SUTRA Version 3.0.0 Release Notes

These release notes provide basic information about the release of SUTRA Version 3.0.0, which was developed from the previous public release, Version 2.2. These notes will be updated as new releases are issued.

Revision history

<u>Version 3.0.0</u>

Major new capabilities and changes relative to Version 2.2:

- Support for "generalized" boundary conditions, a modified implementation of specified pressures and concentrations or temperatures, and lakes. Two new types of "generalized" boundary conditions facilitate simulation of a wide range of hydrologic processes that interact with the groundwater model, such as rivers, drains, and evapotranspiration.
- The way in which two of the original types of SUTRA boundary conditions—specified-pressure and specified-concentration or temperature—are formulated numerically within SUTRA has been modified such that user-specified, conductance-like factors (known as GNUP and GNUU in previous versions of SUTRA) are no longer required.
- A lake capability, which works with all types of SUTRA boundary conditions, including the new generalized boundary conditions, enables simulation of the interaction of groundwater flow and transport with lake water "ponded" on the surface of a three-dimensional model. Coalescence and splitting of lakes is tracked as lake stages increase or decrease, respectively.

Other changes and bug fixes:

- Fixed bugs that affected printing of observations to the OBS and OBC output files on the last time step.
- The second velocity angle (VANG2) was left unset in the case of a two-dimensional (2D) simulation, which could result in meaningless values. That angle is now explicitly set to zero in that case.
- Time-dependent boundary condition flag arrays BCSFL and BCSTR were uninitialized, which could cause anomalous solution cycling. They are now initialized to ".FALSE.".
- The BCS identifier array was uninitialized, which could result in meaningless values. It is now initialized to "" (blank).
- The BCS identifier counter NCID was being reset to zero on every call to subroutine BCSTEP, which could cause improper accounting of BCS identifiers. NCID is now set to zero only one the first call to BCSTEP.

- Fixed a bug in the file-opening routine FOPEN that could result in misidentification of error condition “FIL-4” when checking BCS filenames.
- Fixed a bug that caused observation output to occur before steady-state transport had been solved for.
- Fixed a bug that could cause SUTRA to incorrectly report in the LST output file that time-dependent solute sources/sinks will be set in subroutine BCTIME.
- To avoid the number of observations written per line, NOBLIN, from exceeding the total number of observations, NOBS, which could cause output problems, NOBLIN is now limited to a maximum possible value of NOBS.
- Local array ELAPSD was not being deallocated. It is now deallocated when no longer needed.
- For more appropriate evaluation of the solution error, particularly when specified-pressure of specified-concentration or temperature boundary conditions are used, scaled residuals and right-hand-sides (instead of unscaled residuals and right-hand sides) are now used in evaluating convergence of iterative solutions.
- Setting the maximum number of time step cycles allowed in a schedule, NSMAX in INP dataset 6, to a very large number could result in a very long delay at the start of the run. This issue was resolved by changing from linked-list-based to array-based storage of schedules internally within the code. Input parameters for schedules remain the same, but schedule “TIME_STEPS” must now be defined before any other schedules are defined, and time-step numbers and times must now be listed in ascending order within each ‘STEP LIST’ or ‘TIME LIST’ schedule.
- Refactoring of various sections of code to improve program structure and modularity.

Known issues

- Specified-pressure and specified-concentration or temperature boundary conditions are now incorporated into the matrix equations for pressure and concentration or temperature using a different numerical paradigm that no longer depends on user-input values of GNUP and GNUU. Therefore, SUTRA Version 3.0.0 will typically give slightly different numerical results than previous versions of SUTRA for problems that involve specified-pressure and specified-concentration or temperature boundary conditions. The differences should be minor if GNUP and GNUU were chosen appropriately and the numerical solutions were well converged in the original model runs. This is not a bug; it simply reflects an algorithmic change in the code.
- Because specified-pressure and specified-concentration or temperature boundary conditions are implemented using new method, and because scaled residuals and right-hand-sides (instead of unscaled residuals and right-hand sides) are now used in evaluating convergence of iterative solutions, users will notice different convergence behavior when rerunning old SUTRA simulations using Version 3.0.0. Typically, if the convergence

criteria for the iterative solvers (TOLP and TOLU in INP datasets 7B and 7C) are not changed, simulations rerun with Version 3.0.0 will result in more iterations than with previous versions, but the accuracy of the solution – as measured by the budget errors – will be significantly better (much smaller budget errors) with Version 3.0.0. Test runs to date suggest that relaxing the convergence criteria (using larger values of TOLP and TOLU) to achieve budget errors comparable to those obtained with previous versions results in a roughly comparable number of solver iterations on average. In other words, convergence criteria used with previous versions of SUTRA are often more stringent than necessary for SUTRA 3.0.0 if a comparable solution accuracy is desired.

