SVFlux and ChemFlux: Software for Two-Dimensional/Three-Dimensional Finite Element Variably Saturated Flow and Transport Modeling

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Introduction

SVFlux and ChemFlux are a pair of finite element models designed to simulate the movement of water and contaminants in two and three dimensions under variably saturated conditions. The transport simulator ChemFlux is designed as a companion to the flow simulator SVFlux. SVFlux and ChemFlux are commercial products developed by SoilVision Systems Ltd. and can be purchased via the company's Web site.

SVFlux and ChemFlux run under Microsoft Windows NT/2000/XP operating systems, and require a minimum of 128 MB RAM and approximately 150 MB hard drive space. The software includes Windows-based graphical user interface, numerical model engines, and post-processing programs. SVFlux and ChemFlux are suitable for numerous applications such as modeling of water and transport modeling in aquifers and the unsaturated zone, modeling of seepage across dams and geomembranes, and modeling of infiltration, excess pore water buildup, and dissipation. This article is based on two independent reviews of SVFlux (versions 4.05 and 5.04) and ChemFlux (versions 3.00 and 3.03).

How We Tested

The reviewed software was installed on two platforms, a desktop PC equipped with dual Pentium 4 2 Ghz processors and 512 MB RAM running Windows 2000 Professional; and a laptop PC equipped with a Pentium-M 1.4 Ghz processor and 512 MB RAM running Windows XP Professional. One reviewer used the setup programs for SVFlux

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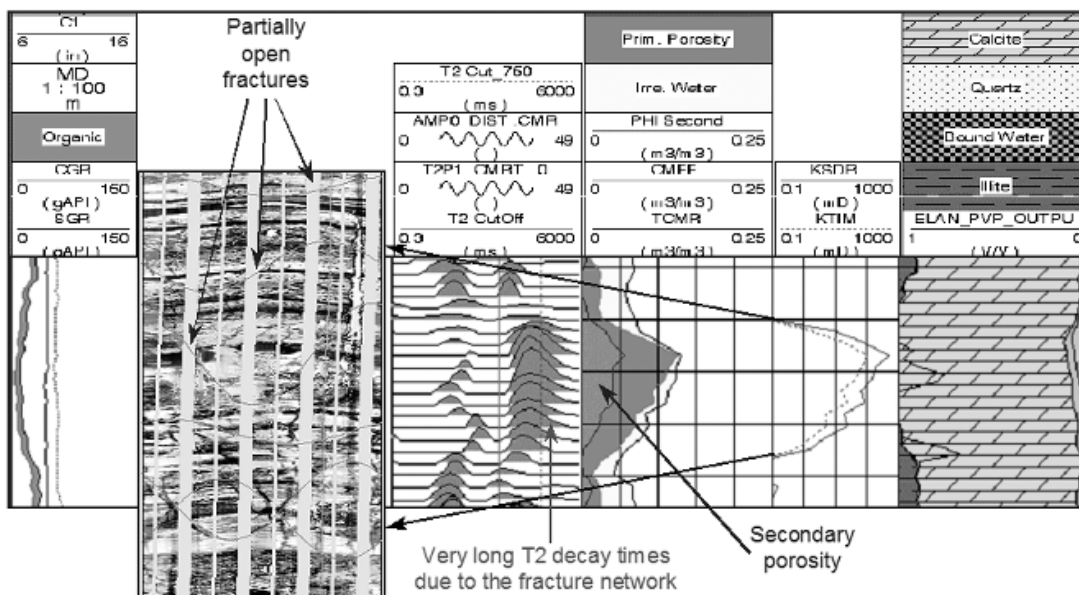[2]Department of Civil, Structural, and Environmental Engineering, State University of New York at Buffalo, 207 Jarvis Hall, Buffalo, NY 14260–4300; lsmatott@buffalo.edu

and ChemFlux, along with their companion solver package, FlexPDE, provided on the distribution CD; the other reviewer downloaded the software from SoilVision's Web site. Installation went smoothly without incident and took an average of less than 10 minutes. Disk usage was 78 MB for SVFlux, 70 MB for ChemFlux, and 6 MB for FlexPDE. After installation, a license for each program must be obtained by filling out a request form at SoilVision's Web site. A license file is then received by e-mail, enabling the user to run the software on a specific computer.

The installation of VisioPlot (a post-processing, two-dimensional visualization program, also available from SoilVision) required an update to the Microsoft .NET Framework. For both SVFlux and ChemFlux, there is a second installation step that occurs when the program is run for the first time. At this point, the user must specify a backend database, and solver and visualizer executables. This procedure was slightly problematic in that the program would report a successful setup, even if an incorrect (e.g., notepad.exe instead of FlexPDE3.exe) or nonexistent file was specified.

What We Found

The software essentially provides a CAD-like front-end graphical user interface (GUI) for FlexPDE, a partial differential equation solver using the finite element method (Figure 1). The software appeared stable, although a nonfatal divide-by-zero error was sometimes reported when the program (either SVFlux or ChemFlux) was opened via the start menu. Users go through a process of project creation (where organizational details like who, where, and when are entered) followed by problem selection (two- or three-dimensional, steady-state or transient, etc.) and problem definition. In the problem definition phase, the user adds soils and materials using a soil manager dialog. Then the user specifies the geometry of individual soil/material objects using the CAD-style interface. Next, boundary conditions and flux output areas are specified. Finally, the user selects from different types of output (e.g., pressure, head, concentration contours) and then runs the solver. Overall, the GUI works well and is fairly intuitive.

