See Section 4.2.2 Control Data of the PEST user manual (5th Edition) for a full discussion of these variables.

15.4.2 Starting PEST

Starting the history matching process is done in a sequence of several steps.

15.4.2.1 Preflight Checks

Before running the model, a sanity check of the PEST setup is recommended. PEST provides several tools (PESTCHEK, TEMPCHEK and INSCHEK) that can be run through the Estimation menu of the FePEST user interface.

These utilities check the most important files of the PEST setup (the control file, the template file and the instruction file) for errors and warnings. Errors will prevent PEST from running, while warnings are indica-

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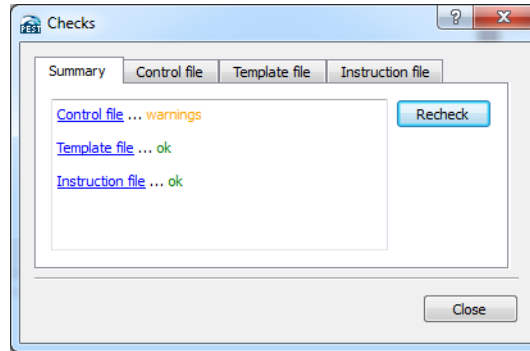


Figure 15.23 The Checks utility in the Estimation menu checks the PEST setup for validity and provides suggestions for improvement.

tions for possible problems and give suggestions for improvements of the setup.

15.4.2.2 Running PEST

PEST is finally started using the Run button in the toolbar. Usually no change needs to be done to the sequence of steps provided in the upcoming dialog (see Figure 15.24).

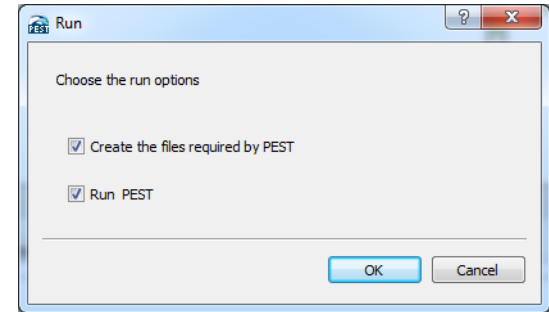


Figure 15.24 The Run dialog. Usually all options will be active.

The sequence is:

- Create the files required by PEST
FePEST generates the required PEST files according to the settings.
- Recalculate Jacobian Matrix
This option is available if the Jacobian matrix is still available from a former PEST run. Advanced users can choose to deactivate this option to save computational effort.
- Start PEST
This finally executes PEST itself and commences the actual history matching process. The FePEST windows display the progress of the PEST iteration.
Users experienced in PEST can choose to generate the PEST files without immediately starting the PEST run itself. See also section 15.7.

It is possible to interrupt (pause) or stop the PEST run. A stopped PEST run can be continued at a later point in time, even if FePEST had to be closed in the

15.4 Parameter Estimation (History Matching/Calibration)

meantime. This is useful if the optimization has to be interrupted, e.g., because the computer is turned off.

15.4.3 Output during PEST Run

During the PEST run, FePEST reads and analyzes the output of PEST and displays key information in several panels and charts:

- **Output**
The primary output of PEST is shown in this window. Users familiar with the output of PEST will find information otherwise omitted in the FePEST output here.
- **Status**
Key information on the status of the PEST run is shown in the Status panel.

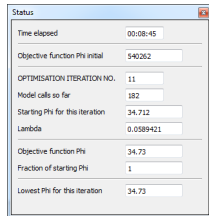


Figure 15.25 The Status panel contains key information about the progress of the optimization.

- **Objective Function**
The history of the objective function shows the progress of the optimization run and allows

identifying the occurrence of problems during the run. Ideally, the function value is shows a continuously falling behavior.

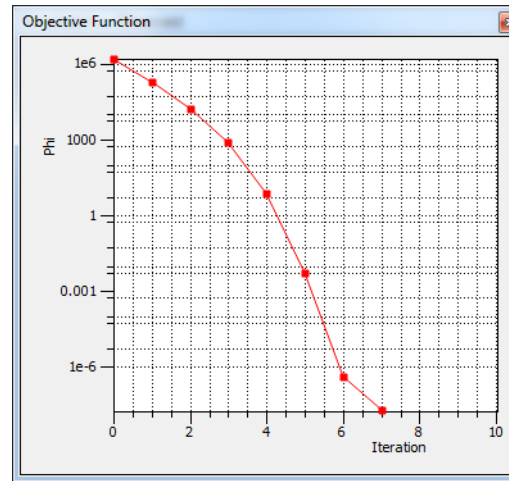


Figure 15.26 The development of the objective function is shown in the correspondent panel.

- **Simulated vs. Observed**
The panel shows a scatter plot that compares the simulated values with their (observed) reference values.
- **Simulated vs. Time**
A graph shows the time-dependent observations in the model. The measured time series is shown for comparison. This panel is not available for steady-state models.
Because the size of the text panels is restricted, they may not contain the complete file. In this case the View

button allows to open the respective file in an external text editor.

15.4.4 Output after PEST Run

PEST provides additional statistics after the history matching process. As already during the run, FePEST displays these and other key information in additional panels.

- **Run Details**

PEST journalizes all important information about setup and results of a PEST run into a run record file, which is shown in full in the Run details panel.

- **Parameter Sensitivities**

For all iterations, PEST journalizes composite parameter sensitivities in the sensitivities file, which is shown in full in the Run Details panel. This information can be used to check for example for hypersensitive parameters. The composite sensitivity of a parameter is a measure of the sensitivity of all model outputs for which there are corresponding observations to this parameter. By inference, it is a measure of the information content of the calibration data set with respect to this parameter.

- **Observation Sensitivities**

PEST writes the observation sensitivities of the last iteration to an observation sensitivities file, which is shown in observation sensitivities.

- **Residuals**

This panel lists the measured and simulated value for each model observation, as well as the difference between these values (the residual).

The native (non-weighted) residuals allow to identify well or poorly calibrated observations. The

weighted residuals (shown separately) are valuable to check for an appropriate choice of observation weights.

The content of this tab is identical to the residuals file created by PEST.

- **Covariance and Correlation matrix**

Covariance and Correlation matrices are only available when not using regularization.

These tables show the covariance and correlation between the parameters, respectively, the latter being normalized to values ranging from 0 (no correlation) to 1 (strong correlation). A color gradient facilitates interpreting the values.

- **Eigenvectors and Eigenvalues**

Eigenvectors and Eigenvalues are only available when running PEST in estimation mode and not using singular value decomposition.

Each observation contains a certain amount of information that contributes to the identification of the calibrated parameters. Because observations and parameters are often correlated, respectively, the information contributed from a particular observation might overlap with the information that was already provided from a different observation. As a result the number of observations is not necessarily proportional to the combined information of these observations.

If the covariance matrix undergoes principle component analysis, orthogonal combinations of parameters can be identified, together with the extent to which these combinations have been informed by the calibration process. These combinations are the eigenvectors of the covariance matrix. If a low eigenvalue is associated with this eigenvector, then its post-calibration variability is low. Conversely, if a high eigenvalue is associated

15.4 Parameter Estimation (History Matching/Calibration)

with an eigenvector, then its post-calibration variability is high.

The ratio of highest to lowest eigenvalue is a measure of the extent to which the inverse problem approaches ill-posedness. If this ratio is more than about $5e-7$ then the problem can be considered to be ill-posed. Furthermore, unless some kind of regularization is being employed (Tikhonov or SVD) PEST will not be able to solve this inverse problem. Instead its behavior will be numerically unstable, and the objective function may not fall at all.

The contents of the text panels can be easily transferred to a spreadsheet program for further processing and visualization.

See section 5.2: The PEST Run Record and section 5.3: Other PEST Output Files of the PEST user manual (5th Edition) for a full discussion of these output files.

15.4.5 Export to FEFLOW

After PEST was able to successfully reduce the objective function to an acceptable level (or another termination criterion was met), it ceases the optimization and FePEST will display a list of resulting parameter values.

To inspect the resulting model more in detail, save it as a new FEM file and open it in FEFLOW.

The found parameter set can also be applied as the initial parameter values, especially if further PEST methods are going to be used.

To return to this dialog at a later point in time, use the Show Results option in the Estimation menu.

15.5 Predictive Analysis

Predictive Analysis requires completion of the fundamental setup, and it is recommended to successfully run a history matching (calibration) process prior to it. The parameter set found as a result of the latter must have been applied as the initial parameter values to the current FePEST setup (in the Show results panel).

For most environmental models it is possible to find a multitude of calibrated models. Unfortunately, even though these model all match the historical data, the predictions made by these models will nonetheless vary at different levels. The prediction given by the particular model that was found during the calibration therefore represents only one out of many possible prediction.

Predictive analysis is a simple tool in PEST for non-linear model predictive error and uncertainty analysis. It searches for the calibrated model with the maximum or minimum key prediction. In this way it is possible to identify the worst-case or best-case scenarios among the set of calibrated models.

However, use of PEST in predictive analysis model is restricted to well-posed problems, where variability arises from measurement noise alone. In case of an ill-posed problem, advanced users may choose to use PEST methods such running PEST in Pareto mode.

Further reading: PEST Manual (5th Ed.) Ch. 6: Predictive Analysis

15.5.1 Required Settings

15.5.1.1 Optimization Control

The required operation mode in PEST is the Predic-

tive analysis mode; the optimization control section of the Problem Settings dialog contains the respective setting.

15.5.1.2 Observation and Type

Predictive analysis aims to either maximize or minimize a key prediction while maintaining the objective function below a user-specified value.

The prediction can be any observation (e.g. a specific hydraulic head) defined during the fundamental problem setup. Usually, a weight of zero will be applied to this particular observation to exclude it from the measurement objective.

The Predictive Analysis section of the problem settings dialog provides the settings for the choice of the prediction whose value must be maximized/minimized, and for the value of the objective function which must not be exceeded.

15.5.1.3 Objective Function Limits

The maximum/minimum prediction is searched under the constraint of maintaining the calibrated state of the model. It is important to define a maximum objective function value below which the model is considered to be calibrated.

For this purpose, Objective function limits are to be chosen. The model is assumed to be calibrated if the value of the objective function is less than the defined Target objective function.

A common choice is a value which is 5...10% greater than that achieved through objective function minimization through the preceding calibration pro-

cess. The choice is however always somewhat subjective and can have significant influence on the result. Where the statistics of measurement noise are well known, this limiting objective function can be set in accordance with theory. See the PEST manual for more details.

See the PEST Manual (5th Ed.), Ch. 6.2.2: PEST Variables used for Predictive Analysis for a full discussion of these variable.

15.5.1.4 Other Settings

The default settings represent recommendations that are meant to be suitable in most cases of a predictive analysis run. The individual settings will not be explained in detail here, but detailed information is provided in the FePEST help system and the PEST documentation.

15.5.2 Starting PEST

To start the predictive analysis, follow the same steps as described for the parameter estimation in section 15.4.

15.5.3 Output during Predictive Analysis

The history of the objective function shows the progress of the optimization run.

In case the initial parameter set does not resemble a calibrated model, PEST will first conduct a calibration to reduce the objective function until it falls below the defined target objective function.

PEST will then start maximizing/minimizing the

model prediction. The objective function during the required iterations will be in the allowed range between target objective function and acceptable objective function. Outputs after the PEST run.

15.5.4 Estimation Results

The first line of the parameter list shows the maximum or minimum prediction value that was found. The found parameter set resembles the calibrated model that is the worst-case (or best-case scenario), and can again be exported to FEM file.

PEST also generates additional statistical data. These are shown in additional panels after the model run.

15.6 Other Tools

15.6.1 Sensitivity Export

Linear sensitivity indicates how strong a parameter influences certain observations. These derivatives are calculated during the optimization and contained in the Jacobian matrix.

The sensitivities are therefore a potentially valuable by-product of the optimization, and can as such be exported for further processing.

15.6.1.1 Required Settings

Export of Sensitivities is possible after a Jacobian matrix was calculated. This is the case whenever an optimization (no matter if parameter estimation or predictive analysis) has been performed (successfully or not).

If no optimization has been performed yet, the NOPTMAX setting in the Termination criterion settings can be set to "Jacobian only" (-1). With this setting PEST will calculate the Jacobian matrix of the first iteration and terminate without any changes to the initial parameter values.

Further reading: PEST Manual (5th Ed.) section 2.2.9: Termination Criteria.

