Training Manual FEFLOW 7.1

Groundwater Modeling with FEFLOW 7.1

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Contents

Preface

0.1 Scope and structure of this manual

This training manual serves as a basis for FEFLOW training courses held by DHI instructors.

It is intended to help you to follow the training more easily, to understand the theoretical background of the program and to be able to repeat the examples at home on your own.

It should neither be considered as an alternative FEFLOW Help System nor as a step-by-step tutorial for personal training.

0.1.1 Terms and notations

This manual has been designed to be as self-explanatory as possible. Still, some notations should be clarified in advance.

At one side of each page you find some white space to take notes related to the contents of the page. The instructor will inform you about helpful details not contained in this manual, and you will probably wish to write down parts of these explanations.

In the manual, you will basically find four different types of content:

- A detailed description of the steps necessary to complete the examples.

- A basic overview of the theoretical or conceptual background of the steps applied.

- Pointers to the most frequent mistakes.

- References to the other parts of the FEFLOW documentation.

0.1.2 Description of the examples

In addition to verbal descriptions of the required screen actions we make use of some icons. They are intended to assist in relating the written description to the graphical information provided by FEFLOW. The icons refer to the kind of setting to be done:

	menu command
	toolbar
	panel
	button
	input box for text or numbers
	switch toggle
	radio button
	check box
	context-menu command

At some points in the text you will find file names printed in color. The respective files are located on the USB memory stick that comes together with this training manual. The exact path of these files is given in the introduction to each chapter.

You may use these files as a starting point for your studies later (if you do not want to start your exercise at the beginning of the chapter again). Please note that DHI WASY does not take any responsibility for the correctness and usability of these data.

Other files (e.g., GIS data or background images) are printed in the same color.

0.1.3 Theoretical / conceptual notes

Notes concerning the theoretical background or the basic concepts in FEFLOW can be found in light blue boxes. They offer a short, practically-oriented overview of the theory related to the described steps. For more detailed information please have a look at the corresponding chapters in the FEFLOW documentation.

0.1.4 Pointers to the most frequent mistakes

The most common mistakes are enclosed in light red boxes.

0.1.5 References

References to other parts of the FEFLOW documentation, such as the Help System or articles of the White Papers are provided in combination with a book sign.

The notation of references is as follows:

WP II 1.3.2

White Papers, Vol. II, Chapter 1.3.2

0.2 Exercise data

Your course material includes a training DVD or a USB memory stick, which contains this training manual and the presentation slides as well as the complete FEFLOW documentation (all PDF format).

All data that you need to create the models discussed in this manual can be found in the folder /model. At the beginning of each exercise, the location of the specific files necessary for the section is indicated.

0.3 Where to find additional information

To get further information, please also refer to other parts of the FEFLOW documentation. The following additional documentation material is available:

0.3.1 The FEFLOW documentation

- License Installation Guideline for Windows

- License Installation Guideline for Linux

- Introductory Tutorial

- Help System: The main core of the FEFLOW documentation is provided via the FEFLOW Help System. The help is available locally (requires user installation) and online. The help gives a detailed description of the user interface. It explains the

essential work steps of model set-up, simulation, post-processing, IFM Programming and Python Interface.

In each chapter, the respective topic is introduced and the relevant FEFLOW tools are presented. The underlying concepts and workflows are described, followed by a tutorial section.

- White Papers Vol. I - V:

A collection of articles about specific modeling approaches and methods used in FEFLOW.

The entire documentation can be found in PDF format in the /documentation folder of the FEFLOW DVD or USB.

0.3.2 The FEFLOW Help system

The Help system provides detailed background information at all stages of modeling. It can be opened from the FEFLOW menu ▦ *Help - Help (Online)* or ▦ *Help - Help (Online)* (requires previous installation).

0.4 Trademark legal notice

All product names, logos, and brands are property of their respective owners. All company, product and service names used in this training manual are for identification purposes only. Use of these names, logos, and brands does not imply endorsement.

1 Box - Fluid Flow

All files related to this exercise can be found on the training USB memory stick in the project folder /models/box_model.

1.1 Objective

By setting up a very simple horizontal 2D model, some basic FEFLOW operations are practiced.

First, the geometry of the model is defined and a finite-element mesh is generated. The model properties - initial, boundary conditions and material properties - are applied.

In a last step, boundary conditions and/or material properties are modified, so that a better understanding of their effects on the model results can be acquired.

1.2 Model Scenario

The model domain is a simple rectangle with an area of approx. 1000 m x 1000 m. The main flow direction follows the hydraulic head gradient from the left (western) to the right (eastern) border.

Two production wells exist within the model area. Recharge is applied as a constant value all over the model domain. Figure 1.1 illustrates the scenario.

1.3 Starting a New Model

Choose ▤ *File - New* from the menu to start with a new model. The upcoming dialog asks you how the model extents should be specified. Choose ◉ *Manual input of the initial domain bounds* and click ⬚ Bu *Next*.

The horizontal and vertical extent of the model domain is ⌗ **1000** m. Enter this number as the maximum value for both the *x-Range* and the *y-Range* (the minimum values remain at the default value of 0 m).
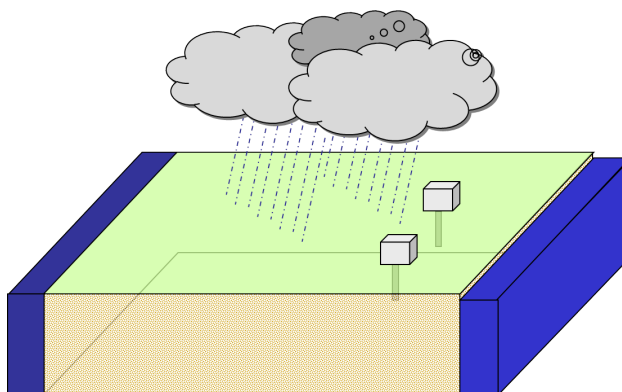

Figure 1.1: Model scenario

With a click on [Bu] *Finish*, a new model is created and a (*Supermesh*) view window is opened.

> Many features of FEFLOW are organized in [▫▫▫] *Toolbars* and [▯] *Panels*. The [▯] *View Components* panel for example contains a list of elements that can be displayed in the currently selected view window.
>
> Panels and toolbars as well as charts can be arranged in the FEFLOW window in an arbitrary manner.
>
> If a panel, toolbar or chart is not visible, it can be activated from the [▭] *View* menu (Figure 1.2).
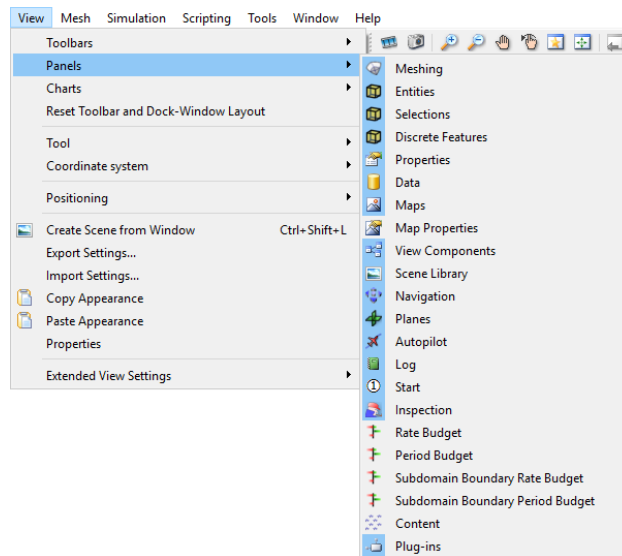

Figure 1.2: Activating a panel

1.4 Supermesh

> The supermesh defines the geometry of the model.
>
> In the simplest case, a supermesh consists of only one polygon that defines the outer boundary. The design of the supermesh also influences the generation of the finite-element mesh. More complex supermeshes contain several polygons and a number of lines and points.

