FEFLOW

Finite Element subsurface FLOW system

Getting Started

FEFLOW

Interactive, Graphics-based Finite-Element Simulation System for Modeling Groundwater Flow, Contaminant Mass and Heat Transport Processes

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Preface

This FEFLOW User's Manual describes a complex simulation system for the analysis of multidimensional, free surface, variably saturated, transient and coupled flow, contaminant mass and heat transport processes in subsurface water resources (groundwater). FEFLOW is an interactive, fully graphics-based software package that runs on Windows 95/NT as well as on the most UNIX color graphics workstations (provided that X Window version 11.4 or later and the OSF/Motif graphics standard version 1.2 or later are available). FEFLOW allows a user with only a technical experience to quickly simulate actual groundwater problems.

The user is requested to inform the developer about any bugs and errors found in the software or in the manual, respectively. Updates are regularly made to include both corrections of errors and improvements of the code. Also, we anticipate upgrades of the simulation system involving computational and software extensions. Requests, error reports, bug reports, and other information should be sent to the system developer at the following address:

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Abstract

FEFLOW (Finite Element subsurface FLOW system) is an interactive, graphics-based groundwater modeling system for **three-dimensional** (3D) and **two-dimensional** (2D) - areal and cross-sectional (horizontal, vertical or axisymmetric) - , fluid **density-coupled**, also **thermohaline**, or uncoupled, **variably saturated, transient** flow, chemical **species and heat transport** in subsurface water resources with or without **free surfaces**. As a computer aided engineering (CAE)-oriented software package for modern UNIX engineering graphics workstations and Windows 95/NT PC's FEFLOW represents an efficient tool of simulation in order to (1) describe the spatial and temporal distribution of groundwater heads and/or contaminants, (2) modeling geothermal processes, (3) analyze moisture dynamics and seepage, (4) estimate the duration and travel times of a pollutant in aquifers, (5) plan and design remediation strategies and interception techniques, and (6) assist in designing alternatives and effective monitoring schemes.

FEFLOW is an interactive, fully graphics-oriented and menu-driven, hierarchically structured software system that contains graphical editors and mesh generators for the geometric design and discretization of possibly complex study areas as well as for the problem attribute specifications. It relies on general computational techniques to solve a wide class of subsurface flow and mass transport problems characterized by flexibility and robustness, and many additional graphical tools to manage the entire solution process and model data.

Databases in form of line-, point-, polygon- and annotation-related formats, such as the the ESRI Shape file format and the ASCII (Generate) format widely used in the **Geographical Information Systems** (GIS) ARC/INFO and ArcView as well as Raster Databases (TIFF) and Hewlett-Packard Graphics Language (HPGL)-formatted data can be imported and applied for purposes of data regionalization and visualization.

FEFLOW employs a fully three- and a two-dimensional finite element method (FEM) to solve the governing partial differential equations that describe the following interdependent processes:

(1) groundwater flow dynamics which can be fluid density-dependent and can involve free surfaces (perched water table)

(2) variably saturated flow and transport (3D and 2D)

(3) convective and dispersive contaminant transport, in which the chemical species may be subjected to: adsorption, hydrodynamic dispersion and first-order chemical reaction.

(4) subsurface heat transport processes, in which fluid-density effects caused by both contaminant mass and temperature fields can occur, so-called thermohaline flow.

The prescription of the initial and boundary conditions can be relatively general so that formulations on arbitrary geometries with different types are possible. Accordingly, it also allows the handling of mixed conditions (e.g., surface water interactions or pumping and injecting well functions) as well as specific mass flux-occupied boundaries (e.g. leaching of substances, diffuse intake of chemicals from landfills, etc.) based on an alternative formulation of the basic equations, so-called divergence form transport formulations. Confined and unconfined aquifers can be handled both as separate and as combined tasks. FEFLOW contains options for combined and separate, nonlinear (fluid density coupled) and linear, fully transient, semi-unsteady and steady-state simulations of the flow and transport. Quadrilateral and triangular spatial discretization schemes of first and second order finite elements are available based on versatile finite element meshing generators. For triangular meshing an advancing front iterative geometry decomposition approach combined with smoothing techniques and a Delaunay based T-MESH generator, supporting Add in's, are utilized, while quadrilateral meshes are generated by using mapped element approach as in form of quadrilateral element mapping and a discrete transfinite mapping with stretching functions. Both first-order and second-order time stepping schemes are incorporated into the simulator. Two principal alternatives exist. Firstly, using fixed (predefined) time steps a fully implicit or the higher order Crank-Nicolson time integration scheme is performed. Secondly, FEFLOW can run predictor-corrector time stepping schemes and aggressive target based time marching strategies which allow a completely automatic control of the transient solution process.

FEFLOW involves three-dimensional graphical tools for a visual analysis of 4D space-time model data. They covers visometric 3D functionality, volume and surface displays, rotation, translation, shading, 3D cursor, arbitrary sections, fence displays, isosurfaces, map integration, pathlines, flow vector patterns and isochrones.

For nonlinear processes FEFLOW uses both an effective Picard iterative scheme having additional features such as relaxation measures and forward projections and the Newton iterative method for either variably saturated problems or density-driven convection processes. Further numerical features as standard or optional are the Galerkin approach and streamline, shock capturing or full upwinding if desired, fast discontinuous and balance improved continuous flow field evaluations, convective and divergence formulations of the governing transport equations for generalized mass/heat-flux boundary conditions, improved particle tracking algorithms and isochrone computations and preconditioned conjugate gradient solution techniques (PCG, Restarted-ORTHOMIN, Restarted-GMRES, CGS, BiCGSTAB and BiCGSTABP applied to symmetric and asymmetric problems) for the solution of the resulting large sparse equation systems. Alternatively, fast direct profile equation system solvers are available using automatic nodal reordering schemes based on the Reverse Cuthill McKee (RCM) algorithm and automatically controlled resolution procedures to minimize the updating effort for the matrix systems.

The simulator FEFLOW is completely written in ANSI C and C++ so that dynamic memory allocation resulting from the interactive capabilities of the system can easily be handled. Thus, no real software limits exist. The problem measures are only restricted by the computer storage capacity available for the user. The dynamic memory monitoring allows

an efficient use of the editors, the mesh generators, the simulator kernel routines, and postprocessing modules. Accordingly, all working arrays, buffers, etc. are allocated and freed during the run time of the computer. All global matrices are compactly stored as vectors. All floating point computations are performed in double precision. More detailed lists of features are given in § 1.6.

FEFLOW employs methods of data regionalization, that means transformation schemes to distribute measured data onto the meshed study area. The kriging method using a spherical model for the variogram computation, an Akima interpolation and extrapolation technique and Inverse Distance Weighting are available to overlay databases for topography, initial conditions, boundary conditions and all relevant model parameters that describe aquifer and fluid materials.

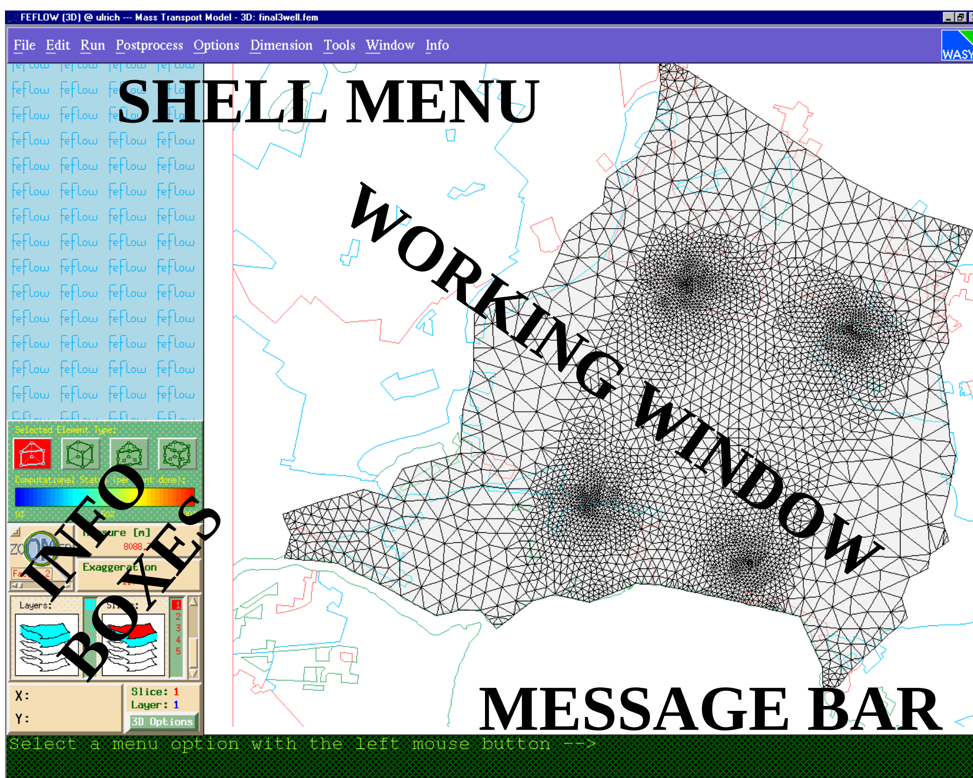
FEFLOW runs under Windows NT/95 using an X-Server and under UNIX and the X Windows and OSF/Motif graphics standard, so that it is available for a wide range of today's engineering graphics workstations. The present FEFLOW version is based on the recent releases of the X Window system (version 11.4 or later) and the OSF/Motif (version 1.2 or later). The interactive graphics with multiple capabilities (windows, icons, dynamic menus) provides good ergonomics and a clear display of the program´s top-down hierarchy. The contents of the windows and menus reflect the progress of user's activities, output of computational results in a graphical style (isolines and fringes, flow patterns, line section, time histories, three-dimensional distributions), support the graphical input (by mouse) and output with zooming and close-up viewing, prompt information about the hierarchy level, basic data, completeness of editing and system options currently valid, and echo multiple messages (instructions on the basic line of the screen, help windows, alert boxes, hourglass for showing the computational status, a running problem summary, and a protocol for the editing and the file data characteristics). FEFLOW provides a hierarchically organized system of defaults and standard procedures, which the user can optionally change, traversing the levels of the system's problem representation hierarchy. Accordingly, the simulation system is oriented to be quite self-explanatory and transparent in its use. For instance, the menu items the system offers are dynamically dependent on the current user's working level and only such menu options need to be used where differences from the defaults are necessary, so that the order of editing steps is widely arbitrary whenever possible and the user is not enforced to work out its problem in a strict top-down, say "Yes/No" manner, where all menu options must be consecutively picked.

The interactive simulation system FEFLOW is modular and built with an open architecture concept as a basic design guide. Thus, this system at any time can be modified or extended at low cost, keeping the simulator open for eventual modifications as suggested with accumulated practical experience.

Contents

Part I

Overview



1 Introduction

1.1 About This Documentation

This documentation describes the use of the interactive Finite-Element Simulation System (FEFLOW) for groundwater flow, solute, and heat transport modeling. Reference information is also provided.
The **installation** of FEFLOW is described in the **booklet** of the CD-ROM.
FEFLOW is ready to run as soon as it is installed. The user is assisted by messages, protocols, help instructions, caution boxes and push-button options in graphics menus. Further detailed information is also included in FEFLOW's online **Help**.
The user should be familiar with groundwater flow theory and the basics of formulating a groundwater model. The manuals are designed for the practicing scientist or engineer in the fields of hydrogeology, groundwater protection, and water resources environmental research, rather than for the theoretician. It provides an overview of the theoretical, numerical, and computational framework of the underlying modeling and solution strategies.
The documentation consists of three handbooks:

Reference Manual

The Reference Manual contains two parts: Physical Basis of Modeling and Applications. **Part I** contains information about the theoretical background behind the FEFLOW simulator. More advanced users will find this manual useful as it contains the different formulations and solution approaches offered by FEFLOW. It includes an introduction to the physical balance laws and methods and derives the governing groundwater flow and transport equations. It also discusses the types of boundary and initial conditions, the set of material conditions which are necessary to describe the different physical and physico-chemical processes and options for the improvement (computational time required, accuracy, and precision) of computational results. This information allows you to move through the simulation system hierarchy more effectively and to understand parameter settings. The **Applications** section presents a series of benchmarks and examples, ranging from simple to more complex model applications. This chapter provides useful examples of technical capabilities as well as verification of FEFLOW results against analytical and other numerical model predictions. These examples illustrate the capabilities, the accuracy, and the flexibility of FEFLOW.

Getting Started

Getting Started consists of two parts. The **Overview** you are reading now offers a short description of the main features and principles of FEFLOW. The second section, **Demonstration Exercise** describes the general procedures which are necessary to create, design, modify, and solve a problem at hand of a real world model. It is recommended for all newcomers to FEFLOW and will guide them through their first three-dimensional flow and mass transport model.

User’s Manual

The User’s Manual starts with a **Menu Guide** through the main menus of FEFLOW including a glossary, a list of defaults and a nomenclature. Additional detailed information on all FEFLOW options is also available through the online **Help** feature. The section **Tutorial** contains an advanced exercise introducing to the more complex features of FEFLOW. You will find a number of hints and tricks which may be useful in your modeling practice.The **Programming Interface** introduces the possibility of linking third party programs or own source codes to FEFLOW. A detailed description for programmers is included on the FEFLOW CD.

1.2 General Overview

FEFLOW is organized on your monitor screen as shown in Figure 1.1. According to the X Window philosophy, the attributes and properties of the screen imitate those of a big window. FEFLOW consists of several menu levels. Each level corresponds to a major functional division of the simulation system.

The system is hierarchically structured. All user actions are controlled by the graphics system Master menu, called the *Shell*. All subordinate levels and menus are accessible from the *Shell menu entries* at the top of the window.

The editing is executed interactively in the *Working window*. It is in this window that the simulator displays the major results (isolines, vector plots, and others). This working window has a local and a global coordinate system. You can assign real dimensions in the form of width measure, vertical exaggeration and the location of the coordinate’s origins. Absolute (global) coordinates are referenced by Gauss-Krüger when handling maps and databases. Besides Cartesian coordinates the user can also work with polar coordinates. The *Information boxes* at the lower left side of the shell are visible in every menu level. They display information about the model, offer tools for zooming and switching between different layers and contain the entry to the **3D Options** menu for 3D analyzing of the model. The *Message bar* at the bottom edge of the shell diplays context sensitive help on the different menu levels. For detailed online help hit the <F1> key or click on the "Help" buttons available in the menus.

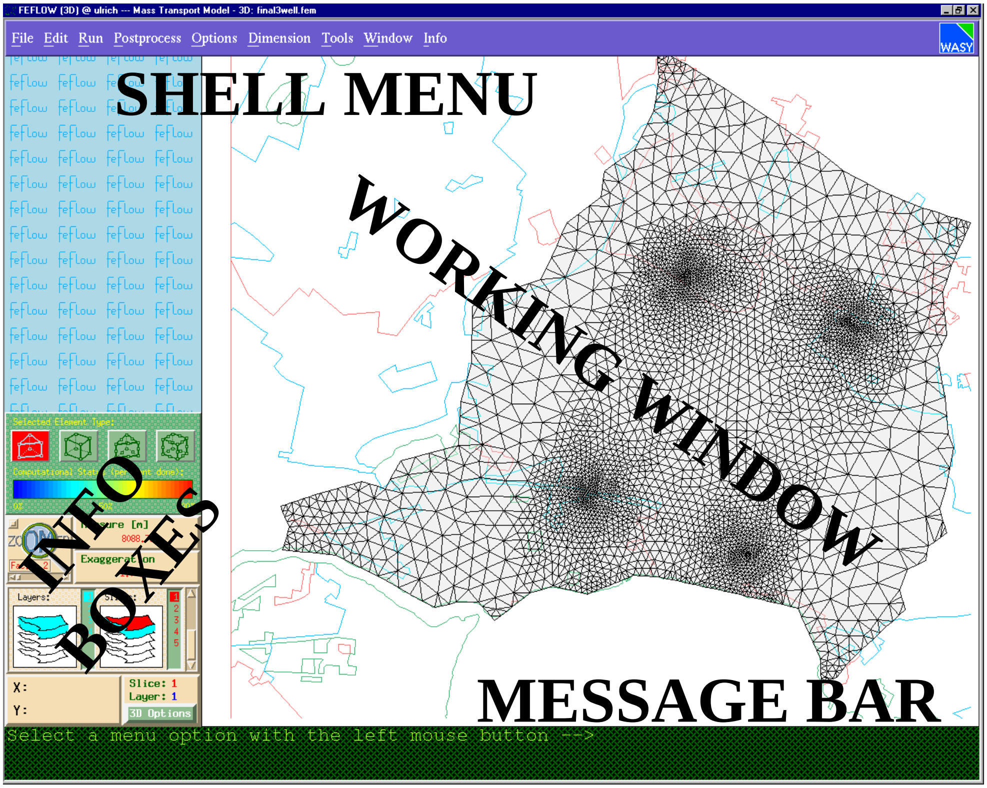


Figure 1.1: Top Level Of The Graphical User Interface

1.3 Structure and System Layout

FEFLOW consists of several menu levels. Each level corresponds to a major functional division of the simulation system. The system is hierarchically structured as depicted in Figure 1.2. All subordinate levels and menus are accessible from the *Shell*. The principal structure is treelike, with the *Shell* on top. For reasons of efficiency, there is sometimes a fast cross-connection between secondary levels. This is discussed in more detail below. The *Shell* contains data interfaces to import and export various data formats (top row of Figure 1.2).

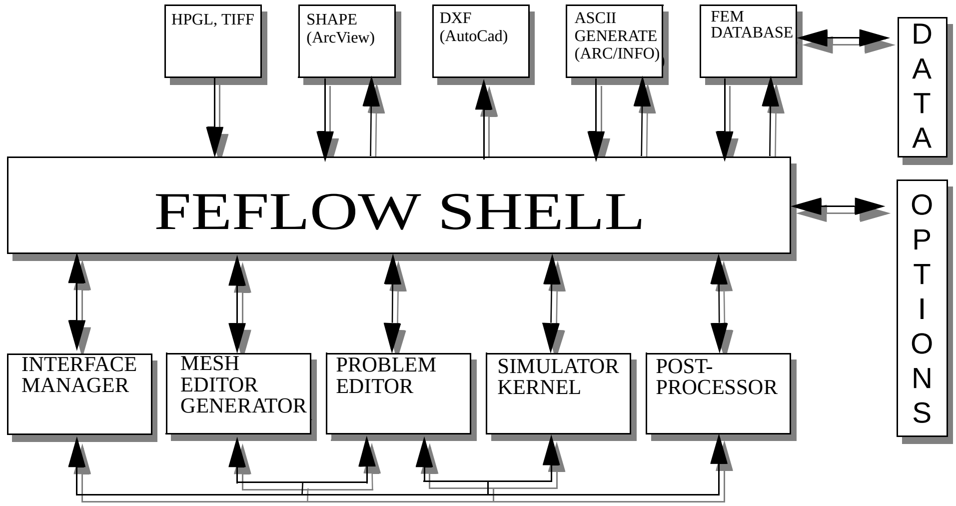


Figure 1.2: General Structure of FEFLOW

Two of the major components in the *Shell*'s pull-down menus are the *Mesh Editor* and *Mesh Generator*, where problems are designed and discretized (bottom row of Figure 1.2). Other major components are the *Problem Editor*, where all non-geometric attributes of the problem are edited, the *Simulator Kernel*, where the computations of the problem are performed and different evaluations of the computed results are possible, and the *Postprocessor*, which is a versatile tool for sifting, graphics evaluation and visualization of the computed response data. Via the *Interface Manager* the linking of external programs with FEFLOW is organized. Your activities are embedded and supported by many auxiliary menu items and procedures, which you can change (options box, Figure 1.2). The next section will summarize the major items.

1.4 FEFLOW History

FEFLOW was initiated in 1979 at the Institute for Mechanics of the former Academy of Sciences of the GDR. FEFLOW was designed as a research-oriented, special purpose, finite-element program for modeling two-dimensional nonlinear flow and mass transport processes in saturated porous media. It was originally written in FORTRAN IV and designed as a typical batch program for mainframes. Since then, FEFLOW has been continuously developed, modified, extended, and improved for a variety of practical tasks and theoretical studies. During its development, FEFLOW has been extensively tested, compared with analytical and numerical solutions, benchmarked with experimental data, and successfully applied to a series of practical groundwater contamination studies and real contamination sites. For more details, see the references (arranged by topic) in Section § 3:

Model developments: 2, 10, 13, 14, 15, 16

Benchmarking: 1, 3, 4, 5, 17, 19, 39, 42, 43, 45, 47, 49

Coupled fields: 4, 5, 8, 9, 11, 14, 15, 19, 21, 22, 25, 33, 39, 41, 42, 43, 44

Unsaturated problems: 10, 16, 47, 48, 49

Remedial and interception techniques: 7, 11, 12, 18, 21, 25

Case studies and applications: 6, 7, 9, 11, 12, 18, 19, 20, 21, 24, 25, 26, 38, 40, 46

Hydrothermal energy: 22, 28, 33, 43

Software developments: 15, 16, 23, 26, 27, 29, 30, 31, 32, 34, 35, 36, 37, 38, 45

FEFLOW has been expanded from an in-house, user-oriented solution program to an interactive, multi-purpose engineering simulation system in several stages (given here by version numbers) as follows:

Version	Date	Description/Highlights
Version 1.x	1979-1986	FORTRAN user-oriented batch program; implementations for IBM 370, EC 1055, BESM-6; limited pre- and postprocessing; about 8,000 lines of FORTRAN source code.
Version 2.x	1987-1990	First interactive prototype for Sun-Workstations , rewritten in about 17,000 C source code statements for the Sun-3 and Sun-4 -workstations as FEFLOW/FEMCAD; PC implementation for the Atari-ST series, GEM graphics, about 25,000 lines of C source code
Version 3.x	1990-1992	X-Windows and OSF/Motif implementation, multiple hardware (platform) installations, additional software tools, about 140,000 lines of C source code.
Version 4.0 - 4.2	1992-1995	3D extensions and developments for flow, mass and heat (thermohaline) transport, 3D visual analysis tools, ARC/INFO GIS interface based on ESRI Shape file and ASCII GENERATE formats, extended capabilities in pre- and postprocessing, also data filtering, about 250,000 lines of C source code
Version 4.5	1996-1997	Extensions regarding numerical capabilities and data interfacing, introducing DSM (data store manager) and FEMAP (map assistant), automatic mesh adaptation in 2D, more features in pre- and postprocessing, about 730,000 lines of C and C++ source code

Version 4.6	1997-1998	Installation on Windows 95/NT, new mesh generator TMESH including Add in's, revision of budget analyzing tools, about 750,000 lines of C and C++ source code
Version 4.7	1998-	Interface Manager for coupling external programs with FEFLOW, unsaturated flow and transport modeling for 2D and 3D, interpolation techniques for time varying data, extended, complete GIS data import of spatial and attribute data, Windows based print tool FEPLOT, about 850,000 lines of C and C++ source code

1.5 Purpose and Scope

Engineers and scientists continually face problems involving groundwater flow and transport. Efficient simulation tools give the opportunity to:

- describe the spatial and temporal distributions of a contaminant or a thermal field,
- analyze moisture dynamics and seepage,
- estimate the duration and travel times of a pollutant,
- plan and design remediation strategies and containment technologies, and
- assist in designing alternatives and effective monitoring schemes.