15.6.1.2 Export of Sensitivities

The Sensitivities feature in the Estimation menu runs the JROW2VEC tool of PEST to extract the sensitivities of parameters for the chosen observations. The resulting table can be

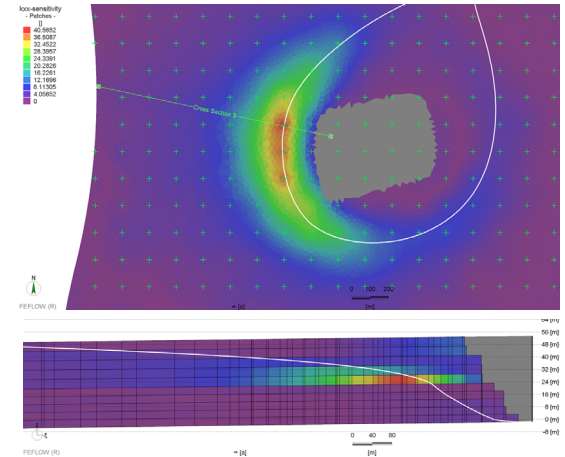


Figure 15.27 Sensitivity maps (plain view of layer 5 and cross-section of indicated line shown.) of hydraulic conductivity in a 3D model. These are created by spatial interpolation of pilot point parameter sensitivity. White line indicates the water table.

- Transferred to a spreadsheet program for further processing (using the Copy option)
- Exported to an ASCII table (dat-) file. Used in conjunction with spatial maps that relate the parameters to their zones or pilot point locations, sensitivity maps can be created in FEFLOW or GIS software (a FEFLOW example is shown in Figure 15.27).

15.6.2 Model Stability Tests (JACT-EST)

As discussed in section 15.2.1.1, it is important that

the numerical model is stable enough to provide reproducible observation - parameter relationships.

As a measure of trouble-shooting, PEST provides a tool (JACTEST) that checks if the model is running sufficiently stable to calculate the Jacobian matrix. This tool can be activated from within FePEST using the Model Stability option in the Estimation menu.

JACTEST will run the model multiple times, each incrementing/decrementing the chosen parameter according to its settings for derivative calculation and plotting the response of the observations.

Further reading: Addendum to the PEST Manual (5th Ed.) section 3.20: JACTEST

15.6.2.1 Using JACTEST

If PEST fails to reduce the objective function and bad derivative calculation is the suspected reason, stop PEST (if it is still running). Open the **Show Results** dialog and **Apply** the latest values as initial parameter values (you may want to save the FPS file now under a different name).

Open the Model Stability dialog from the Estimation menu. The only settings required by the users are:

- Specification of the parameters that are subject to the test.
Those parameters that are suspected to cause instabilities should be chosen here.
- Number of iterations to be performed on each parameter.
A value of 4 should initially suffice to identify parameter-observation relations that show a certain randomness.

After the calculation has finished, the diagram win-

dow shows the resulting observation values. If the slopes are similar or change gradually and monotonously, no problems are indicated. An example for a stable model is shown in Figure 15.28.

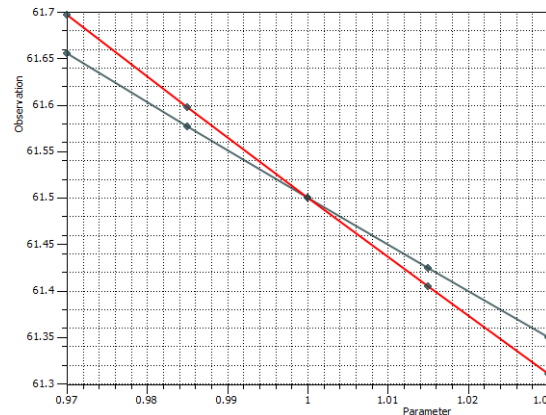


Figure 15.28 JACTEST result indicating stable model behavior. Two parameters are incremented / decremented four times each by 1.5% around the initial value, the resulting values for a particular hydraulic head observation are plotted.

If the parameter values change randomly (and significantly), noise dominates the observation. Identify the affected parameter-observation combinations, and open and run the model in FEFLOW to find and solve the instability issue.

15.7 Customized PEST Setups

PEST is a model-independent parameter estimator and as such easy to integrate with most numerical mod-

15. FePEST

els. The transparent design of its file setup allows the user a lot of customization and to implement own functionality.

One goal in the development of FePEST was to not restrict this flexibility. It provides a convenient user interface to set up the PEST files, but at any time the user is free to abandon the use of FePEST and continue working with PEST in the traditional way (by direct editing its configuration files and running its tools from the command line).

This release of FePEST implements those PEST features that are commonly used for model calibration. As it was discussed before, PEST has a lot more to offer.

Users that are experienced in using PEST might want to make use of features like Pareto methods or Null-Space Monte-Carlo analysis, or to make changes to certain PEST variables or options that are not accessible through the FePEST GUI. Implementation of own pre- or post-processing code (including third-party software and IFM plug-ins) into the PEST iteration loop might also be desired.

To make the best use of both FePEST and traditional PEST, just configure the PEST setup in FePEST as close as possible to the final settings. Then, generate the respective files, which can be edited as desired. Finally PEST can be started (in some cases, this can be done again from within FePEST).

15.7.1 Creating the PEST Setup

The PEST setup files are created when the PEST run is commenced. To be able to edit the files, press the run button, but disable the options for running PEST (and recalculating the Jacobian if applicable) before pressing the OK button (see Figure 15.29).

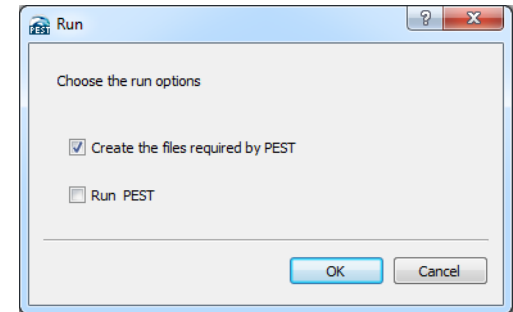


Figure 15.29 Settings in the Run dialog to create the PEST files.

The Checks option will also initiate the creation of the files if these are not present when it is executed.

15.7.2 Convenience Tools

To make the manual editing of the file setup easier, and to allow quick access to the relevant files and locations, the following features become available in the Estimation menu of FePEST after the PEST files have been generated.

- Checks
Runs the PEST error check tools PESTCHEK (checks the control file), INSCHECK (checks the instructions file) and TEMPCHK (checks the template file). Errors and warnings - if raised - will be shown in the dialog.
- Open work folder in explorer
Use this option to open the work folder, operate with files or to open them for editing.
- Open work folder in console window

Use this option to open a new command line window, from where PEST (and other) commands can run.

- Open control file
Directly opens the PEST control (pst) file in the standard editor.
- Show command
Shows a command line string with that the PEST run can be initiated. Use this command if you want to run PEST outside the FePEST GUI.

15.7.3 File Structure

Figure 15.30 shows the basic file structure as it is created by FePEST for the simplest case. Additional files may be present depending on the selected methods.

- PEST script (run_pest.bat)
This script file is executed when the PEST run is started by the user within FePEST. Besides other commands, the PEST executable is called. The content of this script will vary depending on the settings done in FePEST (e.g., SVDAPREP will be run from this script if SVD-Assist is active). Change this script to implement additional commands to the overall PEST process.
- Model script (run_model.bat)
This script is executed by PEST directly to commence a model call (It is cited as the model command in the PEST control file). The actual FEFLOW execution is cited in here.
Add commands to this file that should be executed with every model run.

- FePEST input file (<case>.fpi)
PEST writes parameter values to the FePEST input file (as advised in the respective template file), from where they are read by FePEST. The format is kept very simple, thus that user-specific scripts or plug-ins can access it.
- FePEST output file (<case>.fpo)
FePEST writes observation values to the FePEST output file, from where they are read by PEST (as advised in the respective instructions file). Once again, a very simple format is used thus that user-defined scripts or plug-ins can access this file.
- PEST control file (<case>.pst)
This is the primary PEST control file which defines the configuration of PEST. Edit this file to make changes that are not supported by FePEST.
- SVDA files (super.pst and others)
If SVD-Assist is used, a second pest setup will appear in the directory after SVDAPREP has been executed by the PEST script.
- Supportive files
Other files may appear depending on settings. E.g., several PLPROC files will be generated if the pilot-point method is applied, and a covariance matrix will be created by PPCOV if pilot-points are regularized.

The FePEST help contains a detailed description of these and other files.

15. FePEST

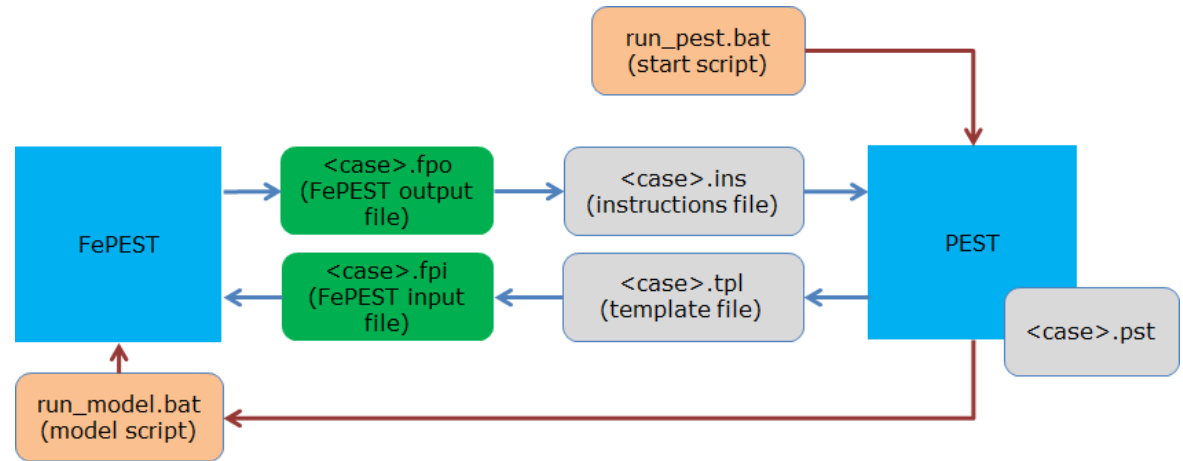


Figure 15.30 PEST file structure created by FePEST. Additional files may be present depending on the used methods (e.g., SVDA or pilot points)

15.7.4 Running Customized PEST Setups

A customized setup of files can be run in two ways: Either from within or outside of FePEST:

- Run from within FePEST
This option is more convenient and should be preferred if applicable. Click on Run again, but deactivate the Create Files option this time (otherwise, the files would be overwritten, see Figure 15.31).

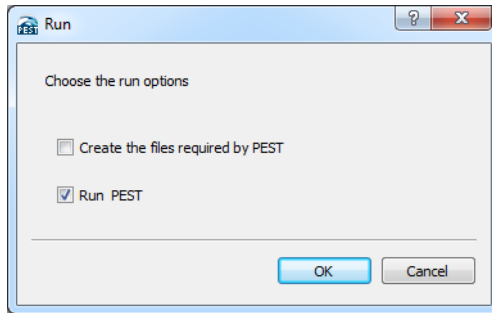


Figure 15.31 Settings in the Run dialog to run PEST without recreating the file setup.

FePEST will commence the PEST run by running the PEST script (run_pest.bat under windows), including all user modifications.

Note that because FePEST parses the primary output of PEST during run-time, FePEST visual feedback might fail partially or completely if the PEST output changes significantly due to the user modifications.

- PEST script from command line
The FePEST is part of a superordinate batch run, the PEST script (or its contents) can be incorporated into another script.
Even though visual feedback cannot be provided any more, FePEST (called in its simulation mode) still ensures that parameters and observations are correctly transferred between FEFLOW and PEST.

15.7.5 Integrating IFM Plug-ins and Third-Party Code

When creating a new observation definition or parameter definition, FePEST offers the type "IFM implemented" to add a specified number of additional parameters to the PEST file setup. These can be directly modified by an IFM plug-In or a third-party code (e.g., a script or another program).