In this simple case, the supermesh consists of one single square polygon with a lateral length of 1000 m as its outer boundary.

Click on [⬡] *Add Polygons* in the [▫▫▫] *Mesh Editor* toolbar.

The polygon is digitized on the display by clicking the left mouse button for each node of the supermesh border. The polygon is closed by either double-clicking the left mouse button or by clicking the first node of the node-string again.

Exact coordinates can be set by pressing the <F2> key on your keyboard instead of clicking the left mouse button. The result should look like the polygon in Figure 1.3.
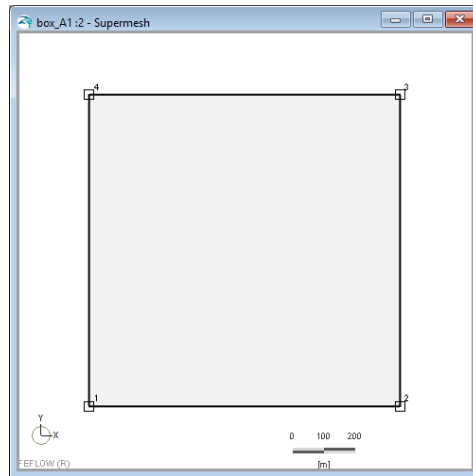
                                                                        [📂] [💾] box.smh

Figure 1.3: Supermesh

1.5 Finite-Element Mesh

FEFLOW provides the different tools to create a finite-element mesh in the 📄 **Meshing** panel.

In the 📄 **Meshing** panel click on **Supermesh** from the panel section **From Supermesh Elements**. This will activate the **Properties** section for all the Supermesh Elements. Enter a number of 🔢 **500** elements in the **Proposed elements** field of the 📄 **Meshing** panel. In the upper section of the panel, select ▾ **Advancing Front** from the drop-down list of generators and click on ⚙ **Generate Mesh** (Figure 1.4).
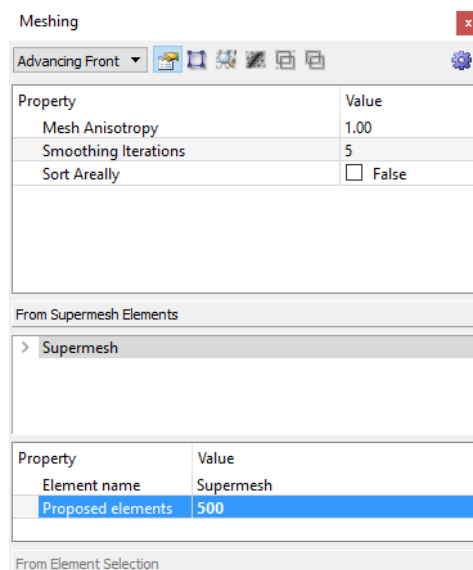

Figure 1.4: Meshing panel.

As a result, you should obtain a mesh similar to the one shown in Figure 1.6.

> 📄 **Meshing** panel:
> This contains all the necessary tools to create the finite-element mesh in 2D or 3D. The finite-element mesh is the basis of the numerical simulation.
> In the case of 2D meshing, FEFLOW can work with quadrilateral as well as with triangular meshes.

Different mesh generators are provided for automatic meshing: ***Transport Mapping*** for quadrilateral; ***Advancing Front***, ***GridBuilder*** and ***Triangle*** for triangles.

Advancing Front produces very regular meshes but neglects line and point features; ***GridBuilder*** overcomes this drawback but may fail under certain circumstances. ***Triangle*** can handle very complex geometries and is extremely fast, but yields elements of slightly lower quality.

The number of finite-elements can be indicated by the ***Proposed elements*** field in the 📃 ***Meshing*** panel, which can be a number either for the entire Supermesh or for a region of the Supermesh.

In the case of 3D meshing, FEFLOW works with the ***TetGen*** mesh generator, which can produce tetrahedral quality meshes. This type of meshes can be either created by meshing directly from a 3D Supermesh or by re-meshing an existing 3D finite-element model.
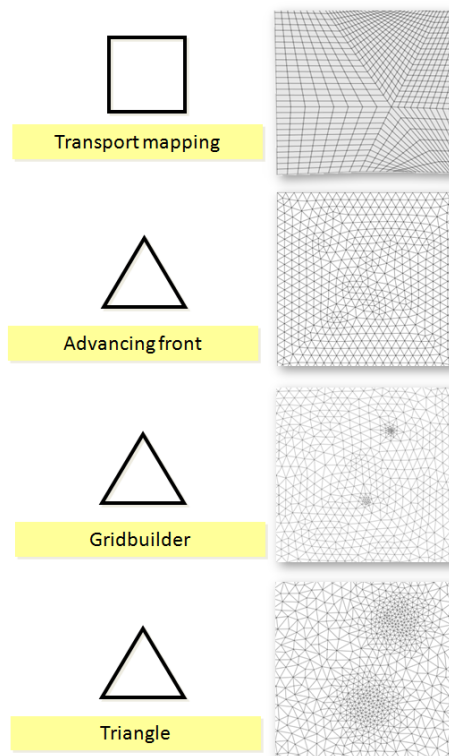

Figure 1.5: Mesh generators in FEFLOW

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1.6 Problem Settings

From the main menu choose 🖿 ***Edit - Problem Settings***.

The ***Problem Settings*** dialog is the control center for all general settings of the model, e.g. the type of the problem (flow only or flow and transport), the temporal domain (steady state or transient) or numerical properties like accuracy settings and the choice of the equation solver.
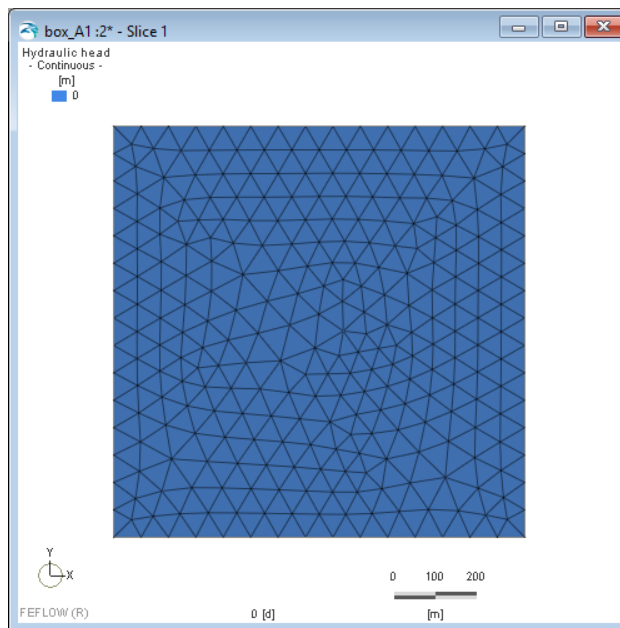
Figure 1.6: The finite-element mesh

The numerous settings of a FEFLOW model are listed in an index on the left side of the dialog.
At the top of the index, you find the **Problem Summary**, which gives information on key properties like the **Problem Class** or the number of nodes and elements. Further down the index, the **Problem Class** category lets you define the type of the model and the respective settings. Other items on the list are the **Equation-System Solver**, **Field-Line Computation** settings and **Editor Settings**.

1.6.1 Problem Class

FEFLOW allows the simulation of flow, groundwater age, mass and heat transport processes in either saturated or variably saturated media. For both flow and transport simulations, a steady-state or a transient solution can be computed.

Saturated/Unsaturated
In saturated mode, unsaturated parts of the model are either excluded or treated in a simplified manner. The Darcy equation is used for the entire model domain. In unsaturated mode, Richards' equation is applied for the unsaturated parts of the model.