For instance a computer simulation generates predictions of groundwater contamination in terms of chemical concentration in time and space. The system must answer questions such as: How does a contaminant plume migrate from its source (e.g., waste dump, waste-well injection, landfill, deposit) through a flowing groundwater field under given geohydrological conditions? Also, which remediation strategies are recommended and how effective are they for the remediation of an aquifer?
Resulting from rapid developments in computer technology, we can utilize computational transport models that were formerly reserved for modeling experts. These developments include: powerful user-system interfaces, interactive graphics, and enhanced computing power of engineering workstations and PCs. Under UNIX, FEFLOW uses the power of the network-based X Window system, together with the X-Toolkit graphics software and the OSF/Motif graphics standard, which are available on most color graphics high resolution UNIX workstations. For PCs, FEFLOW utilizes Xvision, an X-Windows emulator for Windows 95 and Windows NT, to bring this powerful simulation tool to PC users. Reduced Instruction Set Chip (RISC) and Pentium-Pro-based workstations are fast enough to provide quick answers from even complex transport models. This allows the user to interact with the system during computation, making adjustments according to the visual feedback received. The power of the finite element method (FEM) has become more eas-

ily available for non-technical (non-modeling expert) users, who are knowledgeable about a problem's situation, but not necessarily about its technical components and computer technology.

FEFLOW provides simple, symbolic, interactive formats, and intuitive output presentation. This makes the formerly cumbersome and time-consuming task of problem generation, analysis, and simulation reruns for comparative purposes easy to manage. The geometric design, mesh generation, problem attribute specifications, and simulation runs are fully graphics-oriented and menu-driven. By simple mouse clicks and drags, you can quickly select boundary conditions, geometric data and model parameters, taking the emphasis away from the details of the data, and numerical aspects of calculations (see Figure 1.3).

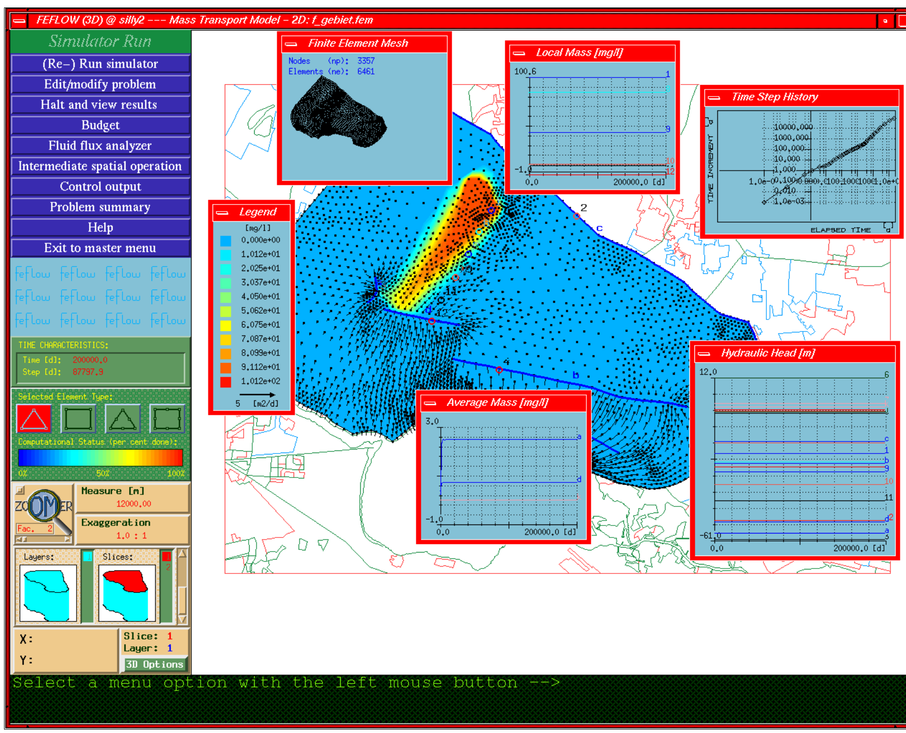


Figure 1.3: Example of the FEFLOW Graphical Interface During Simulation of Contaminant Migration

Groundwater modeling usually demands expertise and considerable experience, because of the complexity of the processes involved, or the difficulty of modeling one or more of these processes. The interactive problem generation and description still requires the ingenuity and experience of an expert to produce a valid FEM model, to interpret the simulation results, and to modify the model when results are questionable or when input data vary. The interactive features of the FEFLOW simulation system play an

important role within this iterative process.
The basic design philosophy of FEFLOW is that you should not have to deal with the numerical intricacies of a model. You can concentrate on specifying the problem and not on solution methods. The FEFLOW simulation system for interactive modeling of flow and transport processes is characterized in three important ways:

1) The complexity of the finite element generation and solution processes are hidden from the user. You are only exposed to a dynamically menu-driven and fully graphics-oriented user interface (see Figure 1.3). You only need to select appropriate options from the menus, and select or position spatially distributed data with a graphics input device, such as a mouse.

2) The system is hierarchically structured. All user actions are controlled by the top level master menu, called the *Shell*. The *Shell* offers the principal options for various problem designs and solution strategies. The customizable commands provide a hierarchically organized system of defaults and standard procedures.

3) The basic system design guideline is an open, modular architecture concept. While it is presently fully operational, the system can be easily and inexpensively modified and extended at any time. This means that the simulator can be modified to adapt to your needs as you become a more experienced user.

The interactive graphics with multiple capabilities (e.g., windows, icons, dynamic menus) results in a user-friendly structuring of the graphics display. The contents of the windows and menus reflect the user's progress, output computational results in a graphical format, prompt for information about the hierarchy level, basic data and system options currently available, and echo many messages (e.g., help messages, instructions, error messages, and hourglass for computational status).
When modeling complex groundwater flow, mass and heat transport processes, you can choose among various degrees of complexity to represent a real life, multilayer hydrogeologic system (Figure 1.4). Three-dimensional (3D) models offer the best approximation of reality, they are often very complex and require a large amount of observational data. However, these data are often not available. The computational effort involved in solving a numerical discretization of the governing 3D equations is also large. Reduction to two-dimensional (2D) aquifer-averaged horizontal, vertical or axisymmetric models is often an appropriate option. Two-dimensional models may have the best starting conditions to allow the investigator to study flow and transport processes, and their major effects and interdependencies. When the 2D models have been shown to be insufficient, they may be expanded to a 3D multi-aquifer system. Therefore, formulation of the problem may proceed from the more complex to the more simple, but the practical modeling approach tends to go from simple to complex.
The modeling approach in the FEFLOW simulation system corresponds to this solution

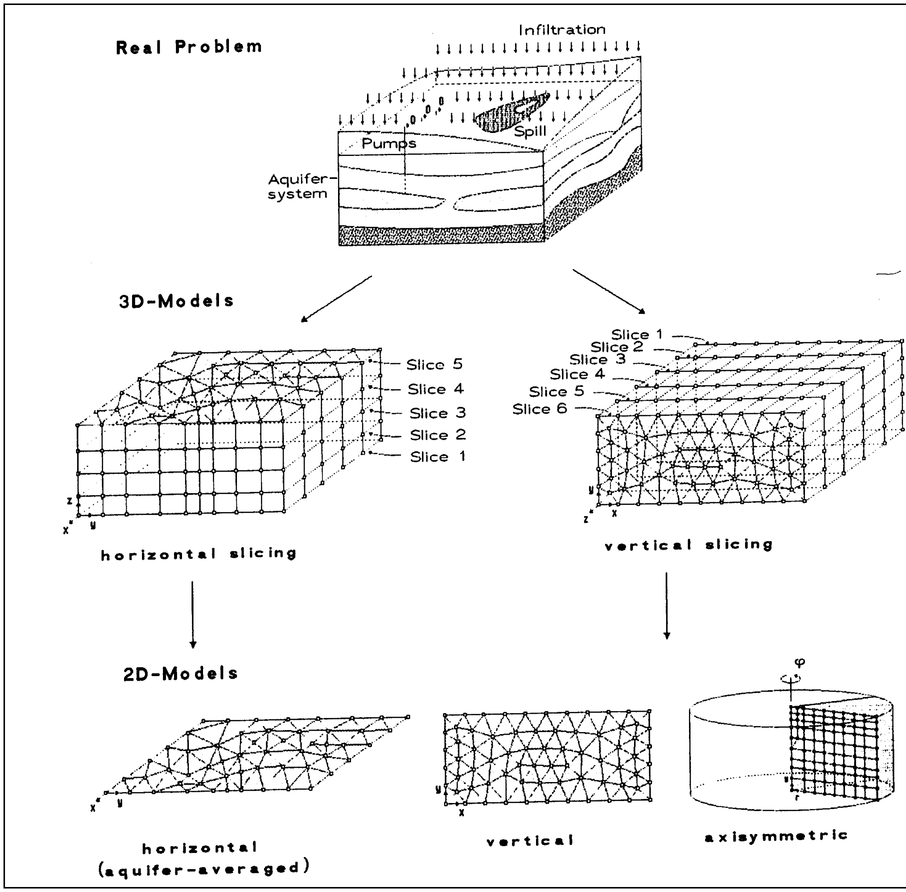


Figure 1.4: Reduced Model Levels Behind FEFLOW

strategy. The current version of the FEFLOW simulator provides all the tools for handling a 2D approach and for managing the extension to a 3D multi-aquifer model.

1.6 Features

The present interactive modeling system FEFLOW solves three-dimensional and two-dimensional problems: plan view and cross-sectional horizontal, vertical, or axisymmetric (2D), fluid density-coupled or uncoupled, variably saturated, transient flow, contaminant mass and heat transport processes in subsurface water resources. Some of the many features and options of FEFLOW are described below:

1.6.1 Physical

- groundwater flow dynamics, which can be fluid density-dependent
- variably saturated flow and transport (3D and 2D) using Van Genuchten, Brooks-Corey, Haverkamp and Exponential parametric models.
- convective and dispersive contaminant transport, in which the chemical species may be subjected to: adsorption (linear Henry sorption isotherm, or nonlinear Freundlich or Langmuir isotherm), hydrodynamic dispersion (Scheidegger-Bear-dispersion model) and first-order chemical reactions, the transport processes can be considered as isothermal or non-isothermal
- convective, conductive and thermodispersive heat transport, thermal processes can be coupled to mass transport (referred to as thermohaline processes)
- fully transient, semi-transient and steady-state flow and transport processes
- heterogeneous and homogeneous aquifers
- anisotropy of aquifers (2D and 3D, not necessarily parallel to Cartesian axes)
- confined and unconfined aquifers, multiple free surfaces in 3D (perched water table)
- temporally and spatially variable material parameters
- free or mixed convection problems, recirculating flow patterns, buoyancy effects
- cellular convection processes (saltwater intrusion, gravity-driven sinking of contaminants, thermally driven convection, double-diffusive convection, etc.)
- extended Boussinesq approximation applied to density-coupled processes involving fluid viscosity effects by contaminant concentrations and temperature
- variable density expansion capable of tackling the 4° C anomaly (also under variable saturation)
- boundary fluxes and transfer conditions (i.e. leaching)
- total (convective plus dispersive) flux boundary conditions
- spatially variable initial hydraulic head, concentration and temperature conditions
- fluid, species concentration, and heat budgets
- multi-layered wells in 3D (well bore conditions)

1.6.2 Numerical

Geometrical

- finite element method (FEM)
- Galerkin-FEM and optional streamline, shock capturing or full upwinding
- central weighting and optional upstream weighting for unsaturated flow.
- in 3D: pentahedral and hexahedral prismatic meshes (6-, 8-, and 20-noded finite elements) of first and second order accuracy
- in 2D: triangular and quadrilateral meshes (3-, 4-, and 8-noded finite elements) of first and second order accuracy

Solving

- unsaturated flow: variable switching technique (variable substitution), optional mixed head-saturation form
- unsaturated flow: evaluation of capacity term with chord slope scheme, time centered analytic or analytic derivative
- automatic time-stepping control:
  - based on predictor-corrector methods, explicit Adams-Bashforth predictor and Trapezoidal-rule corrector (termed as AB/TR-scheme) of second order accuracy and a Forward Euler/Backward Euler (FE/BE) first-order accurate scheme with some modifications
  - based on aggressive target based time marching strategies
- implicit first-order and Crank-Nicolson second-order time discretization schemes for fixed time steps
- first (Dirichlet), second (Neumann), third (Cauchy), and fourth (Single Well) type-boundary conditions for groundwater flow, as well as mass and heat transport
- Newton iteration method for nonlinear problems (unsaturated flow, density-driven convection processes)
- optional Picard iteration method with relaxation and forward projection (integral Euclidean error norm for iteration control)
- constraints for all boundary conditions based on complementary minimum-maximum criteria, all constraints can be time-dependent
- optional full control of free-surface conditions via natural constraint conditions
- optional consistent mass and lumped mass computation

- optional single point integral evaluations
- automatic *h*-adaptive mesh refinement (AMR) strategy based on an *a posteriori error* estimator with two options: (1) equal distribution of global error as proposed by Zienkiewicz and Zhu, and (2) equal distribution of the specific error as proposed by Onate and Bugeda

Other

- optional convective (default) and divergence weak formulations of the governing transport equations to allow a generalized (total) flux boundary conditions
- discontinuous (standard) and continuous, balance-improved Darcy flux approximations and evaluation of fluid and concentration budgets
- Best-Adaptation-to-Stratigraphic-Data (BASD) technique for deformable 3D meshes in free-surface problems
- improved particle tracking algorithms on arbitrary 2D and prismatic 3D meshes for pathline and isochrone computations using either Pollock or 4th-order Runge-Kutta tracking algorithms
- fast streamline integrator based on computed discrete velocity patterns in 2D
- automatically controlled, transient movement of phreatic surfaces in unconfined aquifers

1.6.3 Computational

Mesh

- triangular mesh generation for all-triangle meshes, based on an advancing front iterative geometry decomposition approach with smoothing techniques (mesh regularization) and a Delaunay based T-MESH generator supporting Add in's
- quadrilateral mesh generation for all-quadrilateral meshes using a mapped element approach with discrete transfinite mapping (for special needs)
- layer configurator for 3D prismatic meshes: creating, expanding, and deleting slices and layers, inheriting slice and layer properties

Numerical

- preconditioned conjugate gradient (CG) methods for the solution of large sparse systems of equations: for positive, definite flow equations, an incomplete Gauss factorization preconditioning with the CG technique, for the unsymmetrical transport equations, an incomplete Crout factorization preconditioner and a family of advanced iterative solvers are available: restarted ORTHOMIN (orthogonalizationminimization method), restarted GMRES (generalized minimal residual method), Lanczos CGS (conjugate gradient square method), Lanczos BiCGSTAB (bi-conjugate gradient stable method), and Lanczos BiCGSTABP (postconditioned bi-conjugate gradient stable method); PCG techniques are recommended for large problems

- optional: fast (in-core) direct profile (skyline) equation solvers for symmetrical and asymmetrical sparse matrix systems - recommended for smaller problems
- automatic nodal ordering optimization based on the Reverse Cuthill McKee (RCM) Method to reduce fill-in for the direct equation solvers
- Kriging, Akima and inverse distance weighting interpolation and extrapolation techniques for database regionalization, variogram computations based on a spherical model approach.
- tool for generating time varying material data, boundary and constraint conditions (1D and 2D interpolation) from primary data (measured curves).
- mesh enrichment technique for triangular meshes, based on the red/green meshing strategy proposed by Bank

Memory

- fully dynamic memory monitoring, with no software limitations
- matrices compactly stored as vectors
- double precision arithmetic

Other:

- 3-D visualization (volume and surface displays, rotation, translation, shading, 3-D cursor, cuttings, arbitrary sections, fences, isosurfaces, map integration, pathlines, flow vector patterns, and isochrones)
- computation of Relevant Areas of Influence (RAI)
- fast contouring techniques for labeled isoline contours with many options for refinements
- isoline computations for flow and transport results using an element-wise mapped interpolation technique
- pseudo-3D-projection for graphics displaying results using a fast gridding algorithm with a Newton search and a hidden-line algorithm
- automatic resolution procedure to optimize updating effort in the matrix system assembly

- spatial and temporal operations for computational results: difference maps, standard deviation, cumulative changes, and others
- time histories and breakthroughs of contaminants, temperatures and balance fluxes

Software:

- interactive, graphics-based, completely menu-driven simulation system with computer aided design (CAD) properties
- written in about 850,000 lines of ANSI C and C++ source code
- implemented under UNIX, X Window (version 11.4 or later) and OSF/Motif (version 1.1 or later), or Windows 95/NT with Xvision for graphics workstations and PC's
- hierarchical and modular system structure
- GIS-based interface for importing and exporting background maps and databases in the form of the ESRI Shape file format, ASCII (Arc/Info GENERATE) format, Image (TIF) format, AutoCad DXF format, and the widely applicable HPGL data exchange format. Databases refer to lines, points, polygons, and annotations
- Programming interface for coupling external programs with FEFLOW's pre-/post-processing units and simulator kernel
- data interfaces for the FEFLOW subtools FEPLOT (Windows), XPLOT (UNIX) and FEMAP to manage the entire plotting output and the GIS interconnection.

1.7 System Requirements

FEFLOW requires the following hardware and software:

1.7.1 Hardware

UNIX

- a high resolution color graphics UNIX workstation, providing eight bit-planes (256 simultaneous colors) and full 32-bit or 64-bit virtual memory architecture
- 32 MB main memory (minimum)
- 130 MB hard disk free space (minimum)
- recommended: RISC workstations with1280 x 1024 pixel display

PC

- Pentium 133 or higher
- exactly 256 color video mode with a resolution of 1280 x 1024 or higher
- 32 Mb of RAM (minumum, 64 Mb or higher recommended for 3D)
- 130 Mb of disk space (minimum)
- recommend Pentium Pro processor with high resolution monitor and graphics card (exactly 256 colors, 1280 x 1024 resolution)

1.7.2 Software

UNIX

- UNIX System V (or equivalent) and optional NFS for networking

PC

- Windows NT (4.0 or higher) or Windows 95
- TCP/IP protocol installed
- Xvision X Window server (supplied with FEFLOW)

The source code of FEFLOW is not free for distribution.

Present installations:

- DIGITAL UNIX 4.0+
- Sun Solaris 2.4+
- IRIX 6.2+
- AIX 4.1.4+
- HPUX 9.++, 10.++
- Microsoft Windows 95 and Microsoft Windows NT 4.0 (and higher)

2 Database and GIS-Coupling

2.1 Why GIS?

Numerical models for subsurface flow and transport processes require detailed knowledge of multidimensional parameter fields (conductivity, storativity, dispersivity, reactivity, etc.). Their determination and derivation for complex numerical modeling is often a time-consuming task, that increases the risk of data errors and is more or less subjectively dependent on the modelers.
The development, handling and updating of the entire database consisting of geographical, hydrogeologic, physical and computational data in different forms and formats has been shown to be inexpedient and unproductive without the use of a powerful information system in the form of a Geographical Information System (GIS). Figure 2.1 shows the ArcView visualization of primary GIS data and results exported from FEFLOW.

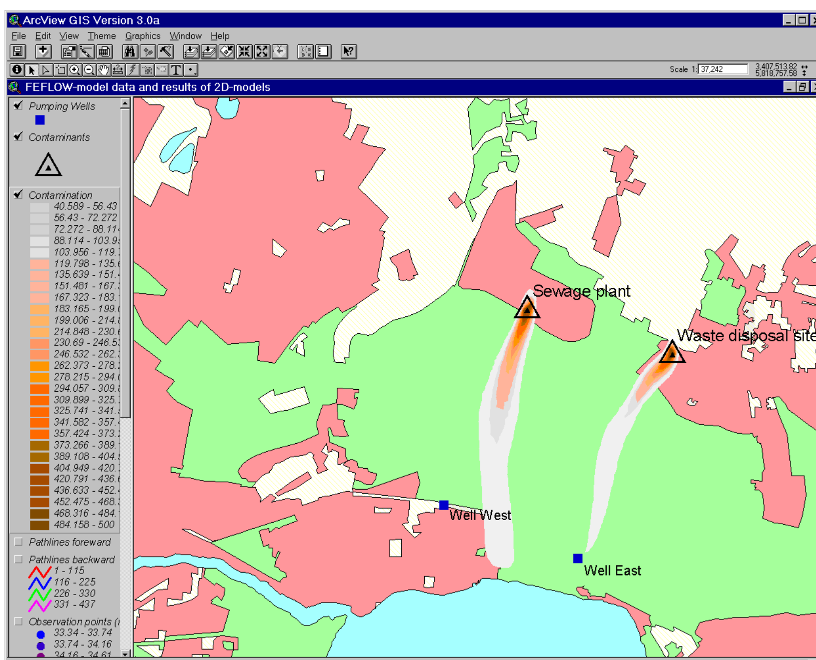


Figure 2.1: GIS data and model results in ArcView

The frequent practice of tailoring the database to a model with specific conditions and requirements (application background, hydrogeologic conceptualization, numerical discret-

ization, computational solution environment, etc.) leads to a rigid dependency of the database upon the numerical model and the computer hardware and software capabilities currently available. This hinders the frequent updating of both the database and the modeling software.
Application of the model often requires extensive work regarding the data preprocessing, model design, and calibration, as well as postprocessing of vast amounts of model results. Effectively, the effort for preprocessing and postprocessing is dominant and exceeds the work needed for the actual computational process.
The advances in computer technology also allow technical planners and decision makers in groundwater management to use numerical transport models. The databases available in these models must frequently be updated to provide effective access to numerical modeling. It is implied that a more general data management system is needed for storing, analyzing, and displaying temporally and spatially distributed data.

