SUTRA Input Data List

This is a complete and up-to-date listing of the SUTRA input datasets. The model version noted below is the latest version in which any input datasets were modified. This listing will be updated continually as input datasets change.

List of Input Data for the File Assignment Input File (**SUTRA.FIL**)

Model Version: ***SUTRA 4.0***

The file "SUTRA.FIL" contains file assignments (one line for each assignment) in the following format:

Variable	Type	Description
FTYPE	Character	File type (within single quotes ' ' as shown below). Valid values are as follows: 'INP' = "**.inp**" input file (main **inp**ut) 'BCS' = "**.bcs**" input file (time-dependent sources and **b**oundary **c**ondition**s**) 'ICS' = "**.ics**" input file (**i**nitial **c**ondition**s**) 'LKIN' = "**.lkin**" input file (**l**a**k**e main **in**put) 'LKBC' = "**.lkbc**" input file (**l**a**k**e-**b**oundary **c**ondition interactions) 'LKAR' = "**.lkar**" input file (**l**a**k**e-**ar**ea nodes) 'LST' = "**.lst**" output file (main output **l**i**st**ing) 'RST' = "**.rst**" output file (**r**e**st**art conditions) 'NOD' = "**.nod**" output file (**nod**ewise results) 'ELE' = "**.ele**" output file (**ele**mentwise results) 'OBS' = "**.obs**" output file (**obs**ervations) 'OBC' = "**.obc**" output file (**ob**servations) 'BCOF' = "**.bcof**" output file (specifications and results at fluid-source/sink nodes) 'BCOS' = "**.bcos**" output file (specifications and results at solute/energy-source/sink nodes) 'BCOP' = "**.bcop**" output file (specifications and results at specified-pressure nodes) 'BCOU' = "**.bcou**" output file (specifications and results at specified-concentration/temperature nodes) 'BCOPG' = "**.bcopg**" output file (specifications and results at generalized-flow nodes) 'BCOUG' = "**.bcoug**" output file (specifications and results at generalized-transport nodes) 'LKBU' = "**.lkbu**" output file (**l**a**k**e **bu**dgets)

		'LKST' = "**.lkst**" output file (**l**a**k**e **st**ages) 'LKRS' = "**.lkrs**" output file (**l**a**k**e **r**e**s**tart) 'LKN' = "**.lkn**" output file (**l**a**k**e **n**umbers for surface nodes) 'LKH' = "**.lkh**" output file (**l**a**k**e **h**ierarchy) 'SMY' = "**.smy**" output file (simulation **s**u**m**mar**y**)
IUNIT	Integer	FORTRAN unit number to be assigned to the file. If IUNIT is not a valid FORTRAN unit number or if it is already assigned to another file, SUTRA will assign the next available unit number after IUNIT. (Unit numbers less than 11 are assumed to be unavailable.)
FNAME	Character	Full name of the file (within single quotes ' ' as shown below).

Notes:

Assignments for the "**.bcs**", "**.nod**", "**.ele**", "**.obs**", "**.obc**", "**.bcof**", "**.bcos**", "**.bcop**", "**.bcou**", and "**.lkst**" files are optional. If any of these assignments are omitted, the corresponding output files will not be created by SUTRA. Assignment for the "**.smy**" file is also optional – if not assigned, it will receive the file name "**SUTRA.SMY**" and an automatically generated unit number, by default. Assignment for the "**.rst**" file is required if ISTORE ≠ 0 in dataset 4, and assignment for the "**.lkrs**" file is required in addition if the lake capability is used. Assignments for the "**.inp**", "**.ics**", and "**.lst**" files are always required. Assignments for the "**.lkin**", "**.lkbc**", **".lkbu**", "**.lkn**", and "**.lkh**" files are always required when the lake capability is used. Assignment for the "**.lkar**" file is optional – if the lake capability is used and the "**.lkar**" file is not assigned, all nodes on the top surface of the model are eligible to form lakes. Assignments may be listed in any order. Assignment of unit numbers is performed by SUTRA in the order in which the files are listed, except for the "**.obs**" and "**.obc**" files. The latter are always assigned last by SUTRA.

