Release Notes for SUTRA Version 2.2

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Summary of release

These Release Notes describe a revision to the U.S. Geological Survey (USGS) **SUTRA** code (Voss, 1984; Voss & Provost, 2002, Versions of June 21, 2003 and June 2, 2008). This revision (*Version 2.2*) adds the ability to specify time-dependent sources and boundary conditions (without programming) and to output information pertaining to source and boundary condition nodes in a convenient format. Utility codes for pre- and post-processing in 2D and 3D are provided with this new version of **SUTRA**. These codes are briefly mentioned herein and are described in more detail in the respective Release Notes for each code. Together, all of these utility codes and **SUTRA** are called **SutraSuite**.

The new code includes changes in the input and output formats. The new input structure is not compatible with previous versions of **SUTRA**. However, **SUTRA** *Version 2.2* can read input files created for use with *Versions 2.0 (2D3D.1)* and *2.1*.

At present, information on **SUTRA** *Version 2.2* includes these Release Notes and the revised **SUTRA** documentation (Voss and Provost, 2002, Version of September 22, 2010), which may be downloaded from a US Geological Survey web site (http://water.usgs.gov/nrp/gwsoftware/sutra.html).

The distribution package for **SUTRA** *Version 2.2* contains Fortran-90 source code and a WindowsTM executable; this informational file; three example 2D simulations that are described in the documentation; and input and output files for three 3D simulation examples, one of which is described in the documentation. The examples also include setup files for the **SutraSuite** pre- and post-processors.

In this release, **SUTRA** is distributed as a 32-bit executable code (compiled with Intel(R) Fortran Compiler Integration for Microsoft Visual Studio 2005, 10.1.3885.2005) that runs under Microsoft Windows[®] XP, 2000, NT, or 95/98 operating systems.

Software Release Notice

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USGS much appreciates your support in reporting any problems that may occur so that the codes can be improved.

Utility codes

SUTRA is included with a number of utility codes for both pre- and post-processing (see table below) in a package called **SutraSuite**. The utility codes are described in detail in separate Release Notes that accompany each code.

SutraGUI (Winston and Voss, 2003, a revision of Voss and others, 1997) is a pre-processor that is applicable to both 2D and 3D problems. **SutraPrep** (Provost, 2002) is a text-based preprocessor that creates 3D input datasets for **SUTRA** *Version 2.0 (2D3D.1)*, which can also be read by **SUTRA** *Versions 2.1 and 2.2*.

There are three post-processors for 2D problems: **SutraPlot** (Souza, 1999); **ModelViewer** (Hsieh and Winston, 2002); and **SutraGUI**. There are two post-processors for 3D problems: **SutraPlot** creates rotatable 3D plots of the mesh, 2D contours of results, and plots of velocity vectors; **ModelViewer** creates rotatable 3D color visualizations of results and plots of velocity vectors.

NOTE: A version of **SutraPlot** that is compatible with **SUTRA** Version 2.2 is currently under development. Please check the web site http://water.usgs.gov/nrp/gwsoftware/sutraplot/sutraplot.html for updates.

Two additional post-processing tools for both 2D and 3D simulations are available. **GW_Chart** can graphically display **SUTRA** fluid, solute and energy budgets, as well as hydrographs for **SUTRA** observation node output, showing pressure, concentration, and temperature as a function of time (Winston, 2000). The utility **CheckMatchBC** aids in setting boundary condition conductances for a **SUTRA** simulation; it checks the match of specified and simulated pressures, concentrations and temperatures and reports the number of matching digits. **GW_Chart** and **CheckMatchBC** are distributed with the installation files for **SutraGUI**.

Examples in 2D and/or 3D for pre-processing and post-processing accompany the utility codes.

All of these codes are available free of charge; however, use of **SutraGUI** requires purchase of a commercial product, ArgusONE™ (http://www.argusint.com).