2.2 FEFLOW Data Interface

The FEFLOW simulation system incorporates a GIS-based data exchange interface. FEFLOW supports the widely used vector-based GIS ARC/INFO and ArcView. The correspondence with GIS takes place by a generalized ASCII-based data exchange format (compatible to the ARC/INFO Generate format) and the shape file format, compatible with ArcView. These formats support the automatic import of attribute data linked to spatial data. Another geometric data import format is the traditional HPGL format. Various techniques for geographic database manipulation (map overlaying, data transformation, data capturing, data regionalization, etc.), previously done exclusively under GIS, have to be supported directly in the FEFLOW modeling environment to maintain the fast dynamic data flow during interactive modeling. The GIS remains a tool for generating, housekeeping, updating, storing, and displaying of measured data. The numerical simulation produces massive data which are mostly of a very transient nature. A number of different simulation cycles may be necessary to get reliable model results (suitable for future use or study) before storing them in the GIS. The diagram shown in Figure 2.2 summarizes the data access and flow for the interactive simulation system, FEFLOW with subtools like XPLOT or FEPLOT in the context of the GIS ARC/INFO and ArcView. Using the *Shell* menu, you can import databases in the form of line-, point-, polygon- and annotation-related ARC/INFO compatible (ASCII) formats as well as the ArcView shape file format, Raster Databases (TIF) and HPGL formatted data. ASCII data formats for temporal power functions, measured results in the form of data triplets, and the complete FEM database (mesh geometry, attributes, functions and others) can also be accessed through the *Shell* menu (import and export). GENERATE formats shape files and dxf files for resulting output are produced by the **Simulator Kernel** and the **Postprocessor**. In this context the FEFLOW subtools XPLOT and the FEPLOT serve as plotter interfaces

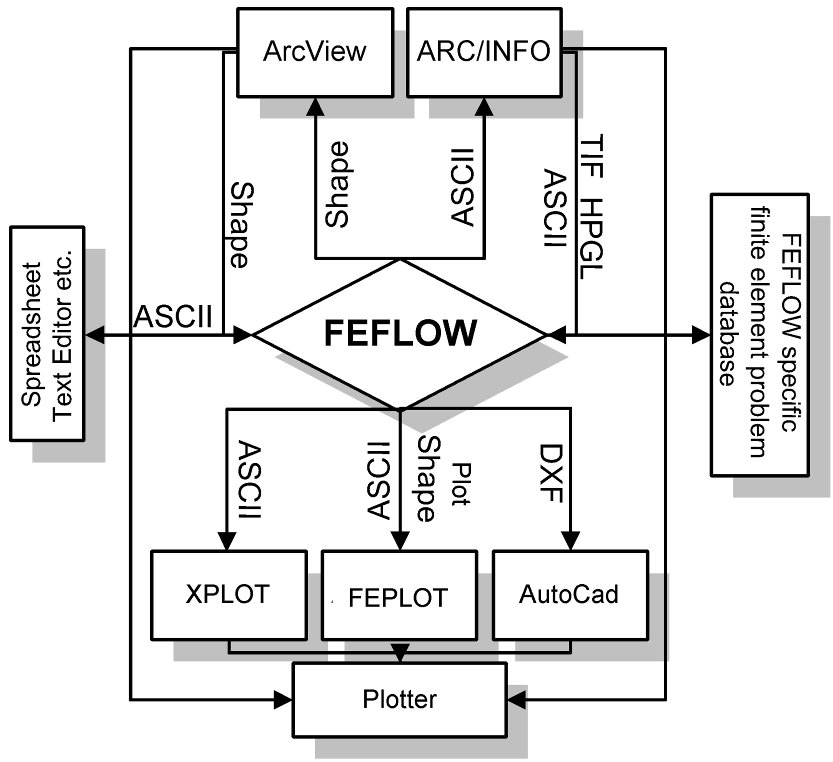


Figure 2.2: FEFLOW Data Access and Interchange

for the computational results of the FEFLOW simulator, as indicated in Figure 2.2. Accordingly, during a simulation or postprocessor run, each interesting result in the corresponding time level can be saved, if desired, in a number of files. These data files may be input either directly to the GIS ARC/INFO or ArcView again or, preferably, to the XPLOT or FEPLOT tool. An example of the FEPLOT interface is shown in Figure 2.3. All data exchange file types used in FEFLOW are summarized in the next section.

2.3 File Handling

Files in the FEFLOW system are stored in a hierarchy of directories. They are assigned to different directories according to the type of information they contain (denoted by different filename extensions). While the subdirectory names are arbitrary, the file extensions are obligatory. Table 2.1 summarizes the file attributes used in FEFLOW. All files can be written as ASCII or binary code. You should note the useful distinction between

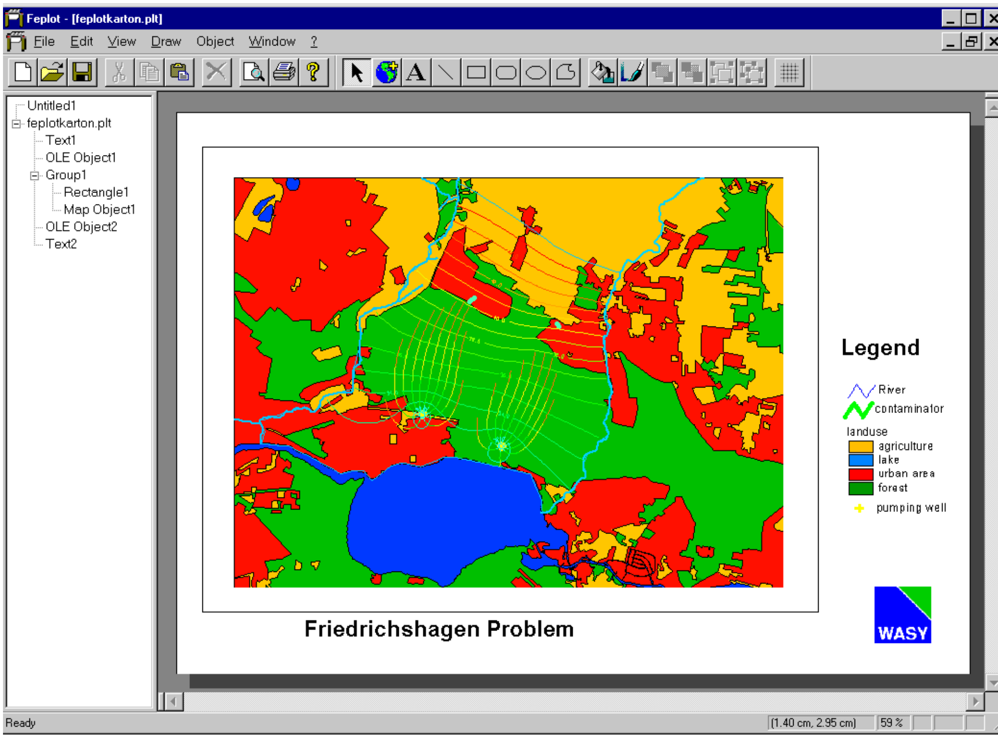
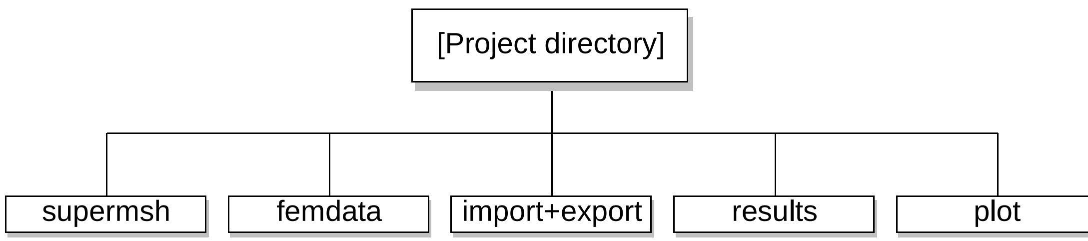


Figure 2.3: FEPLOT.

superelement mesh data (***.smh**) and problem or refined FEM mesh data (***.fem**). For example, the same superelement mesh structure can be the data basis for different finite element meshes. While the superelement mesh data files (***.smh**) contain only the data for the designed coarse superelements (the output from or the input for the **Mesh Editor** and the input for the **Mesh Generator**), the refined FEM problem data (***.fem**) are produced in the **Mesh Generator** and completed using the **Problem Editor**. Only the ***.fem** files are able to run with the **Simulator Kernel**. The **Help** files (***.html**) are read in the FEFLOW online **Help** system.

FEFLOW offers a choice between reduced data (***.dar**) and complete resulting data (***.dac**) for saving the computational results. *.**dar** contains only the computational results for the marked observations points, for single wells if they occur, and for flux boundary sections (e.g. galleries, well screens, outflowing boundary sections) automatically determined in the simulator. ***.dac** contains all output data for each mesh point. This means that a great amount of data can result when working on large problems. The ***.dac** files are the input of the **Postprocessor**. They enable a complete postprocessing for the saved time levels. The resulting data files contain the values for the hydraulic head, the velocity components, the chemical species concentration and the temperatures at the nodes and at the selected time-step level.

The import of background maps is supported by the **Map Assistant**, which is capable of georeferencing and rectifying raster images. The import of background maps is also supported by the **Map Manager**, a program controlling the display of the maps.
Exporting of data in many standard and user-defined formats can be done via the **Data Store Manager**. It allows you to link spatial data with (optional time varying) attribute data. For more detailed information about file handling and file formats, see the **File Format Library** of the online **Help** (enter from the *Shell* menu by hitting <**F1**>).
For uncomplicated file handling you have to organize the modeling data under standardized names:



This enables FEFLOW to open automatically the right directory for importing or exporting data. All path definitions which lead to such a directory group are stored in your **home directory** (UNIX) under the directory *.feflow_prefs/[current version number]/* or in the **registry** (Windows) under *Software/Wasy/Feflow/[current version number]/*, respectively. During the start-up phase, FEFLOW reads the settings and pre-configures the corresponding file streams. The file streams that get pre-configured are for superelement mesh data (***.smh**), the FEM problem data (***.fem**), the resulting data (***.dar**)(***.dac**), the help files (***.html**), and multiple import and export files which are listed in Table 2.1. Now, once you have loaded or saved a finite element problem (*.fem) or a complete results file (*.dac) FEFLOW stores this path and will make it available in all file selection menus for the current session as well as for the next ones.

Table 2.1: The Files Used in Feflow.

Type of Information	Filename Extension	Recommended Subdirectory
Superelement mesh data	*.smh	supermsh/
Problem FEM data	*.fem	femdata/
Help	*.html	help/
Reduced resulting data	*.dar	results/

Table 2.1: The Files Used in Feflow.

Type of Information	Filename Extension	Recommended Subdirectory
Images (Raster Databases)	*.tif	import+export/
HPGL files	*.hpg	import+export/
Line ASCII files	*.lin	import+export/ or plot/
Polygon ASCII files	*.ply	import+export/ or plot/
GRID ASCII files	*.asc	plot/
ESRI shape files	*.shp	import+export/ or plot/
Annotation files	*.txt	import+export/
Point ASCII files	*.pnt	import+export/ or plot/
FEPLOT plot files	*.plx	plot/
FEPLOT plot composition	*.plt	plot/
Time-varying power functions	*.pow	import+export/
Database triplets	*.trp	import+export/
Complete resulting data (postprocessor)	*.dac	results/
AutoCad DXF	*.dxf	plot/
Plot description (readable by XPLOT)	*.fpd	plot/

Selection for file reading or writing in the FEFLOW system is done with the graphics **File Selector** box.The selection box is quite self-explanatory and easy to understand. As soon as it appears, the box displays the files with their extensions and locations. These agree with the paths of the current or formerly used projects. They can also be read from the configuration file (UNIX) or registry entry (Windows NT/95). You can click (with the mouse) on a file from the scroll list and activate its operation by selecting the OK button. A double click on a file will also activate the operation. The **Cancel** button is available if you wish to abandon a selection. To create new files, you can type the file name in a text **Selection** box within the **File Selector** box. The **Filter** button allows you to filter the file entries corresponding to the file extensions.

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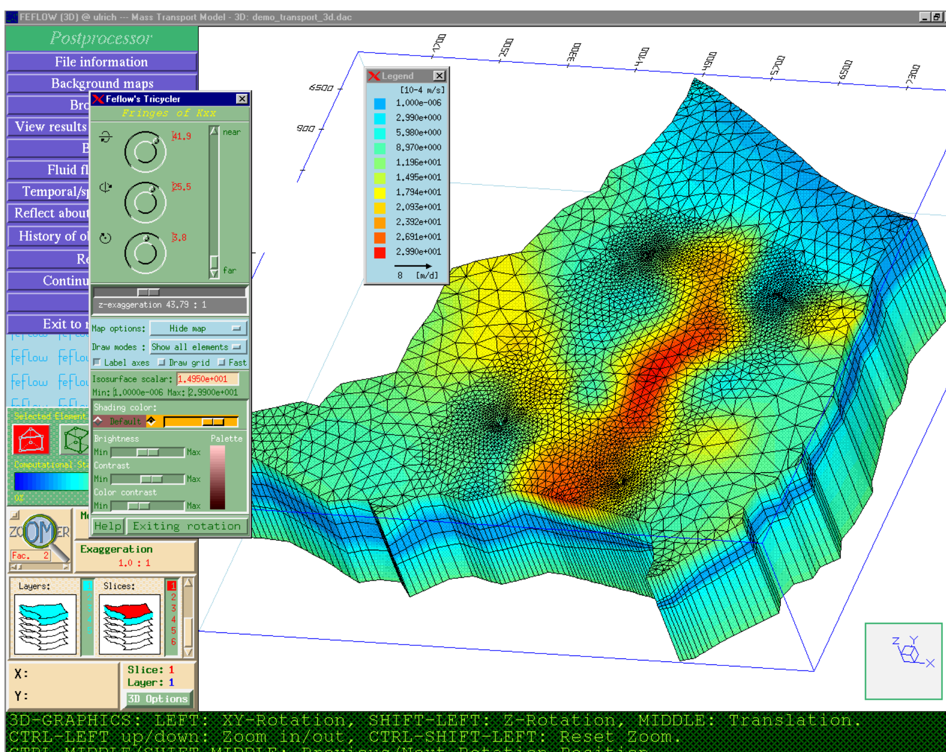
Part II

Demonstration Exercise



1 Scope and Structure

The scope of this tutorial is to introduce the novice user to the philosophy of modeling three dimensional flow and transport problems based on real world data with the help of FEFLOW. The following steps define the tutorial procedure:

Step 1 - Design the basic structure of the model using background maps as templates to generate the supermesh and the finite element mesh.

Step 2 - Develop the model into a 3-Dimensional structure.

Step 3 - Assigning flow initials, boundary conditions, material parameters, etc.

Step 4 - Run the simulation

Step 5 - Postprocessing that features analyzing the model results and data export.

For the installation of FEFLOW please refer to the booklet of the FEFLOW CD-ROM.

Note: You can skip any one of the steps in this excercise by loading the problem files that are already prepared.

1.1 Terms and Notations

For the purposes of this demo, the following terms and notations will be used:

↵	Press the <Enter> key
♦	Click on the toggle beneath the indicated option.
☞	Click the left mouse button where indicated
"Switch"	Switch a button from one option to another, by clicking on it, holding the mouse button down, moving the cursor on the indicated option and releasing the button.

1.2 Starting FEFLOW

On Windows NT/95

Start FEFLOW via the *WASY* entry in the *Programs* folder of the Windows *Start* menu.

☞ "FEFLOW Demo"

FEFLOW will start in the demo mode.

On Unix

Type "feflow -demo" and hit the <Enter> key.

The Main Window of FEFLOW will be displayed on your screen. You are now in the FEFLOW demo mode. The demo mode does not allow you to save any files or to open unregistered files.

1.3 Model Scenario

A fictitious contaminant plume has been detected near the small town of Friedrichshagen, southeast of Berlin, Germany. An increased concentration of a contamination has been found in the town’s two drinking water wells. There are two potential sources of the contamination; the first is the sewage treatment plant located in an industrial area situated to the northwest of the town. The other option is a wastewater disposal site found to the northeast of Friedrichshagen.
For studying the groundwater threat and potential pollution, we need to design, run, and calibrate a three-dimensional groundwater flow and contaminant transport model of the area. First we need to define the model domain. The town is situated in the middle of many natural flow boundaries, such as rivers and lakes. There are two rivers that run north-south on either side of Friedrichshagen that can act as the eastern and western boundaries. The lake Mueggelsee will limit the model domain to the south. The northern boundary runs along an east-west flowline north of the two potential sources of the contaminant.
The geology of the model domain is comprised of Quaternary sediments. The hydrogeologic system concerns two aquifers separated by a clay aquitard. The top hydrostratigraphic unit is considered to be a sandy unconfined aquifer up to 7 meters thick.The second aquifer located below the clayey aquitard has a thickness of 30 meters. The northern part of the model area is primarily used for agriculture, whereas the southern portion is dominated by forest.

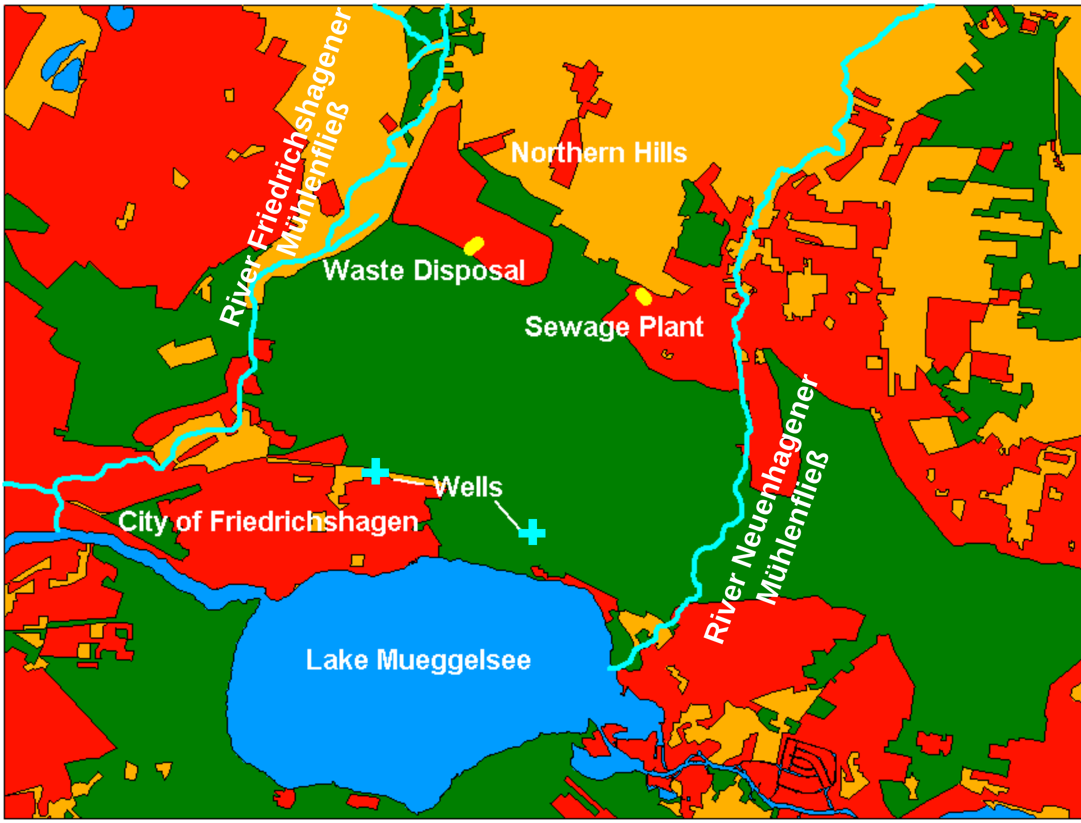


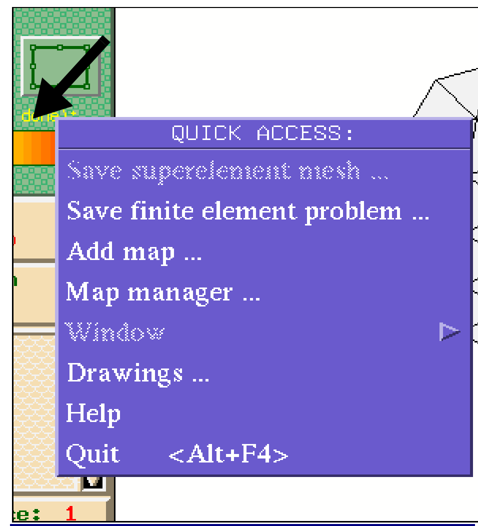
Figure 1.1: Site View of the Model Domain

NOTE: This map was created by importing GIS data for the model into FEPLOT, a plotting & desktop mapping tool made by WASY, which is included on the FEFLOW CDROM. FEFLOW supports the ESRI shape file format, Arc/Info compatible ASCII formats, DXF and FEFLOW specific plot formats for displaying background maps and exporting data.

2 Step 1 - Basic Structure

To define the outer borders of the finite element model, a superelement mesh must be digitized. The superelement mesh will provide the basic structure of the model. Designing the superelement mesh is accomplished via the **Mesh Editor** located in the **Edit** menu of the Shell.