For the observation output files ("**.obs**" and "**.obc**"), FNAME is a base filename from which the actual filenames are automatically derived by SUTRA. SUTRA generates one observation output file for each combination of schedule and output format that appears in the observation specifications in dataset 8D of the main input ("**.inp**") file. For an example of this, see the description of dataset 8D.

Multiple **".bcs"** files may be assigned. At the beginning of each time step, SUTRA checks each **".bcs"** file and reads in any boundary condition specifications that pertain to that time step. The **".bcs"** files are checked in the order in which they are listed in "**SUTRA.FIL**". If the **".bcs"** files contain multiple specifications of the same kind, at the same node, on the same time step, the specification read in last overrides any previous specifications.

Example:

'INP'	50	'project.inp'
'BCS'	52	'project.bcs'
'ICS'	55	'project.ics'
'LST'	60	'project.lst'
'RST'	66	'project.rst'
'NOD'	70	'project.nod'
'ELE'	75	'project.ele'
'OBS'	80	'project.obs'
'OBC'	85	'project.obc'
'BCOF'	91	'project.bcof'
'BCOS'	93	'project.bcos'
'BCOP'	92	'project.bcop'
'BCOU'	94	'project.bcou'
'BCOPG'	95	'project.bcopg'
'BCOUG'	96	'project.bcoug'
'SMY'	98	'project.smy'
'LKIN'	40	'project.lkin'
'LKBC'	41	'project.lkbc'
'LKAR'	42	'project.lkar'
'LKBU'	43	'project.lkbu'
'LKST'	44	'project.lkst'
'LKRS'	45	'project.lkrs'
'LKN'	46	'project.lkn'
'LKH'	47	'project.lkh'

General Format of the "**.inp**", "**.bcs**", and "**.ics**" Input Files

SUTRA reads the "**.inp**", "**.bcs**", and "**.ics**" input files in a list-directed fashion (except for dataset 1 of the "**.inp**" file):

- Input data appearing on the same line should be space- or tab-separated.

- As a rule, any data that are not optional must be given values in the input file (blanks are not sufficient) and must appear within the first 1,000 characters of a line. SUTRA reads only the first 1,000 characters of each line; subsequent characters are ignored. The exception to this rule is dataset 8D, in which lists of times or time steps may extend beyond the 1,000-character limit.

- Enclose input variables of "character" type in single quotation marks (unless specified otherwise) to provide maximum compatibility across computing platforms.

- Comment lines may be placed within the "**.inp**", "**.bcs**", and "**.ics**" files, subject to the following restrictions:
  - Comment lines must either
    - be empty (i.e., contain only a carriage return), or
    - have a pound sign, #, in the first column.
  - Comment lines can be placed before or after any dataset.
  - Comment lines can be placed within any dataset except those in which a single line of data can be optionally broken up over multiple lines, namely, time or time step lists in dataset 6 of the main input ("**.inp**") file, datasets 2 and 3 of the initial conditions ("**.ics**") file, and the "restart" information that follows dataset 3 in a "**.rst**" (restart) file being used as a "**.ics**" (initial conditions) file.

- Comments (or any text) can be appended to the end of any line of input data, provided all the required parameters have first been entered on that line. (In the case of a line of input that is optionally continued over multiple lines, only the last line would meet this requirement.) Be sure to leave at least one space or tab between the last required parameter and the beginning of the comment.

- Data contained in separate files can be "inserted" into the main ("**.inp**"), time-dependent sources and boundary conditions ("**.bcs**"), and initial conditions ("**.ics**") input files using the "@INSERT" command.

  - For example, including the line

    ```
    @INSERT  52  'project.inp7'
    ```

    in the "**.inp**" file causes SUTRA to open file "project.inp7" on FORTRAN unit 52 (or the next available unit number, according to the convention for files listed in "**SUTRA.FIL**") and begin reading input data from it as though it were reading from the "**.inp**" file. When the end of the inserted file is reached, SUTRA closes it and resumes reading from the "**.inp**" file.
  - "Inserts" can be nested, i.e., a file that contains an "@INSERT" statement can itself be "inserted" into another file. Nesting can be up to twenty levels deep.

- Like comment lines, “inserts” can be placed within any dataset except time or time step lists in dataset 8D of the main input (“**.inp**”) file, dataset 2 or 3 of the initial conditions (“**.ics**”) file, or the “restart” information that follows dataset 3 in a “**.rst**” (restart) file being used as a “**.ics**” (initial conditions) file.