Distribution file, installation, and compilation

The SUTRA Version 3.0.0 release is contained in two distribution files, which are available for download at https://doi.org/10.5066/P9PPEHHM. The first file, "SUTRA_3_0_0.zip", contains executable code, documentation, and source code in the following directory structure, which parallels the directory structure of recent SUTRA releases:

```
SutraSuite/
     SUTRA_3_0/
          bin/
          documentation/
          source/
```

These release notes ("ReleaseNotes_SUTRA_3_0_0.pdf") are contained in the SUTRA_3_0 subdirectory. The second file, "SUTRA_3_0_Examples.zip", contains examples created to test and demonstrate the new features in SUTRA Version 3.0. The directory structure of the second file is

```
SutraSuite/
     SUTRA_3_0/
          Examples/
               2D/
                    Dam/
               3D/
                    Lakes/
```

To install SUTRA Version 3.0.0, simply unzip the distribution files. The "SutraSuite/" directory structure may already exist on your computer from previous installations of SUTRA. To install SUTRA Version 3.0 within the existing directory structure, unzip each of the distribution files to the directory that contains the top-level “SutraSuite/” directory (typically “C:/”).

The SUTRA executable code provided in the “bin/” subdirectory is compiled for 64-bit Windows® using the Intel® Visual Fortran Compiler 19.0.3.203. SUTRA Version 3.0.0 can be recompiled using any compiler that supports standard Fortran 90 source code.

Documentation

The “documentation/” subdirectory contains the SUTRA documentation for Versions 2.2 and 3.0.0:

Version 2.2:
Voss, C.I., and Provost, A.M., 2002 (Version of September 22, 2010), 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, 291 p., http://pubs.er.usgs.gov/publication/wri024231.

Version 3.0.0:
Provost, A.M., and Voss, C.I., 2019, SUTRA, a model for saturated-unsaturated, variable-density groundwater flow with solute or energy transport—Documentation of generalized boundary conditions, a modified implementation of specified pressures and concentrations or temperatures, and the lake capability: U.S. Geological Survey Techniques and Methods, book 6, chap. A52, 62 p., https://doi.org/10.3133/tm6A52.

Appendix B of the SUTRA Version 2.2 documentation contains a complete set of the input instructions for that version. Appendix 3 of the SUTRA Version 3.0.0 documentation describes modifications and additions to the input instructions introduced in Version 3.0.0.

Execution

To perform a SUTRA simulation, first prepare the requisite input files according the input instruction in the SUTRA documentation. Required input files include “SUTRA.FIL”, which points to the remaining input files. To run the simulation, run the SUTRA executable in the directory that contains “SUTRA.FIL.” The example problems included in the distribution each come with the requisite input files and a batch file, “RUNSUTRA.BAT”, that calls the SUTRA executable. To run SUTRA on an example problem, double-click on “RUNSUTRA.BAT” or open a command window, navigate to the example directory, and enter “RUNSUTRA.BAT” on the command line.

Example problems

Two example problems demonstrate the new features in SUTRA Version 3.0. Both examples are documented in detail in the SUTRA Version 3.0.0 documentation.

The first example, which is in the “Dam/” subdirectory and is summarized in “Dam-readme.pdf”, is a two-dimensional (2D), saturated-unsaturated problem that simulates flow through a dam with vertical sides. The seepage face through which water exits is modeled using generalized-flow boundary conditions.

The second example, which is in the “Lakes/” subdirectory and is summarized in “Lakes-readme.pdf”, demonstrates the formation, coalescence, and splitting of lakes that form on the surface of a three-dimensional (3D) groundwater model. As they evolve, the lakes exchange water and solute with the groundwater model.

Both examples test the new paradigm for enforcing specified-pressure boundary conditions introduced in SUTRA Version 3.0.0. In the dam problem, specified-pressure boundary conditions are specified on the upstream side of the dam, and the generalized-flow boundary conditions on the downstream seepage face act as specified-pressure boundary conditions when water is discharging from the face. In the lakes problem, specified-pressure boundary conditions are specified over the top surface of the model.

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