To enter the **Mesh Editor**,



☞ **Edit** in the top bar of the Shell menu

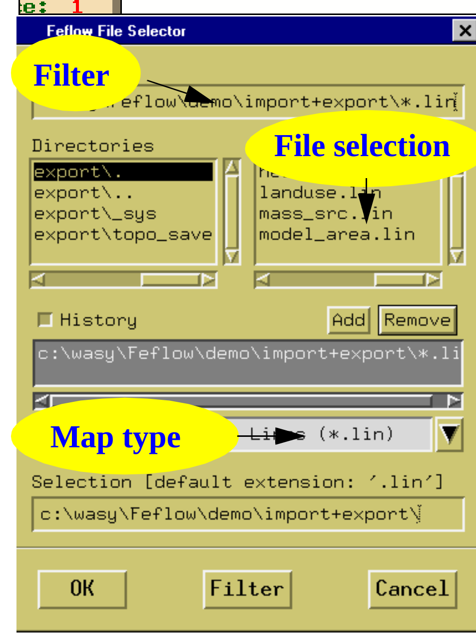
☞ **Design superelement mesh**

The **Mesh Editor** menu appears along the left hand side of the window.To construct the superelement mesh, we need to load the background maps and use them as templates. This can be accomplished by using the Quick Access menu. Click anywhere on the green colored part of the screen. The **Quick Access** menu should appear.

Holding the left mouse button, select "***Add map ...***" from the menu.

The FEFLOW **File Selector** appears. The uppermost field, called the ***Filter***, displays the current directory path. FEFLOW automatically searches for data in the directory called ***import+export***. The ***Map type*** field allows you to choose between different map formats.

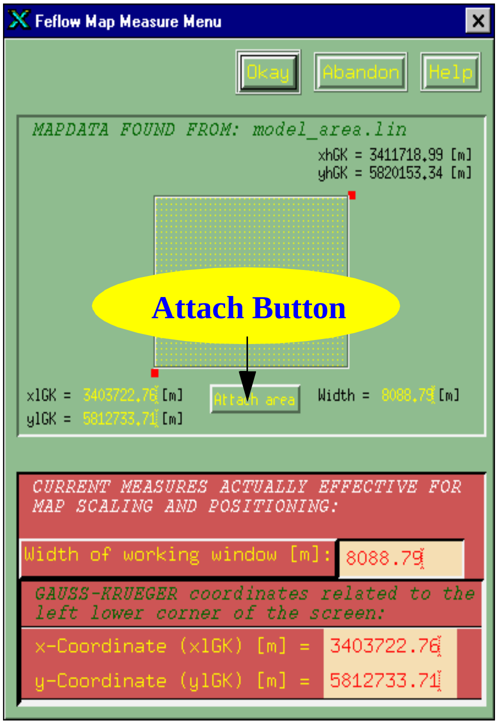
The ***Files*** field displays all the available files of the seleced map type.



☞ ***model_area.lin*** in the *Files* list.

☞ **[OK]**

The **Map Measure Menu** appears. The **Map Measure Menu** allows you to define the extent of the background maps and the co-ordinates of the Working Window.



☞ **[Attach area]** in the middle of the window. The attach area button references all additional maps to the attached map co-ordinates.

☞ **[Okay]** to import the map.

FEFLOW executes an automatic georeferencing and scaling utility of the working window to the co-ordinates of the background map and displays the map in the working window. Next we will import a map showing the landuse of the area.

Click anywhere on the green colored part on the left of the screen. The **Quick Access** menu appears.

Holding the left mouse button, select ***Add map ...*** from the menu. The FEFLOW **File Selector** pops up.

☞ ***landuse.lin*** in the *Files* list.

☞ **[Okay]**

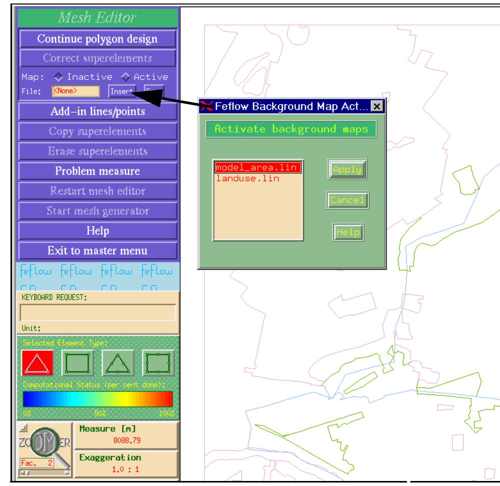
The **Map Measure** menu pops up.

☞ **[Okay]** to import the map. **Do not** attach the area a second time.

We have now imported the required model area and landuse maps for our investigation. If more background maps are required, FEFLOW can import raster images. If necessary, images can be referenced via the FEMAP Assistant that is included with FEFLOW. Saving is possible in Arc/Info, ArcView, MapInfo and FEFLOW compatible formats. To save time, we will skip this and begin generating our superelement mesh.

2.1 Designing the Superelement mesh

Before starting with the construction, activate the background map ***model_area.lin*** as the template for the superelement.



☞ **[Insert]** button in the *Map* field on the left of the working window, below the **[Correct superelements]** button.The background map activator pops up listing all generated line and point files you have imported.

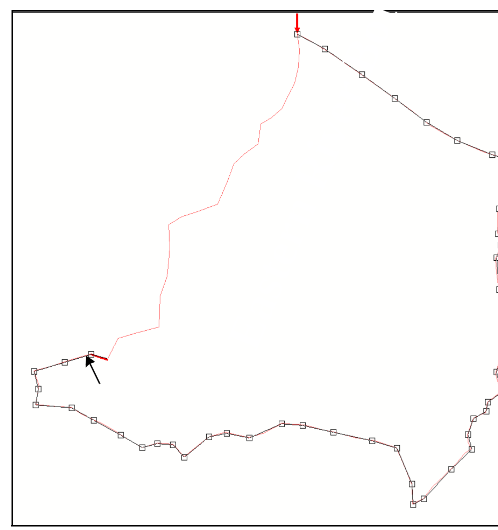
☞ ***model_area.lin*** as the background map.

☞ **[Apply]** to exit the map activator.

♦ **Active** The map is now activated.

We must now define the outside boundary of our model.

☞ **[Continue polygon design]** (The cursor becomes a cross-hair.)



Move the cursor to the outline of the ***model_area.lin*** map in the working window. If the cursor is within the snap distance to the map, a part of the map outline becomes red.

Nodes need to be set at fairly equal intervals around the perimeter of the model area. Define the nodes, by clicking the left mouse button along the model outline.

Digitize around the model area. When you return to the first node, close the polygon by clicking a second time on the first node (marked by a red arrow). The polygon will become shaded gray.

Note: You can undo the last digitized nodes by clicking the middle mouse button For a two-button mouse: click both buttons simultaneously.

To exit the superelement mesh module, click the right mouse button in the model area.

By creating the polygon, you have now defined the outer border of the model. Next we will import the so called **Add In's**. Add In's are lines or points which FEFLOW uses as focal points to create finite element nodes during the mesh generation. Add In’s are very useful to position boundary conditions like contaminant mass sources or wells in exact locations. First we have to load the Add In’s as background maps:

Click anywhere on the green colored part of the screen. The **Quick Access** menu should appear.

Holding the left mouse button, select "***Add map ..."*** from the menu.The FEFLOW **File Selector** appears. The uppermost field, called the ***Filter***, displays the current directory path.The ***Files*** field displays all the available files of the seleced map type.

☞ ***mass_src.lin*** in the *Files* list, the background map which describes the locations of the contaminant sources at the sewage treatment plant and the waste disposal.

☞ **[OK]**.The **Map Measure Menu** appears.

☞ **[Okay]** to load the map. Two small lines are displayed on the model.

Repeat the steps described above for the background map ***demo_wells.pnt*** for visualizing the ASCII point map of the well locations. You have to select **ASCII Point (*.pnt)** from the ***Map type*** field in the **File Selector** (see page 33):

☞  at the ***Map Type*** list. The list pops up. Select **ASCII Point (*.pnt)**

Now we activate the two background maps as Add in’s like before for the polygon design:

☞ **[Insert]** button in the *Map* field on the left of the working window**.** The background map activator pops up listing all generated line and point files you have imported.

☞ ***mass_src.lin*** as the background map.

☞ **[Apply]** to exit the map activator.

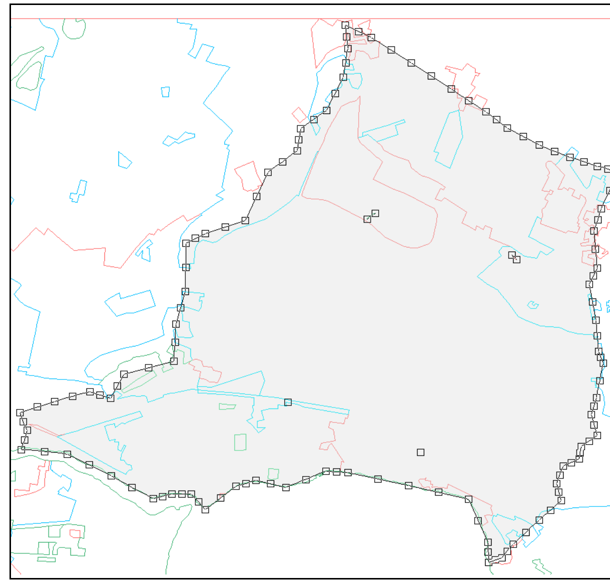
♦ **Active** The map is now activated.

☞ **"Add lines from map".** The lines are imported as Add in's automatically.

Repeat these steps to include two pumping wells located in the southern portion of the map. Use ***demo_wells.pnt*** the dynamically renamed button **[Add point from map]**. The mesh should look like the figure to the right.

☞ **[Continue mesh design]**

☞ **[Exit to master menu]**



2.2 Generating the Finite Element Mesh

If you have skipped the previous steps, please load the file ***demo.smh*** via the **Load super element mesh** option in the **File** menu before beginning this exercise. Please note that loading this file brings you directly to the Mesh Generator Menu.

The finite element mesh is generated in the **Mesh Generator Menu**.

☞ **Edit**

☞ **Generate Finite Element Mesh**

☞ **Generate automatically** (The **Mesh density input** menu pops up.)

Enter an element number of "**500**" . The element number is an educated estimate based on the size and type of model.

☞ **[Start]**

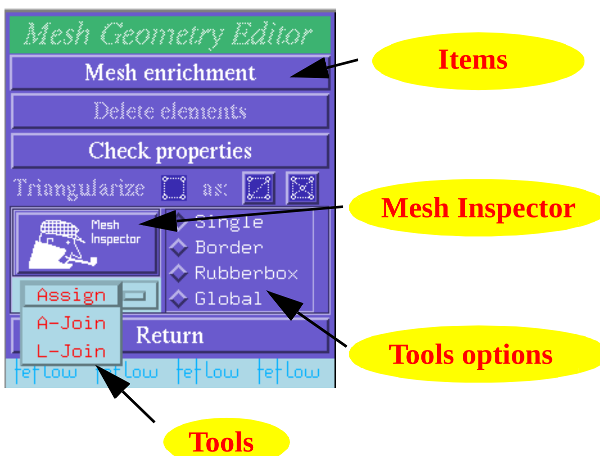
The TMesh generator is an extremely accurate tool that creates precise meshes based on your Add In's and boundary design. It does however take more time for generating compared to the other two mesh generators available with FEFLOW.

2.3 Mesh Geometry

For our mass transport simulation, the mesh is too coarse in the area where the contaminant will be distributed. Therefore the mesh must to be partially refined.

☞ **[Mesh geometry]**

You will enter the **Mesh Geometry Editor**. Before starting the mesh refinement, please note these fundamental rules for using the FEFLOW tools: (see next page)



When refining the model...

1. Choose a tool.
2. Select 1 of the options offered.
3. Choose the item/parameter you want to edit.
4. Start editing.
5. Exit the function by clicking the right mouse button.

The menu functions are listed on the left of the working window. The upper buttons define the items [Mesh Enrichment], [Delete elements] and [Check properties]. The icon showing a man's face activates the **Mesh Inspector** which gives you information about the parameters assigned to each node/element. The **tools** can be selected by clicking on the light blue button below the mesh inspector. Having selected a tool, different options are offered in the field right of the tools button. If you are going to change the global value settings, a red alert box will warn you and ask for confirmation.
To refine your mesh, you need to import a polygon background map which shows the area that you want to redefine. To do this,

Click anywhere on the green colored part on the left of the screen ('Selected Element type' and 'Computational status' icon). The **Quick Access** menu appears.

Holding the left mouse button, select ***Add map ...*** from the menu. The FEFLOW **File Selector** appears.

☞  at the *Map Type* list. The list pops up. The *Map Type* feature allows you to search for file extensions more efficiently.

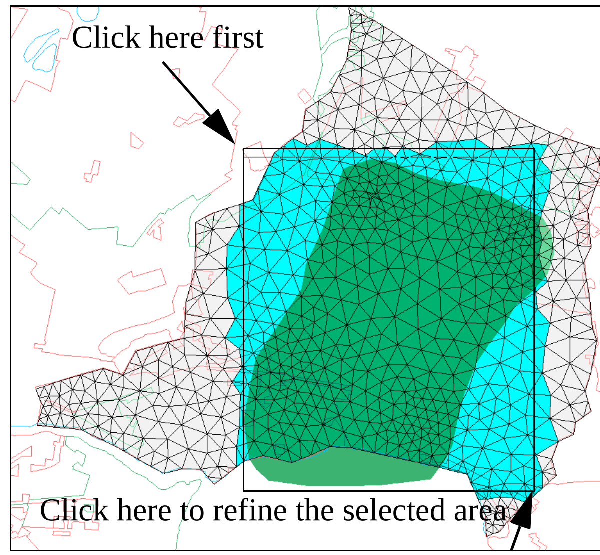
☞ **"ASCII Polys (*.ply)"**

☞ ***demo_refine.ply*** in the *Files* list.

☞ **[Okay]**. The **Map Measure Menu** appears.

☞ **[Okay]** to import the map. The area that we will refine is shown as a green colored polygon. There are several different possibilities for refining the mesh. To save time, we will use the **"*Rubberbox*"** option.

The tools button is set on "**Assign"** by default.



♦ **Rubberbox**

☞ **[Mesh Enrichment]** and hold the left mouse button.

Select **Refine** from the small pop up menu and release the left mouse button.

Click on the screen to set the upper left corner of the rubberbox.

Move the cursor over the model until the light blue rubberbox covers the area of the polygon background map.

Click the screen to set the lower right corner of the rubberbox. The mesh refinement is executed. To undo the mesh refinement, repeat the steps. However select **"Derefine"** to undo the grid refinement to the regions which lie inside the polygon.

Note: You can also refine the mesh using the polygon background map. Selecting the "active" template, click on (A-Join tool). Select polygons and load *demo_refine.ply*.

You can switch the background maps off by selecting the **Map Manager** from the **Quick Access** menu.

☞ **[Return]**

☞ **[Exit to master menu]**

3 Step 2 - The 3rd Dimension

If you have skipped the previous steps, please load the file ***demo_2d.fem*** via the **Load finite element problem** option from the **File** menu before beginning this exercise.

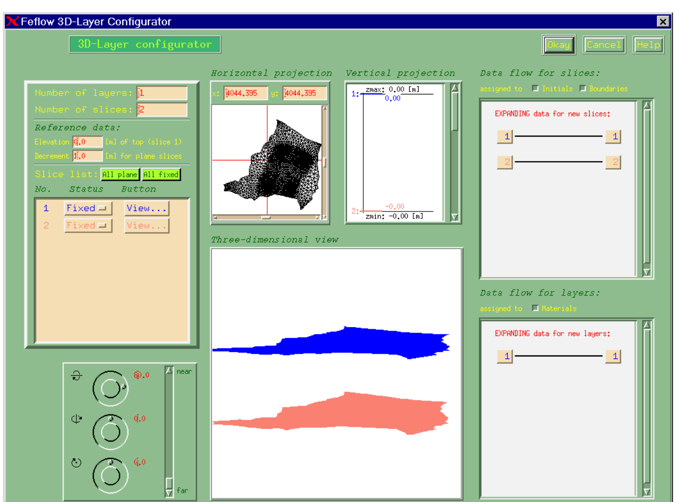
Until now, you have only designed a two-dimensional model. The following steps describe how to introduce the third dimension into your model using FEFLOW. A three-dimensional finite element model is built up by a number of nodal planes, called **slices**. These slices can be regarded as the top or bottom planes of the (geological) **layers**.

Note: When modeling one layer you need two slices, the top and bottom slice. When modeling two layers you need three slices, the top slice, the dividing slice between the two layers and the bottom slice. Initial conditions and boundary conditions are assigned on slices, while material parameters are assigned to layers.

3.1 Designing Slices and Layers

☞ **Dimension**.

♦ **"Three-dimensional (3D)"**. The **3D-Layer Configurator** pops up. See figure below.



The 3D-Layer Configurator controls the basic settings for the 3D model. Assigning the number of layers and slices, assigning the data flow between slices and assigning the relative position between the slices. For this exercise, we will import the topographic data in the **3D-Slice elevation menu** later.

You will now define the number of layers/slices you need for the this model. The upper aquifer is limited by the ground surface and by an aquitard at the bottom. The second aquifer lies below the aquitard, underlain by a clay layer of unknown vertical extension. We will first create the slices necessary for the stratigraphy of the existing area.:

In the *Reference data box,* enter an elevation for the top slice at "**1000m"** in the *Elevation field* and a decrement of "**100m"** in the *Decrement field*.

This will set the top slice of the model at an elevation of 1000 m, with all remaining slices set with a vertical distance of 100m apart. These settings will prevent problems of slices intersecting when assigning real z-elevations from borehole data. We will now assign the 3D layers.

In the *Number of layers* input box, insert a value of "3".

Note: The number of slices automatically changes to 4 slices.

↵ to add the layers.

As you can see, the 3D-Layer Configurator offers many other tools such as the FEFLOW Slice Partitioner for defining layers. The online **Help** supplies you with more detailed information about this menu. For this demonstration exercise, we will not need these tools.

☞ **"Okay"** to exit the menu.

4 Step 3 - Editing Model Parameters

> If you have skipped the previous steps, please load the file "**demo_3d.fem**" via the "Load finite element problem" option of the File menu.

We will define the parameters of the model by entering the **Problem Editor Menu.** The existing parameters already have default values set. To save time, we will only modify some of these parameters. Enter the Problem Editor.

☞ **Edit**

☞ **"Edit problem attributes.. "**. The **Problem Editor** appears.

According to the FEFLOW philosophy, the most efficient procedure to develop a model is to work from the uppermost option down to the lower ones.

4.1 Problem Class

In the Problem Class Menu we will define the principle model type of the model. Our model will be a transient flow with mass transport for unconfined aquifers using the **BASD** moving-grid technique. For information about BASD click on the **"Help"** buton in the **Free surface editor** and follow the link to the **"Theory"** button.

☞ **"Problem class"** to enter the Problem Classifier.

Since we are conducting a transient flow/ transient mass transport model, click on;

♦ **Flow and Mass Transport**.

♦ **Unconfined (phreatic) aquifer(s)**.

☞ **"Edit free surface(s)"**. The **Free surfaces editor** appears. This will allow us to define the hydrogeologic properties of the slices.

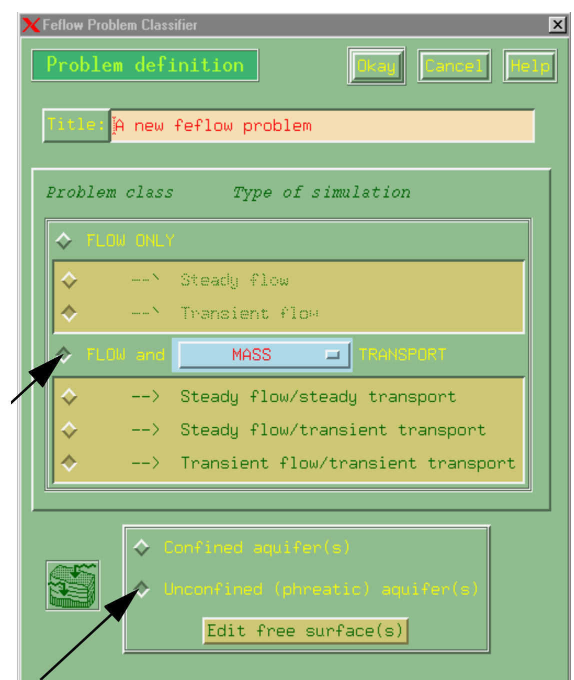
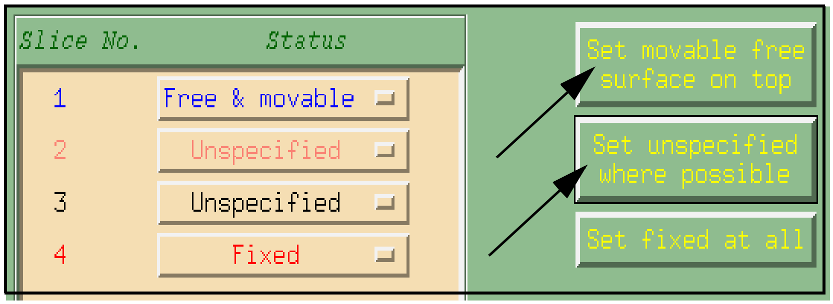


Figure 4.1: Feflow Problem Classifier

☞ "**Set movable free surface on top"**. Now the top slice will follow the groundwater surface..