List of Input Data for the Main Input File (**.inp**)

Model Version: ***SUTRA 4.0***

DATASET 1: Output Heading (two lines)

Variable	Type	Description
TITLE1	Character	First line of heading for the input data set.
TITLE2	Character	Second line of heading for the input data set. The first 80 characters of each line are printed as a heading on SUTRA output. In this dataset, the character inputs need not be enclosed in quotation marks.

DATASET 2A: Simulation Type (one line)

Variable	Type	Description
SIMULA	Character	Four words [If the version specification is omitted, SUTRA will read all input datasets in the version 2.0 (2D3D.1) format]. The first word must be "SUTRA". The second and third words indicate the SUTRA version number and must be "VERSION X.X, " where X.X is "4.0," "3.0," "2.2," "2.1," "2.0," or "2D3D.1." The fourth word indicates the type of transport and must be either "ENERGY," FREEZING," or "SOLUTE." Freezing is not supported in versions prior to 4.0. Any additional words are ignored by SUTRA.

Examples:
For an energy-transport simulation without freezing, one may write the following:
'SUTRA VERSION 4.0 ENERGY TRANSPORT'

For an energy-transport simulation with freezing, one may write the following:
'SUTRA VERSION 4.0 FREEZING TRANSPORT'

For a solute-transport simulation, one may write the following:
'SUTRA VERSION 4.0 SOLUTE TRANSPORT'

In these examples, the word "TRANSPORT" is ignored by SUTRA but is included to make the input more readable.

DATASET 2B: Mesh Structure (four lines)

This information is input for convenience of post-processing only. Except for the difference between 2D and 3D, calculations in the SUTRA code itself are not influenced by the mesh structure. Calculations in SUTRA for all mesh structures are handled as though the mesh were fully irregular.

Variable	Type	Description
Line 1:		
MSHSTR	Character	Two words. The first word indicates the dimensionality of the mesh, and must be either "2D" or "3D". The second word indicates the regularity of the mesh, and must be either "REGULAR", "BLOCKWISE", "LAYERED", or "IRREGULAR". Any additional words are ignored by SUTRA. By definition, a LAYERED mesh must be 3D. (See note at the end of this dataset for descriptions of the four types of mesh.)
For a REGULAR mesh:		
NN1	Integer	Number of nodes in the first numbering direction. Must have NN1≥2.
NN2	Integer	Number of nodes in the second numbering direction. Must have NN2≥2.
NN3	Integer	For a 3D mesh, the number of nodes in the third numbering direction. Must have NN3≥2. May be omitted if the mesh is 2D.
For a LAYERED mesh:		
NLAYS	Integer	Number of layers of nodes in the mesh. Must have NLAYS≥2.
NNLAY	Integer	Number of nodes in a layer. Must have NNLAY≥4.
NELAY	Integer	Number of elements in a layer. Must have NELAY≥1.

		In this context, the "number of elements in a layer" is the number of quadrilateral element faces defined by the nodes in a layer. One other words, if a layer is viewed as a 2D SUTRA mesh, then NELAY is the number of "2D elements" in a layer.
LAYSTR	Character	One word. Must be either 'ACROSS' or 'WITHIN'. Indicates whether node numbering proceeds first across layers or within a layer.

For an IRREGULAR mesh:

(No additional information required on Line 1.)

Omit lines 2 – 4 if mesh is NOT BLOCKWISE.

Line 2:

NBLK1	Integer	Number of blocks in the first numbering direction.
LDIV1	Integer	A list of the number of elements into which to divide each of the NBLK1 blocks along the first numbering direction.

Line 3:

NBLK2	Integer	Number of blocks in the second numbering direction.
LDIV2	Integer	A list of the number of elements into which to divide each of the NBLK2 blocks along the second numbering direction.

Line 4:

NBLK3	Integer	Number of blocks in the third numbering direction.
LDIV3	Integer	A list of the number of elements into which to divide each of the NBLK3 blocks along the third numbering direction.