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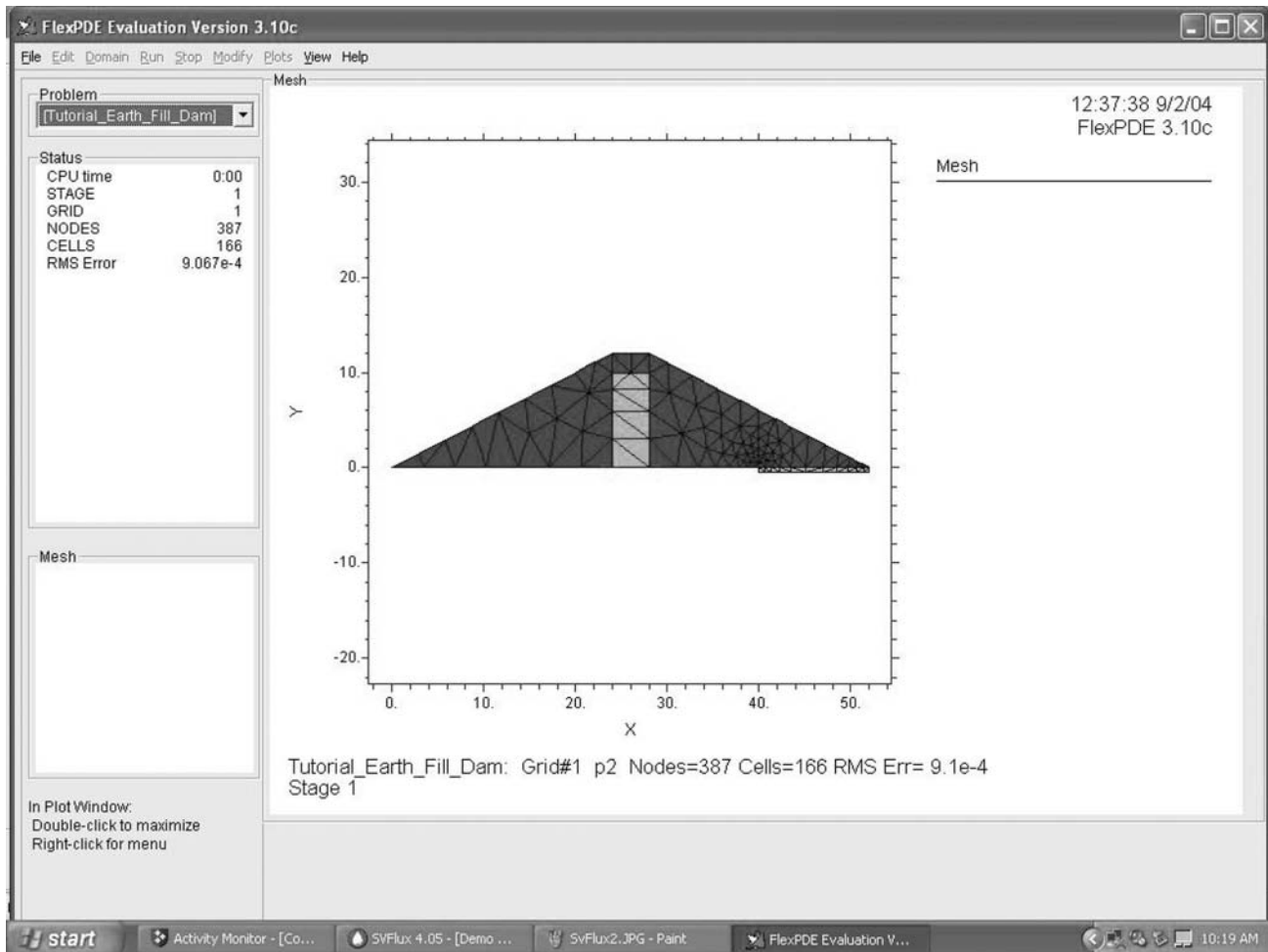www.slb.com/waterservices

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Figure 1. A screen capture of a program window for the SVFlux software.

The strength of the software lies in the automatic mesh generation, mesh refinement during the solution process, and automatic time step control. Two-dimensional problems can be quickly set up in SVFlux by drawing regions and assigning soil properties, boundary, and initial conditions. Three-dimensional problems are set up as a stack of layers. After the problem is set up, the user clicks the "Analyze" button to run the simulation. What actually happens behind the scene is that SVFlux generates a script for the specified problem and launches FlexPDE. To simulate transport, the flow simulation is first run using SVFlux, and then the problem geometry and the computed fluxes are imported to ChemFlux. ChemFlux can model the transport of a single solute and simulates advection, dispersion, adsorption, and decay. The current version of ChemFlux only handles steady-state flow results from SVFlux.