☞ "**Set unspecified where possible"**. These slices will be distributed according to the moving groundwater surface and the stratigraphy

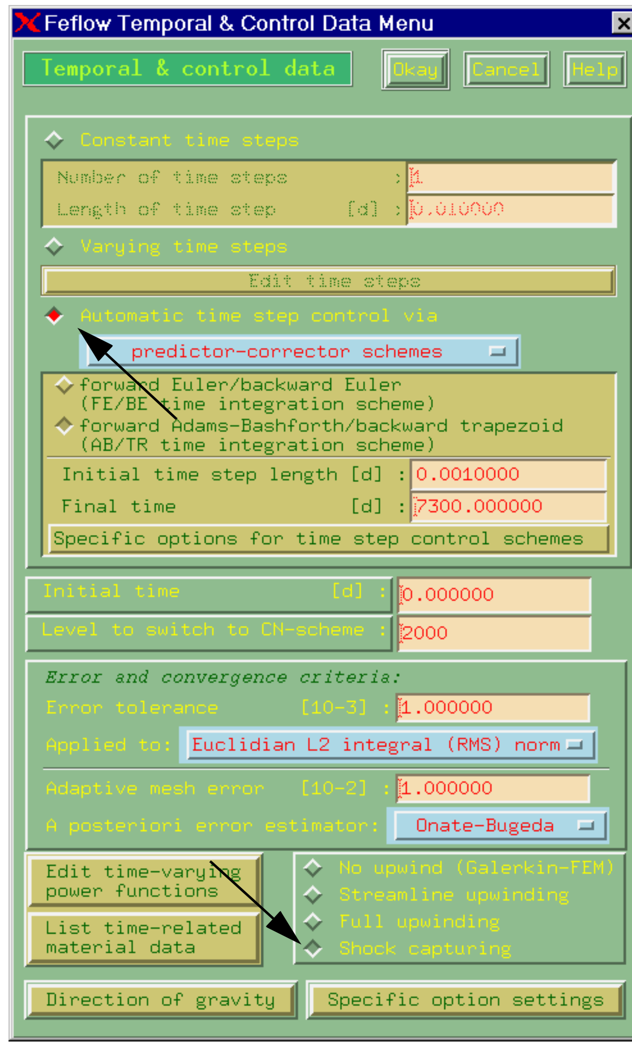
.☞ **"Apply"**



☞ **"Okay"** to exit the Problem Classifier.

The model now describes an unconfined flow & mass transport problem with moving grid properties, i.e). the mesh will follow the moving groundwater table according to the BASD technique for avoiding dry fallen elements.

4.2 Temporal & Control Data



In the Temporal & Control Data Menu, all parameters regarding time and time varying functions are defined or imported. Also, the error norms and the upwinding technique for suppressing numerical oscillations are specified here.

For our purpose, we will set the parameters for the time steps during the simulation run. The simulation should run over 20 years by using the automatic time step control option and the shock-capturing upwinding method for the mass transport simulation:

☞ **"Temporal & Control Data"** to open the menu

♦ **Automatic time step control via predictor-corrector scheme**.

Input an **initial time step length** of "**0.001"** days.

Input a **final time** of "**7300"** days.

We will now select the **Shock capturing** upwinding method which adds a nonlinear anisotropic damping factor to stabilize convection-dominant transport processes. It provides a powerful method to remove numerical oscillations around abrupt layers or fronts of the solution with a minimal amount of numerical dispersion. Numerical damping is only performed in the vicinity of sharp gradients. Outside the fronts numerical dispersion vanishes or becomes significantly reduced

♦ **Shock capturing** upwinding method at the lower right corner of the menu.

☞ **"Okay"** and exit the **Temporal & Control Data Menu** .

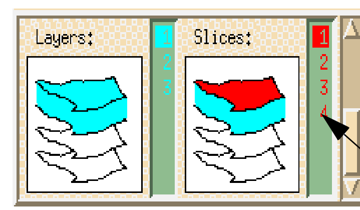
4.3 3D- Slice Elevation

The 3D-Slice Elevation Menu allows you to define the slices based on real-world **z-**elevations by regionalization of irregularly distributed data points, i.e. from borehole logging. Database regionalization of all initial values, boundary conditions and material parameters can be assigned on the model as described for the z-elevations of the slices.

☞ **"3D- Slice elevation"** to enter the Slice Elevations Menu.

In the **Layer configurator** (Section 3.1) we had set the top slice on 1000 m and the lower slices with and vertical spacing of 100 m. Now we will “pull down” the slices on their real-world elevations by assigning the corresponding z-elevations. For avoiding intersection we will assign the data on the lowest slice first:

Select slice **"4"** by clicking on the corresponding number in the Layers & Slices browser at the lower left side of the screen. In the browser, the left column lists the numbers of layers while the right column lists the number of slices.

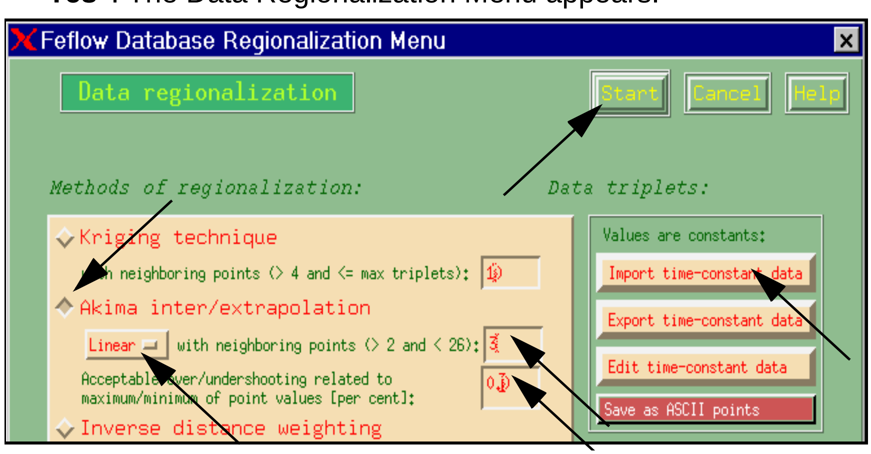


To import z-elevations of the slice based on borehole data, we must enter the **Database Regionalization Menu**.

♦ "***Database"*** option (left of the mesh inspector).

☞ **"z-Coordinates"**. An alert box pops up asking if you want to overwrite the existing values.

☞ **"Yes"**. The Data Regionalization Menu appears.



♦ ***Akima inter/extrapolation***.

Switch the drop down button from **"*Cubic*"** to the ***Linear*** method by clicking the left mouse button and holding.

In the ***neighboring points*** field, type **3.** Only the nearest three neighboring data points will be used for the interpolation.

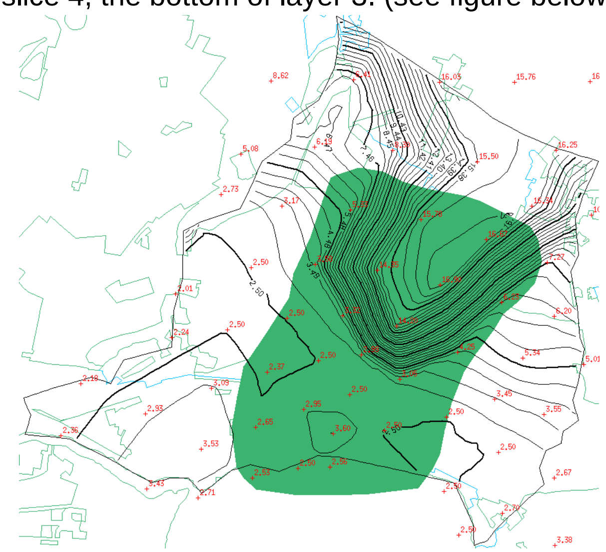
In the ***Acceptable over/undershooting*** field, type **0**. This assures that the interpolation will be executed, without smoothing the resulting surface.

☞ "**Import time-constant data**". The file selector appears and allows you to select your regional information.

☞ **[bot_san2.trp]** in the *Files* list. This ASCII file has an *x-coordinate, y-coordinate, function-value* format.

☞ **"Okay"**

☞ **"Start"** in the Database Regionalization Menu and FEFLOW creates contours for the slice 4, the bottom of layer 3. (see figure below)



Exit the Assign database function by clicking the right mouse button in the model domain.

Browse to the next upper slice using the Layer & Slices browser and repeat the above steps assigning the data files according to the list located on the next page.

Table 4.1: Regionalization of Z-Elevations

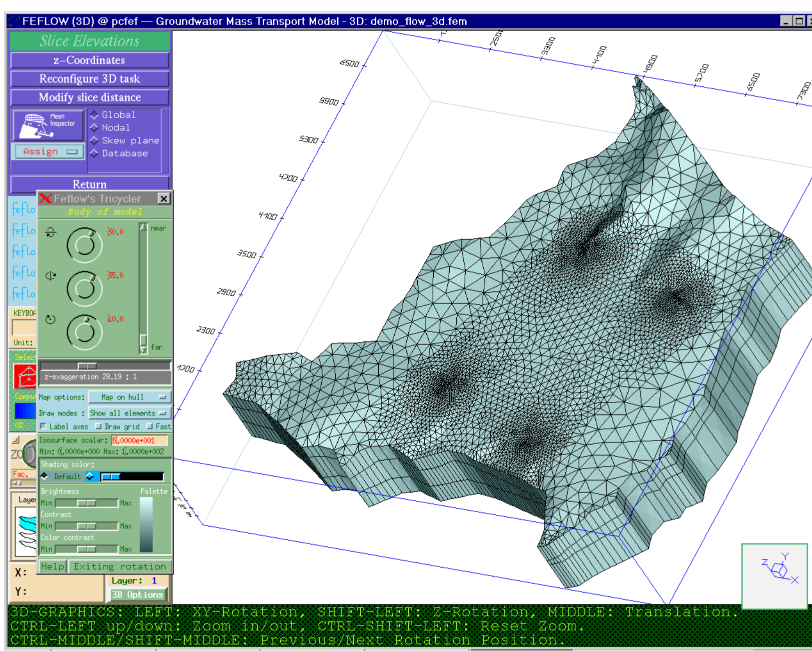
slice	database
4 (bottom of lower aquifer)	bot_san2.trp
3 (top of lower aquifer/bottom of aquitard)	bot_clay.trp
2 (top of aquitard/bottom of upper aquifer)	bot_san1.trp
1 (relief)	demo_relief.trp

You can display the model in a 3D view:

☞ 3D-Options button on the lower left side of the screen and hold the mouse button. A small menu pops up

Move the cursor to the ***Visualize*** item. A second menu pops up.

Move the cursor on ***Body*** and release the mouse button. The Tricycler Menu pops up and the model is displayed in 3-dimensional view. (see figure.)



Move, rotate and zoom on the model as described in the green message area below the working window.

☞ **"Exiting rotation"** in the Tricycler menu .

4.4 Flow Data

The Flow Data section controls all the necessary input parameters for the groundwater flow model. The Flow data menu is consists of 3 submenus: the **Flow initials**, the **Flow boundaries** and the **Flow materials** menus. Click on the corresponding buttons to enter the submenus.

☞ **"Flow Data"** to enter the first level of the **Flow Data Menu**.

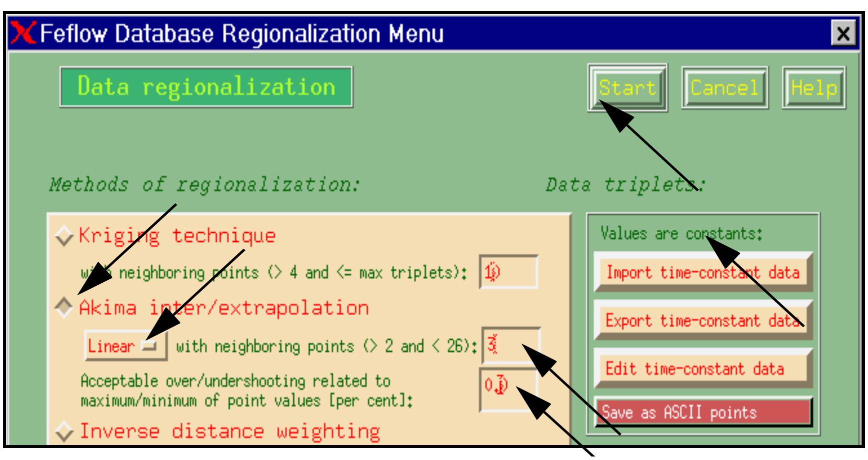
4.4.1 Flow Initials

The Flow initials menu allows you to assign the groundwater surface for the start of your simulation run.

☞ **"Flow initials**"

♦ "***Database"*** to import previously collected data points.

☞ **"Hydraulic head"**. The **Database regionalization** menu pops up.



In the *Methods of regionalization,* we will select the Akima interpolation technique.

♦ ***Akima inter/extrapolation***.

Switch the drop down button to "***Linear"***.

In the ***neighboring points*** field, type "**3**".

In the ***Acceptable over/undershooting*** field, type **"0"**.

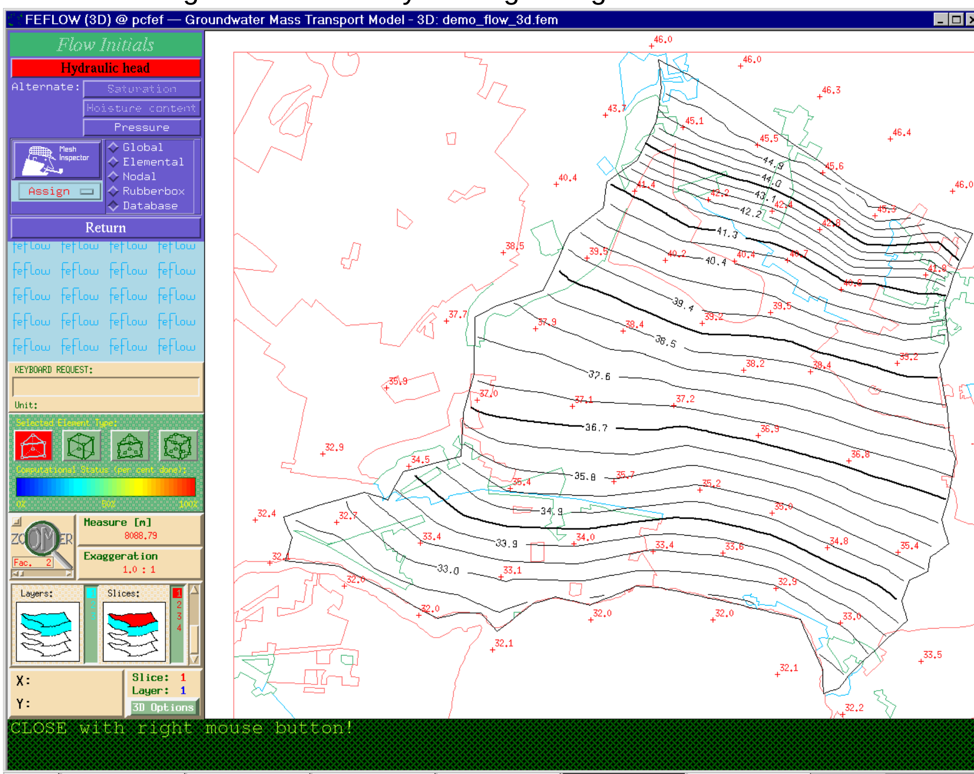
☞ "**Import database**". The file selector appears.

☞ **[demo_head_ini.trp]** from the *Files* list. This ASCII file has the format *x-coordinate, y-coordinate, function-value.*

☞ "**Okay**"

☞ "**Start**". The regionalization will execute the interpolation of the data we have just imported (see resulting contours in the figure below).

Exit the Assign tool function by clicking the right mouse button in the model domain..



You can visualize the results.

☞ **"Assign"** and switch it to **"Show"**.

☞ **"Hydraulic head"**. FEFLOW shows the hydraulic head distribution as colored fringes.

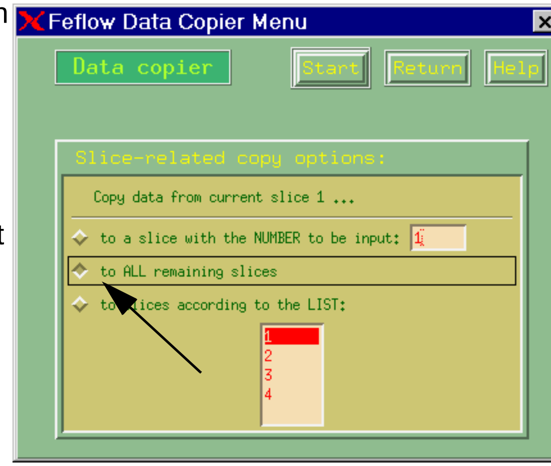
Click with right mouse button to exit the visualization.

☞ **"Show"** and switch it to **"Vanish"**.

☞ **"Hydraulic head"**. FEFLOW resets to normal view.

We will now copy the initial values to all the remaining slices.

Go to the **Mesh Inspector** icon and switch the light blue Tools button to **"Copy"**..



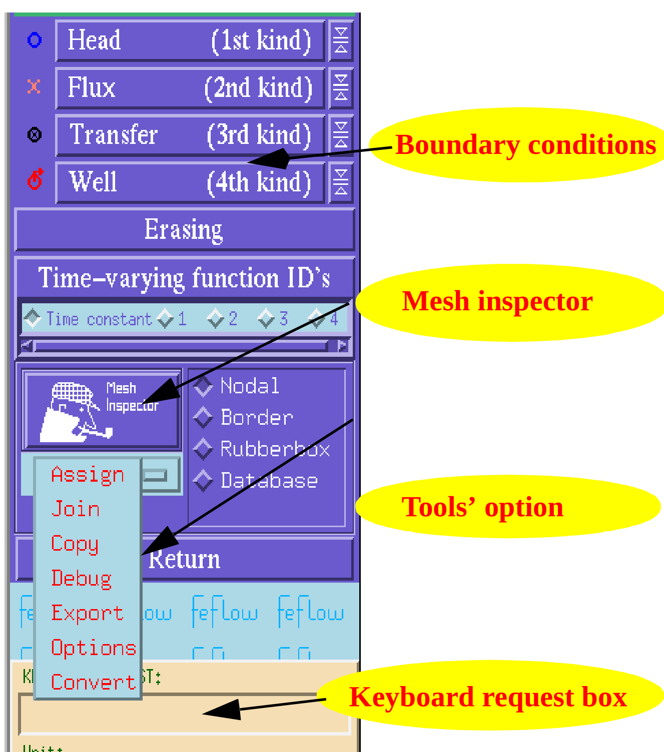
- ☞ **"Hydraulic head"**. The **Copier** menu appears.
- ♦ "**Copy to ALL remaining slices**"
- ☞ **"Start"**. You will be asked by an alert box if you really want to overwrite the current values.
- ☞ **"Yes"**

Click on **"Return"** to close the Copier menu.

- ☞ **"Return"** to exit Flow Initials Menu.

4.4.2 Flow Boundaries

We must now enter the Flow boundaries menu and set the boundary conditions for our model. The picture below shows you all options of the menu.



The submenu's functions are listed on the left of the working window. These input features have been strategically designed to assist you with developing the model in a more intuitive manner.

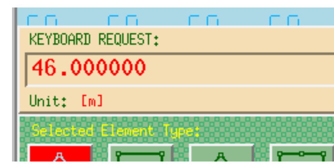
Note: FEFLOW as a finite-element based program uses boundary conditions which have to be fixed at nodes, unlike finite-difference models that assign the center of a cell as the location of boundary conditions.

We must now set the northern boundary condition which describes the northern hills. In this exercise, for the sake of simplicity, we will assume a reasonable hydraulic potential along this border. Therefore we will set a constant hydraulic head of 46 m.

Go to the mesh inspector icon.

Switch to the **"Assign"** tool.

♦ ***Border***



☞ **"Head (1st kind)"**

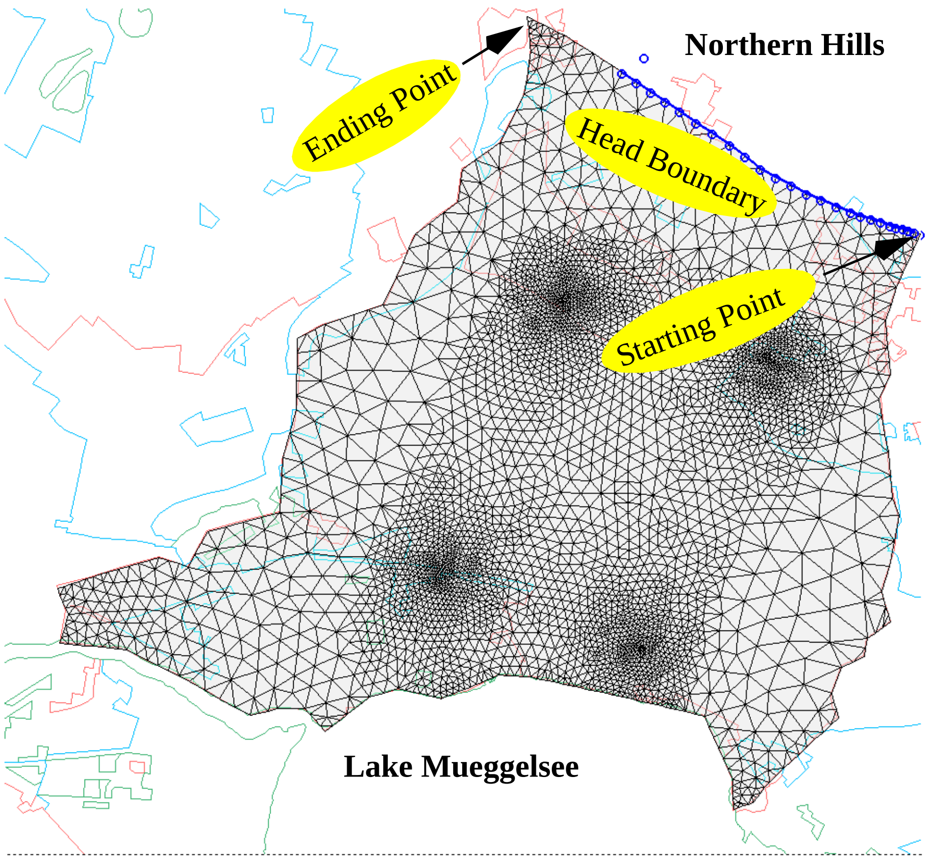
To clear the **Keyboard request box,** hit **<Esc>**. A red flashing light prompts you to enter a new head value. Type "**46"** in the Keyboard Request box.

↵

Move the cursor to the working window. Click and hold the left mouse button over the northeastern corner of the model domain. Still holding the left mouse button, move the cursor along the northern boundary to secure the assignment direct and release the left mouse button. Notice all nodes have been assigned a head value of 46 m a indicated by blue circles.

Continue along the northern boundary and stop at the northwestern boundary.

Click the right mouse button to set the end point.



Note: If you have assigned too many nodes, simply select the "Nodal" option in the "Assign" tool, click on the "Hydraulic Head" button, go to the head boundary conditions you want to delete and click on each unwanted node. Click the right mouse button to exit.