Notes:

A REGULAR mesh is a logically rectangular 2D or 3D mesh. Node numbering starts at a node at one of the eight "corners" of the mesh and proceeds in a "natural" order along rows, columns, and vertical strings of nodes. (Because the logically rectangular mesh can be geometrically deformed, "vertical" strings of nodes need not lie strictly along the Z-direction, and rows and columns need not lie strictly within an X-Y plane. As used here, "vertical" implies a numbering direction that is effectively perpendicular to the "horizontal" directions defined by the rows and columns.) For example, numbering might proceed first along a vertical string of nodes, continue with successive vertical strings until all nodes within the first row are numbered, and then continue row-by-row until all nodes are numbered. In this case, the nodes would be said to be numbered first along vertical strings (across layers), then along rows, and finally along columns.

A BLOCKWISE mesh is a special type of REGULAR mesh that is created by the preprocessor SutraPrep (Provost, 2002), which creates input datasets for SUTRA version 2.0.

A LAYERED mesh is a 3D mesh that can be thought of as being formed from a vertical stack of 2D meshes. Each 2D mesh in the stack has the same connectivity, though that connectivity need not be logically rectangular. Node numbering starts at a node that lies in either the top or the bottom layer of the stack and proceeds in either of two ways:

- across the layers, i.e., along the vertical string of nodes until the opposite (bottom or top) layer is reached, or
- within a layer, i.e., along nodes in the same layer as the starting node.

Once numbering within a vertical string or layer is complete, it continues with another string or the next layer above or below. The order in which nodes are numbered within each string or layer is analogous to that in the first string or layer.

An IRREGULAR mesh is a 2D or 3D mesh that lacks the special structural features possessed by the other three mesh types. Nodes may be numbered in any order.

SUTRA uses the information in dataset 2B as follows:

- It checks that the mesh dimensions specified in datasets 2B and 3 are valid and mutually consistent.
- It writes mesh structure information and dimensions to output files, when they can be read by postprocessing software.

If the structure of the mesh is not known or is not of interest for postprocessing, the user may simply specify the mesh to be IRREGULAR, regardless of the actual structure. This will affect neither the way in which SUTRA solves the numerical problem nor the solution that is obtained.

Examples:

For a 3D, regular (logically rectangular), 10x20x30-node mesh, one may write the following:

```
'3D REGULAR MESH'  10  20  30
```

For a layered mesh with 10 layers of nodes, each containing 2560 nodes and 2210 elements, and with node numbering proceeding first across the layers, one may write:

```
'3D LAYERED MESH'  10  2560  2210  'ACROSS'
```

For a 2D, irregular mesh, one may write the following:

```
'2D IRREGULAR MESH'
```

In these examples, the word "MESH" is ignored by SUTRA but is included to make the input more readable.

DATASET 3: Simulation Control Numbers (one line)

Variable	Type	Description
NN	Integer	Exact number of nodes in finite element mesh.
NE	Integer	Exact number of elements in finite element mesh.
NPBC	Integer	Exact number of nodes at which pressure is a specified constant value or function of time.
NUBC	Integer	Exact number of nodes at which temperature or concentration is a specified constant value or function of time.
NSOP	Integer	Exact number of nodes at which a fluid source/sink is a specified constant value or function of time.
NSOU	Integer	Exact number of nodes at which an energy or solute mass source/sink is a specified constant value or function of time.
NPBG	Integer	Exact number of nodes at which a generalized-flow condition is specified.
NUBG	Integer	Exact number of nodes at which a generalized-transport condition is specified.
NOBS	Integer	Exact number of points at which observations will be made. Set to zero for no observations.

Note:

The order in which NPBC, NUBC, NSOP, and NSOU are listed above is *different* from the order in which the corresponding datasets (19, 20, 17, and 18) appear in the **".inp"** file.