- IFM plug-ins
An IFM plug-in must be attached to the FEFLOW model and registered in FEFLOW before the PEST run is started. If parallelization is used that involves remote servers, the plug-in must be installed on all remote machine as well (these will not be transferred automatically).
It opens the fpi-file during run-time of the model to read parameters, and opens the fpo-file to save observations.
- Scripts and third-party software
Any program used for additional postprocessing can access the fpi (to read parameters) and fpo file (to save observations) accordingly. To include them in the optimization, they have to be started appropriately from one of the batch files (either the model batch file or the pest run batch file).
For user-defined parameters, consider creating a new parameter group with appropriate settings for the derivative calculation.

15.8 FePEST Tutorial

For this exercise, a new FEFLOW file **fepest_fri_1.fem** is created based on the original demonstration-exercise file **exercise_fri_13.fem**. In this stage, all boundary conditions, material properties and problem settings have already been assigned. The file is located in the folder femdata in the tutorial section.

While a steady-state flow problem is considered here, the same workflow can be followed for other FEFLOW problem classes (including transient simulations) as well. The tutorial covers the four main steps that apply to any FePEST problem:

- Definition of observation points (in FEFLOW and/or FePEST)
- Definition of parameters zones (in FEFLOW)
- Definition of PEST problem (in FePEST)
- Post-processing of PEST results (in FePEST and FEFLOW)

15.8.1 Conceptual Model

The material property **Conductivity K_{xx}** is calibrated in this FePEST demo exercise. Conductivity measurements were taken in different locations at the surface level (*Slice 1* in FEFLOW). Initially, the spatial distribution of conductivity in FEFLOW for this slice was computed by means of a **Linear Akima regionalization** method. Using existing information of conductivity measurements, structure parameters of semivariogram (or variogram) were identified. Methods for variogram fitting are outside of the scopes of this chapter. Therefore, additional bibliography is recommended.

Two sets of field measurements (**Hydraulic Head**) are used for the parameter estimation problem.

Pilot points together with a regularization approach are applied to estimate the final conductivity distribution in *Slice 1*. Simple **Prior knowledge** is used to incorporate existing information of conductivity in the regularization techniques.

15.8.2 Field Measurements and Reference Data

Seven **Observations Points** are already defined in **fepest_fri_1.fem**. Together with four additional observation points to be included later in FePEST, they will be used for the calibration of **K_{xx}** . Details of observation-points manipulation will be discussed in this chapter.

Distribution of measured conductivity is shown in Figure 15.32. Here, a first overview gives an idea of the wide range of conductivity values in the model domain. A classical approach in this situation is to apply a log-transformation to the distribution of **K_{xx}** . From the measurement distribution, a variogram structure can be estimated using geostatistical methods. In our case, the distribution of **$\log(K_{xx})$** is well represented by a spherical variogram with nugget = 0, sill = 0.58, and range = 4200. This information will be implemented in the FePEST problem.

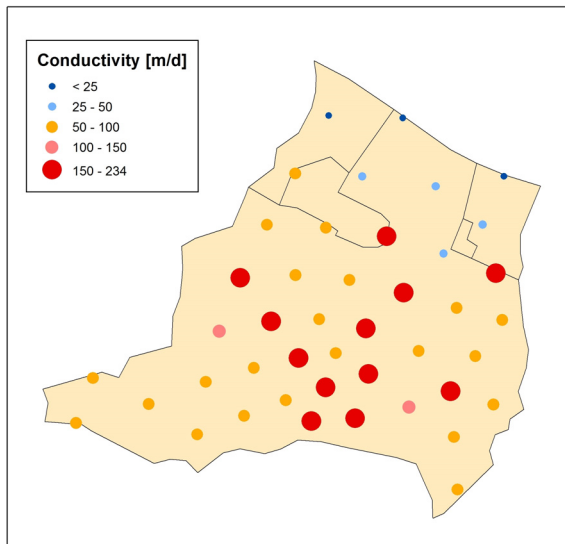



Figure 15.32Field measurements of conductivity in Friedrichshagen FEFLOW model domain.


15.8.3 FEFLOW Model Preparation

If the parameter estimation considers only a specific zone of the FEFLOW model domain (e.g., a layer, slice, or arbitrary subdomain), some preliminary steps are needed in FEFLOW before initiating FePEST.

In this FePEST demo exercise, conductivity is calibrated in slice 1 only; therefore, an element selection of this area is created first after opening **fepest_fri_1.fem** in FEFLOW 6.2:


- In the active view, go to **Slice 1**.
- In the  **Selection** toolbar, indicate as selection target **Elements**.

- Click on  **Select All**.

- In the  **Spatial Units** panel, store the element selection and rename it as **Slice_1**.

This element selection **Slice_1** will be available in FePEST as a **Zone** for the parameter estimation.

The **Observation Points** already included in the FEFLOW problem can be verified by opening the **Observation Point Properties** dialog (Figure 15.33). The same dialog is also used to assign measurement time series to observation points.

Click on  **OK** to leave the dialog without any changes. In the **Slice** view, navigate through the different slices. Notice that **Observation Points** are situated on slices 1 and 4 of the FEFLOW model while the actual parameter estimation in this example will be limited to the first slice. Observation wells to be included for the calibration problem can be still defined later in FePEST.

Save the fem file as **fepest_fri_1.fem**.

15. FePEST

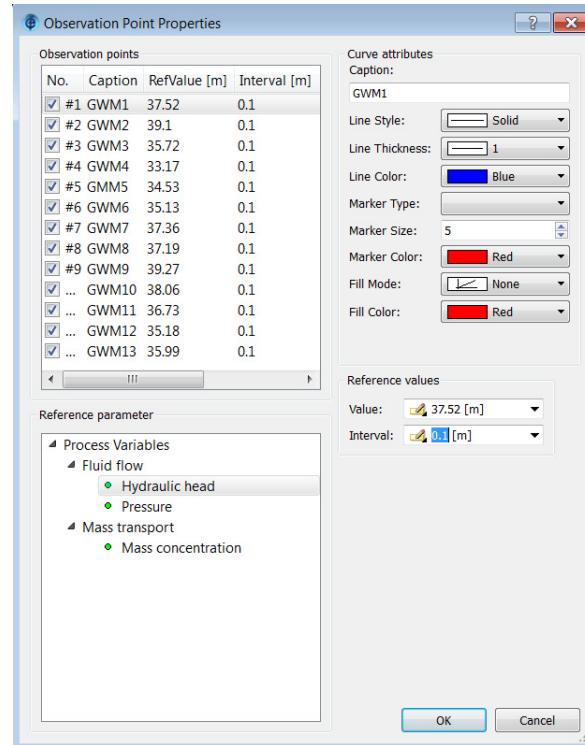


Figure 15.33 Observation Point Properties dialog.

15.8.4 FePEST Initial Configuration

FePEST is the graphical user interface for PEST. Although FePEST provides full communication between FEFLOW 6.2 and PEST (main program and PEST utilities), the user has the option to manually update the PEST program files and thus to control which PEST version is used in FePEST. During FEFLOW 6.2 installation, PEST program files are

automatically installed as well. Their location is controlled via the menu **Tools > Options** in FePEST (Figure 15.34).

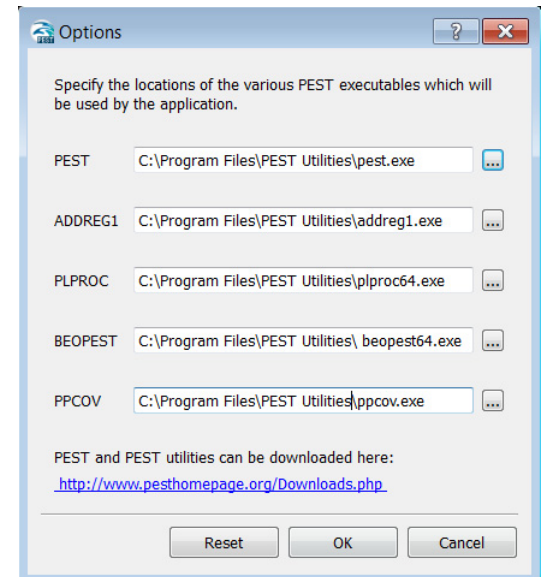


Figure 15.34 Location of main PEST files and PEST utilities.

15.8.5 Definition of a New FePEST Problem

Open FePEST and create a new problem from the menu **File > New**. A dialog prompts for the location of the FEFLOW fem file that will be used for FePEST optimization (Figure 15.35). Specify the previously saved file

\tutorial\femdata\fepest_fri_1.fem

Click on **OK** to create a new FePEST problem.

FePEST now automatically retrieves all important information from the FEFLOW model such as problem class (flow, mass, heat and/or age), material properties, observation points with their corresponding time series (if applicable), stored element selections, etc.

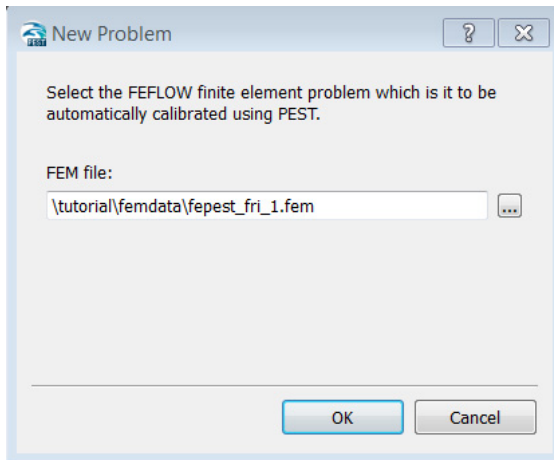


Figure 15.35 Definition of new FePEST problem.

15.8.6 Optimization Settings

Next, the FePEST *Problem Settings* dialog will prompt for the information needed to define the PEST problem and to create the main PEST files:

- Optimization Control
- Parameters
- Observations
- Prior Knowledge
- Subspace Regularization
- Predictive Analysis
- Parallelization

Experienced PEST users will recognize the traditional code names of the PEST parameters shown in bold letters.

While for most groundwater models, the default values suggested by the PEST manual and indicated in the Problem Settings dialog should be appropriate, some modifications may be needed for highly-parameterized FEFLOW models.

In the *Optimization Control* section, the PEST operation mode is indicated. For the case of this exercise, PEST runs in Estimation operation mode. This is the default mode in FePEST

Click on **Bu** *APPLY* to confirm changes.

In *Optimization Control > Termination Criteria* (Figure 15.36), the different criteria to terminate PEST execution are listed. A maximum number of PEST iterations (*NOPTMAX*) of 30 is recommended. It is worthy to notice that a single PEST iteration includes several FEFLOW model runs. The total number of FEFLOW runs depends on the number of parameter to be calibrated and the selected kind of PEST statistics. The most-demanding PEST operation is the computation of the *Jacobian Matrix*.

Other termination criteria are the relative reduction of the objective function (*PHIREDSTP*), the maximum number of consecutive iterations which failed to lower the objective function (*NPHINORED*), the maximum relative parameter change (*RELPARSTP*), and the maximum number of consecutive iterations with minimal parameter change (*NRELPAR*).

The value of *NOPTMAX* in FePEST also defines the type of action to undertake in the current PEST run. In a classical PEST configuration (no FePEST interface), a value of *NOPTMAX* equal to 0 means that PEST runs only once to compute the measurement

objective function. A value of -1 computes the Jacobian matrix and statistics, and a value of -2 the Jacobian matrix only. In FePEST these options are controlled via the combo box below *NOPTMAX* in the **Termination Criteria** section.

The type of optimization statistics (covariance matrix, correlation matrix and eigenvalues) for the final PEST run needs to be indicated in the **Optimization Control > Optimization Statistics** section.

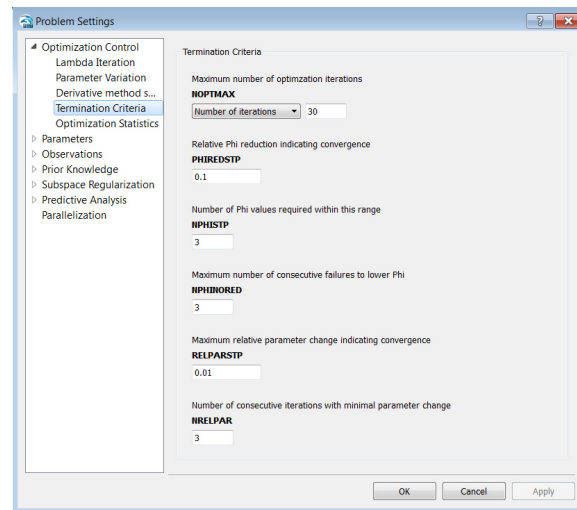


Figure 15.36 Problem Settings dialog: Termination Criteria.