Now define the southern boundary conditions describing the shoreline of Lake Mueggelsee. We recommend using a **Head** boundary condition with a hydraulic head of "**32.1"** meters which you have to assign on every border node with the **"Assign-border tool"** as described previously for the northern boundary.

The western and eastern borders of the model have not been assigned any values, therefore the finite element model will consider the "natural boundary condition" of "**0"** flux across both borders.

Once we have assigned the head boundary conditions for the northern and southern borders of our model, we will assign the wells describing the pumping schedule of the City of Friedrichshagen.

Switch to the **"Join"** tool from the light blue button..

♦ ***"Supermesh"***

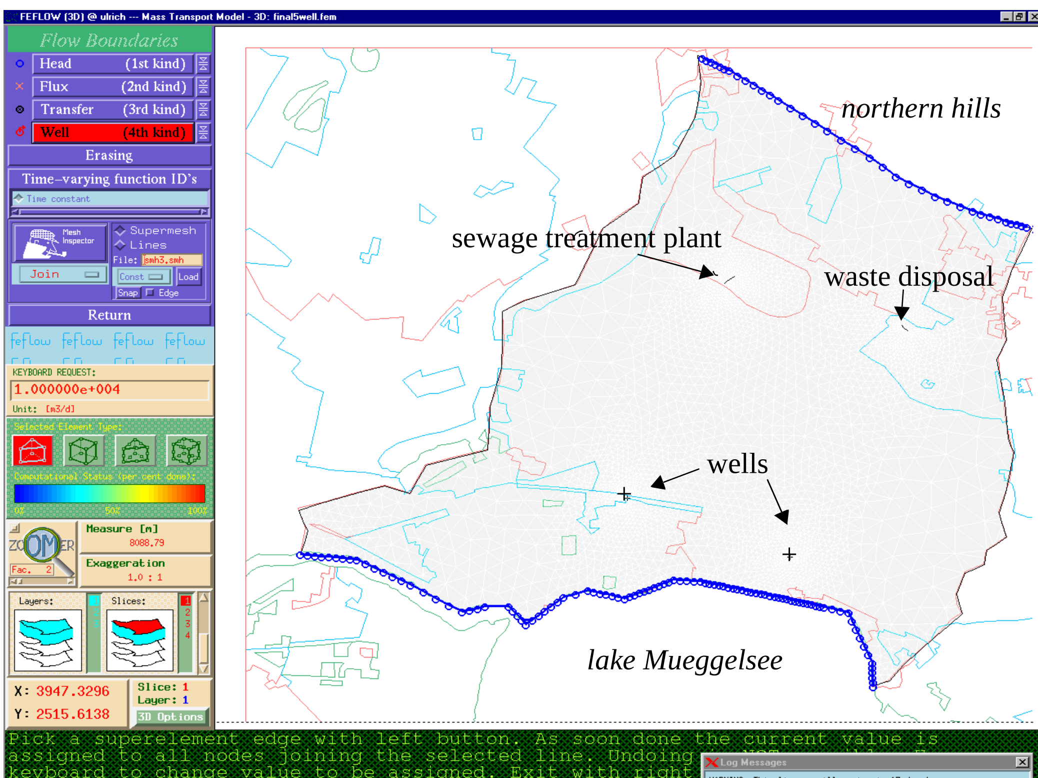
☞ **"Load"** button below the *Supermesh* option. The file selector appears.

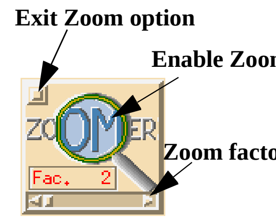
The selected supermesh will act as a frame for the finite element mesh. It contains the polygon describing the outer boundaries of the model and the Add In’s for the exact positioning of the pumping wells and the contaminant sources (waste disposal site, sewage treatment plant).

☞ **[demo.smh]** in the *Files* list.

☞ **"Okay"**

Now the imported supermesh including the Add In’s is displayed on the working window (see figure).





The wells (boundary conditions) should be set on the southern part of the model where the two Add In points are positioned. For a more accurate setting of the wells, you can zoom into this area using the zoomer icon found among the information boxes.

Move the horizontal slider bar in the Zoomer icon by clicking on the right arrow until you get the zoom "**factor 4**".

Click on the Zoomer icon. The cursor becomes a rectangle. Move the cursor to the southern part of the model where the two Add In's describing the wells are positioned. Click with the middle mouse button (for 2 button mouse: both buttons). The zoom is executed.

We will now set the wells as boundary conditions of 4th kind with a discharge rate of 10000 m^3/d. Since the wells are screened through all slices, the actual discharge rate can be set on the uppermost node.The underlying nodes will get a value of zero (0) for the discharge rate. FEFLOW will then automatically distribute the discharge rate along the whole screen.

☞ **"Well (4th kind)"**

Hit **<Esc>** in order to clear the Keyboard Request box.

Enter a value of "**10000"** (discharge rates are positive!).

↵

Move the cursor over one of the Add In's. The underlying mesh node should be highlighted by a red box.

Click on the left mouse button to set the boundary condition with the discharge rate of **10000 m^3/d** exactly on the Add In.

Repeat this step for the second Add In.

Once completed, click the right mouse button to exit this function.

We will now assign all other slices a value of zero (0).

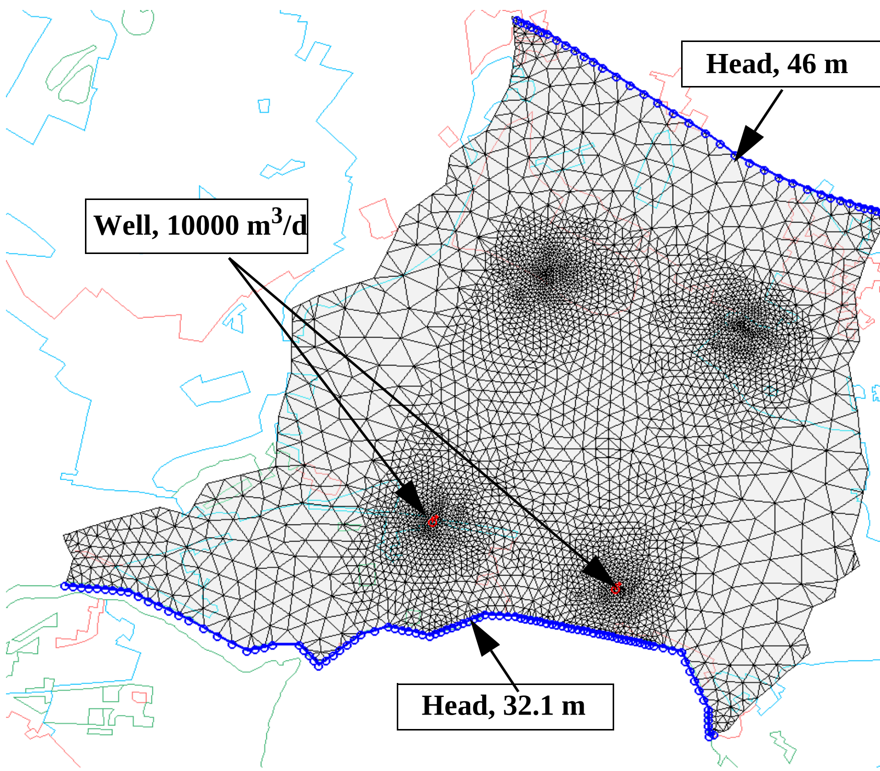
Select the next slice in the Layer/Slices menu located below the Zoom option by clicking on the **"*Slices:*"** number.

Repeat the previous steps for each slice using a value of 0 for the wells or assign the 10000 cubic meters for each slice.

To zoom out, click on the small toggle button in the upper left edge of the Zoomer icon.

Click on **"Return"** to exit the **Flow boundaries** menu.

Note: You can verify the input data by using the mesh inspector. Click on the mesh inspector icon and move the cursor into the model domain. Move directly over the wells. The actual values will be displayed in the Inspector Echo window.



4.4.3 Flow materials

The **Flow Materials Menu** allows you to edit all material parameters which have to be set for modeling a groundwater flow problem.

☞ **"Flow materials".** The menu's structure is similar to the **Flow Data** menu.

Upper Aquifer

The upper aquifer's conductivity will be imported from borehole samples stored in an ASCII database (syntax: X-coordinate, Y-coordinate, Conductivity). The method used is similar to assigning z-elevations in the 3D-Slice elevation menu.

Ensure the **"Assign"** tool is set on the light blue button under the mesh inspector.

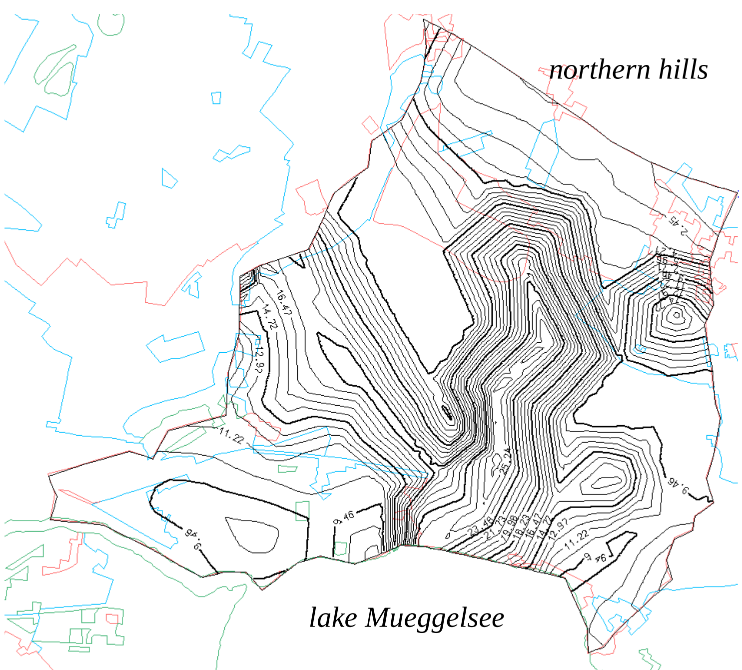
- ♦ ***Database*** option.
- ☞ **"Conductivity [Kxx]"**, the Database regionalization Menu appears.
- ♦ ***Akima inter/extrapolation***

Set the number of neighbors to "**3**" and the over/undershooting to **"0 %"**.

- ☞ "**Import time-constant data**"
- ☞ **[conduc2d.trp]** in the "Files" list.
- ☞ **"Okay"**
- ☞ **"Start"** in the Data regionalization Menu.

FEFLOW will now inter/extrapolate from the borehole data and will display the resulting distribution as a contour map of conductivities.(see figure below) The contours of our example show low conductivities near the northern hills and a high conductivity flow channel going down from the north to the south dividing the model domain into two equal halfs.

Click the right mouse button after the interpolation is finished.



You can visualize the interpolation in high resolution color.

Switch the light blue button to the **"Show"** tool. The value distribution is displayed as colored fringes

☞ **"Show"** and switch it to **"Vanish"**.

☞ **"Conductivity Kxx"**. FEFLOW resets to normal view.

We will now specify the storativity for the layer.

Switch the light blue button to the **"Assign"** tool.

♦ **"Global"** option. This will assign the same value to the entire layer.

☞ "**Storativity (drain/fillable)"**.

An alert box pops up asking if you are sure to overwrite the data. Select **"Yes"**.

Hit **<Esc>** to clear the Keyboard request box.

Input a value of "**0.1"** in the Keyboard request box.

↵

Exit the function by clicking the right mouse button.

Aquitard

Our next step is to assign the conductivity properities of the Aquitard. Select ***Layer* 2** in the Layers & Slices browser.

Switch the light blue button to the **"Assign"** tool.

♦ ***Global*** option. This will assign the same value on the entire layer.

☞ **"Conductivity [Kxx]"**. An alert box pops up asking if you really want to overwrite the current values.

☞ **"Yes"**

Hit **<Esc>.** Input a value of "**1e-6"** in the Keyboard request box similar to the unit box showing 1e-4 m/s.

↵ Exit the function by clicking the right mouse button.

We will assign a new storativity value due to the low conductivity we have just created.

Switch light blue button to the **"Assign"** tool.

♦ **"Global"** option.

☞ "**Storativity (drain/fillable)"**

An alert box pops up asking if you are sure to overwrite the data. Select **"Yes"**.

Hit **<Esc>** to clear the Keyboard request box. Input a value of "**0.01"** in the Keyboard request box.

↵ Quit the function by clicking the right mouse button.

Bottom Aquifer

On the bottom aquifer we leave the default conductivity of 10 e-4 m/s.

☞ ***"Layers:"*** "**3**" in the "Layers/Slices" browser.

Switch light blue button to the **"Show"** tool.

☞ **"Conductivity [Kxx]"**. The distribution is displayed.

Swith to the**"Vanish"** tool.

☞ **"Conductivity [Kxx]"**. The mesh is redrawn.

Now for all layers copy K[xx] values to the K[yy] and K[zz] parameter to create isotropic conductivities.

Switch the light blue button from “Vanish” to the **"Copy"** tool.

☞ **"Conductivity Kxx"**. The **Copier** menu appears..

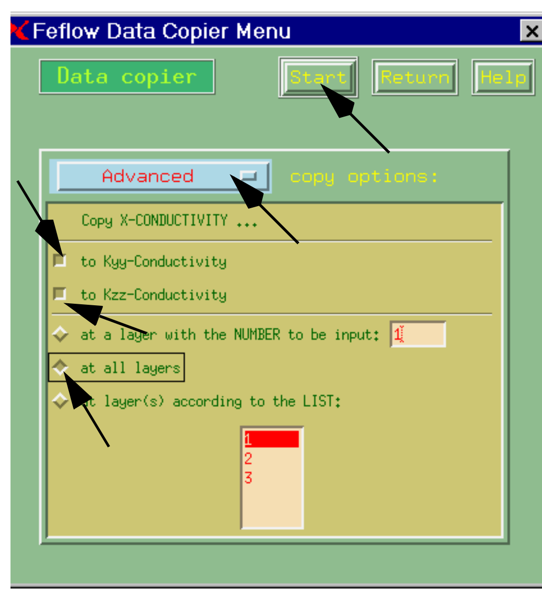
Switch the light blue button from **“Layer-Related”** to **Advanced**

Ensure that the "**Copy to Kyy-Conductivity"** and "**Copy to Kzz-Conductivity"** butttons are selected in the upper part of the menu

♦ **at all layers** in the lower part of the menu.

☞ **"Start"**

You will be asked by an alert box twice if you really want to overwrite the current values.

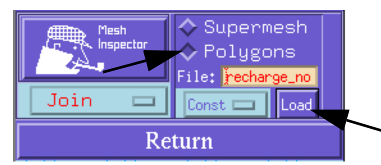


Select **"Yes"** both times

☞ **"Return"** to close the "Copier" menu.

Groundwater Recharge

The assignment of the groundwater recharge will be executed using a template showing the areas of different landuses and a ASCII database containing the attribute data. The polygon file contains is linked with the database:.



☞ "*Layers:"* **1** in the "Layers/Slices" browser

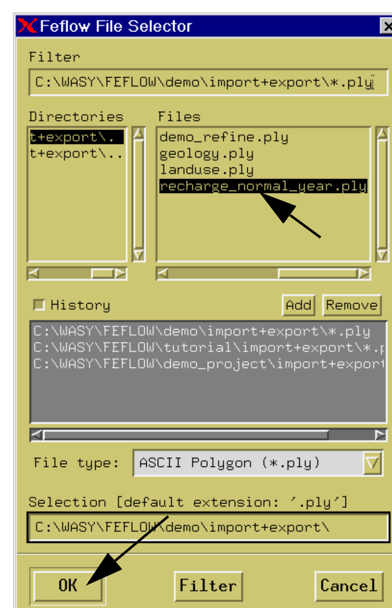
Switch light blue button to **Join** tool.

♦ "Polygon" option.

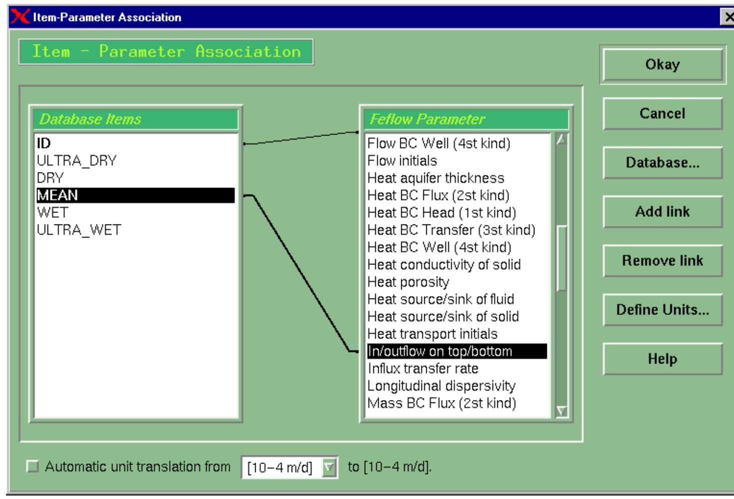
☞ “Load” below the "Polygon" option. The **File Selector** pops up.

☞ **[recharge_normal_year.ply]** in the "Files" list.

☞ "**Okay**" button to leave this file selector.



Now the **Parameter Association** menu becomes visible. On the left hand side the field names of the database are listed. On the right hand side the FEFLOW parameters are shown. Two pipelines connect the right hand list with the left hand side. The polygon Id's are linked with the field "id" of the database. The data of the **"MEAN"** field is linked to the FEFLOW parameter **"In/outflow on top/ bottom"**.

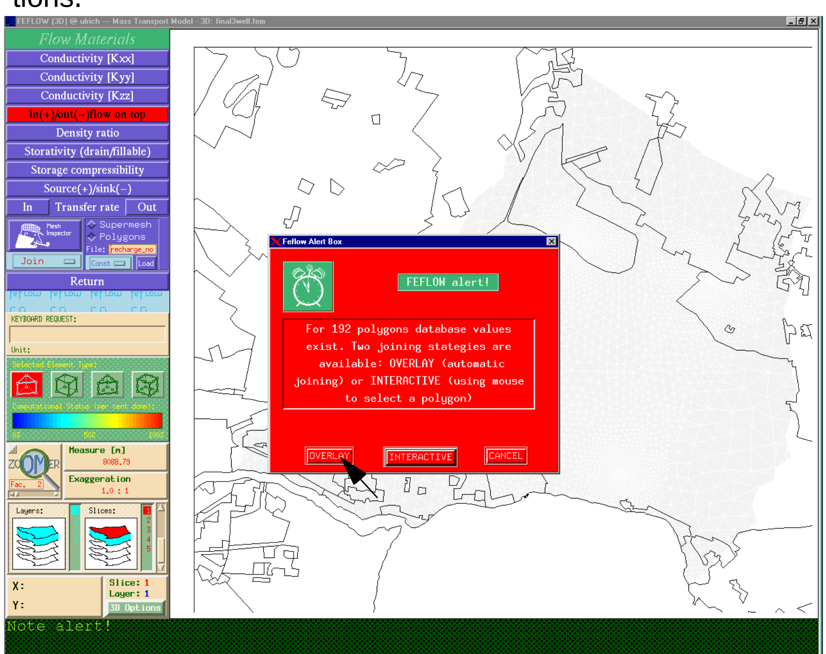


You can add and remove links. However, for this demo exercise just

☞ **"Okay"**.

The polygon file is displayed as template in the working window

☞ "In(+)/out(-) flow on top". An alert box appears telling you the database link options.



☞ "**Overlay**" in the alert box. The database values will automatically be assigned to the model. For detailed information about this database link see the FEFLOW online help (top/file formats library/polygon files).

☞ the right mouse button.

☞ **"Return"** to leave the **Flow materials** menu.

☞ **"Return"** to leave the **Flow data** menu.

You have now created an executable transient flow problem. Changing the problem class to "flow only" allows you to make a first trial on the simulation and skip the next sections regarding the transport parameter settings.

4.5 Transport Data

If you have skipped the previous steps, please load the file **"demo_flow_3d.fem"** via the "Load finite element problem" option of the File menu before beginning this exercise.

Enter the **Transport Data** menu in the Problem Editor. This menu contains all editors for defining mass and heat transport parameters. Its structure is similar to the Flow Data menu, i.e. you can set initial values, boundary conditions and material parameters.
The **Mass transport initials,** which describe the initial concentration of the model**,** remains on the default value 0 mg/l.

4.5.4 Mass Transport Boundaries

In the **Mass transport boundaries** Menu, "fresh water" conditions - at very low concentrations - will be assigned for the outer borders where water can enter the model. The contaminant sources lie on the top slice.
Click on **"Mass transport boundaries"** to enter the menu.

Switch to the **"Assign"** tool .

♦ ***Border*** option.

☞ **"Mass (1st kind)"**

Hit **<Esc>**. The Keyboard request box is active now. Type the value of "**1e-12".**

↵

Move the cursor on the working window to the north eastern corner of the model.

Click and hold the left mouse button on the first node on the northeastern border.

Move the cursor along the northern boundary still holding the left mouse button. Free the left mouse button. All border nodes you have passed should be marked by a blue circle.

Having marked the last node of the northern boundary, click the right mouse button. The northern boundary to the northern hills is now set for freshwater conditions.

Repeat this step for the southern boundary, the lake's shoreline.

☞ left mouse button and assign the boundary conditions along the southern border.

Note: You have defined that only fresh water enters the model. Enabling higher levels of contaminated water leaving the model can be computed exactly, however you should set additional constraints. See the FEFLOW online Help by hitting <F1> in the Mass transport boundaries menu and follow the hyperlink to the <u>Constraints</u> section of the Theory.

Next we will assign the boundary conditions for the two contamination sources, the sewage water treatment plant and the waste disposal site, which are placed in the northern part of the model.

Switch **"Join"** tool on the light blue button.

♦ "***Supermesh"*** option.

☞ **"Load"** button below the Supermesh option. The file selector pops up.

☞ **[demo.smh]** in the *Files* list

☞ **"Okay"** button. Now the supermesh including the Add In's are displayed.