DATASET 4: Simulation Mode Options (one line)

Variable	Type	Description
CUNSAT	Character	One word. Set to 'SATURATED' to simulate only saturated flow. Set to 'UNSATURATED' to simulate unsaturated/saturated ground-water flow.
CSSFLO	Character	One word. Set to 'TRANSIENT' for simulation of transient ground-water flow. Set to 'STEADY' for simulation of steady-state flow. (Note: Variable-density simulations generally require TRANSIENT flow.)
CSSTRA	Character	One word. Set to 'TRANSIENT' for simulation of transient solute or energy transport. Set to 'STEADY' for simulation of steady-state transport. (Note: Steady-state transport requires a steady-state flow field. So, if CSSTRA = 'STEADY', then also set CSSFLO = 'STEADY'.)
CREAD	Character	One word. Set to 'COLD' to read initial condition data ("**.ics**" file) for a "cold start" (the very first time step of a simulation). Set to 'WARM' to read initial condition data ("**.ics**" file) for a "warm restart" of a simulation using data that were previously stored by SUTRA in a "**.rst**" file. A "warm restart" is used only when continuing a previous simulation as though it had never been interrupted and with no changes in problem specification (except for changing time step size and extending simulation time). Beginning with SUTRA Version 2.2, a "warm restart" results in continuation of time stepping as in the original simulation. For example, a simulation that is restarted using a "warm start" from results stored at the end of time step 5 will continue numbering the time steps 6, 7, 8, etc. If restarted using a "cold start," it will number the time steps 1, 2, 3, etc. (In previous versions of SUTRA, the time step numbering was reset for both "cold" and "warm" starts).
ISTORE	Integer	To store results each ISTORE time steps in the "**.rst**" file for later use as initial conditions on a restart, set to +1 or greater value. To cancel storage, set to 0. This option is recommended as a backup for storage of results of intermediate time steps during long simulations. Should the execution halt unexpectedly, it may be restarted with initial conditions consisting of results of the last successfully completed time step stored in the "**.rst**" file. When

ISTORE > 0, results are always stored in the "**.rst**" file after the last time step of a simulation regardless of whether the step is an even multiple of ISTORE. For this option to be used, the "**.rst**" file must be listed in file "**SUTRA.FIL**".

Any extra words included in the character variables in this dataset are ignored by SUTRA.

Example:

To simulate saturated, steady-state ground-water flow with transient solute or energy transport from a cold start, storing intermediate results every 10 time steps, one may write the following:

```
'SATURATED FLOW'   'STEADY FLOW'   'TRANSIENT TRANSPORT'  'COLD START'   10
```

In this example, the words "FLOW", "TRANSPORT", and "START" are ignored by SUTRA but may be included to make the input more readable.

DATASET 5: Upstream Weighting Parameter (one line)

Variable	Type	Description
UP	Real	Fractional upstream weight for stabilization of oscillations in results due to highly advective transport or unsaturated flow. UP may be given any value from 0.0 to +1.0. UP = 0.0 implies no upstream weighting (Galerkin method). UP = 0.5 implies 50% upstream weighting. UP = 1.0 implies full (100%) upstream weighting. Recommended value is zero. WARNING: Upstream weighting increases the local effective longitudinal dispersivity of the simulation by approximately UP* (ΔL_L)/2 where ΔL_L is the local distance between element sides along the direction of flow (see section 7.2 of the main SUTRA documentation (Voss and Provost, 2002). Note that the amount of this increase varies from place to place, depending on flow direction and element size. Thus, a nonzero value for UP actually changes the value of longitudinal dispersivity used by the simulation and broadens otherwise sharp concentration, temperature, or saturation fronts.

DATASET 6: Temporal Control and Solution Cycling Data (one line, followed by one* line for for each schedule, plus one line)

(Lists of times or time steps may be continued over multiple lines in TIME LIST and STEP LIST schedules.)*

Variable	Type	Description
Line 1:		
NSCH	Integer	Number of schedules. In the case of steady transport, NSCH may be set to zero to avoid unnecessarily defining schedules. Zero is allowed only if transport is steady-state, i.e., CSSTRA='STEADY' in dataset 4. See note at the end of this dataset for details.
NPCYC	Integer	Number of time steps in pressure solution cycle. Pressure is solved on time steps numbered: n(NPCYC), where n is a positive integer, as well as on initial time step.
NUCYC	Integer	Number of time steps in temperature/concentration solution cycle. Transport equation is solved on time steps numbered: n(NUCYC), where n is a positive integer, as well as on initial time step. Either NPCYC or NUCYC must be set to 1.

NOTE: Schedule "TIME_STEPS" must be defined before any other schedules are defined.