15.8.7 Parameter Definition

Parameters in a FePEST optimization problem can be defined either as homogeneous zones, or as spatially variable using pilot points. In both cases, material properties (so-called *Parameter definitions*) are specified for *Zones* (or for the entire model domain). Typi-

cally, zones reflect different geological units with respective FEFLOW material properties.

Zones correspond to stored element sections in a FEFLOW *.fem file. After opening the file with FePEST, all existing element selections will be listed in the *Zones* section of the *Parameter definition* dialog.

In the *Parameters* section of the *Problem Settings* dialog, click on **Bu** *New* to create a new parameter definition. The *Parameter definition* dialog (Figure 15.37) shows that the FEFLOW file contains an element selection named *Slice_1*.

In the *Parameter definition* dialog (Figure 15.37), select *Slice_1* as *Zone*, choose *K_xx* as *Parameter type* and *Interpolate from pilot points* as the *assignment method*.

The assignment method via *#IFM implemented#* is for advanced users with experience in FEFLOW interface programming. A FEFLOW plug-in module (previously attached and registered in FEFLOW 6.2) can be made responsible for transferring parameter values to FePEST. This is a powerful option to calibrate FEFLOW parameters not available via the FePEST graphical interface, e.g., boundary conditions.

After defining *Interpolate from pilot points* as the assignment method, the *Parameter definition* dialog slightly changes (Figure 15.38).

Now the locations of pilot points need to be specified using as reference a specific geographical position (X, Y, Z), slice number, or layer number.

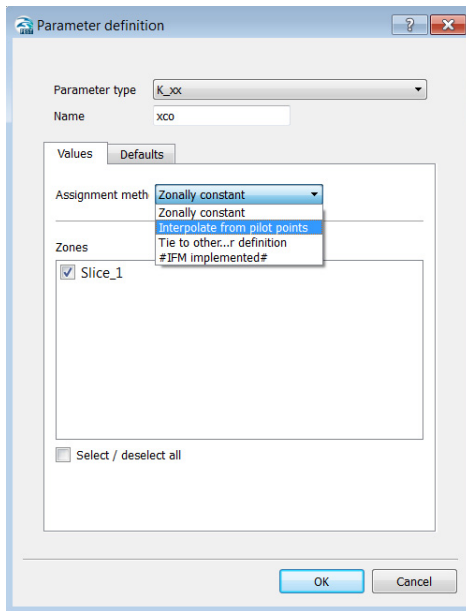


Figure 15.37 Parameter definition dialog.

FePEST provides a very convenient automatic generator of pilot points. Click on **Bu** *Generate* to open the *Pilot point generation* dialog (Figure 15.39) which will prompt for the number of points desired. For this exercise, enter a value of 1^{23} **60**. Pilot points can be distributed in one of three automatic patterns: *uniform*, *stagger rows* and *stagger columns*.

Choose the option *uniform* and close the dialog by clicking **Bu** *OK*.

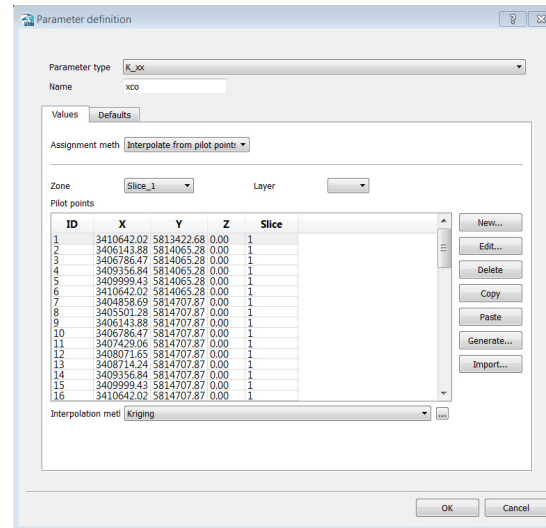


Figure 15.38 Parameter definition dialog in pilot point mode.

Notice that the actual number of pilot points will depend on the geometry of the FEFLOW model domain and pattern specified. Indeed, the final number of pilot points in our case is 61. If the automatic generation was not satisfactory, pilot points can be edited and/or deleted in the *Parameter definition* dialog.

PEST will calibrate parameter values at each individual pilot point. Subsequently, PEST interpolates (and/or extrapolates) parameter values over the entire *Zone* specified as pilot-point domain. *Kriging* or *Radial basis functions* are available as interpolation methods.

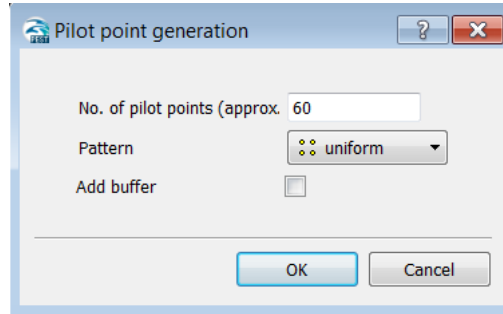


Figure 15.39 Pilot point generation dialog.

For this exercise, the *Kriging* interpolation method is used.

Click on *Interpolation method properties* to assign properties of the experimental variogram. In the Kriging configuration dialog (Figure 15.40), four well-known variogram types are available (*Spherical*, *Exponential*, *Gaussian* and *Power*). In Geostatistics, these are called theoretical variograms (or semivariograms) and they represent the spatial structure of a measured property, in particular, how field measurements are correlated depending on sampling distance. Notice that all the variogram properties (*range*, *sill*, *nugget*, etc.) have to be set up in FePEST and the uncertainty of these parameters will be also reflected in the parameter estimation.

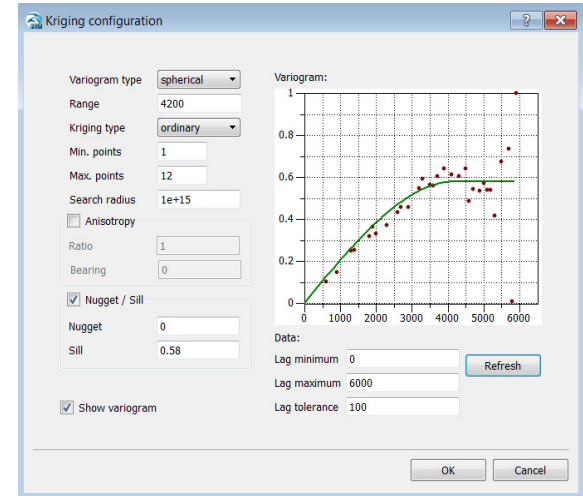


Figure 15.40 Kriging configuration dialog.

After a click on *Show variogram* and on *Refresh*, FePEST computes the experimental variogram (dots) and theoretical variogram (continuous line) in the chart (Figure 15.40). FePEST can also compute variograms for different *lag tolerances*. This feature gives a faster overview about the goodness-of-fit between experimental and theoretical variograms. Chart information can be exported by choosing the *Properties* option from the context menu.

For this exercise, use the values presented in Figure 15.40. Click on *OK* to confirm changes in the *Kriging configuration* dialog.

Next, click on the *Defaults* tab in the *Parameter definition* dialog. Depending on the material property, a parameter log-transformation may improve the PEST optimization result. Parameters such as conductivity and transmissivity are typically log-transformed

because they can change several orders of magnitude within a given model domain.

FePEST offers four possibilities to define a PEST parameter (*none*, *log*, *fixed* and *tied*):

- **None:** Parameter calibration is carried out without any transformation of the parameter.
- **Log:** A log-transformation is applied to the parameter before PEST is executed. PEST statistics are presented based on transformed parameters.
- **Fixed:** The parameter is listed within the PEST control file, but is not modified during PEST optimization. Fixed parameters do not influence the objective function.
- **Tied:** The parameter is tied to a so-called “parent” parameter and its value will depend on the current value of the parent. Tied parameters will be updated during the PEST run with the same ratio as given by the initial parameter values.

In this exercise, *Initial value* is set as *current*, i.e., FePEST will retrieve automatically all parameter K_{xx} values from the FEFLOW *.fem file.

In a first PEST run, it is always recommended to provide wide bounds for the parameter to be estimated so that the PEST optimization would not be influenced. Here, modify *Upper Bound* to a value of 10^{23} 500 m/d. In further PEST runs, parameter bounds can be adjusted based on parameter tendency observed from previous runs.

Click on **OK** to close the dialog.

Since our FEFLOW model contains information in three dimensions, values of conductivity in K_{yy} and K_{zz} are also available in the fem file. However, these two material properties in FEFLOW are related to values of K_{xx} , i.e. $K_{yy} = K_{xx}$ and $K_{zz} = K_{xx} / 10$. Therefore, PEST and FePEST should also update the

spatial distributions of K_{yy} and K_{zz} according to the modifications of K_{xx} . This is accomplished by defining K_{yy} and K_{zz} as *tied* parameters, with parent parameter K_{xx} .

Click on **New** to create a new parameter definition. Indicate conductivity K_{yy} as parameter type. In the *Assignment method*, choose **Tied to other parameter definition**. Indicate *xco* (Conductivity K_{xx}) in the field *Tied to*. In the *Defaults* tab, modify *Upper Bound* to a value of 10^{23} 500 m/d. Click on **OK** to confirm changes. FePEST automatically creates 61 pilot points to compute the distribution of K_{yy} based on the distribution of the parent-parameter pilot points.

Repeat the steps for K_{zz} .

Click on **Apply** to assign all changes made in the *Parameter* section.

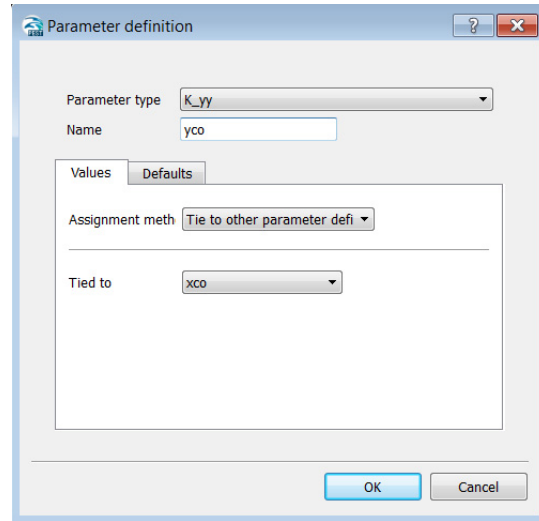


Figure 15.41PEST parameters for parameter definition (tied parameters).

15.8.8 Observations Definition

In the **Observations** section of the **Problem Settings** dialog, all field measurements (**Hydraulic head**, **Mass concentration**, **Temperature**, **Groundwater age**, etc.) to be used in the PEST optimization problem are specified.

Create a new observation definition by clicking on the **New** button. In the **Observation definition** dialog, indicate **Hydraulic head** as **Observation type**. As Source method, select **Reference values in the**

FEM (Figure 15.42). This option will automatically retrieve the information for all **Observation Points** (Figure 15.33) from the FEFLOW file.

In the **Defaults** tab in the **Observation definition** dialog, indicate a **Weight** of 10^{-3} **10** for this observation group. The weight value will reflect how much an observation group affects the measurement objective function. Different **Weights** can be used between observation groups to include different uncertainty of the measurements. As a “rule of thumb”, observation weights can be calculated as the inverse of the measurement standard deviation.

Click on **BU OK** to add this observation group to the FePEST problem (Figure 15.42).

Since also the Observation Points located on Slice 4 were retrieved into FePEST, they need to be deactivated so that they do not influence the objective function. Double-click on the observation line corresponding to **GWM2** and change **Weight** to 10^{-3} **0**. Click on **BU OK** to confirm modifications. Repeat these steps for **GWM5**, **GWM8**, **GMW10**, **GMW11** and **GMW12**.

The second set of observation points is added directly using an external file. This group has a higher uncertainty (standard deviation of 0.35 m).

- Click on **BU New** to create a second observation definition. Define **Hydraulic head** as **Observation type**.
- Select **External file** as **Source** for importing observation points.
- In the file dialog, select the **FEFLOW triplet file** named **new_observations.trp**.
- In the **Defaults** tab, insert a **Weight** of 10^{-3} **2.86** (1/0.35) as shown in Figure 15.42.

- Click on **Bu** **OK** to complete definition of this second observation group.