Flow/Transport
FEFLOW can simulate the flow regime exclusively, or in combination with a transport simulation. For transport, you can choose between groundwater age, mass (contaminant) transport, heat transport or any combination of the three. We recommend to always set up a flow model first to check its usability. In a subsequent step, it can be extended to a flow and transport model.

Steady state/Transient
In steady state mode, FEFLOW calculates the state of a model with time-constant

> boundary conditions and material properties after an infinitely long time, e.g. to simulate average conditions for an aquifer. In transient mode, the simulation is done for a specified time period. This time period is divided into time steps for which results are computed (temporal discretization).
>
> The steady flow/transient transport mode requires a steady state solution of the flow simulation as initial condition!

Open the **Problem Settings** dialog via the ▬ **Edit** menu. Choose the **Problem Class** item from the index on the left-hand side of the dialog. Switch to ⦿ **Steady** for **Fluid flow**. No further changes are required (see the settings in Figure 1.7).
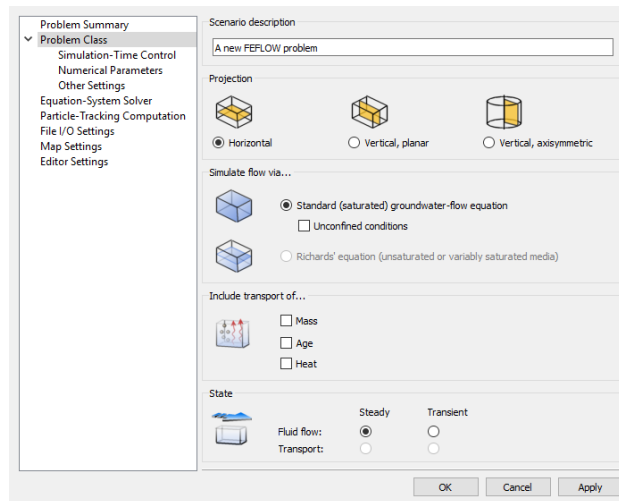Close the window with ⸤Bu⸥ **OK** and confirm the changes with ⸤Bu⸥ **Yes**.

Figure 1.7: Defining the problem class in the Problem Settings dialog

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1.7 Model Properties

The model properties reflect the physical conditions in the model area. This includes initial conditions, boundary conditions and material properties. All model properties can be found in the 📄 **Data** panel (Figure 1.8).

1.7.1 Initial Conditions

In the 📄 **Data** panel, all model properties are organized in seven major categories (**Geometry**, **Process Variables**, **Boundary Conditions**, **Material Properties**, **Auxiliary Data**, **User Data** and **Discrete Features**).
The **Process Variables** include the primary variables (piezometric head for the flow model, mean age, lifetime expectancy, exit probability, concentration and temperature for transport models) and secondary (derived) variables (like Darcy flux, saturation, etc.).
The state of the primary variables at the beginning of the simulation reflects the initial conditions of the model.
With a double-click on **Hydraulic head**, this property is plotted in the currently active view window. The default initial head is 0 m and will be used for this simple steady-state example. No changes are necessary.
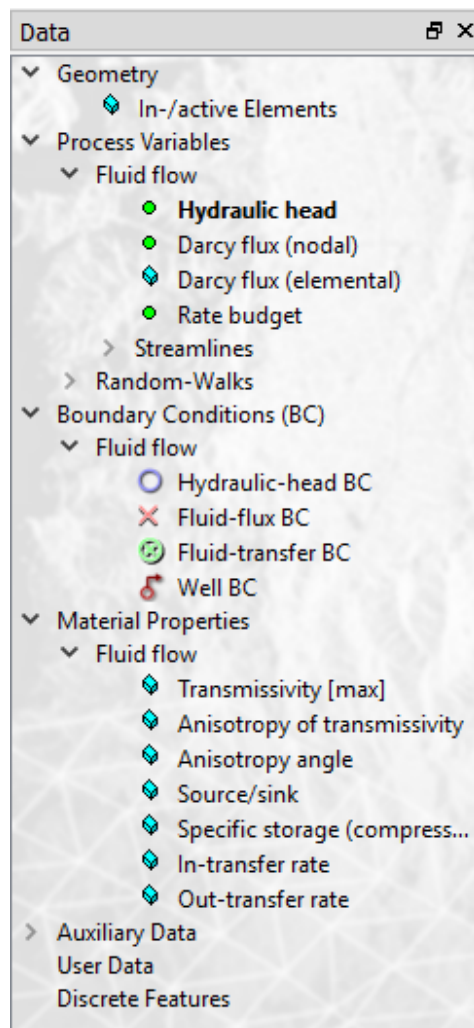
Figure 1.8: Model properties shown in the Data panel

1.7.2 Boundary Conditions

For the purpose of this exercise, a fixed hydraulic head will be assigned to both the left (30 m) and the right borders (29.85 m).

Activate **Hydraulic-head BC** from the ▨ **Data** panel (**Boundary Conditions - Fluid flow**) by double-clicking on it. The model turns grey, indicating that no boundary conditions have been assigned yet.

> By default, all boundaries of a FEFLOW model are impervious.
> To allow an interaction of the model domain with its environment, boundary conditions have to be specified. In FEFLOW, there are five different types of flow boundary conditions: **Hydraulic-head BC**, **Fluid-flux BC**, **Fluid-transfer BC**, **Well BC** and **Multilayer-well BC**.

Boundary and initial conditions of a finite-element model are node-based parameters. Before the boundary conditions can be assigned, a selection of nodes must be created as assignment target. In this example, the left border will be selected first.

Choose the ◢ **Select Nodes Along a Border** tool from the drop-down list in the ▱ **Selection** toolbar.

Move the mouse cursor to the bottom-most node of the left border. Press and hold the left mouse button. Move the mouse cursor to the topmost node of the left border and

release the mouse button again. You should see that the nodes of the left border are se-
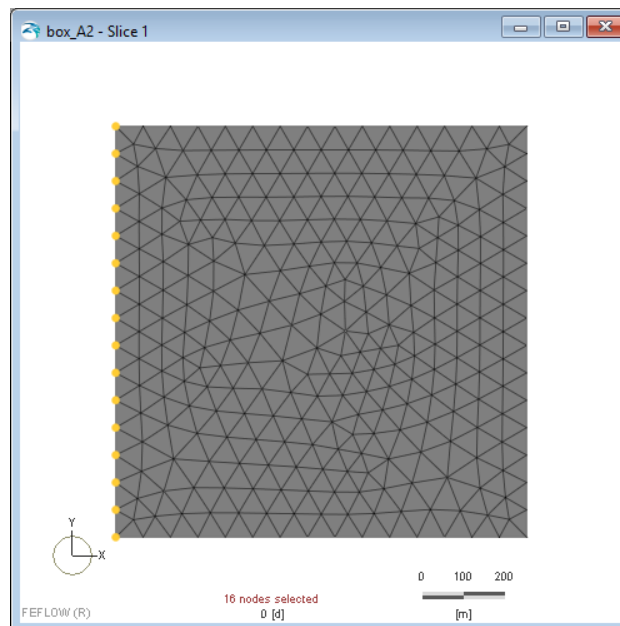lected, indicated by yellow markers as shown in Figure 1.9.

Figure 1.9: Selection of nodes along the left border

In the ▫▫▫ **Editor** toolbar, enter a value of 🔢 **30** m into the input box. Click on ✅ **As-
sign** to assign the BC value. The boundary conditions on the left side should now be
visible and highlighted as blue circles.
To check the value of the boundary conditions that have just been assigned, activate the
🔍 **Inspect Nodal/Elemental Values** tool in the ▫▫▫ **Inspection** toolbar. Move the magni-
fying glass over the node that you want to check, and the value of the boundary condition
is displayed in the 📄 **Inspection** panel (Figure 1.10).
Before repeating the same steps for the right model border it is necessary to clear the
current selection (otherwise the boundary conditions that have already been set at the
active selection would be overwritten). Go to the ▫▫▫ **Selection** toolbar and click on
❎ **Clear Selection**. Now, repeat the steps for the right border. Choose the ◣ **Select
Nodes Along a Border** tool from the ▫▫▫ **Selection** toolbar again and select the nodes
between the bottom-most and the topmost node of the right border.

