

# Release Notes for SUTRA-MS Version 1.1

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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 1.1 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 1.1 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 archive file for SUTRA-MS Version 1.1 contains Fortran-90 source code and 32- and 64-bit Windows™ executables; this informational file; documentation for SUTRA-MS, and documentation for two additional heat and solute transport SUTRA-MS simulations. An additional archive file containing three 2D and one 3D example SUTRA-MS simulations that are described in the documentation and two additional 2D heat and solute transport simulations is also available.

In this release, SUTRA-MS is distributed as an executable code (compiled with Intel® Visual Fortran Version 14.0.1.139 Build 20131008) that runs under the Microsoft Windows 7 operating system.

## Software Release Notice

SUTRA-MS is public-domain software and is released to you cost-free by USGS for any purpose you choose. This is a general public release.

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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 1.1 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, C:\WRDAPP\SUTRA-MS\_1.1\. If a directory other than the default directory was selected, \SUTRA-MS\_1.1 will not be located directly under C:\WRDAPP, but the directory structure below \SUTRA-MS\_1.1 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 Version 1.1 installation archive is extracted, all of associated files will be in a new directory, C:\WRDAPP\SUTRA-MS\_1.1. If a typical extracted was performed, this directory will contain four subdirectories:

1. `\src`, which contains the Fortran source files and an example `makefile` that can be modified to be used with other Fortran compilers (for example `gfortran`)
2. `\msvs`, which contains a Microsoft Visual Studio 2012 solution and Intel® Visual Fortran project file
3. `\doc`, which contains this `ReleaseNotes_SUTRA-MS_v1.1.pdf` file, a pdf of the SUTRA-MS user's manual (`OFR2004-1207.pdf`)
4. `\bin`, which contains the 32- and 64-bit versions of the SUTRA-MS executable file, `SUTRA-MS_1.1.exe` and `SUTRA-MS_1.1_x64.exe`, and an icon file for this executable file. The system `PATH` statement can be modified to include the `SUTRA-MS_1.1\bin` subdirectory so that SUTRA-MS Version 1.1 may be run from the command line without specifying the complete path to `SUTRA-MS_1.1.exe` and `SUTRA-MS_1.1_x64.exe`.

If the Example Problems archive is downloaded and extracted the `SUTRA-MS_1.1` subdirectory will also contain:

1. `\data`, which contains input files for the example problem datasets.
2. `\output_test`, which contains output SUTRA-MS list files from running the example files with the 32-bit version of SUTRA-MS version 1.1. These files can be used to evaluate correct execution of the precompiled and (or) user-compiled 32-bit executable.
3. `\output_test_x64`, which contains output SUTRA-MS list files from running the example files with the 64-bit version of SUTRA-MS version 1.1. These files can be used to evaluate correct execution of the precompiled and (or) user-compiled 64-bit executable.

The Example Problems archive should be extracted to the same location as the SUTRA-MS Version 1.1 executable, documentation, and source code file (i.e., `C:\WRDAPP\SUTRA-MS_1.1\`).

### **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_1.1.exe
```

or

```
SUTRA-MS_1.1_x64.exe
```

3. 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. Examples of batch files are included in each of the example problem subdirectories.
4. Create a Windows shortcut to the SUTRA-MS\_1.1.exe and (or) SUTRA-MS\_1.1\_x64.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). Item (1) above pre-suppose that the PATH statement was modified 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 time steps.

- 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 is 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 data***

- 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 user's manual (Hughes and Sanford, 2004) are the primary documentation of the code. The SUTRA-MS user's manual is also available, free of charge, in electronic (pdf) format from the USGS website <http://water.usgs.gov/nrp/gwsoftware/SUTRA.html>. Documentation for two additional coupled heat- and solute-transport problems has also been included in pdf format (`SUTRA-MS_ThermalSolute.pdf`) in this release.

`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*

Five example 2D simulations are provided in sub-directories of the `data` directory. All input files for each problem are included there. Output list files generated using the 32- and 64-bit versions of SUTRA-MS have been included in the `output_test` and `output_test_x64` directories, respectively. Other output files have not been included to reduce the file size of the Example Problems archive.

The examples may be run manually [see 'Running SUTRA-MS', above]. The 2D examples include:

1. the Henry and Hilleke problem (`data\01_HenryAndHilleke\`)
2. the Pringle, Glass, and Cooper problem (`\data\02_PringleGlassCooper\`)
3. the Henry seawater intrusion problem with additional species problem (`\data\03_HenryWithAdditionalSpecies\2D\`)
4. the coupled Gelhar and Collins (1971) constant density heat and solute transport problem (`\data\04_TSRAD\`)
5. the coupled density-dependent heat and solute transport problem based on Gelhar and Collins (1971) (`\data\04_TSRADVD\`)

Information on the setup of the 2D examples may be found in the SUTRA-MS documentation (Hughes and Sanford, 2004) and `SUTRA-MS_ThermalSolute.pdf` document in the `doc` directory. In addition, the `03_HenryWithAdditionalSpecies` example is provided for comparison with the 3D version described below.

### *3D examples provided*

One example 3D simulation is provided in the (`\data\03_HenryWithAdditionalSpecies\3D\`) sub-directory. All input files and the output list files generated using the 32- and 64-bit versions of SUTRA-MS have been included.

The example may be run manually [see 'Running SUTRA-MS', above]. The 02\_HenryWithAdditionalSpecies problem is described in the SUTRA-MS documentation (Hughes and Sanford, 2004).

### **SUTRA-MS version 1.1 enhancements and bug fixes**

SUTRA-MS version 1.1 retains all of the features of SUTRA-MS Version 2004.1. Enhancements and bug fixes included in SUTRA-MS version 1.1 include:

#### ***Enhancements***

- Nodal and Elemental aquifer parameters can be specified using zones defined in the main SUTRA-MS input data file (sutra.inp) using the NREG and LREG parameters in DataSets 14B and 15B and aquifer parameters specified in a separate input data file (sutra.zon).
- Optional output of nodal and elemental data to ASCII Tecplot® files. Specified using TPN and TPE keywords in sutra.fil. Output frequency based on output control in main file (sutra.inp) or in user specified output times file (sutra.otm).

#### ***Bug fixes***

1. Fixed error in initialization of CS1 array in InData1.f90 for multi-species energy and solute transport problems.
2. Fixed error when using a steady-state flow solution and backsolving for multi-species simulations (NSPE>1). The issue is UMAT cannot be reused for multi-species simulation. The solution is to always zero and refill UMAT prior to solving for each species (i.e., backsolving is not used).

### **Input file modifications for SUTRA-MS version 1.1**

#### ***Specification of Nodal Adsorption and Production***

The following additions need to be made to SUTRA-MS input data sets to specify spatially varying adsorption and production parameters.

#### ***Data Set 14C***

Data Set 14C is added after Data Set 14B only if ADSMOD is not specified to be 'NONE' in Data Set 11 for at least one species for SOLUTE transport (NSPE >= 1) and SOLUTE and ENERGY transport simulations (NSPE > 1). Data Set 14C is not specified for ENERGY transport simulations (NSPE = 1).