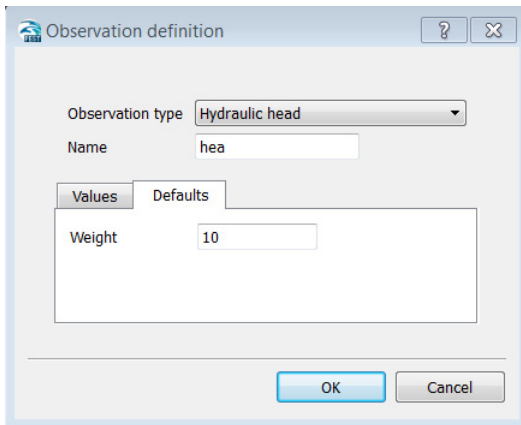
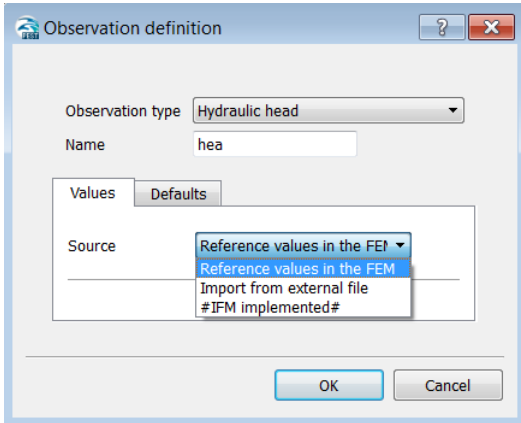


Figure 15.42 Observation definition dialog.

A FEFLOW triplet file can be easily prepared in a spreadsheet or text editor. This file type has a very simple structure and can accommodate geographical coor-

dinates and observation values, as shown in Figure 15.43. Further details can be found in the FEFLOW Help System.

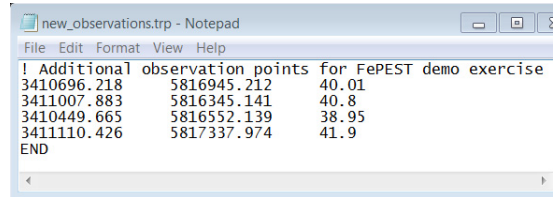


Figure 15.43 Structure of a FEFLOW triplet file used to import observations.

Information for all the observations considered in the FePEST optimization problem is given in the lower part of the **Observation** section in the **Problem Settings** dialog (Figure 15.44), including observation type, name, coordinates, value, weights, etc. Any time series associated with FEFLOW **Observation Points** would also be listed here.

Observation items can be edited directly within FePEST. Additionally, FePEST provides the possibility to edit all or some of the observations in an external spreadsheet. Clicking **Bu** **Copy** will generate a copy of the entire observation list (this also applies for the parameter list).

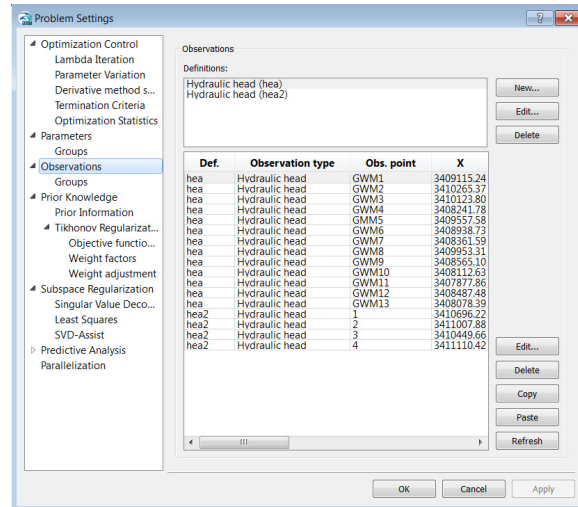


Figure 15.44 Final list of observations used for PEST optimization.

15.8.9 Parallelization Mode

FePEST allows a PEST run in parallel mode. FePEST uses BeoPEST (third-part software) as tool for the communication between slaves and master.

In the *Parallelization* section of the *Problem Settings* dialog, click on **bu** *New* to create a *Slave definition*. In the *Slave definition* dialog, the server to be used is specified under *Host name*. In this exercise, *localhost* is used for sake of simplicity. This means that multiple FEFLOW executions will simultaneously run on different cores of the same computer. As *No. of slaves*, insert a value of 10^{23} **3**. Make sure *Active* is selected (Figure 15.45).

Click **bu** *OK* to close the *Slave definition* dialog. Click **bu** *Apply* to confirm the changes in the *Parallelization* section.

Similarly, slave definitions can be created if multiple slave servers are available. Status (*Active* or *Inactive*) of a slave definition can be modified any time before the PEST problem is initiated.

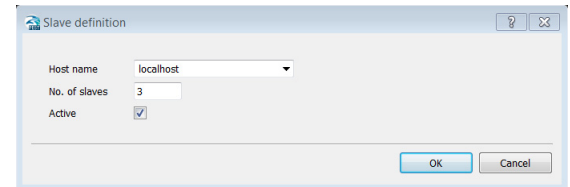


Figure 15.45 Definition of slaves for a PEST run in parallel mode.

For reference, all the FePEST runs in this exercise were computed using a Intel(R) Core™ i7 – 3840 QM CPU with 2.80 GHz and 16.0 GB RAM. Depending on hardware, FePEST running times may vary.

15.8.10 Estimation Method and Regularization Setup

PEST provides two approaches for the PEST estimation mode (parameter calibration):

- No regularization methods
- Regularization methods
 - Tikhonov Regularization
 - Singular Value Decomposition (SVD)
 - SVD-Assist
 - Least Squares Regularization (LSQR)

By default, FePEST uses *Singular Value Decomposition*. This is a very powerful option for FEFLOW models, as discussed in the theoretical part of this chapter. For this exercise, scenarios are implemented with and without regularization. The options *Least Squares* and *SVD-Assist* are not covered in this chapter. All the PEST runs considered are listed in Table 15.1.

Table 15.1 Summary of FePEST projects with different PEST setups: no regularization, Tikhonov regularization and Singular Value Decomposition (SVD), and with/without inclusion of observation error.

Case	Setup
A	No Regularization + Observation Error
B1	Tikhonov (Setup 1) + Observation Error
B2	Tikhonov (Setup 2) + Observation Error
C	SVD + Observation Error
D	Tikhonov + SVD + Observation Error
E	Tikhonov + SVD

15.8.10.1 No Regularization Setup

For a PEST run without use of regularization techniques, the default option of Singular Value Decomposition needs to be deactivated. In the *Problem Settings* dialog, *Subspace Regularization* > *Singular Value Decomposition*, uncheck the option for *Singular Value Decomposition* (Figure 15.46). Click **Bu** *Apply* and **Bu** *OK* to confirm changes.

Save the FePEST project under the name **fest_fri_A.fps**.

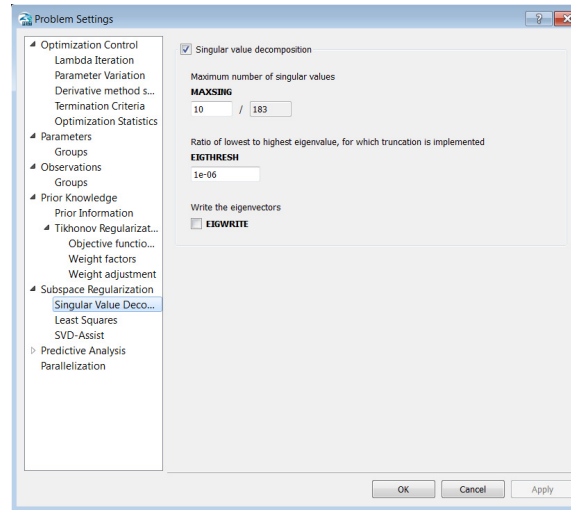


Figure 15.46 Subspace regularization: Singular Value Decomposition.

15.8.10.2 Tikhonov Regularization Setup

In FePEST open the project named **fest_fri_A.fps** from the menu *File* > *Open*. Save the file as **fest_fri_B1.fps**.

Click **Bu** *Control* to open the *Problem Settings* dialog. For a PEST run with Tikhonov regularization only, go to section *Prior Knowledge* > *Tikhonov Regularization*, activate *Tikhonov regularization* and include *Add simple regularization prior information equations based on initial parameter value*

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(Figure 15.47). In the *Objective function* settings of *Tikhonov Regularization*, specify values of 10^{17} , **17.85** and **0.1** for the PEST parameters *PHIMLIM*, *PHIMACCEPT*, and *FRACPHIM*, respectively.

Click on **Apply** and **OK** to confirm changes.

Save changes under same FePEST project name **fest_fri_B1.fps**.

Now the same Tikhonov regularization is applied for case B2; however *Objective function* parameters are changed for a different handling between measurement objective function and regularization objective function, as discussed previously in section 15.2.4.

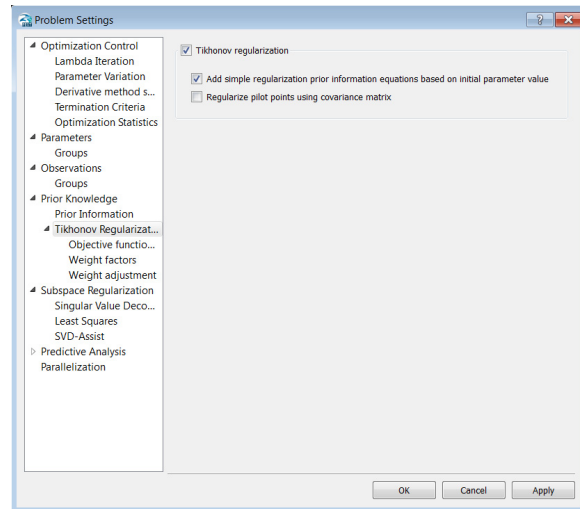


Figure 15.47 Activating Tikhonov regularization mode.

The FePEST project named **fest_fri_B1.fps** is saved as **fest_fri_B2.fps** to create a second project file without overwriting first one.

Click on **Control** to open *Problem Settings* dialog, go to section *Prior Knowledge > Tikhonov Regularization > Objective function* and define the following values:

PHIMLIM 10^{17} **1e-10**

PHIMACCEPT 10^{17} **1.05e-10**

FRACPHIM 10^{17} **0.1**

Click **Apply** and **OK** to confirm changes.

Save changes under FePEST project name **fest_fri_B2.fps**.

15.8.10.3 Singular Value Decomposition Set-up

Open the FePEST project named **fest_fri_A.fps**.

Save this file as **fest_fri_C.fps**. So far, the file contains no regularization techniques. Click **Control** to open the *Problem Settings* dialog. For a PEST run with SVD regularization only, go to section *Subspace Regularization > Singular Value Decomposition* and activate with *Singular value decomposition*. Leave the default parameter values.

Click on **Apply** and **OK** to confirm changes.

Save the changes to **fest_fri_C.fps**.

15.8.10.4 Singular Value Decomposition and Tikhonov Regularization

Open the FePEST project named **fest_fri_C.fps** and save as **fest_fri_D.fps**.

Click **Control** to open the *Problem Settings*

dialog, go to section *Prior Knowledge > Tikhonov Regularization*, activate *Tikhonov regularization* and *Add simple regularization prior information equations based on initial parameter value*.

Click on *Apply* and *OK* to confirm changes.

Save the changes to **fest_fri_D.fps**.

Now a final FePEST project is created with reduced noise in the second observation group. Click *Control* to open the *Problem Settings* dialog. In the *Observations* section, modify the *Value* entry for the last four observations (those belonging to group *head2*): Enter **40.1**, **40.8**, **38.95** and **41.9** for observation points 1, 2, 3 and 4, respectively. Modify the *Weight* to a value of **10**. Now all observations will equally affect the measurement objective function. Click *Apply* and *OK* to confirm changes.

Save the changes to a new FePEST project **fest_fri_E.fps**.

15.8.11 Running PEST

In the previous section, a number of FePEST projects were prepared for different regularization techniques:

- **fest_fri_A.fps**
- **fest_fri_B1.fps**
- **fest_fri_B2.fps**
- **fest_fri_C.fps**
- **fest_fri_D.fps**
- **fest_fri_E.fps**

Next, it is described how these files can be run.

First, open the file named **fest_fri_A.fps**. In the active view FePEST shows pilot points, observation

points and parameter zones (Figure 15.48), as indicated in the *Problem Settings* dialog.

Navigation through different slices and layers of the FEFLOW domain is possible via *Map Contents* panel (if not visible, this is found in menu *View > Map Contents*).