☞ **"Mass (1st kind)".** Zoom on each contaminant source and assign the concentration of **500 mg/l.**

Hit **<Esc>** in order to clear the Keyboard Request box.

Enter a value of "**500 "** to represent contaminant release at the sewage treatment plant to the west and the waste disposal site to the east.

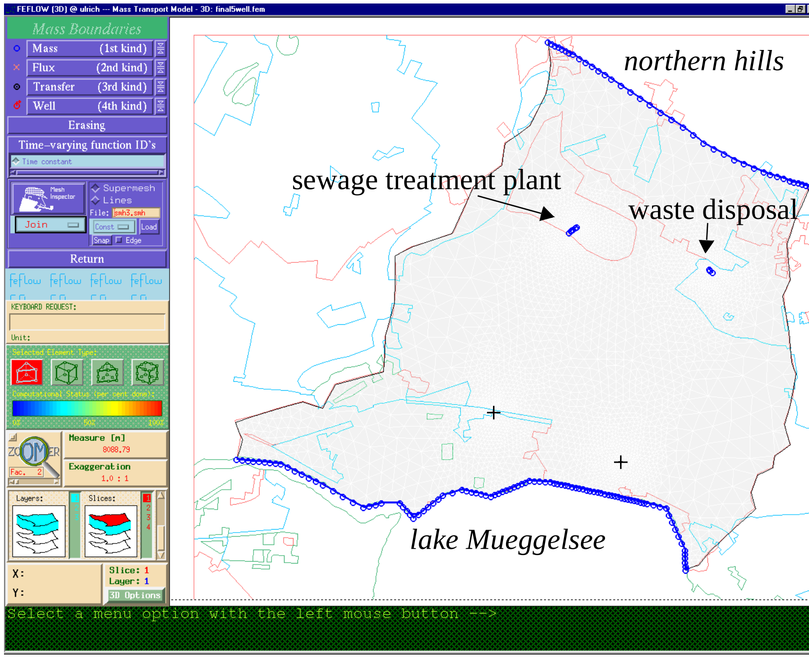
↵

First, move the cursor to the sewage facility (west side) directly over the Add In line. Notice that the line becomes highlighted.

Click the left mouse button to assign the contaminant concentration.

Repeat these steps for the waste disposal facility (east side).

Click with the right mouse button to exit the function.



We will now copy these boundary conditions on all remaining slices.

Switch light blue button to **"Copy"**.

☞ **"Mass (1st kind)"**. The **Copier** menu appears.

♦ **"Copy to ALL remaining slices"**

☞ **"Start"**

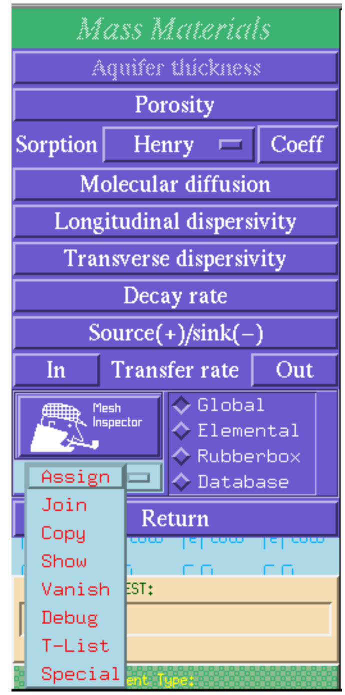
A FEFLOW alert box pops up. Select **"Yes"** to overwrite the values.

☞ **"Return"** to exit the Copier menu.

We will now leave the **Boundaries** menu and enter the **Mass transport materials** menu.

☞ **"Return"**

4.5.5 Mass transport materials



All material parameters concerning mass transport are set in the Mass Transport Materials Menu. We will first assign the values for the total porosity of the aquifer for the top layer:

Switch the light blue button to the **"Assign"** tool.

Click on the toggle for the **"Global"** option.

Click on **"Porosity"**

A FEFLOW alert box appears. Select **"Yes"** to overwrite the default value.

Hit **<Escape>** to clear the Keyboard request box.

Input a value of **"0.2"** in the Keyboard request box .

↵

Exit the function by clicking the right mouse button.

We must now specify the contaminant mass transport dispersivity for our model. Switch the light blue button to **"Assign"** tool.

♦ ***Global*** option.

☞ **"Longitudinal dispersivity"**. An alert box pops up asking you if you really want to change the values.

☞ **"Yes"**

Hit **<Esc>,** and input a longitudinal dispersivity value of "**70"** in the Keyboard request box.

↵

Quit the function by clicking the right mouse button.

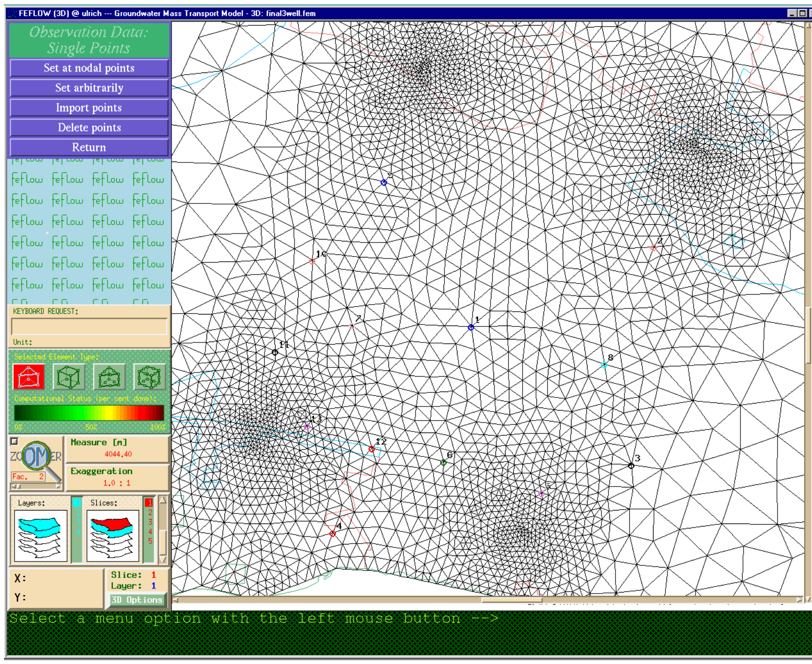
Repeat the steps for **"Transverse dispersivity"**, assigning a value of **"2.5"**

Copy the dispersivity values to all layers using the "**Copy"** tool.

Exit the **Transport data** menu by selecting **"Return"** and go up to the **Problem Editor Menu**.

4.6 Setting Reference Data

At last you should set some observation points on the top slice. For the points, all resulting data such as hydraulic heads or contaminant concentrations are visualized online in diagrams during the simulation run.



- ☞ **"Points, Groups & Fences"**. We will now enter the **Reference data editor**.
- ☞ **"Observation single points"**.
- ☞ **"Import points"**. The file selector pops up. Now you will import the observation points from an ASCII database (Arc/Info compatible Generate format).
- ☞ **[demo_obs_pnts.pnt]**
- ☞ **"OK"**. The points are loaded and visualized as colored circles.

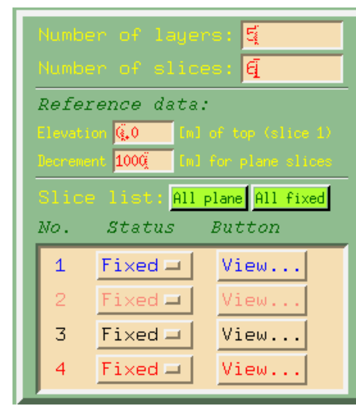
Leave the **Problem editor** for the top **Shell** menu by clicking on the various **"Return"** buttons.

4.7 Reconfigure 3D Task

The basic model parameters are now assigned, but we will add one additional layer to increase the accuracy of modeling the aquitard. Therefore we have to re-enter the **Layer configurator** via the **3D-Slice elevations menu**.

☞ "**3D-Slice elevations**" in the **Problem Editor** menu.

☞ "**Reconfigure 3D Task**" .

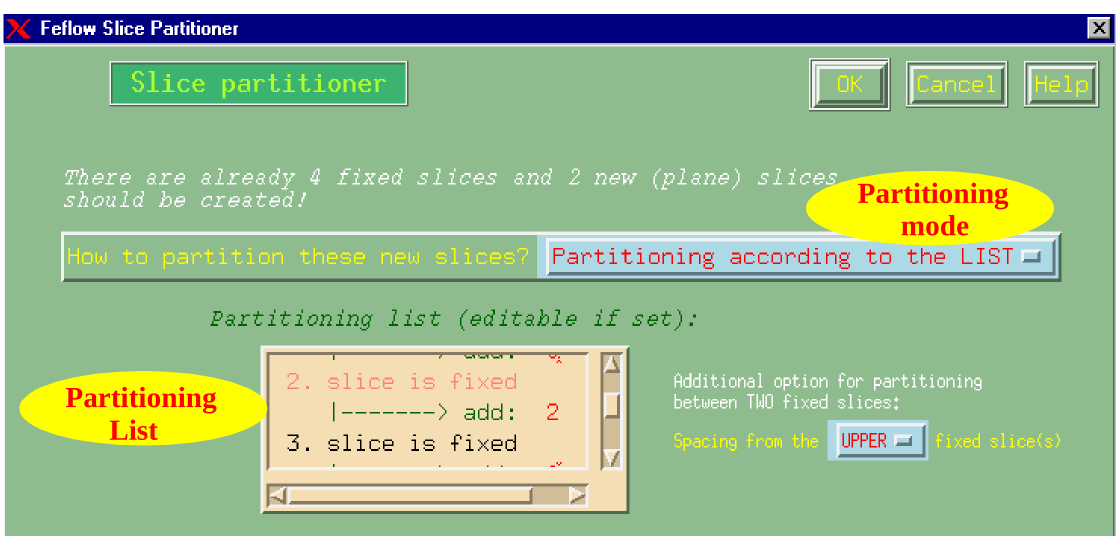


Type a decrement of **“1000”** in the **Reference data** ***Decrement*** box .This unrealistic high decrement makes FEFLOW place the new slice exactly in the middle of the top and bottom slice of the aquitard dividing it in two equal layers.

Change the ***Number of layers*** in the input box at the upper left corner of the menu to "**5**".

↵

The **Slice Partitioner** pops up



Switch light blue button beside the "How to partition these new slices?" to the **"Partitioning according to the list"** option.

Move the cursor on the ***Partitioning list***.

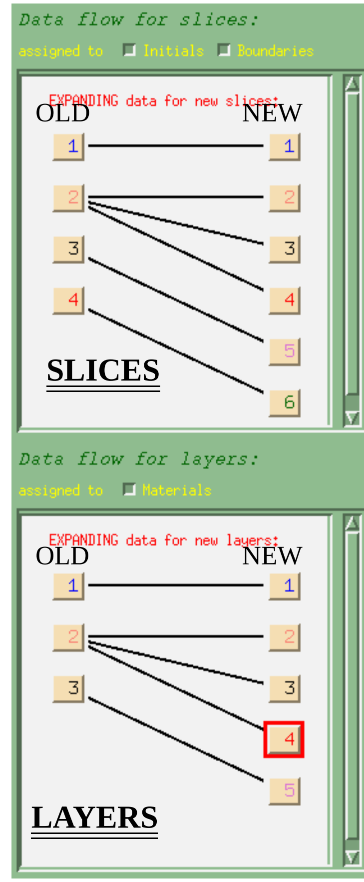
Scroll the ***Partioning list*** using the vertical slider button on the right of the menu and replace the **“2”** automatically set by FEFLOW under *4. slice fixed* by a **"0"**.

Between the *2. slice is fixed* and *3. slice is fixed* replace the "**0"** by **"2"**. The new slice’s z-elevations are interpolated from the nodal values of the upper and lower slice. Therefore the new slice will divide the aquitard exactly in the middle.

☞ **"OK"**

Now the aquitard is divided in three layers. To ensure that the data copied is executed correctly from the old to the new slices, we will utilize the Data Flow lists on the right of the **3D-Layer configurator** menu. As shown in the next picture, there are two lists that allow you to control data between various layers. The upper control called "*Data flow for slices*" describes the data flow of the initial conditions and boundary settings from the old slices. These are shown as number buttons in the left column with the new slices in the right column. The data flow is symbolized by lines connecting the old with the new slices. The lower list, "*Data flow for layers*" describes the data flow for all material data from the old to the new layers.

Note: The initial and boundary condtions are set on slices (nodal planes) while material parameters are set on layers (3D elements).



The data flow in the upper list for the initial and boundary conditions is set automatically by FEFLOW. The information of the old slice 2 will be inherited by the new slices 2, 3 and 4. The data flow in the lower list for the materials data describes the same data characteristics from the old bottom layer (lower aquifer) to the new layers 2, 3 and 4. For our example, we will change the links.

Go to the lower "*Data flow for layers*" list.

☞ 

in the left column. (represents the aquitard)

☞ 

in the right column. A line will now connect the old layer 2 with the new layer 3. The data are inherited.

☞ 

in the right colum. A line will now connect the old layer 2 with the new layer 4.

The resulting data flow lists should look like the figure to the right.

☞ **"OK"** to exit the Layer configurator.

Exit the **Problem editor** for the top **Shell** menu by clicking on the various **"Return"** buttons.

5 Step 4 - The Simulator

If you have skipped the previous steps, please load the file **demo_transport_3d.fem** via the "Load finite element problem" option of the **File** menu before beginning this exercise.

Enter the simulator via the **Simulator** shell menu by selecting **Run ....**
Start the simulation by clicking on the "**(Re-)Run simulator**" button. Notice that FEFLOW automatically generates various windows that detail the ongoing results for the wells, observation points, hydraulic head and contaminant concentrations. These windows will be displayed as diagrams.

Note: You can stop the simulation by holding the right mouse button until the simulator stops. This may require a few minutes. Restart by clicking on "(Re-)Run simulator".

The simulation will require approximately 1/2 to 1 hour on a Pentium 133Mhz. Since you cannot save the results in the demo version of FEFLOW, we have prepared a results file, which you can view in the **Postprocessor Menu**.
Having interrupted the simulation, you can now analyze the results of the current time steps with the options offered in the Halt & View Results menu (isoline maps, velocities, particle tracking, data export), the Budget analyzer, the Fluid flux analyzer or in the spatial operations menu. The same menu's are available in the Postprocessor, where analyzing is enabled over different time steps.

☞ **"Return"** to exit the **Simulator**.

6 Step 5 - The Postprocessor

The postprocessor allows the users to evaluate, analyze and export the computational results. Additionally, the Postprocessor Menu controls each saved time step of the simulation and allows a continuation of the simulation from the last time stage..
To use the postprocessor, you must have saved the simulation results in a so called "**dac"** file. Because the demo version of FEFLOW does not allow you to save the results, we have prepared a special demo **"dac"** file.

☞ **Postprocessor** shell menu.

☞ **"Load and run ...".** The file selector appears.

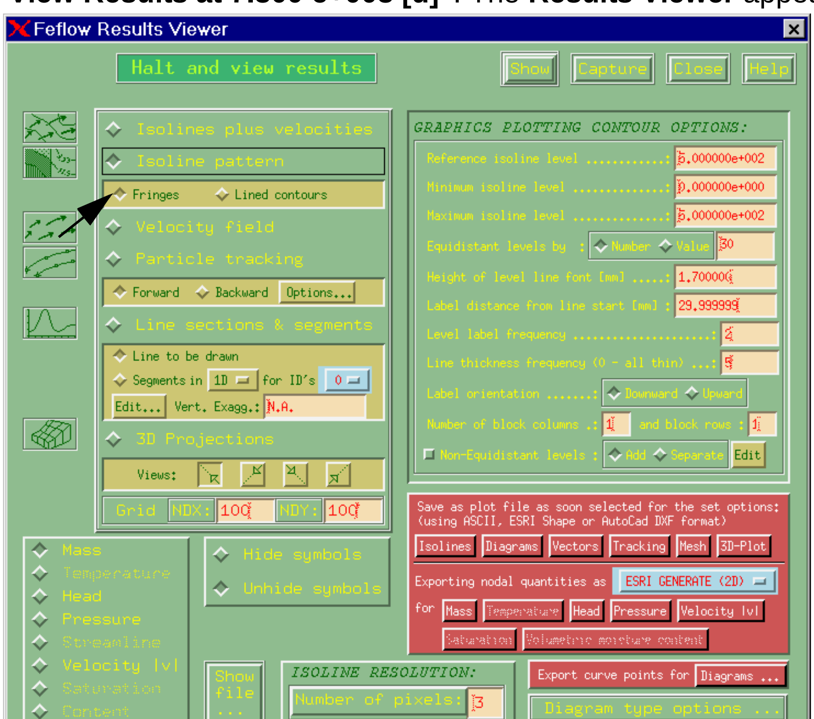
☞ **[demo_transport_3d.dac]** in the *Files* list.

An alert box pops up asking if you want to abandon the current fem file. Select **"Yes"**.

The **[demo_transport_3d.dac]** file is loaded and you will enter the Postprocessor.

To get an idea of the final results, start with the 2D visualization tools:

☞ **"View Results at 7.300 e+003 [d]"**. The **Results Viewer** appears.

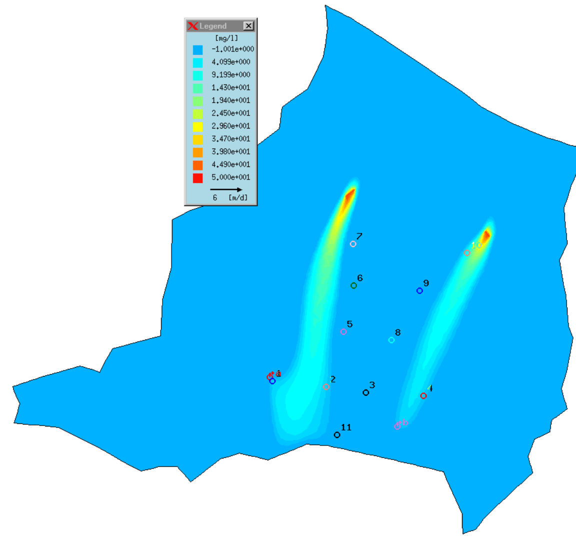


♦ *Isoline pattern* in the upper right part of the menu.

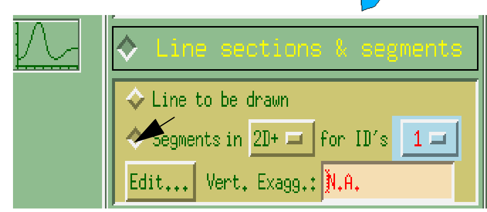
☞ **"Show"**. The mass distribution for the current slice is visualized

Click with the right mouse button. The **Results Viewer** reappears.

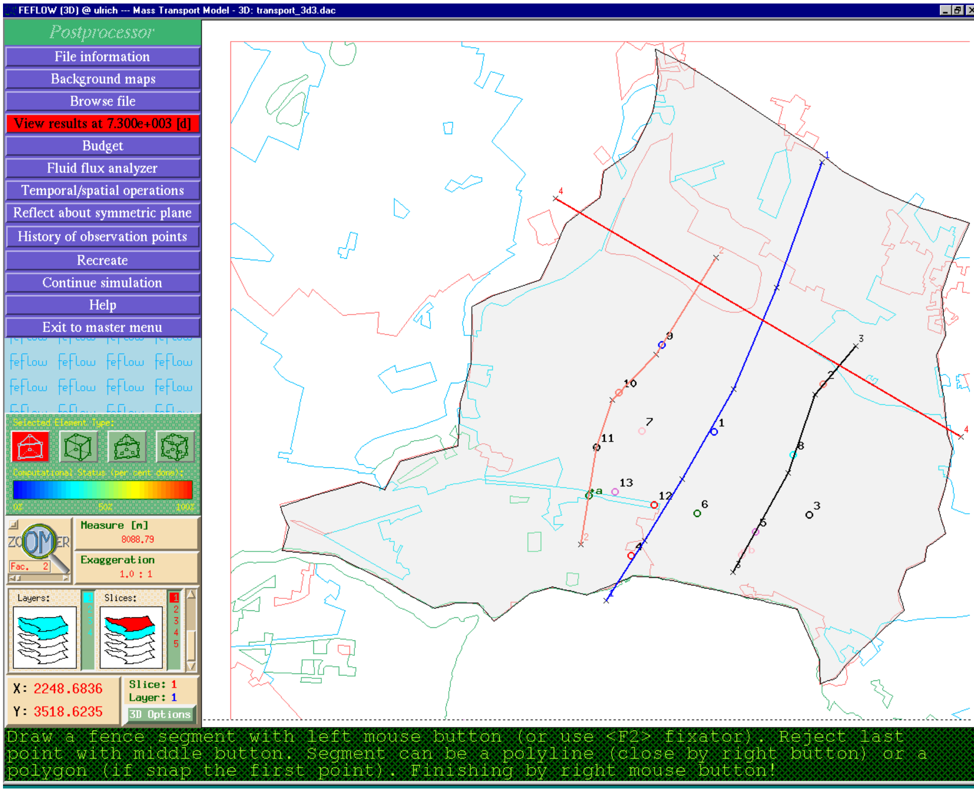
The cross sections can be visualized for all parameter distributions along lines which can be drawn on the working window or imported as ASCII Generate files. First draw a cross section:



☞ **"Edit.."** below the **Line sections & segments** entry and hold the mouse button.



Move the cursor on **"Draw segments"** and release the mouse button. Now you have to draw the line for the cross section on the working window. Refer to the follow figure:

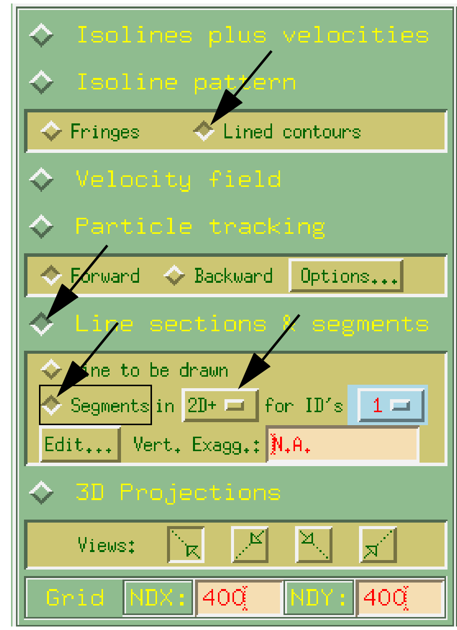


☞ on the start point for the cross section on the model. Digitize the cross section by clicking on the model.

