Release Notes for
SUTRA-MS Version 2004.1

December, 2004

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Summary of release

These Release Notes describe a version of SUTRA modified to simulate heat and multiple-solute transport (SUTRA-MS). Modifications for SUTRA-MS were made to Version 2D3D.1 of SUTRA that included both 2D and 3D simulation capability (Voss and Provost, 2002). SUTRA-MS was modified such that standard SUTRA simulations could be run in addition to heat and multiple-solute transport simulations. SUTRA-MS version 2004.1 was verified to correctly simulate all represented processes under saturated conditions in a number of tests that appear in the documentation.

At present, information on SUTRA-MS Version 2004.1 includes these Release Notes and the SUTRA-MS documentation (Hughes and Sanford, 2004), which may be downloaded from a US Geological Survey web site (http://water.usgs.gov/nrp/gwsoftware/sutra.html). Additional information on SUTRA and documentation for SUTRA Version 2D3D.1 may also be downloaded from a US Geological Survey web site (http://water.usgs.gov/nrp/gwsoftware/sutra.html).

The distribution package for SUTRA-MS Version 2004.1 contains Fortran-90 source code and a Windows™ executable; this informational file; and documentation for SUTRA-MS. An additional installation package containing three 2D and one 3D example SUTRA-MS simulations that are described in the documentation is also available.

In this release, SUTRA-MS is distributed as an executable code (compiled with Compaq® Visual Fortran Version 6.6.C) that runs under Microsoft Windows® XP, 2000, NT, or 95/98 operating systems.

Software Release Notice

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The user assumes all risk for any damages whatsoever resulting from loss of use, data, or profits arising in connection with the access, use, quality, or performance of this software.

The USGS would appreciate your support in reporting any problems that may occur so that SUTRA-MS can be improved.

Utility codes

No specific utility codes have been developed for SUTRA-MS Version 2004.1 but program output can easily be modified to be consistent with standard SUTRA output in order to use utilities codes provided with SUTRA in the package called SutraSuite. SUTRA-MS users are referred to the Release Notes for SUTRA and associated utility codes available at http://water.usgs.gov/nrp/gwsoftware/sutra.html.

For the examples presented in the documentation for SUTRA-MS, the SutraGUI (Winston and Voss, 2003) was used to develop standard SUTRA input files for each simulated species and SUTRA-MS input datasets were manually created using the standard SUTRA input files and a text editor. SutraPrep, a text-based preprocessor (Provost, 2002), can also be used to develop input datasets for each simulated species.

All of the SUTRA utility codes, including SUTRA-Prep, are available free of charge; however, use of SutraGUI requires purchase of a commercial product, ArgusONE™ (http://www.argusint.com).

General Instructions

Except where stated otherwise, the following instructions assume that SUTRA-MS has been installed into the default directory recommended during the installation process, C:\SutraSuite\SUTRA-MS. If a directory other than the default directory was selected, \SUTRA-MS will not be located directly under C:\USGS, but the directory structure below \SUTRA-MS 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-MS code (Version 2004.1) is installed, all of associated files will be in a new directory, C:\ SutraSuite\SUTRA-MS. If a typical installation was performed, this directory contains three subdirectories: \Source, which contains the Fortran source files; \Documentation, which contains this ReleaseNotes_SUTRA-MS_v2004.1.pdf file and a pdf of the SUTRA-MS users manual (OFR2004-1207.pdf); and \bin, which contains the SUTRA-MS executable file, SUTRA-MS.exe, and an icon file for this executable file. Please note that the \Source subdirectory will not be present unless the typical installation is performed or a custom installation is performed and this item is selected. During installation of SUTRA-MS, the system PATH statement is modified to include the SUTRA-MS\bin subdirectory so that SUTRA-MS may be run from the command line without specifying the complete path to SUTRA-MS.exe. After installation of SUTRA-MS, the PATH statement should be checked to confirm that it has been correctly modified.

If the Example Problems installation package is downloaded and installed the SUTRA-MS subdirectory will also contain an \Examples subdirectory, which contains input and output files for the example datasets. For convenience, the Example Problems should be installed in the same location as SUTRA-MS executable, documentation, and source code file (*i.e.,* C:\ SutraSuite\SUTRA-MS\).