SutraSuite utilities

Utility code	Pre- processor	Post- processor	Description
SutraPrep	<i>3D</i>		Generates 3D, regular SUTRA meshes and creates input data files for SUTRA <i>Version 2.0</i> [2D3D.1], which can be read by SUTRA <i>Versions 2.1 and 2.2. Instructions for using</i> SutraPrep can be found in the documentation that accompanies the code.
SutraGUI	2D and 3D	20	Graphical environment for setting up and executing 2D and 3D SUTRA runs, and for visualizing results from 2D SUTRA runs. Instructions for using SutraGUI can be found in the documentation that accompanies the code.
SutraPlot		2D and 3D	Creates 2D and rotatable 3D plots from 2D and 3D SUTRA output data. <i>Instructions for using SutraPlot can be found in the documentation that accompanies the code.</i> NOTE: A version of SutraPlot that is compatible with SUTRA <i>Version 2.2</i> is currently under development. Please check the web site http://water.usgs.gov/nrp/gwsoftware/sutraplot/sutraplot.html for updates.
Model Viewer		2D (fishnet meshes only) and 3D	Creates rotatable 3D color visualizations and animations from 2D and 3D SUTRA output data. <i>Instructions for using Model Viewer can be displayed by accessing the Help menu.</i>
GW_Chart		2D and 3D	Graphical display of fluid, solute and energy budgets and observation node output, showing pressure, concentration, and temperature as a function of time (hydrographs). <i>Instructions for using</i> GW_Chart can be displayed by accessing the Help menu.
CheckMatchBC		2D and 3D	Checks match of specified and simulated pressures, concentrations and temperatures and reports number of matching digits. This aids in setting boundary condition conductances.

General Instructions

Except where stated otherwise, the following instructions assume that **SUTRA** has been installed into the default directory recommended during the installation process, <u>c:\SutraSuite\SUTRA 2 2</u>. If a directory other than the default directory was selected, <u>\SutraSuite</u> will not be located directly under <u>c:\</u>, but the directory structure below <u>\SutraSuite</u> will remain as described below.

Instructions that involve mouse clicks refer to clicking on file names or icons displayed under the Windows Explorer file manager. For example, to "double-click on *file.txt*", use Windows Explorer to display the contents of the directory (folder) that contains the file *file.txt*, then click twice (in rapid succession) on the file name *file.txt* or its corresponding icon using the left mouse button. To "right-click", click once using the right mouse button.

Installation

After the **SUTRA** code (*Version 2.2*) is unzipped, most of the associated files will be in a new directory, c:\SutraSuite\SUTRA 2 2. This directory contains four subdirectories: \source, which contains the Fortran source files; \examples, which contains example datasets; \documentation, which contains this *ReleaseNotes.doc* file; and \bin, which contains the **SUTRA** executable file, *sutra_2_2.exe*, and a shortcut to this executable file. Please note that the \examples subdirectory will be empty until the large zipped example files are separately downloaded and installed.

In <u>c:\SutraSuite\SUTRA 2 2</u>, there is a file called *RunSUTRA.bat*, which is used to run the SUTRA code. *RunSUTRA.bat* contains the line

```
C:\SutraSuite\SUTRA 2 2\bin\sutra 2 2.exe
```

which provides the path for the **SUTRA** executable file, *sutra_2_2.exe*. If **SUTRA** was installed into a directory other than the default directory, please make certain that this line contains the correct pathname to where *SUTRA_2_2.exe* is located. Use a text editor to change the line if necessary.

Running SUTRA

To run **SUTRA** manually, create the file SUTRA filename assignments file, *SUTRA.FIL*, in the desired working directory. There are two ways to run **SUTRA**. 1- Double-click on the *RunSUTRA.bat* in the same directory. 2- Create a *Windows shortcut* to the *sutra_2_2.exe* file in the directory in which you will work, and then double click the shortcut to run **SUTRA**. For both methods, a window will appear indicating that the **SUTRA** code is running.