This time, enter a value of 🔢 **29.85** m in the input box of the ▫▫▫ **Editor** toolbar. Click on
✅ **Assign** to assign the boundary condition. Next, use the 🔍 **Inspect Nodal/Elemental
Values** tool a second time to make sure that the values are correct and clear the selection
again (❎ **Clear Selection**).

The last boundary conditions to be set are the two wells. The production wells are
located within the eastern part of the model, each having a pumping rate of 500 m^3/d. The
steps for assigning well boundary conditions are the same as for the previous boundary
condition: First, select (double-click) **Well BC** in the 📄 **Data** panel. Second, create a
selection that contains two nodes within the right part of the model. An appropriate tool
for creating a selection of single nodes is the ↗ **Select Individual Mesh Items** tool
that can be found in the left drop-down list of the ▫▫▫ **Selection** toolbar. Make sure
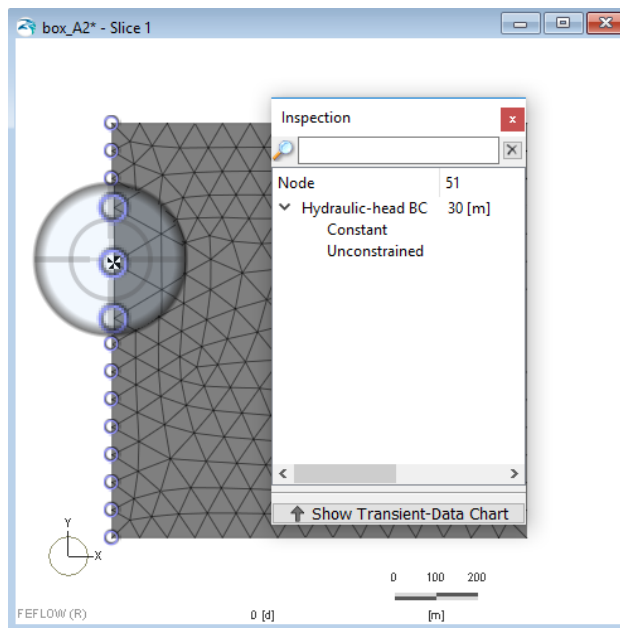
Figure 1.10: Boundary conditions checked with the Inspect Nodal/Elemental Values tool

that the selection mode ⊞ **Add to Selection** is active (second drop-down list in the 🔳 **Selection** toolbar). Choose two arbitrary nodes in the right part of the model, and click on each of them once. Two yellow markers indicate the active selection.

Finally, enter a pumping rate of ₁₂³ **500** m³/d in the 🔳 **Editor** toolbar and click on ✅ **Assign**.

All required boundary conditions have now been assigned to the model. For a final check, clear the selection by clicking ⊠ **Clear Selection** and double-click on **Boundary Conditions - Fluid flow** in the 📋 **Data** panel to display all types of boundary conditions at the same time. The result should look similar to Figure 1.11.

> For Fluid-flux BC and Well BC type boundary conditions positive values define outflow from the model, negative ones define inflow.

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1.7.3 Material Properties

When a new model is created, FEFLOW assigns default values for all material properties. Except for transmissivity and recharge, these default values will be used for this simple example. Double-click on **Material Properties - Fluid flow - Transmissivity [max]** in the 📋 **Data** panel.

In a finite-element model, all material properties are elemental values. Both transmissivity and recharge are considered as homogeneous. Therefore, a selection containing all elements is to be created for the following data-assignment steps.

Click on 🔲 **Select All** in the 🔳 **Selection** toolbar (the keyboard shortcut <CTRL + A> has the same effect). Enter a value of ₁₂³ **170** in the 🔳 **Editor** toolbar and click on ✅ **Assign** (the FEFLOW default unit is [m²/d]).

One way of representing recharge in a FEFLOW model is using the **Source/sink** parameter. Double-click on this entry in the 📋 **Data** panel to plot the current distribution in the active view.
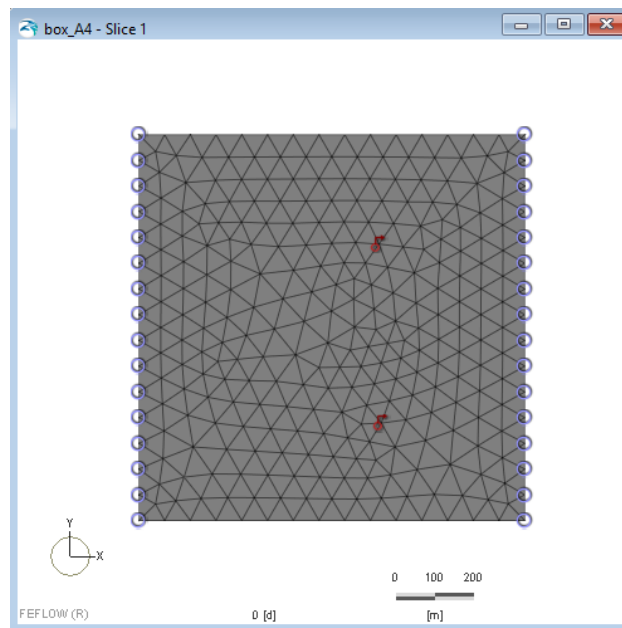
Figure 1.11: All boundary conditions shown in the view window

Type a value of 🔢 **5e-4** m/d into the input box of the 🔲 *Editor* toolbar, click on ✅ *Assign* again and clear the selection with ❎ *Clear Selection* afterwards.

📂 💾 boxA4.fem

1.8 Simulation Run

To see the changes in the model results while the simulation is being performed, plot the hydraulic-head distribution in the active view by double-clicking on *Process Variables - Fluid flow - Hydraulic head* in the 📄 *Data* panel. Now, go to the 🔲 *Simulation* toolbar and click on ▶ *Start*. After a few seconds, a colored distribution of the resulting hydraulic head is shown in the active view (Figure 1.12).
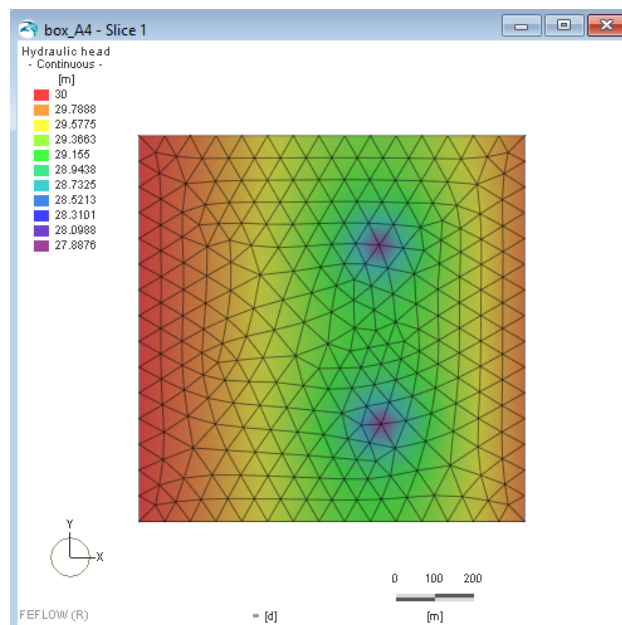
Figure 1.12: The hydraulic head field as calculated during the model run

1.9 Postprocessing

To study the results in more detail, we use the 🗐 **View Components** panel. This panel contains a list of all properties that are currently displayed in the active view. The components are sorted in different categories, in this case **Geometry** and **Hydraulic head**.