For the most part, the solver worked quite impressively. However, one reviewer encountered cases where the solver took very small time steps in a transient run, thus requiring a very long computation time. The reviewer did not have enough time to experiment with modifying the finite element method control parameters to reduce the computation time.

The reviewers' learning process on how to use the software was at times hampered by outdated or inadequate information in the user's manual, or minor bugs in the program. However, software support (via e-mail communica-tion) was excellent in answering one reviewer's questions. After several e-mail exchanges, the reviewer was able to use the software effectively. The software evaluation took approximately 30 hours.

The problem setup schematics drawn in SVFlux and ChemFlux can be exported as dxf, emf, or wmf files (the last two are Windows meta files). For two-dimensional problems, this is quite adequate. For three-dimensional problems, the program can display wire frame representations of surfaces used to define model layers. When several surfaces are displayed together, the wire frame lines result in a cluttered picture that is difficult to interpret. The graphical output capability of the solver FlexPDE is quite limited. A more useful option is to save the results to a file in a format that can be imported to Tecplot or AcuMesh (SoilVision's own three-dimensional visualization program). For three-dimensional problems, this is almost essential, but requires the additional graphics software.

Documentation (user's manual, tutorial manual, etc.) were provided in three-ring binders and also available in the form of Adobe Acrobat PDF files. Unfortunately, at the time of the software review, the vendor had just released SVFlux version 5 but the documentation was still for version 4. Some of the new features or parameter requirements were not described in the documentation. Although the user's manual was quite lengthy (230 pages), it did not cover all the details. Consequently, although the reviewers

were able to get a good overall knowledge of how the program works, there were occasions when one reviewer could not find the necessary information and was unable to proceed until he got an e-mail response from the vendor's support staff.

What We Liked

The finite element solver automatically generates the mesh and refines it during the simulation. This is probably the biggest strength of the software. A problem can be set up quickly by drawing regions and assigning soil properties to regions. Reviewers like the ability to specify boundary conditions using the "equation builder." For example, the user can specify the head along a boundary by something such as "if $t <= 10$ then $50 + 0.1*t$ else 60." This would specify the head to increase linearly from 50 at $t = 0$ to 60 at $t = 10$, and then remain at 60 afterwards.

A very nice feature was the ability to fit a number of empirical equations (such as van Genuchten and Maulem) to laboratory data of suction vs. water content or hydraulic conductivity. All the soil properties go into a database, which makes it easy to use the soil properties entered from another problem. Another nice feature was the ability to compute volumetric flow across a user-specified line (in a two-dimensional model) or a plane (in a three-dimensional model).

The material in the manuals is quite informative; users can quickly get up to speed by reading through one of the many tutorials provided. In addition to the tutorials, there is (1) a user's manual, which describes the use of each program in detail, (2) a theory manual, which describes the mathematics of the physical processes modeled by the program, and (3) a verification manual, which compares each software package against established counterparts (SVFlux is compared with Seep/W and ChemFlux is compared with MODFLOW/MT3DMS and CTRAN/W).

What We Did Not Like

One reviewer was quite frustrated when initially learning to use the software due to program quirks and outdated documentation. Once the reviewer learned the program idiosyncrasies and various workarounds, he began to appreciate the power of the software. Learning to use the software would be substantially enhanced by thoroughly updated documentation. For three-dimensional problems, better three-dimensional visualization capabilities would greatly help in setting up the problem.

The graphical output generated by FlexPDE was limited and uninspiring. The graphical settings are made prior to running the simulation. The plots generated by the solver are saved to a file for later viewing, but graphical settings (for example, contour intervals) cannot be changed after the run. The contours are sometimes choppy and the color schemes do not come out very well on the computer screen. Furthermore, contours are labeled with letters (referencing a legend), rather than numerical values, and units are not

included in axis labels. The reviewers would also like better guidance on how to set the parameters for the finite element method so that transient simulations do not run with tiny time steps, thus taking a long time to complete.

Overall

SVFlux and ChemFlux do a good job of providing a front-end GUI to the underlying finite element solver Flex-PDE. The procedure for creating a project and specifying a problem is straightforward. Automatic mesh generation and refinement are impressive. The SVFlux/ChemFlux/Flex-PDE programs should be very useful for modeling flow and transport under variably saturated conditions. It is apparent that the developers put a lot of thought and effort into building the software to meet a wide variety of user needs.

Rankings

The reviewers ranked the software's capability, reliability, ease of use, and technical support on a scale of 1 (worst) to 5 (best). The following rankings are the average of three sets of scores from both reviewers and the editor.

Capability	3.5
Reliability	4.0
Ease of use	4.0
Technical support	5.0

How to Obtain the Software

For more information on how to purchase SVFlux and ChemFlux, visit the Web site of SoilVision Systems at *www.soilvision.com*. The company is located at 2109 McKinnon Ave. S., Saskatoon, SK, Canada S7J 1N3; (306) 477–3324; fax (306) 955–4575. The commercial price for three-dimensional versions of SVFlux and ChemFlux is $5995 with a 25% educational discount. A student edition limited to 800 nodes is available at no cost.

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