Lines 2 to NSCH+1:		
SCHNAM	Character	Schedule name. May be up to 10 characters long and may include spaces. A given schedule name may not be defined more than once. The names "STEP_0", "STEP_1", and "STEPS_1&UP" are reserved (see "Notes" below) and may not be used for user-defined schedules. If transport is transient, the user must define a schedule named "TIME_STEPS", which specifies the starting time for the simulation and the sequence of times at which time steps end.

		Schedule "TIME_STEPS": must contain two or more time values, including the starting time.
SCHTYP	Character	One or two words. Schedule type. (See note at the end of this dataset for descriptions of the various schedule types.) Valid values are: 'TIME LIST' = a list of times 'TIME CYCLE' = a sequence of times generated at specified intervals 'STEP LIST' = a list of time steps 'STEP CYCLE' = a sequence of time steps generated at specified intervals Schedule "TIME_STEPS": must be defined using a time-based schedule type, i.e., either a 'TIME LIST' or a 'TIME CYCLE'.

For a TIME LIST schedule:

CREFT	Character	One word. To define the schedule in terms of absolute time (simulation clock time), specify 'ABSOLUTE'. To define the schedule in terms of elapsed time (time relative to the simulation starting time), specify 'ELAPSED'.
SCALT	Real	Scale factor to be applied to each time value in the list.
NTLIST	Integer	The number of times in the list.
TLIST	Real	The list of times in ascending order. (May be continued over multiple lines of input.) Schedule "TIME_STEPS": If schedule "TIME_STEPS" is defined as a TIME LIST in terms of ELAPSED times, the times in TLIST are assumed to be relative to time TICS specified in dataset 1 of the initial conditions ("**.ics**") file. In that case, the first time in TLIST must be set to zero for schedule "TIME_STEPS", and TICS becomes the (absolute) starting time of the simulation.

For a TIME CYCLE schedule:

CREFT	Character	One word. To define the schedule in terms of absolute time (simulation clock time), specify 'ABSOLUTE'. To define the schedule in terms of elapsed time (time relative to the simulation starting time), specify 'ELAPSED'.
SCALT	Real	Scale factor to be applied to each time value in the list.

NTMAX	Integer	Maximum number of time cycles allowed, i.e., the maximum number of times allowed in the schedule, not including the initial time.
TIMEI	Real	Initial time. Cycling begins at time = TIMEI. Schedule "TIME_STEPS": if defined as a TIME CYCLE in terms of ELAPSED times, then TIMEI and TIMEL (see below) are assumed to be relative to time TICS specified in dataset 1 of the initial conditions ("**.ics**") file. In that case, the TIMEI must be set to zero for schedule "TIME_STEPS", and TICS becomes the (absolute) starting time of the simulation.
TIMEL	Real	Limiting time. Cycling continues until time ≥ TIMEL.
TIMEC	Real	Initial time increment.
NTCYC	Integer	Number of cycles after which the time increment is updated. The current time increment is multiplied by TCMULT (see below) after every NTCYC cycles. (The value of the time increment is limited by TCMIN and TCMAX; see below.)
TCMULT	Real	Factor by which the time increment is multiplied after every NTCYC cycles.
TCMIN	Real	Minimum time increment allowed.
TCMAX	Real	Maximum time increment allowed.

For a STEP LIST schedule:

NSLIST	Integer	The number of time steps in the list.
ISLIST	Integer	The list of (integer) time steps in ascending order. (May be continued over multiple lines of input.)

For a STEP CYCLE schedule:

NSMAX	Integer	Maximum number of time step cycles allowed, i.e., the maximum number of time steps allowed in the schedule, not including the initial time step.
ISTEPI	Integer	Initial time step. Cycling begins at time step = ISTEPI.
ISTEPL	Integer	Limiting time step. Cycling continues until time step ≥ ISTEPL.
ISTEPC	Integer	Time step increment.

Last line:

Character	A single dash, '-', must be placed on the line below the last schedule.

Notes:

The schedules defined in this dataset determine the sequence of time steps (via schedule "TIME_STEPS") and control the timing of observation output (see also dataset 8D). Time or time step values may not be repeated, i.e., each value must be unique, within a given schedule.