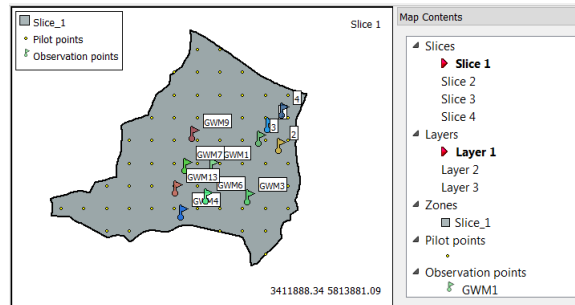


Figure 15.48 FEFLOW model with assigned pilot points, observation points and for FePEST project.

Before initiating a PEST run, all configuration files need to be created. Click on *Checks* to generate the three PEST main files (Control file, Template file and Instruction file) and batch files for FEFLOW and PEST runs. At the same time, the PEST check tools **PEST-CHEK**, **TEMPCHEK**, and **INSCHEK** are executed. A dialog in FePEST will show any errors and/or warnings found.

If errors are found, modifications can be made via the *Problem Settings* dialog. As general recommendation, the *Checks* tools should be always run after any modification to the FePEST project.

PEST is initiated with a click on *Run*. FePEST still provides the possibility to re-create PEST files if modification have been made in the *Problem Settings*

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dialog. If a FePEST project involves the use of pilot points, this option should be marked, as pilot-point files *PLPROC* are not automatically created by *Checks* tool.

In the *Run* dialog, activate *Create the files required by PEST* and click *OK* to initiate the PEST optimization.

Output panels appear after PEST initialization. In the case of running PEST in parallel mode, additional *Output* panels will appear on the master display for each slave. The information presented in the *Output* panels is identical to that appearing on the console in a classic command-line PEST execution.

In a similar manner the rest of FePEST projects can be executed.

15.8.12 Postprocessing PEST Results

Immediately after the first FEFLOW model execution, FePEST provides graphical feedback of the optimization problem and the status of the objective function (Figure 15.49). In the *Simulated vs. Observed* panel, the current misfit between FEFLOW results and observation is shown.

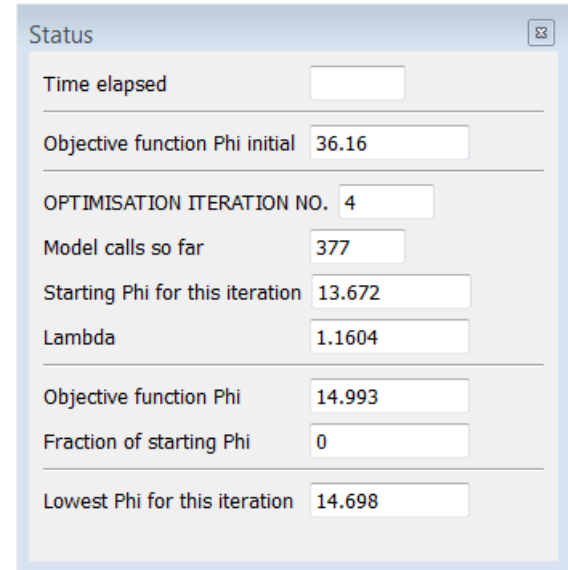


Figure 15.49 Status panel in FePEST with current PEST iteration information.

Open the file **fest_fri_A.fps**, which considers a parameter estimation without regularization and run it. After the PEST optimization process has finished, results are available via the *Estimation > Show results* menu.

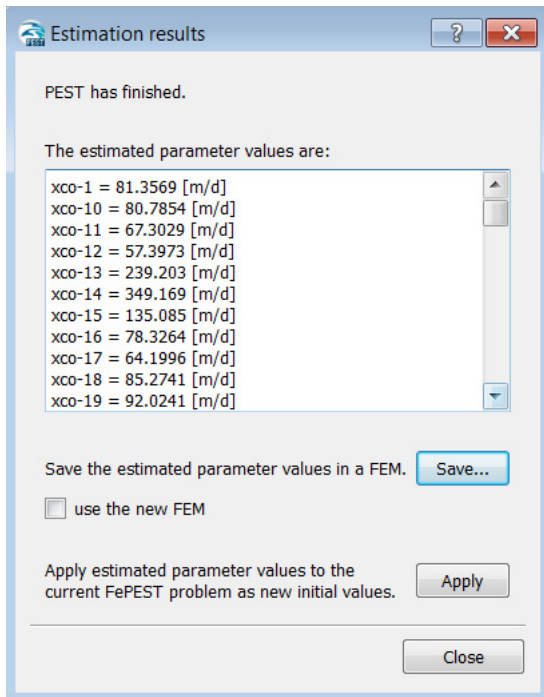


Figure 15.50 Estimation results and different export options.

In the *Estimation results* dialog, the final estimated value of K_{xx} for each pilot point is shown. From here, several options are available:

- Click **Save** to save results in a FEFLOW *.fem file with final parameter estimates (automatic assignment of material properties in FEFLOW).
- Click **Save** and **Use the new FEM** to connect a new FEFLOW *.fem file (with new

material properties) to the current FePEST project.

- Click **Apply** to create a new FePEST project based on the final parameter estimates.

Use the first option to review PEST results directly in FEFLOW. Save the new file as **fepest_fri_1a.fem** and open it in FEFLOW 6.2. Make sure that *Slice 1* is selected in the **Spatial Units** panel. Double-click on K_{xx} under *Material Properties* > *Fluid Flow* > *Conductivity* in the **Data** panel to plot this parameter in the *Slice* view.

In the **Map** panel, right-click on *ASCII Table Files* and choose *Add Map(s) to folder ASCII Table Files*. Select **new_observation_wells.dat** to include a file with new observation points (second group in FePEST).

Right-click on this new entry and choose option *Convert to* > *Observation Points*. Click **OK** to accept the defaults settings.

Double-click *Observation Points* in the **Spatial Units** panel to plot them in the active view.

The distribution of K_{xx} estimated by PEST is shown in Figure 15.51. Observation points *NEW1-NEW4* strongly influence the conductivity values.

15. FePEST

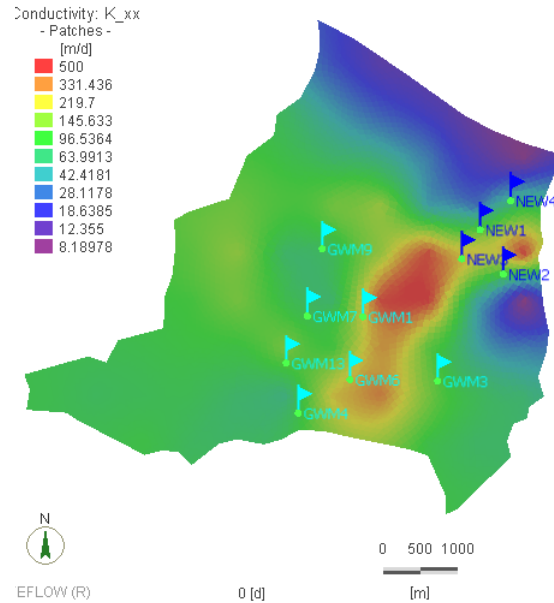


Figure 15.51 Distribution of conductivity K_{xx} estimated by PEST without regularization techniques.

Areas of high conductivity (shown in red in Figure 15.51) are mainly overestimated. Here, K_{xx} coincides with **Upper Bound** defined in the **Parameter definition** dialog in FePEST. The sole criterion in PEST was to match measured observations only.

The initial distribution of conductivity K_{xx} has been previously stored as a **User Data > cond_original** in the **Data** panel. Double-click on **cond_original** to plot its distribution in the **Slice** view. By default, **User Data** are plotted using a linear color mapping. Double-click on **cond_original** in the **View Components** panel to open the **Properties** panel. Here, change to the **Logarithmic** option and click **Bu Apply**

to confirm. The distribution of the original (initial) conductivity K_{xx} is shown in Figure 15.52.

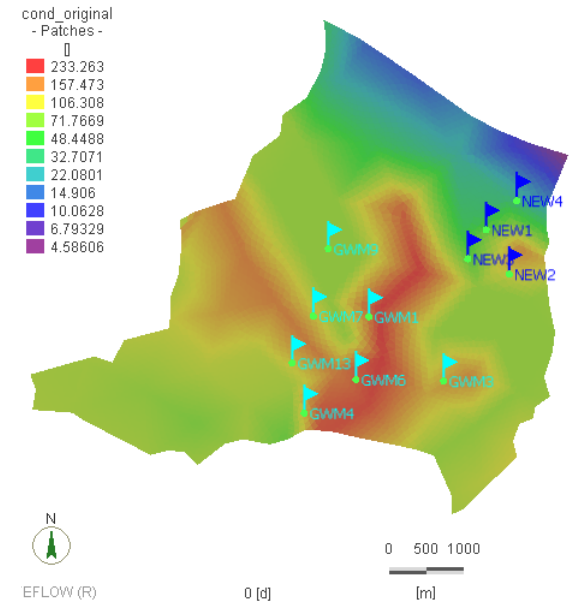


Figure 15.52 Distribution of initial conductivity K_{xx} interpolated by a Akima regionalization technique.

The initial distribution of conductivity K_{xx} looks somewhat “bumpy” due to the Akima regionalization applied.

To compute the “parameter error”, the initial distribution **cond_original** is used as reference. In the **Data** panel, right-click on **User Data** to open the context menu and select **Add Elemental Expression**. Rename this elemental expression to **error**. Right-click on **error** to open its context menu and select **Edit Parameter Expression**. In the **Expression Editor**, write the same expression as shown in

Figure 15.53.

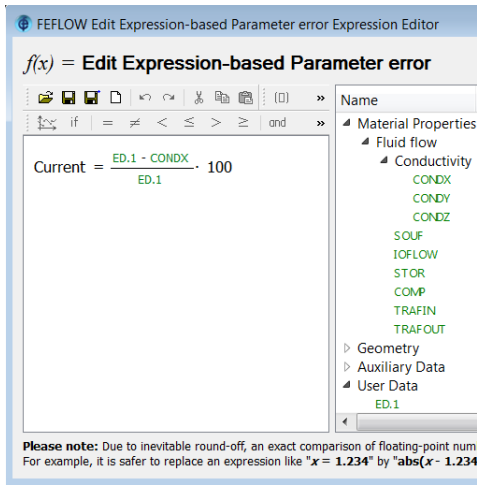


Figure 15.53 Use of Expression Editor in FEFLOW 6.2 to compute the parameter error.

Click to confirm the changes, leave the dialog and plot the element expression in the active view (Figure 15.54).

The distribution of the error given in Figure 15.54. shows that the approach without regularization techniques did not find convincing parameter estimates, and that the values computed by PEST differ significantly from initial distribution and K_{xx} measurements.

In similar manner, the distribution of estimated K_{xx} and of the error can be analyzed for all other FePEST projects.

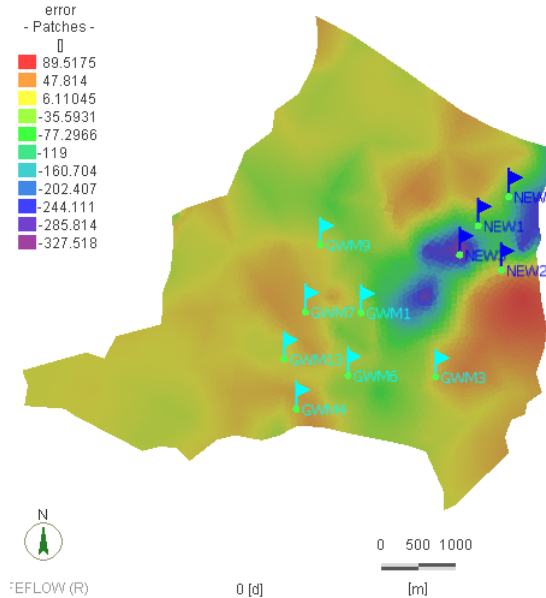


Figure 15.54 Distribution of error parameter for case without regularization techniques.

Open the FePEST project named **fpest_fri_D.fps**, which applies a combination of *Tikhonov* and *Singular Value Decomposition* regularizations. Repeat the previous steps to compute the parameter error as *User Data*.

The distribution of conductivity K_{xx} for case D with *Tikhonov* and *Singular Value Decomposition* is shown in Figure 15.55. Note that the estimated distribution is significantly smoother due to the regularization techniques. Still, higher noise and uncertainty is found around the four observation wells (*NEW1-NEW4*), accompanied by a significant overestimation

of K_{xx} .