For **Hydraulic head**, different plot styles are available. The default style is a **Continuous**, interpolated color distribution. To change to a **Fringes** or **Isolines** plot style, deactivate the check mark in front of ☑ **Continuous** and activate the ☑ **Fringes** or ☑ **Isolines** style instead. Finally, the water balance of the model should be checked. Bring the 🗐 **Rate-Budget** panel to the front which is located to the lower right of the FEFLOW interface by default. To start the budget calculation, use the ☑ **Active** check box (Figure 1.13).
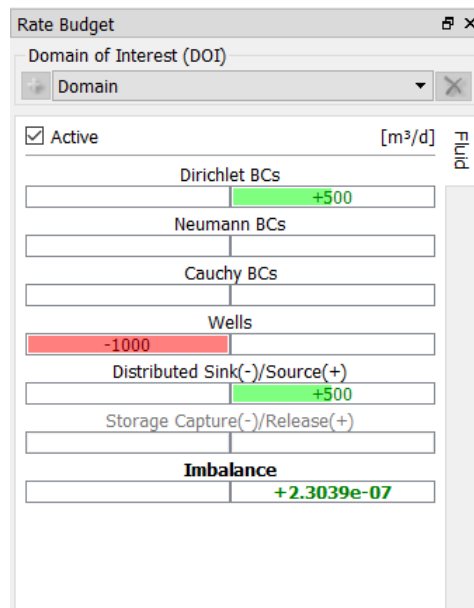
Figure 1.13: The water balance of the model is shown in the Rate-Budget panel

> The **Imbalance** term in the 🗐 **Rate Budget** panel reflects the solver residual error and the numerical error due to 1) mesh discretization in the case of steady-state problems and 2) both mesh and temporal discretizations in the case of transient problems. For steady-state problems, the imbalance should be close to zero.

1.10 Additional Practice

For additional practice of the methods used so far, try to change some parameters, such as the pumping rates of the wells, the transmissivity, etc., and compare the results.

2 Box - Solute Transport

All files related to this exercise can be found on the training USB memory stick in the project folder /models/box_model.

2.1 Objective

In this exercise, the 2D flow model is extended to a 2D mass-transport model. Basic concepts of mass-transport modeling including boundary conditions and material properties are explained.

Common problems in transport modeling, such as oscillations and numerical dispersion, and their prevention strategies are explained and discussed. Boundary constraints are introduced during the exercise.

2.2 Model Scenario

Two contaminant sources that are located upstream of the wells can potentially affect the water quality. Therefore, contaminant concentrations at the wells should be determined. For our model, this is done by a steady-state simulation for a worst-case scenario. The scenario is shown in Figure 2.1.

2.3 Problem Settings

2.3.1 Problem Class

Load the previously created 2D flow model or open boxA4.fem from the training USB stick or DVD. Open the **Problem Settings** dialog located in the **Edit** menu.

Choose **Problem Class** from the index and activate the option **Include transport of...** **Mass** (Figure 2.2).

To finish, click Bu **OK** and confirm the changes with Bu **Yes**.

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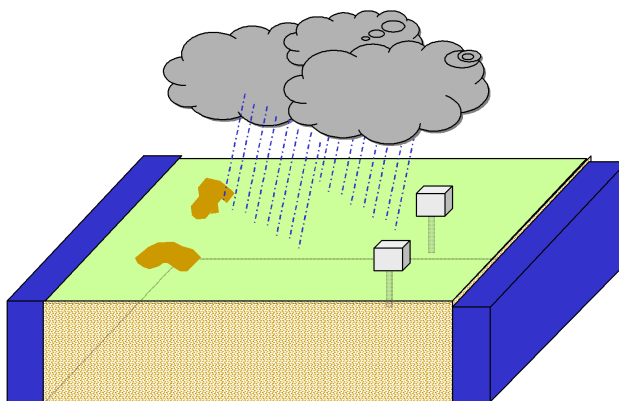
Figure 2.1: Model scenario
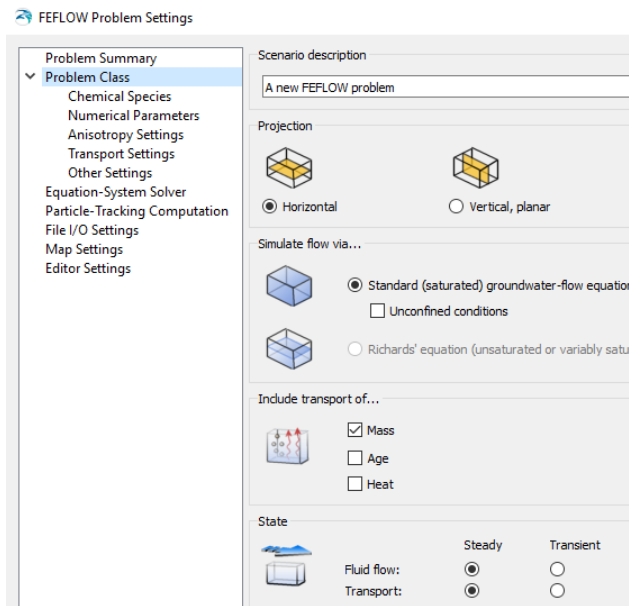
Figure 2.2: Problem-class settings for steady mass transport

Sign	Boundary condition	Geometry	Unit
○	**Mass-concentration BC** 1st kind / Dirichlet BC -> fixed concentration	node	mg/l

✕	**Mass-flux BC**
	  2nd kind / Neumann BC
	   -> in/outflux
		line (2D)
		area (3D)
			g/m/d
			g/m²/d

◉	**Mass-transfer BC**
	  3rd kind / Leakage / Cauchy BC
	   -> reference concentration + resistance
		line (2D)
		area (3D)
			mg/l

𝄞	**Mass nodal sink/source BC**
	  4th kind
	   -> nodal extraction/injection
		node	g/d

Figure 2.3: Available types of mass-transport boundary conditions

2.4 Model Properties

After the problem class has been changed, additional model properties related to the transport model appear in the 📄 **Data** panel. This includes initial and boundary conditions, as well as material properties.

2.4.1 Initial Conditions

In the 📄 **Data** panel, double click on **Process Variables - Mass transport - Mass concentration**.

The state of the process variables at the start of the simulation reflects the initial conditions of the model. The default initial condition of 0 mg/l is accepted without changes.

2.4.2 Boundary Conditions

The mass-transport boundary conditions are of a similar type as the flow BCs. Figure 2.3 gives an overview of the available boundary-condition types.

The model domain contains two contamination sources. The easiest and probably most conservative approach - using a fixed concentration - will be used to represent these two sources.
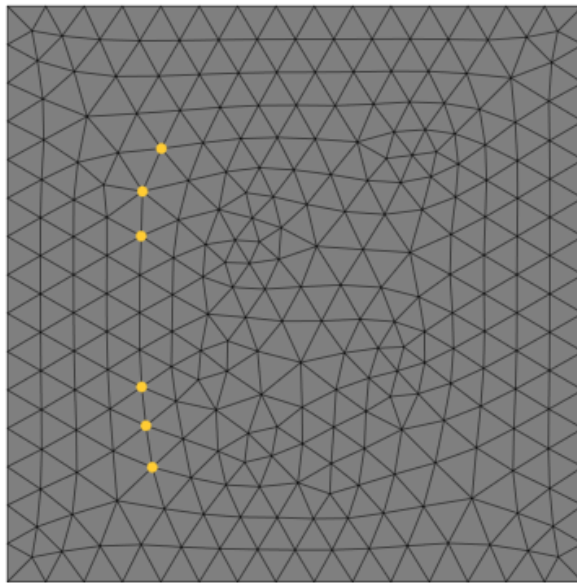
Figure 2.4: Selection for contamination sources

In the 📄 **Data** panel double-click on **Boundary Conditions - Mass transport - Mass-concentration BC**.