Running SUTRA-MS

To run SUTRA-MS manually, create the file SUTRA-MS filename assignments file, SUTRA.FIL, as described in the documentation in the desired working directory after creating SUTRA-MS input files. There are three ways to run SUTRA.

1. Open a command prompt (Start⇒Run⇒Cmd.exe), navigate to the directory with the SUTRA.FIL file and associated SUTRA-MS input files, and type `SUTRA-MS`.

2. Create a batch file in the same directory as the SUTRA.FIL file and associated SUTRA-MS input files. At a minimum, the batch file should contain the following command:

```
SUTRA-MS
```

The batch file can include any necessary pre- and post-processing commands (*i.e.,* copy, del, *etc.*). Double-click on the batch file in Windows Explorer.

3. Create a Windows shortcut to the SUTRA-MS.exe file in the directory that contains the SUTRA.FIL file and associated SUTRA-MS input files, and then double click the shortcut to run SUTRA-MS.

A DOS window will appear indicating that the SUTRA-MS code is running for items 2) and 3). Items 1) and 2) above pre-suppose that the PATH statement was correctly set during the installation process to include the SUTRA-MS\bin subdirectory. Control-s can be used to pause execution of SUTRA-MS.

SUTRA-MS Modifications to SUTRA Version 2D3D.1
SUTRA-MS retains all of the features of SUTRA Version 2D3D.1, including variably saturated to fully saturated flow, advection, and production and decay of simulated species. The principal modification in SUTRA-MS is an extension of existing numerical methods to solve for the transport of multiple species and allow for dependence of density and viscosity on any of the simulated species. Users are referred to the documentation for SUTRA for more information on the capabilities of SUTRA (Voss, 1984; Voss and Provost, 2002).

Additional SUTRA-MS modifications include:
- Ability to specify spatially varying solid matrix thermal conductivities values.
- Ability to use either a volumetric average or geometric-mean approximation for bulk thermal conductivity.
- Ability to simulate simple time-varying boundary conditions (SUTRA-MS TBC Option) without the need for problem specific code modifications and compilation as is necessary with the SUTRA (Version 2D3D.1).
- Ability to output nodal- and element-simulation data at user-specified times (SUTRA-MS OTM Option). This option provides users with more control over when simulated results are saved in output files and the size of simulated output files.
- Ability to use a simplified automatic time-stepping algorithm to adjust time steps based on solution convergence (SUTRA-MS ATS Option). This option also includes the capability to rerun a time step if user-specified iteration criteria are not met. Use of this option can reduce the possibility that a non-convergent solution will occur for well-posed problems using excessive timesteps.
- Ability to enter observation locations using spatial coordinates instead of node numbers (SUTRA-MS SOB Option). This option makes it easier to explore different horizontal and vertical discretizations since this option finds the closest node to the specified location in a given SUTRA-MS input dataset.
- Hydraulic parameters can be specified in a separate file for zones defined in the main SUTRA-MS input file (SUTRA-MS ZON option). Use of this option reduces memory requirements for large two- and three-dimensional problems and facilitates the use of generic parameter-estimation codes such as UCODE (Poeter and Hill, 1998).

The current modifications do not place an arbitrary limit on the number of species that can be simulated. The number of species that can be simulated is a function of the problem size and the amount of available random access memory (RAM). Furthermore, the modifications are such that more complicated relationships between solute concentration and system state (e.g., density, etc.) can be easily incorporated.

FILE NAMES

There are now a number file types directly associated with the SUTRA-MS. The filename extensions for all types are standardized and are listed below. In order to maintain consistency with SUTRA Version 2D3D.1 it is suggested that these standard extensions be used for SUTRA-MS datasets. All of the changes to input and output files indicated below are also consistent with SUTRA Version 2D3D.1.