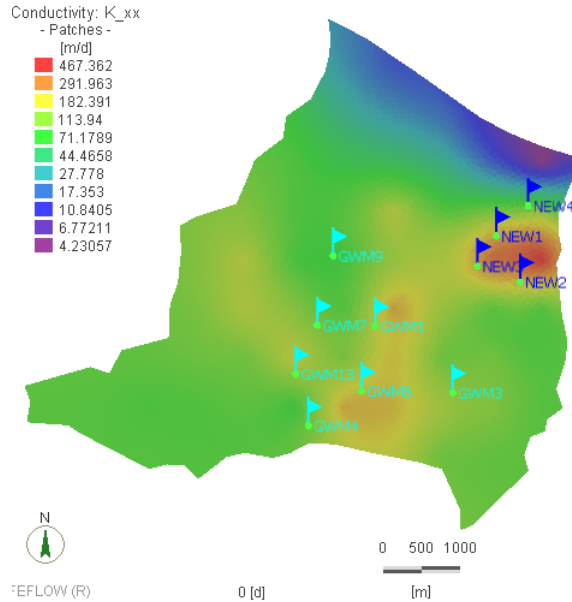




Figure 15.55 Distribution of conductivity K_{xx} estimated by PEST with Tikhonov and Singular Value Decomposition regularization techniques for case D (with observation error).

The option  *Select by Expression* in the  *Selection* toolbar provides a direct means to identify areas with a specific parameter deviation. Use the Expression Editor (Figure 15.56) to display areas with a parameter deviation higher than 30% (Figure 15.57). Again it can be seen that the second group of observation points located at the northeast corner dominates the parameter estimates.

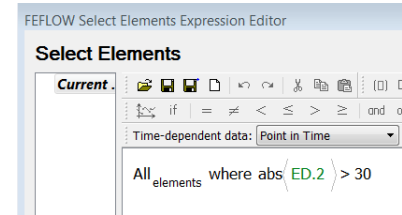


Figure 15.56 Selection of areas with parameter deviation higher than 30%. Notice the absolute operator applied to elemental distribution ED.2 named *error*.

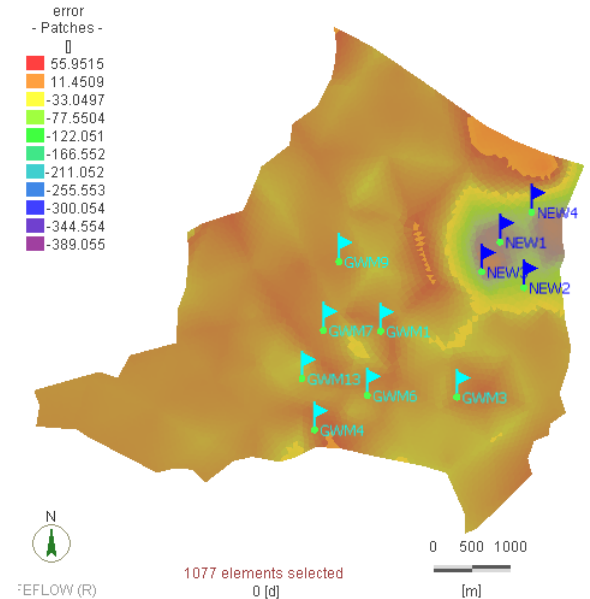


Figure 15.57 Distribution of error parameter for case D with Tikhonov and Singular Value Decomposition regularization techniques (with observation error). Notice area selected with an absolute deviation higher than 30%.

Save the changes in FEFLOW 6.2 to **fpest_fri_1d.fem**.

Open the last project case **fest_fri_E.fps** in FePEST and execute as described in the previous section. Observe the final match between simulated values and observed values in the **Simulated vs. Observed** panel (Figure 15.58). Exact numbers can be visualized faster using the **Tooltip** option (activated via right-click on the chart), and placing the mouse cursor over a data point in the chart.

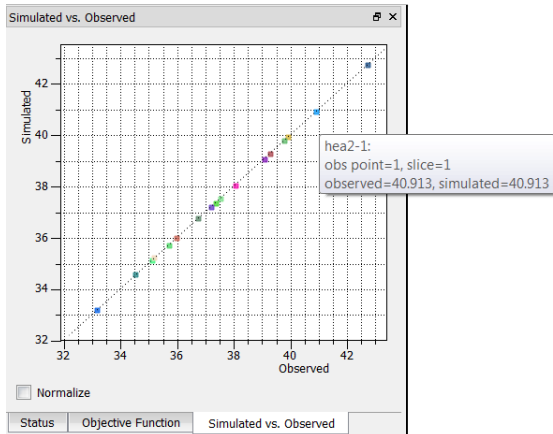


Figure 15.58 Simulated versus observed values in FePEST project fest_fri_E.fps.

The final misfit can be reviewed in the **Residuals** panel (Figure 15.59), which also contains information on the weighted residuals.

Output	Run details	Parameter sensitivities	Observation sensitivities	Residuals	Covariance matrix
Name	Group	Measured	Modelled	Residual	
hea-0	heagp	37.52000	37.51930	7.0000000E-04	
hea-1	heagp	39.10000	39.04660	5.3400000E-02	
hea-2	heagp	39.72000	39.72030	-3.0000000E-04	
hea-3	heagp	39.17000	39.18200	-1.2000000E-02	
hea-4	heagp	34.53000	34.59450	-6.4500000E-02	
hea-5	heagp	35.13000	35.12690	3.1000000E-03	
hea-6	heagp	37.36000	37.36480	-4.8000000E-03	
hea-7	heagp	37.19000	37.20870	-1.8700000E-02	
hea-8	heagp	39.27000	39.26920	8.0000000E-04	
hea-9	heagp	38.06000	38.05700	3.0000000E-03	
hea-10	heagp	36.73000	36.75220	-2.2200000E-02	
hea-11	heagp	35.18000	35.22750	-4.7500000E-02	
hea-12	heagp	35.99000	35.98370	6.3000000E-03	
hea2-1	hea2gp	40.91300	40.91300	0.0000000	
hea2-2	hea2gp	39.92100	39.92150	-5.0000000E-04	
hea2-3	hea2gp	39.79100	39.79040	6.0000000E-04	
hea2-4	hea2gp	42.73000	42.73000	0.0000000	

Figure 15.59 Residuals panels shows the final misfit between FEFLOW simulated values and measured values.

Next, the sensitivity distribution will be computed. Using the **JROW2VEC** PEST utility, FePEST extracts information from the **Jacobian Matrix** to compute the sensitivity distribution. In the **Estimation** menu, open the **Sensitivities** dialog (Figure 15.60) and check **Select / deselect all** to consider all the observations. Click **Bu OK** to initiate the calculation. Select **Interpolate from pilot points** as **Assignment method**.

Click **Bu Export** to save the results to **pilot_point_sensitivities.dat**.

Open the **Estimation results** dialog via menu **Estimation > Show results**. Export the results for FEFLOW as **fpest_fri_1e.fem**.

Open FEFLOW and load **fpest_fri_1e.fem**. Double-click on **K_xx** under **Material Properties > Fluid Flow > Conductivity** in the **Data** panel to plot estimated conductivity (Figure 15.60). This time the distribution of conductivity **K_xx** appears more realistic and estimated values are closer to those measured in the field.

15. FePEST

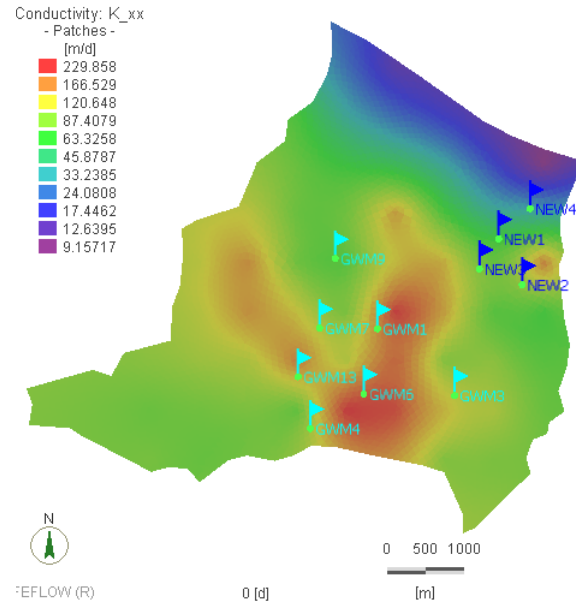


Figure 15.60 Distribution of conductivity K_{xx} estimated by PEST with Tikhonov and Singular Value Decomposition regularization techniques for case E (without observation error).

As before, create a new *Elemental Expression* distribution named *error* in *User Data* and compute the parameter deviation (Figure 15.53). The distribution is displayed in Figure 15.61.

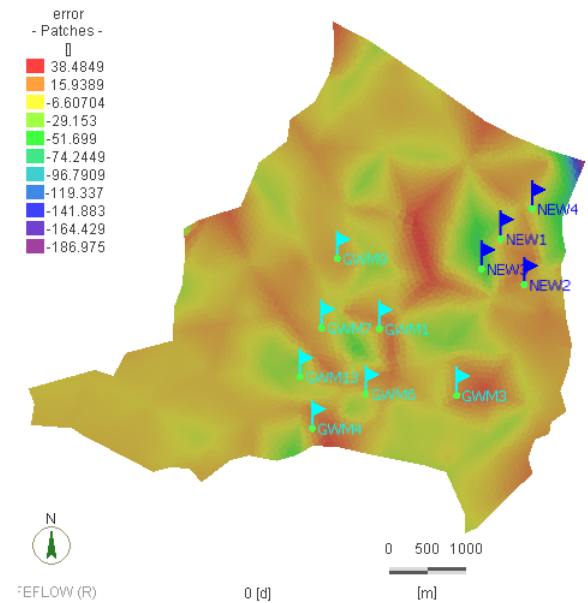













Figure 15.61 Distribution of error parameter for case E with Tikhonov and Singular Value Decomposition regularization techniques (without observation error).

To plot in FEFLOW the sensitivity distribution computed in FePEST, follow these steps:

- Click  **Add Nodal Distribution** under *User Data* in the  **Data** panel and name the new entry “*sensitivity*”.
- In the  **Maps** panel, right-click on **ASCII Table Files** and select  **Add Map(s) to Folder ASCII Table Files**. Choose the file **pilot_point_sensitivities.dat**. Right-click on this

new file and select  **Link to Parameter(s)**. In the **Parameter association** dialog, create a link between **HEA-9** and **User Data > sensitivity**. Leave the default settings (**Regionalization method Inverse distance, Neighbors 4 and Exponent 2**). Click  **OK** to confirm the changes.

- Activate the link with a double-click on **HEA-9** -> **sensitivity**. Select **Slice 1** in the  **Spatial Units** panel and select all  nodes with a click on  **Select All**. Reduce the **Snap distance** to 10^3 **0 m** in the  **Snap-Distance** toolbar and click  **Assign**.

The sensitivity distribution for observation **HEA-9**, corresponding to observation point named **GWM9**, is plotted in Figure 15.62. The distribution of sensitivity from the **Jacobian Matrix** reveals that **K_{xx}** values from pilot points placed on the southern border (around observation points **GWM13**, **GWM6** and **GWM4**) highly influence the values for observation **HEA-9**.

The negative sensitivity values reflect the tendency of a decreasing **Hydraulic Head** in **HEA-9** with increasing **K_{xx}** in these pilot points.

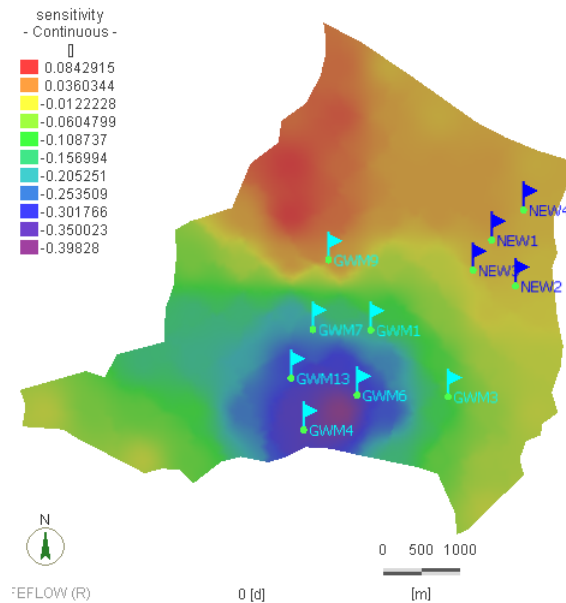


Figure 15.62 Distribution of sensitivity for observation point GWM9.