Choose the ➚ **Select Individual Mesh Items** tool from the ▭▭▭ **Selection** toolbar. Move the mouse cursor into the view window and select several mesh nodes in the upper left side of the model with single left-mouse clicks.

Repeat these steps to select a second area in the lower left side of the model. If a selection has been created erroneously, use ⊠ **Clear Selection**, ↺ **Undo Last Selection Step** or ↻ **Redo Last Selection Step** buttons of the ▭▭▭ **Selection** toolbar. The result should look similar to the selection shown in Figure 2.4.

Finally, enter a value of ₁₂₃ **100** mg/l into the input field of the ▭▭▭ **Editor** toolbar and click on ✓ **Assign** to set the boundary conditions. The mass-boundary conditions are displayed with the same blue symbols that indicate a **Hydraulic-head BC**.

To check the values of the boundary condition, use the 🔍 **Inspect Nodal/Elemental Values** tool again.

Finally, click on ⊠ **Clear Selection** to avoid that these boundary conditions are over-written during the following operations. During the next steps, the boundary conditions for the left and right border are assigned.

At any border with advective inflow, the concentration of the water entering the domain should be specified. For this model, it is assumed that the inflowing water is freshwater with a concentration of 0 mg/l.

Choose the 🔺 **Select Nodes Along a Border** tool from the ▭▭▭ **Selection** toolbar. Move the mouse cursor to the bottommost node of the left border. Press and hold the left mouse button. Move the mouse cursor to the topmost node of the left border and release the mouse button again. You should see that the nodes of the left border are selected, indicated by yellow markers.

Repeat these steps for the right border. The nodes of the left and the right border are highlighted in yellow. Go to the ▭▭▭ **Editor** toolbar and enter a value of ₁₂₃ **0** mg/l into the input field. Click on ✓ **Assign** to assign the values. The boundary conditions on the left and right side should now be visible as blue circles (Figure 2.5).

To check the values of the boundary condition, activate the 🔍 **Inspect Nodal/Elemental Values** again. Move the magnifying glass over the nodes to check the assigned value of
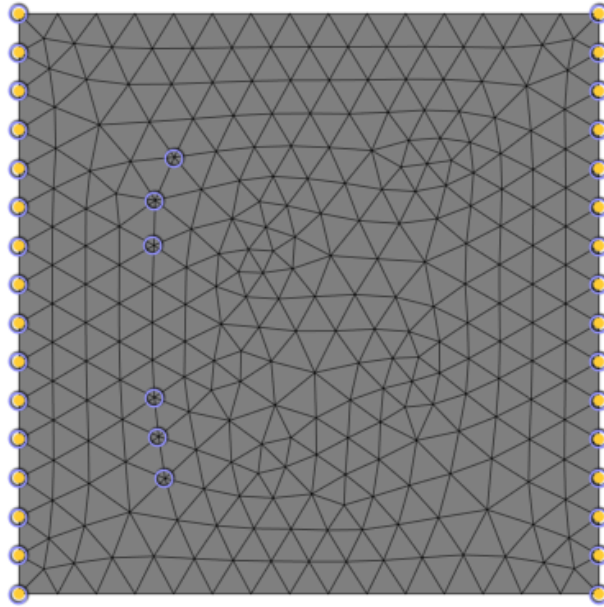
Figure 2.5: Nodal selection and mass boundary condition

the boundary condition.

🗁 💾 boxB2.fem

Constraints

The flow-boundary conditions assigned to the model (***Hydraulic-head BC*** at left and right border) potentially allow for both in- and outflow.

In a transport simulation, borders with an inward-flow direction have to be treated in a different way than borders with an outward-flow direction. In the former case, the concentration at the border should be fixed, while in the latter case, free advective outflow is required, and the mass-boundary condition therefore has to be deactivated. This can be achieved by a second, complementary condition that is called a ***Constraint*** in FEFLOW.

> Constraints limit the application of boundary conditions.
>
> A good example is a well with a constant pumping rate, whose drawdown should be limited to a certain level (Figure 2.6). The minimum hydraulic head to which dewatering is allowed is defined as a constraint. If the hydraulic head at the well node is above the minimum head, the well-boundary condition is applied. If the hydraulic head would drop below the minimum head, the well-boundary condition is internally turned into a head-boundary condition with the value of the minimum head.
>
> Please note that when using the settings mentioned above for a well-boundary condition limited by a minimum head, it is possible that the groundwater level drops below the minimum head due to effects in the surroundings of the well. In that specific case, the well will be turned - most likely unwanted - into a head-boundary condition which will lead to an infiltration of water instead of a reduction of the pumping rate. To avoid this, a well can be set up with a different boundary condition/constraint combination: Use a head-boundary condition with a value of the minimum head and limit the outflow using a minimum flow-rate constraint with a value of the pumping rate of the well. To avoid any inflow, use a maximum flow-rate constraint of 0 at the same time.
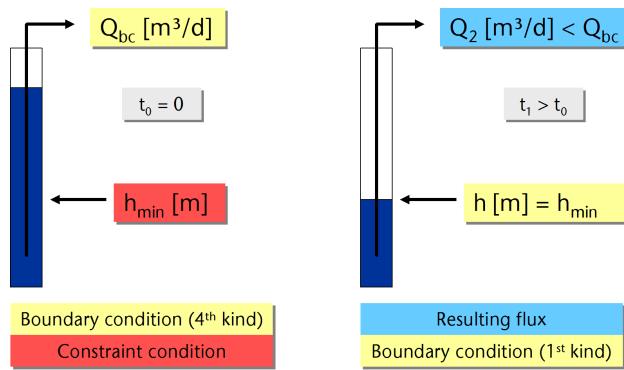
Figure 2.6: A pumping well with limited screen depth as an application example for constraints
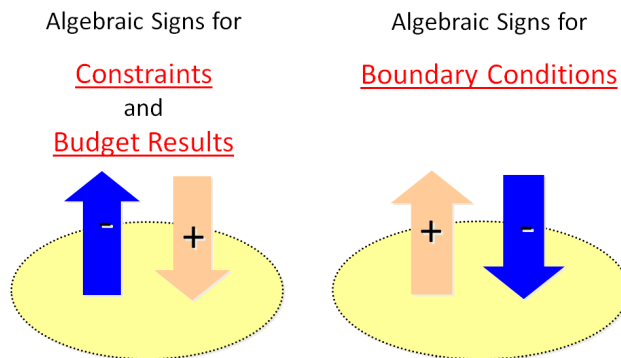

Figure 2.7: Comparison of the sign convention for budget results, constraints and boundary conditions

Note: Unlike the definition for boundary conditions, for constraint conditions of flux type, positive values define an inflow into the model, negative ones an outflow (Figure 2.7).

By default, constraints are not shown as a parameter in the 🗐 **Data** panel and have to be made visible first. Use the right mouse button to open the context menu of the item **Boundary Conditions - Mass transport - Mass-concentration BC** in the 🗐 **Data** panel. Choose 🗎 **Add Parameter - Min. mass-flow constraint**.

Double-click on the new parameter to activate it for assignment (Figure 2.8). Go to the 🔲 **Editor** toolbar and enter a value of 🔢 **0** g/d into the input field. Finish the assignment with a click on ✅ **Assign**.

The constraints are now indicated in the view window by horizontal bars below the boundary-condition symbols.

As a last step, click on ❎ **Clear Selection** in the 🔲 **Selection** toolbar.