INPUT DATA

- All input files (".inp", ".ics", ".tbc", ".otm", ".ats", ".sob", and ".zon") for SUTRA-MS consist primarily of unformatted data. This allows the user to decide on any columnization of data that seems useful. All character data must be enclosed by quotes.
- Comment lines are allowed before and after each individual dataset in all input files (".inp", ".ics", ".tbc", ".otm", ".ats", ".sob", and ".zon"), making the files easier to read.
- The main input file (".inp") includes a description of the mesh type (2D or 3D, IRREGULAR, REGULAR or BLOCKWISE). For REGULAR or BLOCKWISE meshes, it also includes the number of nodes in each mesh direction, and for BLOCKWISE meshes, it also includes the number of elements in each strip of blocks in each direction.
- Matrix equation solvers are selected in the main input file (".inp") for the flow solution and for the transport solution (either DIRECT, CG, GMRES or ORTHOMIN). Parameters are also provided for the iterative solvers.
- Uniform initial conditions can be specified in the initial conditions file (".ics") for pressure, temperature, and/or solute concentration(s) by specifying only a keyword (UNIFORM) and the constant value.
- The new format of the name file, SUTRA.FIL, that lists file types, assigned unit numbers, and filenames (in free format) is:

'INP'	51	'project.inp'
'ICS'	52	'project.ics'
'TBC'	53	'project.tbc'
'OTM'	54	'project.otm'
'ATS'	55	'project.ats'
'SOB'	56	'project.sob'
'ZON'	57	'project.zon'
'LST'	61	'project.lst'
'RST'	62	'project.rst'
'NOD'	63	'project.nod'
'ELE'	64	'project.ele'
'OBS'	65	'project.obs'
'SMY'	66	'project.smy'

  The order of SUTRA file types need not be exactly as shown here and it is suggested that the filenames have the indicated extensions. The unit numbers are user-selectable, and the ones given are only a suggestion. These should generally be chosen in the range 11-99 to avoid conflicts with pre-defined Fortran units. The "project" prefixes are also user-selectable, and these need not all be identical, though this is often desired to unify the naming of a simulation's input and output files.

OUTPUT

- The frequency of output for each output file may now be controlled independently and specific output times can be specified through use of the SUTRA-MS OTM option. The order and content of columns in the columnar nodewise and elementwise output files is now controlled by data in the main input file (".inp"). If the OTM option is used, data specified in the OTM input file (".otm") overrides parameters specified in the main input file (".inp") to control output of nodewise and elementwise data.
- Observation node output from a SUTRA-MS run has been moved from the main output file to a separate observation file with extension ".obs". This applies with the standard method for specifying observation locations by nodes or the SUTRA-MS SOB option is used.

- The file project.smy or (by default) SUTRA.SMY keeps a simulation summary, which includes a running report of the simulation's progress and an iterative solver convergence log for each iteration on every time step.

Documentation

These Release Notes and the SUTRA-MS users manual (Hughes and Sanford, 2004) are the primary documentation of the code. The SUTRA-MS users manual is also available, free of charge, in electronic (pdf) format from the USGS website http://water.usgs.gov/nrp/gwsoftware/sutra.html.

Control-s can be used to pause execution of SUTRA-MS and may be required to review run-time information for all but one of the 2D example problems.

2D examples provided

Three example 2D simulations are provided in sub-directories of the directory SutraSuite\SUTRA-MS\Examples. All input for each problem are included there. All output files, except the restart (".rst") files, have been included in the v2004.1_Results subdirectory in the directory containing the input files for each example problem. The restart (".rst") files have been excluded to reduce the file size of the Examples installation program.

The examples may be run manually [see 'RUNNING SUTRA-MS', above]. The 2D examples include the Henry and Hilleke problem (Examples\HenryAndHilleke), the Pringle, Glass, and Cooper problem (\Examples\PringleGlassCooper\), and the Henry seawater intrusion problem with additional species problem (\HenryWithAdditionalSpecies). Information on the setup of the 2D examples may be found in the SUTRA-MS documentation (Hughes and Sanford, 2004). In addition, the HenryWithAdditionalSpecies example is provided for comparison with the 3D version described below.

3D examples provided

One example 3D simulation is provided in sub-directories of the directory, SutraSuite\SUTRA-MS\Examples. This may be found in the \HenryWithAdditionalSpecies subdirectory. All input and output files (except the restart (".rst") files for the reasons listed above) for the problem are included there.

The example may be run manually [see 'RUNNING SUTRA-MS', above]. The HenryWithAdditionalSpecies problem is described in the SUTRA-MS documentation (Hughes and Sanford, 2004).

References

Hughes, J.D. and Sanford, W.E., 2004, SUTRA—MS: A Version of SUTRA Modified to Simulate Heat and Multiple-Solute Transport: U.S. Geological Survey Open-File Report 2004-1207, 141 p.
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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

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http://water.usgs.gov/nrp/gwsoftware/sutra.html