```
#
#Data Set 14C - Nodal Sorption Parameters
# NODE      CHI1(1) CHI2(1) CHI1(2) CHI2(2)
      1         0         0 700431.      0
      2000      0         0 700431.      0
      0
```

where:



- Only nodes that differ from the default values in Data Set 11 need to be specified
- CHI1 and CHI2 values have to be specified for each node specified in Data Set 14C regardless of the sorption model (this is consistent with the approach used in Data Set 11)
- CHI1 and CHI2 values are specified using the same rules defined for Data Set 11
- Data for Data Set 14C is terminated with a 0 node number and a termination line is required for all SUTRA-MS simulations that do not use a `sutra.zon` file and simulate adsorption
- An error condition is returned if NODE is greater than NN

### Data Set 14D

Data Set 14D is specified after Data Set 14B and 14C (if required) only if one of the production terms in Data Set 12 is non-zero for at least one species.

```
#
##Data Set 14D - Nodal Production Parameters
# NODE   PRODF0(1) PRODS0(1) PRODF1(1) PRODS1(1) PRODF0(2) PRODS0(2) PRODF1(2) PRODS1(2)
    1         0         0         0         0         1.         0. -1.37e-11 -1.37e-11
  2000         0         0         0         0         1.         0. -1.37e-11 -1.37e-11
0
```

where:

- only nodes that differ from the default values in Data Set 11 need to be specified
- PRODF0, PRODS0, PRODF1, PRODS1 values have to be specified for each specified node (this is consistent with the approach used in Data Set 12)
- PRODF0, PRODS0, PRODF1, PRODS1 values are specified using the same rules defined for Data Set 12 data
- Data Set 14D is terminated with a 0 node number and a termination line is required for all SUTRA-MS simulations that do not use a `sutra.zon` file
- an error condition is returned if NODE is greater than NN

### Data Set ZON2B

Data set ZON2B is specified for each SUTRA-MS simulation that uses a `sutra.zon` file

```
## Zone Data Set ZON2B
## Sorption and Production
## ZONE SPECIES   CHI1      CHI1  PRODF0  PRODS0  PRODF1  PRODS1
    1         3         0         0 1.667D-02      0         0         0
    1         1         0         0         0         0         0
    1         2         0         0         0         0         0
0
```

where:

- CHI1, CHI2, PRODF0, PRODS0, PRODF1, PRODS1 values have to be specified for each species and each zone (this is consistent with the approach used in Data Sets 11 and 12)
- CHI1, CHI2, PRODF0, PRODS0, PRODF1, PRODS1 values are specified using the same rules defined for Data Sets 11 and 12

- Zone Data Set ZON2B is terminated with a 0 node number and is required
- an error condition is returned if ZONE is greater than NodeZones
- an error condition is returned if the number of ZON2B lines is less than NSPE \* NodeZones

### Creating Tecplot output

The following additions need to be made to a SUTRA-MS input data sets to create ASCII nodal and (or) elemental output files.

### *sutra.fil*

The following additions are made to `sutra.inp` to create ASCII nodal and (or) elemental Tecplot output files for data specified in Data Sets 8B and 8C, respectively.

```
TPN 35 Results\HenryAndHilleke.nod.dat
TPE 36 Results\HenryAndHilleke.ele.dat
```

where:

- TPN is the Tecplot nodal data file which is similar to the standard nodal data file and includes output items described in Data Set 8B. The Tecplot nodal data file can also include the additional data items described below for Data Set 8B
- TPE is the Tecplot elemental data file which is identical to the standard elemental data file and includes output items described in Data Set 8C

### ***Additional Data Set 8B options***

The following optional output items can be saved to ASCII nodal Tecplot output files.

```
201 'X' 'Y' 'P' 'U' 'R' 'H' 'V' 'S' '-' 'Data Set 8B'
```

where:

- 'R' outputs the fluid density at the node to the Tecplot nodal data file
- 'H' outputs the total head at the node to the Tecplot nodal data file
- 'V' outputs the two (2D) or three (3D) velocity components at the node to the Tecplot nodal data file

None, some, or all of these data items can be output the ASCII nodal Tecplot data file. These data items are not output to the standard nodal output file.

## **References**

Gelhar, L.W., and Collins, M.A., 1971, General analysis of longitudinal dispersion in nonuniform flow: Water Resources Research, v. 7, no. 6, 1511-1521.

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