When using constraints, it is recommended to use a transient model approach. The reason for doing so is the fact that the check whether the boundary condition or the constraint should be active is done at every time step for a transient run. In a steady-state model, this check is only done for the first iteration and then kept for the subsequent iterations.
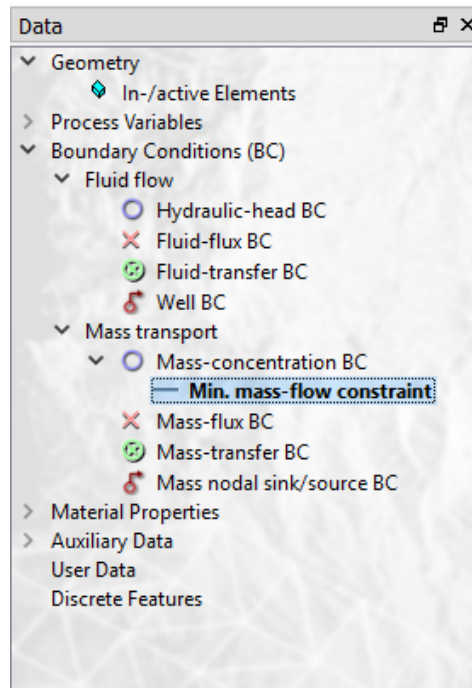
💾 boxB3.fem

Figure 2.8: Data panel showing the minimum mass-flow constraint

2.4.3 Material Properties

For the simulation of a mass-transport problem, additional material properties are available, including sorption isotherms and reaction terms.

For the sake of simplicity, default parameters are used for this model. Please note: For practical applications, you should at least adapt porosity and dispersivity values to local conditions. The default values are 30 % for porosity, 5 m for the longitudinal and 0.5 m for the transverse dispersivity.

Three different mechanisms need to be considered for contaminant transport within a porous medium:

- Advection,

- Molecular diffusion and

- Dispersion.

Dispersion occurs due to differences in transport velocities caused by matrix variations (microdispersivity, Figure 2.9) and by geological inhomogeneities of larger spatial scales (macrodispersivity).

Dispersion is usually considered by applying the linear Bear-Scheidegger dispersivity law, which distinguishes between a dispersivity parameter in flow direction (longitudinal dispersivity) and a dispersivity parameter perpendicular to the flow direction (transverse dispersivity). The longitudinal dispersivity depends on the length scale of the phenomenon. Figure 2.10 shows a chart of measured longitudinal dispersivities in relation to the spatial scale.

In comparison to longitudinal dispersivity, much less is known about transverse dispersivity, and often, the ratio a_t/a_l of transverse over longitudinal dispersivities is assumed to be 0.1. However, even that factor varies widely in laboratory and field experiments.
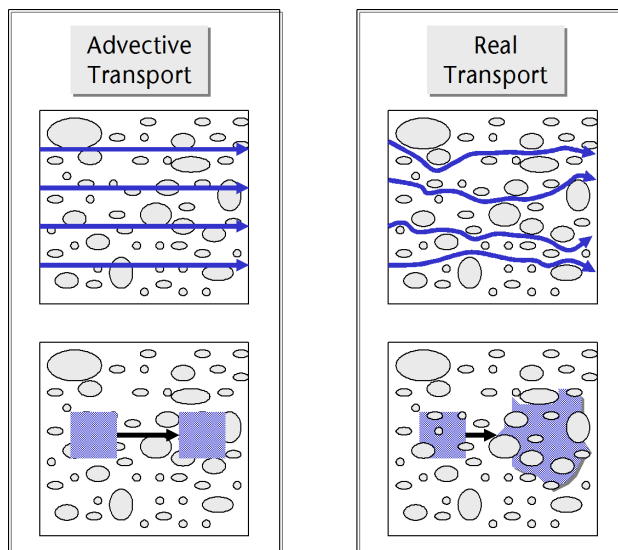
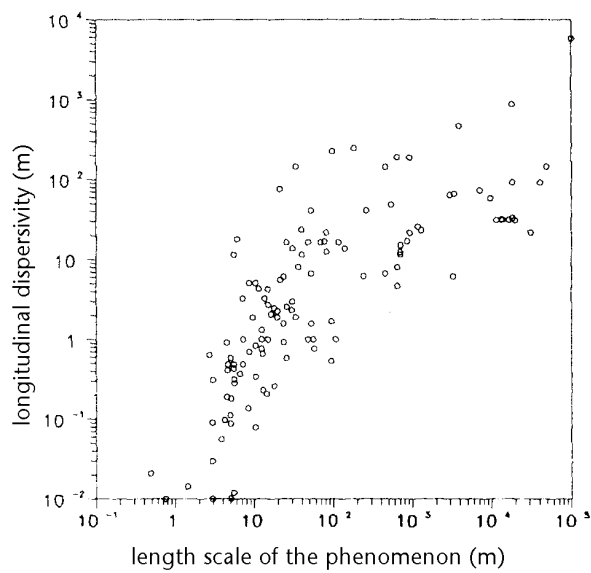Figure 2.9: Comparison of purely advective and real mass transport (taken from: [**?**])

Figure 2.10: Longitudinal dispersivity vs. scale of phenomenon (taken from: [**?**])
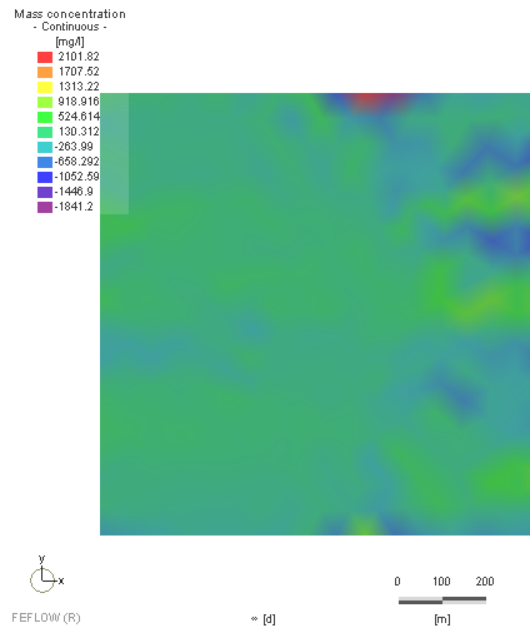
Figure 2.11: Result of mass-transport simulation (coarse mesh)

2.5 Simulation Run

Plot the initial concentration in the active view by double-clicking on **Process Variables - Mass transport - Mass concentration** in the 🗎 **Data** panel.

To start the simulation run, click on ▶ **Start** in the ▦ **Simulation** toolbar. After a short time, the result is shown. To turn the display of element edges off in the current view, use the check mark in front of ☑ **Geometry - Edges** in the 🗎 **View Components** panel.

As Figure 2.11 shows, the current model setup results in negative concentrations. This is a clear indication for model instability; the reason for this being an insufficiently fine spatial discretization.

To improve the model result, the mesh has to be refined.

Before any further changes can be done, the simulation must be stopped by clicking on ■ **Stop** in the ▦ **Simulation** toolbar.

Create a selection of all nodes using ▣ **Select All** in the ▦ **Selection** toolbar (or press <Ctrl + A> on your keyboard). Click on ⬢ **Refine Elements** in the ▦ **Mesh Geometry** toolbar twice to refine the mesh.

⊠ **Clear Selection** and run the simulation again.

The two contamination plumes should now be visible in the resulting concentration field. When checking the results in more detail, one finds that negative results still occur at the fronts of the contaminant plume. Figure 2.12 shows a close-up of the contamination source (the element edges have been reactivated for this figure). Upstream of the contaminant sources, high and low concentrations change at regular intervals.

This is a typical oscillation pattern in transport models.