SUTRA may also be run directly from the **SutraGUI** preprocessing utility and directions for doing this may be found in the **SutraGUI** documentation (Winston and Voss, 2003) and in some example simulations, including step-by-step instructions (see Rocky and Henry examples) provided in the directory \SUTRA 2 2\examples.

New in SUTRA Version 2.2

A brief description of the main changes in Version 2.2 follows:

TIME-DEPENDENT BOUNDARY CONDITIONS WITHOUT PROGRAMMING

In the previous version of **SUTRA** (*Version 2.1*), the user was required to program into subroutine BCTIME (in Fortran) any time-dependent boundary conditions. In *Version 2.2*, programming is not required to implement time-dependent boundary conditions; they can be specified using one or more ".bcs" input files.

BOUNDARY CONDITION OUTPUT FILES

SUTRA *Version 2.2* offers a set of four new output files (".bcof", "bcop", ".bcos", and ".bcou"), which summarize specifications and results at the four types of boundary condition nodes: fluid sources and sinks, specified pressure, sources and sinks of solute mass or energy, and specified concentration or temperature.

Documentation

These Release Notes and the **SUTRA** manual (Voss and Provost, 2002, Version of September 22, 2010) are the primary documentation of the code. The **SUTRA** manual is available, free of charge, in electronic (*pdf*) format from the USGS website http://water.usqs.gov/nrp/qwsoftware/sutra.html.

2D examples provided

Three example 2D simulations are provided in sub-directories of the directory SutraSuite\SUTRA 2 2\examples. All input and output files for each problem are included there. (The examples may be run manually [see 'RUNNING SUTRA', above] or may be recreated using the preprocessor described in the *ReadMe* file that accompanies each example and run through the preprocessor.) It is recommended that the utility and input files be copied to a new working directory for testing runs, so that the user's new *SUTRA* output does not overwrite the existing output files that were downloaded. The 2D examples include the Rocky Mountain Arsenal contaminant plume problem (\\Rocky), and the Henry seawater intrusion problem (\\Henry). The input files were created with the utility *SutraGUI*. Information on the setup of the 2D examples may be found in the *SUTRA* documentation (Voss and Provost, 2002, Version of September 22, 2010) and in the respective *ReadMe* files that accompany each example. Users are also encouraged to download, install, and try using *Model Viewer* to view results of these runs. Creation of the input files and post-processing using *SutraGUI* is described in the *SutraGUI* Release Notes. Also provided is the Island2D example, in which the mesh has been modified since the previous release to facilitate comparison with the updated 3D version described just below.

3D examples provided

Three example 3D simulations are provided in sub-directories of the directory, SutraSuite\Sutra 2\examples. These may be found in sub-directories \Bf., \Pond, and \Island3D. All input and output files for each problem are included there. (The examples may be run manually [see 'RUNNING SUTRA', above] or may be recreated using the pre-processor described in the *ReadMe* file that accompanies each example and run through the pre-processor). The island problem is described in the SUTRA documentation (Voss and Provost, 2002, Version of September 22, 2010), and the other two problems are described in the ReadMe file that accompanies each example. The Island3D problem has been modified since the previous release to feature an irregular 3D mesh. It is recommended that the utility and input files be copied to a new working directory for testing runs so that the user's new **SUTRA** output does not overwrite the existing output files that were downloaded. Users are encouraged to download, install, and try using **Model Viewer** to view results of these runs. (This tool also comes with examples.)

References

Burnett, R.D., and Frind, E.O., 1987, Simulation of contaminant transport in three dimensions 2. dimensionality effects, Water Resources Research, 23(4), 695-705.