Click with the right mouse button to end the editing of a line. The line gets an ID number.

Click with the right mouse button a second time. The **Results Viewer** appears.

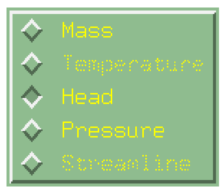
Now we will define an isoline contour for the hydraulic head along the cross section that also shows the velocities at the nodes:



- ***Lined contours*** in the upper right part of the menu.
- ***Line sections & segments***
- ***Segments***

Switch the small button from ***1D to 2D+*** for the velocities at the nodes.

- **Head** in the lower left part of the menu for analyzing the hydraulic head distribution.



☞ **"Show"**. A vertical cross section of the hydraulic head distribution is displayed.

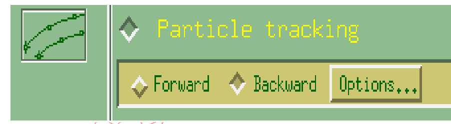
Click with the right mouse button. The **Results Viewer** reappears.

We will now analyze the flow pathlines to the wells using particle tracking :

☞ ***Slice* 3** in the Layers & Slices browser at the lower left side of the screen to start the pathlines from this nodal plain.

♦ **"Particle tracking"**

♦ **"Backward"**

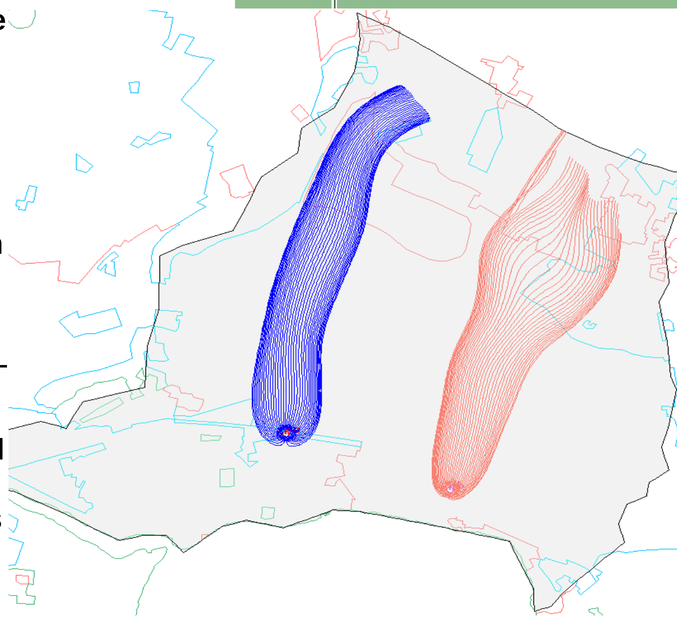


☞ "**Options...**". The **Pathline editor** appears.

♦ "**multiple pathlines around a single well**" in the left row. This option allows you to start multiple pathlines exactly from a well to create capture zones.

☞ "**Close**" to leave the Pathline editor.

☞ "**Show**" to activate the tool menu. The working window displays the model's border and symbols for the wells.



☞ on a well location to create the backward (reverse) particle tracking.

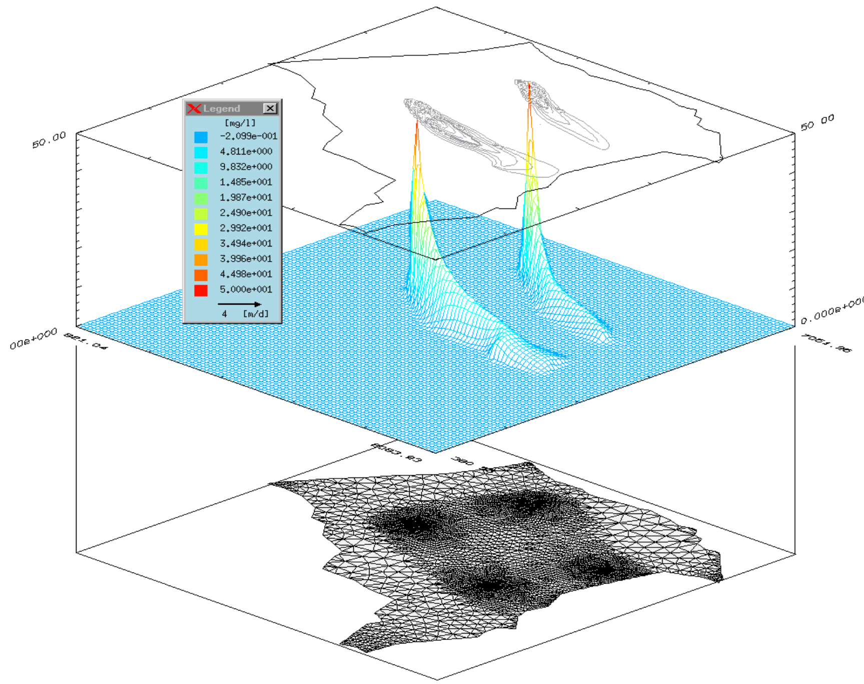
Click with the right mouse button to exit the function. The Results Viewer reappears.

At last try out the Pseudo 3D Visualization for parameter distribution:

♦ **3D Projections**.

♦ ***Mass*** in the lower left part of the menu.

☞ **"Show"**. The mass distribution is visualized as a 3D plot, where the quantity of mass concentration is visualized as Z elevation.



Click with the right mouse button to exit the function. The Results Viewer reappears.

☞ **"Exit"** to close the Results Viewer.

The Budget analyzer calculates the water, mass and heat balancing for the entire model, single slices or subregions to be defined by interactive input or import of lines or polygons in ASCII format. The budget can be analyzed for a special time step or over a time period.

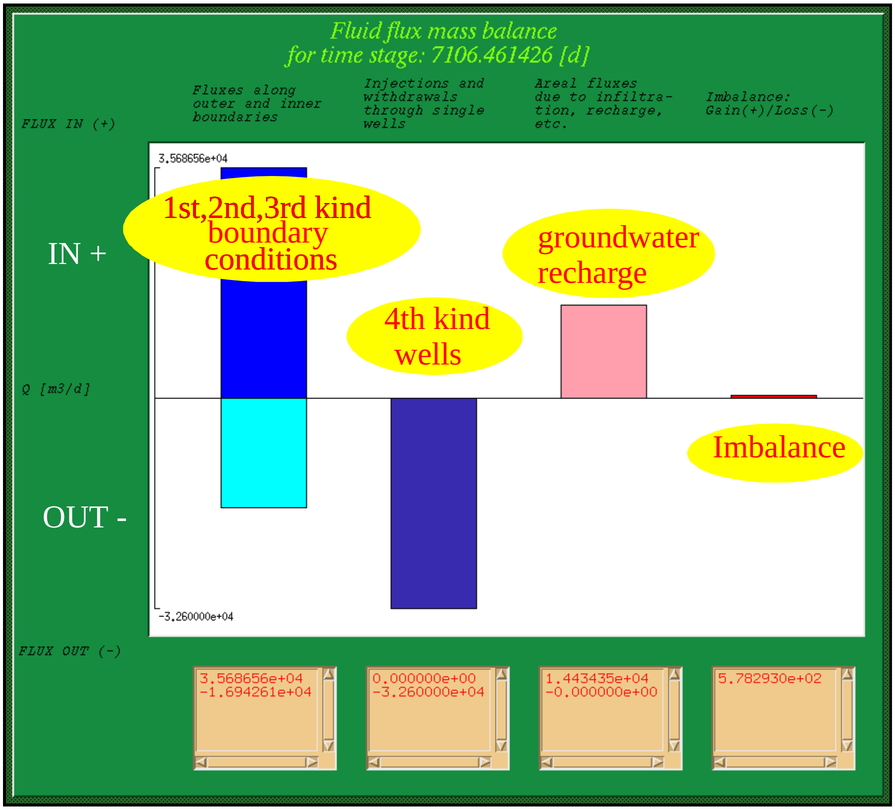
☞ **"Budget analyzer"**. The **Budget analyzer** opens. As default, **Fluid flux mass** and **Total balancing on all inner and outer boundaries (balance checking)** is selected.

☞ **"Start"**. The total balancing of the model for the current time step is executed.

Click the right mouse button to exit the budget function..

Note that FEFLOW has drawn blue and red circles on the model. Red circles show nodes where water enters the model and blue circles indicate water leaving the model. The diameter of the circles shows the relative quantity.
In addition, a diagram has popped up displaying block diagrams for the in (+) and out (-) flow due to the different boundary conditions and groundwater recharge. The last column

shows the imbalance (loss or surplus) of the model.

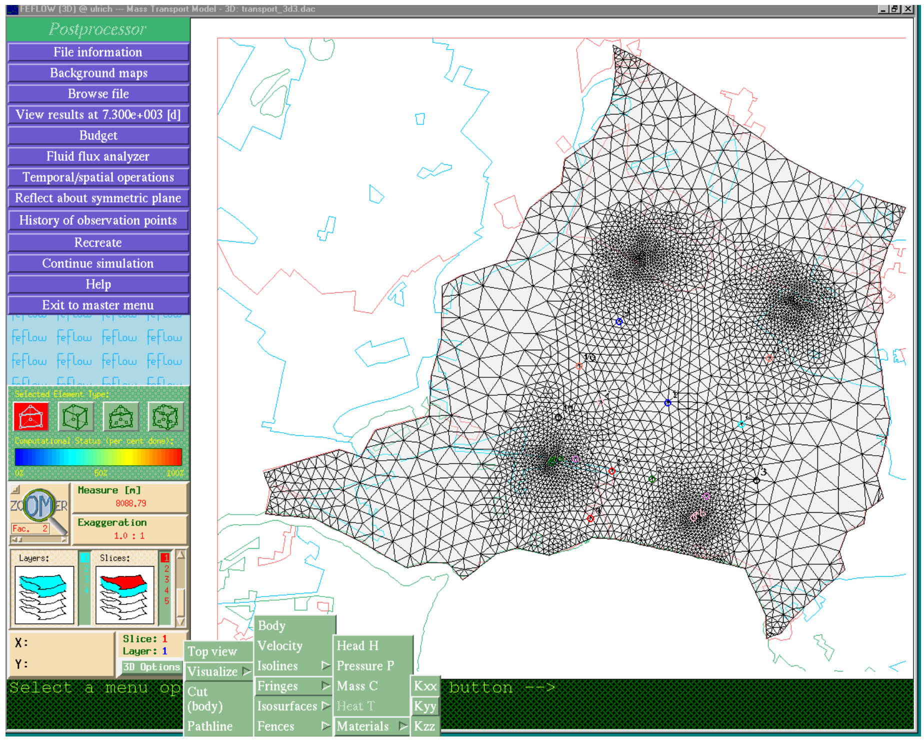


6.1 3D-Options Menu

For a detailed 3D description of our model, and to review all parameters, we will exit to the main menu and go to the 3D Options button located below the Layer/Slices browser. You can enter the menu from the either the ***Shell*** menu or the ***Problem Editor.*** You enter the 3D Options menu via the green **"3D Options"** button at the lower left side of the screen, below the "Layers & Slices" browser.

Go to the lower left corner of the working window.

☞ **"3D Options"** and hold the mouse button.

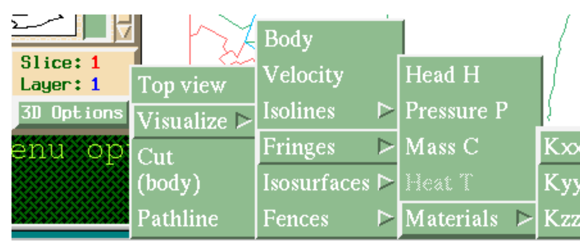


Click and hold the **"Visualize"** button and release.

☞ **"Fringes"**

☞ **"Materials"**

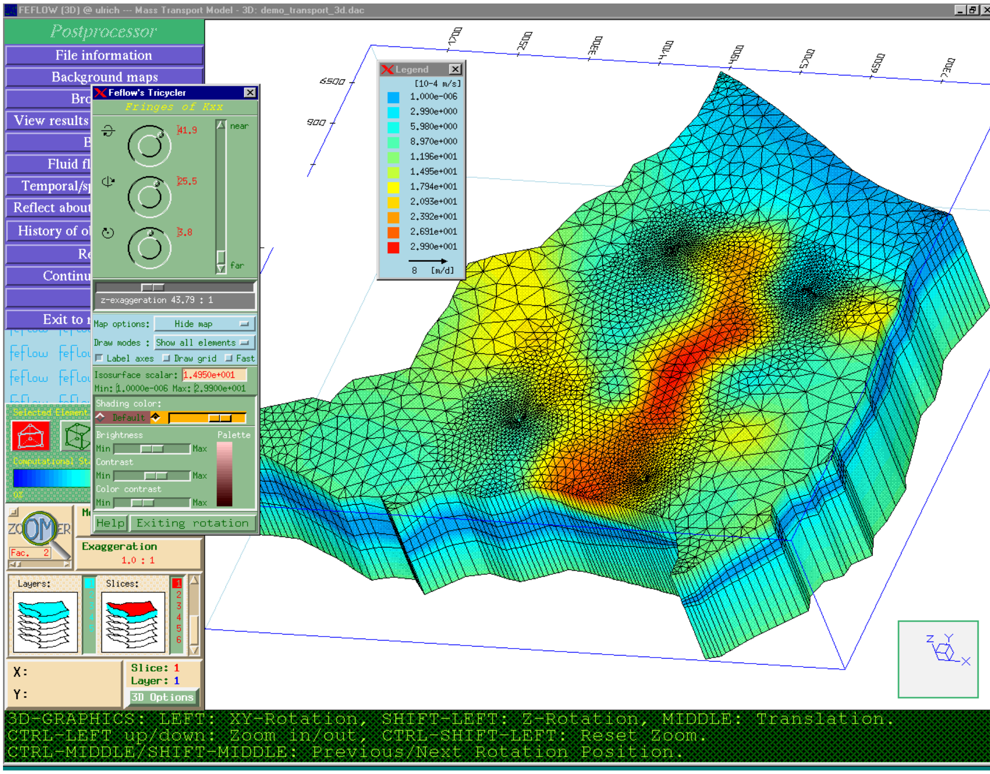
☞ **"Kxx"**



The conductivity in the x-direction is visualized as a 3D object. Additionally the **Tricycler** menu appears.

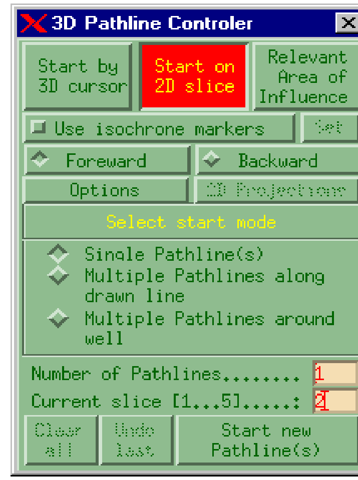
☞ on the model, hold the left mouse button and move the mouse in order to rotate the model.

Press the **<Ctrl>** key and move the mouse up and down to zoom in or out. Click the middle mouse botton to move the model.



6.1.1 3D Pathline Analyzer

One of the main 3D-analyzing tools FEFLOW offers is the 3D pathlines visualization. You can start the pathlines by positioning the starting point via the 3D cursor on the model (move the red handlers), by starting them from a specified slice or by importing an ASCII file for the computation of the Relevant Area of Influence (RAI) for a well.



We will start now some pathlines from the second slice.

☞ **"3D-Options"** and hold the mouse button.

Go to Pathlines and release the mouse button. The **3D Pathline Controller** appears.

☞ **"Start on 2D slice"**

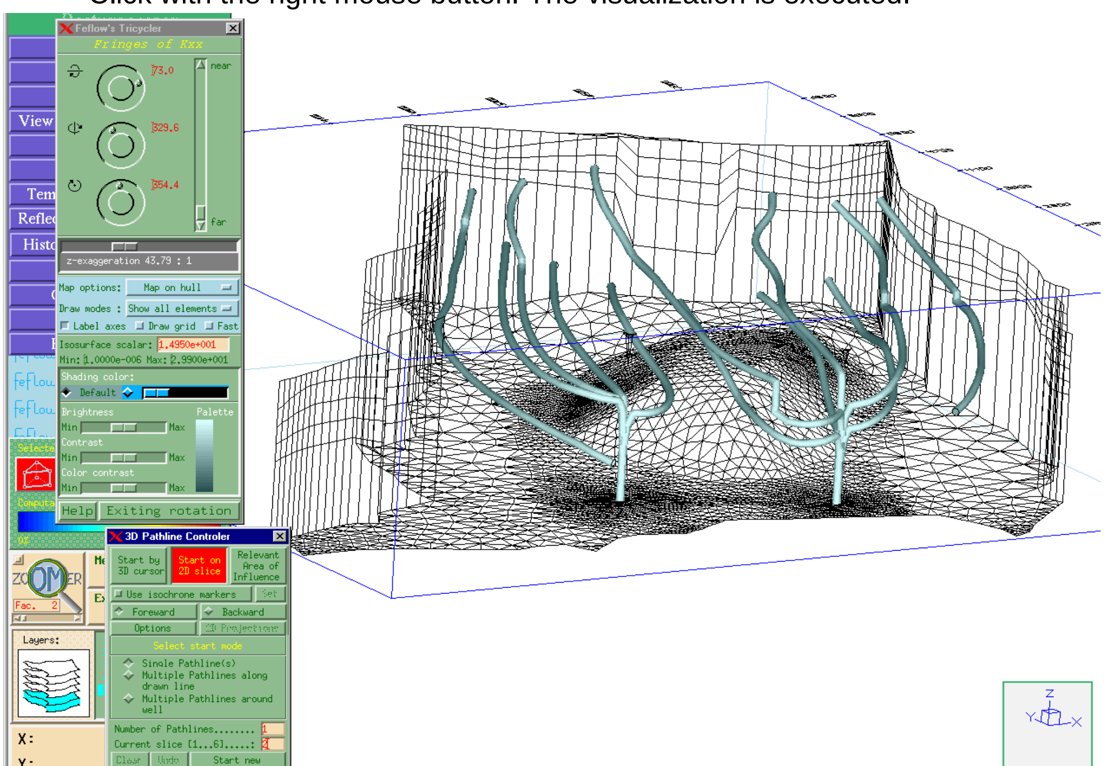
Insert **"2"** in the "*Current slice"* field

☞ **"Start new pathlines".** The selected slice is visualized. The cursor is in the zoom mode.

Click with the right mouse button to deactivate the zoomer.

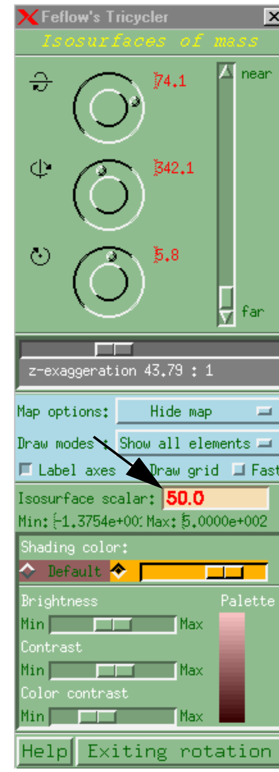
☞ on any arbitrary point on the northern part of the model. Each point will be a starting point for a pathline.

Click with the right mouse button. The visualization is executed.



The visualization of isosurfaces gives the predicted pathline of the contaminant plume. Insert a value of "**50**" in the *Isosurface scalar* field in the **Tricycler menu**.

☞ **"3D Options".** Hold the mouse button.:

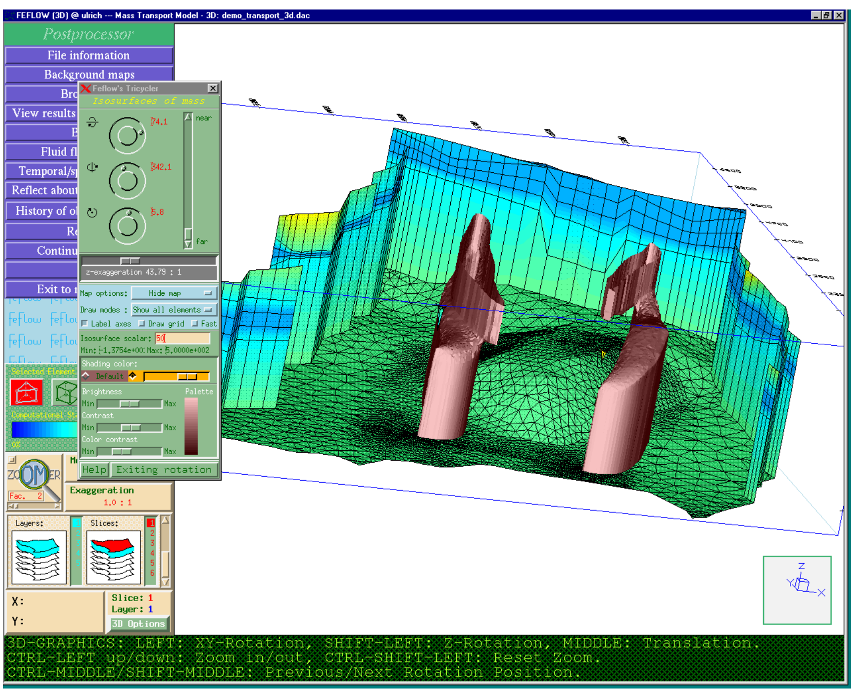


Go to **"Visualize"** and release the mouse button.

☞ **"Isosurfaces"**

☞ **"Mass C"**

The isosurfaces for the 50 mg/l mass concentration are visualized.
To exit the 3D Options menu, simply click on the Exit rotation button located in the lower right corner of the Tricycler menu.)



7 Final Remarks

This completes the FEFLOW DEMO. Please take some time to familiarize yourself with the many features FEFLOW offers. If you have questions, please refer to the online Help found in all menus by hitting <F1> or clicking on the "Help" button. If you have any further questions please contact your local distributor.