> Oscillations in a transport simulation can occur if the discretization is insufficient, i.e., if the mesh is too coarse or if time steps are too large. There are three major strategies to reduce oscillations:
>
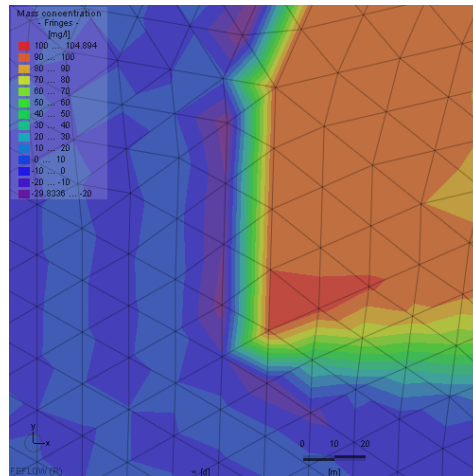>   • Mesh refinement
>
>   • Upwind techniques

Figure 2.12: Concentration distribution near the contamination sources

- Increasing dispersivity values

The first approach always is the preferable solution as mesh refinement does not change the physical properties of the model. However, in some cases, mesh refinement might not be an option due to restrictions in memory and/or computation time.

Upwind techniques add numerical dispersion to the model, the most general one - full upwinding - in all directions, the most restricted one - shock capturing - only where it is necessary. Upwind techniques always change the dispersivity applied to a model, and therefore lead to a larger contaminant plume.

Increasing the dispersivity also leads to a more stable simulation as gradients in concentration or temperature are reduced. However, increasing dispersivity values artificially changes the physical properties of the system.

2.6 Oscillation Prevention

As the oscillations in the model are too high, all of the following solution approaches should be tried in order to reduce the oscillations.

2.6.1 Mesh Refinement

Repeat the steps described in section 2.5 to refine the mesh several times. As a result, the oscillations become smaller and the shape of the concentration plume can be reproduced. Additionally, concentration over- and undershoots are gradually reduced or removed completely. In further steps, it is possible to refine the mesh locally by selecting the nodes around the contamination sources using the ☐ *Select in Rectangular Region* tool. The selection and the result are shown in Figures 2.13 and 2.14.

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. The dimensionless Péclet

Number relates the Darcy velocity, characteristic length of the finite element and dispersivity values.
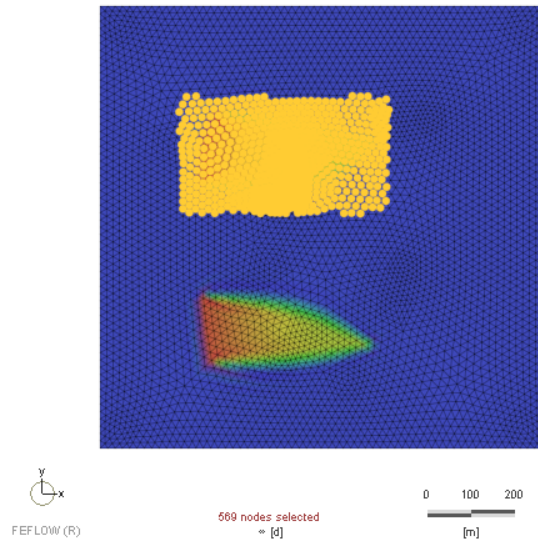

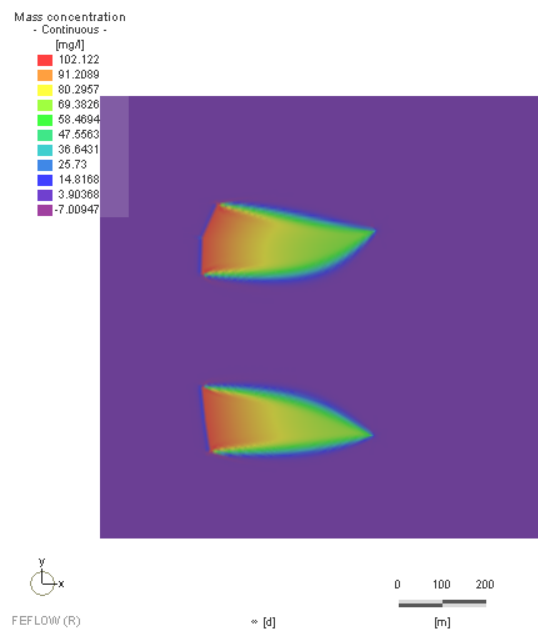Figure 2.13: Local refinement for mass-transport simulation

Figure 2.14: Result of mass-transport simulation (fine mesh with approx. 10,000 elements)

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2.6.2 Upwinding

To activate an upwinding technique, open the **Problem Settings** dialog via the **Edit** menu.

Here, open **Problem Class - Numerical Parameters**. Choose ● **Full upwinding**. Press ⎣Bu⎦ **OK** and confirm the changes with ⎣Bu⎦ **Yes**.

Run the simulation again. In the best case, there will be no negative values in the resulting concentration field. However, it can be seen that the sharp fronts of the plume are artificially smoothed as a result of the extra numerical dispersion (Figure 2.15).
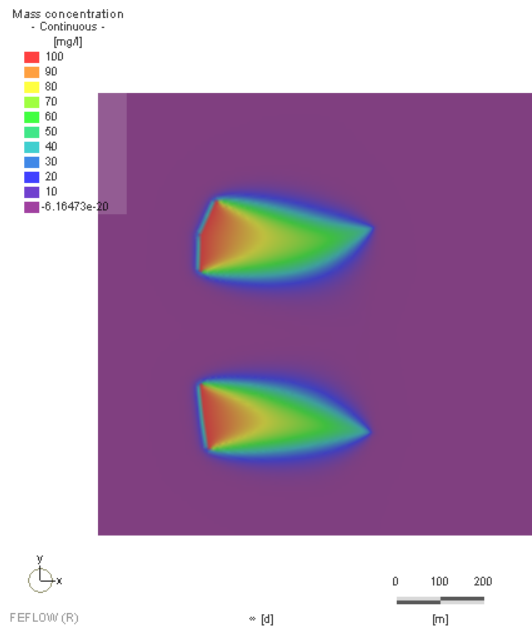

Figure 2.15: Result of mass-transport simulation with Full Upwinding

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2.6.3 Increasing Dispersivity Values

Reload the model BoxB3a.fem via **File - Open**. In the **Data** panel, double-click on **Material Properties - Mass transport - Longitudinal dispersivity** and create a selection of all elements by clicking on **Select All** in the **Selection** toolbar (or press <Ctrl+A> on your keyboard). Enter a value of **50** m into the input field of the **Editor** toolbar and click on **Assign**.

Repeat these steps for the **Transverse dispersivity** and assign a value of **5** m.

After running the simulation again, the result looks similar to the one of the simulation with full upwinding but the spreading of the contaminant plume in both longitudinal and transverse flow direction is even larger(Figure 2.16).
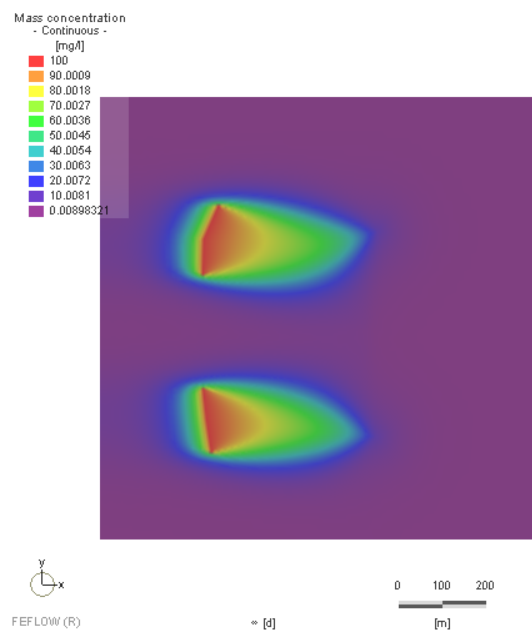
boxB3c.fem

Figure 2.16: Result of mass-transport simulation with increased dispersivity values