Save the changes to the FEFLOW file **fepest_fri_1e.fem**.

15. FePEST

Plug-ins and Interface Manager IFM

Extending FEFLOW's functionality by using and programming plug-ins

16.1 Introduction

FEFLOW covers a broad range of functionality for porous-media flow and transport simulation, accessible via a comprehensive user interface.

Nevertheless there are cases in which extended user control over the internal processes in the software is desired and useful. Typical examples include data import from user-defined sources, coupled simulations with other software, extended interdependencies between parameters, specific physical processes, and user-specific output formats.

Many of these cases can be accommodated by the FEFLOW plug-in concept and its open programming interface controlled by the FEFLOW Interface Manager (IFM).

While the use of available plug-ins does not require any programming skills, the IFM also provides support for coding of own plug-ins by advanced modelers with some programming experience.

16.2 Plug-ins for Users

Plug-ins for FEFLOW typically come as a set of three files:

- a *.dll (Windows) or *.so (Linux) file
- a *.html file with a description
- a *.txt file with a copyright statement

For the plug-in functionality, only the first file is important. Plug-ins are automatically registered to FEFLOW when they are located in the modules32 (32-bit version of FEFLOW) or modules64 (64-bit version) folder in the FEFLOW installation directory.

The *Plug-ins* panel is used to manage the plug-ins. Additional plug-ins in other than the above described locations can be registered, and any registered plug-in can be added to the current model. There is no limitation in the number of plug-ins in a model. Their execution order is based on the list order in the *Plug-ins* panel.

Some of the plug-ins have functionality that is invoked by clicking the *Edit* button in the panel or by choosing *Activate* from the context menu of the plug-in. Plug-ins with their own user interface typically bring up the interface when hitting the *Edit* button.

Plug-ins also have the ability to store their own data

16. Plug-ins and Interface Manager IFM

into the *.fem file. Thus data input to the plug-in can be saved with the model file.

When deactivating a plug-in in the panel, it is no longer executed, but its data are kept. In contrast, removing the plug-in from the current model also removes its data from the FEFLOW model.

16.3 Technology

Plug-ins are compiled into Dynamic Link Libraries (DLL) on Windows operating systems, and into Dynamic Shared Objects (DSO) on Linux. With these, it is possible to extend the capabilities of FEFLOW without modifying its source code. The Interface Manager (IFM) uses a technique based on jump-tables that are provided in source code, which supersedes the use of object code or libraries. The jump tables are internally implemented by FEFLOW, so that plug-ins have no external references to FEFLOW's code or data. The plug-ins are thus largely shielded from changes within FEFLOW. In particular, they are not bound to a specific version of FEFLOW, making plug-in management independent from FEFLOW.

The set of API functions provided by the IFM ensures read and write access to nearly all parameters and settings in FEFLOW, along with functionality to influence the course of simulation runs.

16.4 IFM for Programmers

The backbone of the programming interface are the above-mentioned API functions together with callbacks, the possible entry points for plug-in code. Each of the callback functions is called at a specific point of FEFLOW's internal code sequence. For example, the PreTimeStep callback function is called immediately

before a new time step of the simulation is started.



For each callback to be implemented by the plug-in, a separate C/C++ function stub can be automatically generated. While C and C++ are the 'native' languages for coding FEFLOW plug-ins, code in other programming languages can also be included via mixed-language programming.


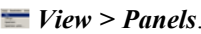

On Windows systems, Microsoft Visual Studio is often used for plug-in development, either as the commercial or as the free Express edition. To be able to develop plug-ins, the IFM Development Kit has to be installed as part of the FEFLOW installation. With this software development kit (SDK), a wizard for Microsoft Visual Studio is installed. This wizard provides a graphically supported, efficient way to generate the frame code for a new FEFLOW plug-in project, including all required project and solution settings. The programmer 'only' has to fill in the user-specific code and compile the plug-in. Even the registration of the plug-in to FEFLOW is done automatically during the compilation process.


16.5 Tutorial

16.5.1 Using Plug-ins



To show the capabilities of plug-ins in FEFLOW, we attach and use the *Check Mesh Properties* plug-in, which is part of the FEFLOW installation. The plug-in calculates the occurring minimum and maximum angle of each finite element of a 2D mesh to check the mesh quality.


Start a new FEFLOW document and create an arbitrary supermesh polygon using the  **Add Polygons** tool. When the polygon is finished, click  **Generate Mesh** to generate a finite-element mesh.

Open the  **Plug-ins** panel via . In the list of available plug-ins, right click on **Check Mesh Properties** and choose  **Attach** from the context menu. The plug-in will now appear in the list of attached plug-ins.

When the **Check Mesh Properties** plug-in is attached, it creates two reference distributions **Mesh-Properties:MaxAngle** and **MeshProperties:MinAngle** in the  **Data** panel and two additional charts are displayed.

Double-click on one of these reference distributions to visualize the angles in the active view.

Whenever the mesh is changed (e.g., when applying  **Smooth Mesh** in the  **Mesh-Geometry** toolbar), the values in the reference distribution are updated.

If a mesh contains a large number of elements, the computation time for the updating process may become unacceptably long. In this case, the plug-in can be temporarily disabled by removing its checkmark in the  **Plug-ins** panel.

16.5.2 Programming Plug-ins

The widely used Microsoft Visual Studio development environment has been found suitable for the development of plug-ins. The basic version, Visual Studio Express, is available free of charge (<http://www.microsoft.com/express/>).

The following example is based on Microsoft Visual Studio 2010 Standard/Professional Edition. The approach differs slightly from other versions of Microsoft Visual Studio and the free Microsoft Visual Studio 2010 Express Edition.

Before starting the plug-in development, the following items have to be installed:

- Microsoft Visual Studio Standard/Professional or Microsoft Visual Studio Express Edition with C++ support
- FEFLOW IFM SDK (the respective package in the FEFLOW setup has to be selected)



Microsoft Visual Studio has to be installed prior to the IFM SDK to allow the installation of the template.

16.5.2.1 Starting the IFM Wizard

To start with a new plug-in, open Visual Studio 2010 and choose **New > Project** from the **File** menu.

In the tree on the left side of the dialog, click on **FEFLOW 6.2 Projects**. Next, click on the **FEFLOW 6.2 IFM Plug-in** template. Remove the **Create directory for solution** check mark at the bottom of the window. After entering the name (HelloWorld) and the target location for the new plug-in, click **OK** to proceed.

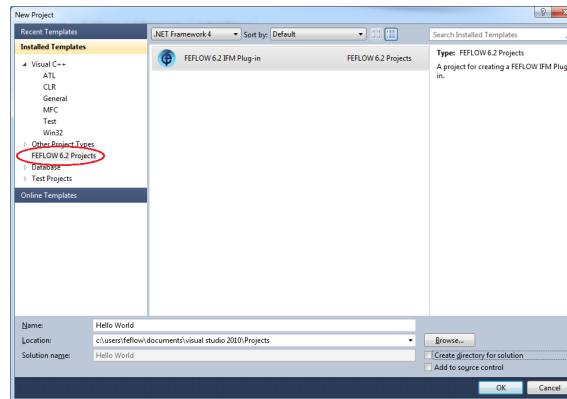


Figure 16.1 Choosing an IFM plug-in template.



Microsoft Visual Studio Express and versions older than Visual Studio 2010 only allow compiling x64 versions of a plug-in if additional Microsoft tools are installed.

16. Plug-ins and Interface Manager IFM

16.5.2.2 Initial Plug-In Settings

On the *Welcome page*, click *Next*.

The following *Plug-in Name* page asks for a plug-in ID (which is its unique identifier), its display name (the name to be shown in FEFLOW) and the plug-in version number.

By default, *Plug-In ID* and *Display Name* are set according to the project name given before. We accept the default. The value of the *Register Proc* field should not be modified.

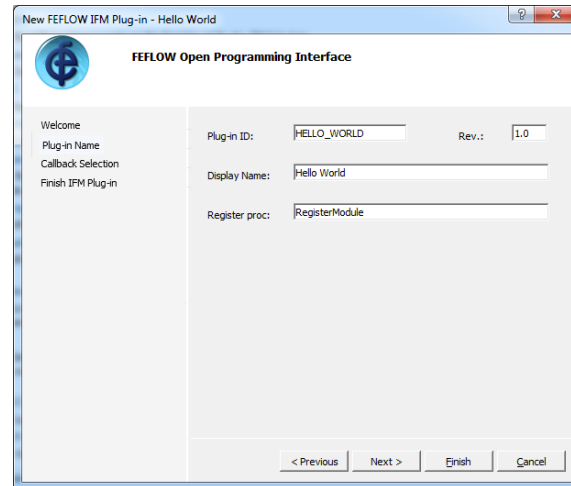


Figure 16.2 Plug-in Name page.

Clicking *Next* leads to the *Callback Selection* page. Place the mouse cursor over a callback to get detailed information in a tooltip window. Activate the callback *OnEditDocument*.

Click on *Finish* to start the generation of the plug-in frame code and of the Visual Studio files.

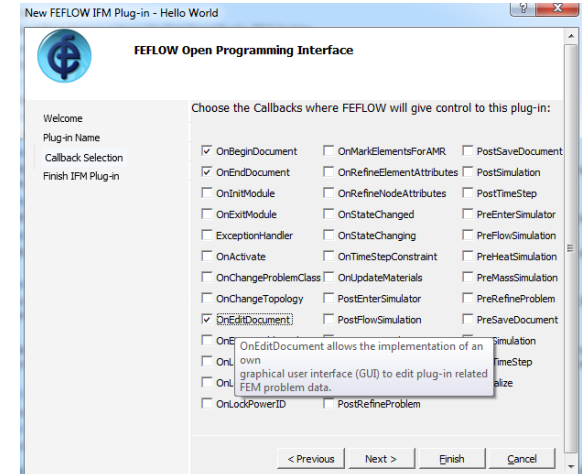


Figure 16.3 Callback Selection page.

16.5.2.3 Implementing the Functionality

With a double-click, open the primary source code file **HelloWorld.cpp** from the tree in the *Solution Explorer* panel.

Scroll down to

```
// Callbacks  
void CHelloWorld::OnEditDocument...
```

and replace the lines

```

/*
 * TODO: Add your own code here...
 */

```

by the command

```
IfmInfo(pDoc, "Hello World!");
```

according to Figure 16.4.

```

// Callbacks
void CHelloWorld::OnEditDocument (IfmDocument pDoc, Widget wParent)
{
    IfmInfo(pDoc, "Hello World!");
}

```

Figure 16.4 Example code.

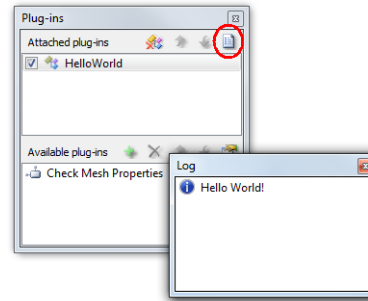


Figure 16.5 Log window message “Hello World!”.

16.5.2.4 Compiling and Debugging

Build the plug-in by pressing <F7> and then start debugging with <F5>. Visual Studio starts FEFLOW as a child process in debugging mode. FEFLOW automatically lists the plug-in in the **Plug-ins** panel.

Load an arbitrary FEFLOW model, attach the plug-in as described in Chapter 16.5.1, and click **Edit plug-in properties** in the **Plug-ins** panel. The message “Hello World” appears in the **Log** panel.

Compiling release and x64 versions

By default, a debug dynamic link library is compiled, which allows debugging (e.g., using breakpoints in the plug-in code), but has reduced performance.

To build a more efficient release version, change the **Configuration** as shown in Figure 16.6. In case that FEFLOW is still open, make sure to close it in order to return to Visual Studio.

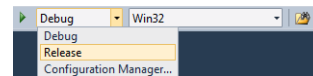


Figure 16.6 Changing the configuration.

In the same way the platform can be changed to x64, providing the means to build plug-ins suitable for the 64-bit version of FEFLOW (Figure 16.7).

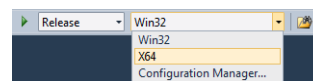


Figure 16.7 Changing the platform.

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