Hsieh, P.A., and Winston, R.B., 2002, User's guide to **Model Viewer**, a program for three-dimensional visualization of ground-water model results: U.S. Geological Survey Open-File Report 02-106, 18 p. http://water.usqs.gov/nrp/gwsoftware/modelviewer/ModelViewer.html

Provost, A.M., 2002, **SutraPrep**, a pre-processor for SUTRA, a model for ground-water flow with solute or energy transport: U.S. Geological Survey Open-File Report 02-376, 43 p. http://water.usgs.gov/nrp/gwsoftware/sutra.html

Souza, W.R., 1999, **SutraPlot**, a graphical post-processor for SUTRA, a model for ground-water flow with solute or energy transport: U.S. Geological Survey Open-File Report 99-220, 30 p. http://water.usgs.gov/nrp/gwsoftware/sutra.html

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Voss, C. I., and Provost, A.M., 2002 (Version of June 21, 2003), **SUTRA**, A model for saturated-unsaturated variable-density ground-water flow with solute or energy transport, U.S. Geological Survey Water-Resources Investigations Report 02-4231, 250 p.

Voss, C. I., and Provost, A.M., 2002 (Version of June 2, 2008), **SUTRA**, A model for saturated-unsaturated variable-density ground-water flow with solute or energy transport, U.S. Geological Survey Water-Resources Investigations Report 02-4231, 270 p. http://water.usgs.gov/nrp/qwsoftware/sutra.html

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Voss, Clifford I., Boldt, David, and Shapiro, Allen, 1997, **SUTRA-GUI**, A graphical-user interface for the U.S. Geological Survey's SUTRA code using ArgusONE, U.S. Geological Survey Open-File Report 97-421, 106p.

Winston, R.B., 2000, Graphical User Interface for MODFLOW, Version 4: U.S. Geological Survey Open-File Report 00-315, 27 p. http://water.usgs.gov/nrp/gwsoftware/modflow.html

Winston, R.B. and Voss, C.I., 2003, **SutraGUI**, a graphical-user interface for SUTRA, a model for ground-water flow with solute or energy transport: U.S. Geological Survey Open-File Report 03-285, 114 p. http://water.usgs.gov/nrp/gwsoftware/sutra.html

File types for SUTRA Version 2.2 and associated codes

Code	File types for current SUTRA version (2.1) and Version 2.0 (2D3D.1)	Content
SUTRA input	SUTRA.FIL .inp .ics .bcs (<i>Version 2.2</i> only)	file assignments main input initial conditions time-dependent boundary conditions
output	.smy (defaults to SUTRA.SMY) .lst .rst .nod .ele .obs .obc (Versions after 2.0 only) .bcof (Version 2.2 only) .bcop (Version 2.2 only) .bcos (Version 2.2 only) .bcos (Version 2.2 only)	simulation summary or file assignment errors main results listing restart file nodewise results elementwise results observation results observation results fluid source/sink node information specified-pressure node information solute-mass or energy source/sink node information specified-concentration or temperature node information
SutraPrep* input	.prp .inp	main input existing SUTRA .inp file
	.prl	SutraPrep log
output	.inp .ics .wrl	3D blocks or mesh in VRML
SutraGUI input	.nod .ele	
output	.inp .ics	
SutraPlot**		
input	.inp .nod .ele	
output	.gr2 .gr3 .spl	2D grid of results 3D grid of results plot layout
Model Viewer	156.	
input	.inp .nod .ele	
output	.mvb .wrl .bmp	Binary version of .nod & .ele 3D view of image bitmap of image
GW_Chart	ionip	Signap of image
input	.obs .lst	For hydrographs For budget charts
output	.wmf	Saved image
CheckMatchBC input	.inp .nod	
output		

(Uppercase names are not user-selectable.)

^{*}SutraPrep creates input for SUTRA Version 2.0 (2D3D.1), which can be read by SUTRA Versions 2.1 and 2.2.

^{**}A version of **SutraPlot** that is compatible with **SUTRA** *Versions 2.1 and 2.2* is currently under development. Please check the web site http://water.usgs.gov/nrp/gwsoftware/sutraplot/sutraplot.html for updates.