For a time-based schedule (TIME LIST or TIME CYCLE), the scale factor SCALT is applied to all numeric time values in the schedule definition. This feature is useful for converting time units. For example, in the definition of a TIME LIST, the list of times TLIST could be input in terms of days and converted to seconds by setting SCALT=86400.

The method of defining a TIME CYCLE is similar to that used to specify time stepping in the SUTRA Version 2.1 (2D3D.1) input format. After the scale factor SCALT has been applied, NTMAX, TIMEL, TIMEC, NTCYC, TCMULT, and TCMAX are analogous to ITMAX, TMAX, DELT, ITCYC, DTMULT, and DTMAX, respectively. However, there are two important differences. First, in a TIME CYCLE, the user specifies the initial time TIMEI; in the former method, it is assumed to be TICS (formerly called TSTART). Second, in a TIME CYCLE, a new time increment size is begun when the cycle number minus one is an integer multiple of NTCYC; the former method begins a new time step size when the time step number is an integer multiple of ITCYC. This second difference is illustrated in the following example, in which DELT=TIMEC=1., DTMULT=TCMULT=2., and ITCYC=NTCYC=5:

Time step or cycle number	Time step or time increment size	
	Old time stepping method	TIME CYCLE method
1	1.	1.
2	1.	1.
3	1.	1.
4	1.	1.
5	2.	1.
6	2.	2.
7	2.	2.
8	2.	2.
9	2.	2.
10	4.	2.

If transport is steady-state, no schedules need be defined, and NSCH may be set to 0. In this case, SUTRA will not read the remainder of Line 1, as this information is not needed. Reading will commence with the next line of data. However, the end-of-list marker, '-',

is still required. If any user-defined schedules are listed, they are ignored by SUTRA, and schedule "TIME_STEPS" is automatically defined as consisting only of time steps 0 and 1.

SUTRA automatically defines three schedules that can be useful for specifying steady-state and time-dependent sources and boundary conditions using optional **".bcs"** files:

- "STEP_0", which consists only of time step 0,
- "STEP_1", which consists only of time step 1, and
- "STEPS_1&UP", which consists of all time steps after time step 0.

Examples:

The following examples assume that time is ultimately specified in seconds. The scale factor 3.15576e+7 is used to convert from years to seconds.

To define a schedule named "TIME_STEPS" (which controls time stepping in the simulation), starting at (absolute) time TICS and taking fifty 1-year time steps followed by fifty 2-year time steps, one may write the following:

```
'TIME_STEPS'  'TIME CYCLE'  'ELAPSED'  3.15576e+7  100  0.  1e+99  1.  50  2.  0.  1e+99
```

To define a schedule named "A" that consists of five absolute times, 10., 25., 30., 40., and 75. years, one may write the following:

```
'A'  'TIME LIST'  'ABSOLUTE'  3.15576e+7  5  10.  25.  30.  40.  75.
```

To define a schedule named "B" that consists of four time steps, 5, 10, 90, and 95, one may write the following:

```
'B'  'STEP LIST'  4  5  10  90  95
```

To define a schedule named "C" that begins at time step 40 and includes every 2nd time step up to and including time step 80, one may write the following:

```
'C'  'STEP CYCLE'  20  40  9999  2
```

DATASET 7A: Iteration Controls for Resolving Nonlinearities (one line)

Variable	Type	Description
ITRMAX	Integer	Maximum number of iterations allowed per time step to resolve nonlinearities. Set to a value of +1 for noniterative solution. Noniterative solution may be used for saturated aquifers when density variability of the fluid is small or for unsaturated aquifers when time steps are chosen to be small.
RPMAX	Real	Absolute iteration convergence criterion for pressure solution. Pressure solution has converged when largest pressure change from the previous iteration's solution at every node in mesh is less then RPMAX. May be omitted for noniterative solution.
RUMAX	Real	Absolute iteration convergence criterion for transport solution. Transport solution has converged when largest concentration or temperature change from the previous iteration's solution at every node in mesh is less than RUMAX. May be omitted for noniterative solution.

DATASET 7B: Matrix Equation Solver Controls for Pressure Solution (one line)

Variable	Type	Description
CSOLVP	Character	Name of solver to be used to obtain the pressure solution. Select one of the following: 'DIRECT' = Banded Gaussian elimination 'CG' = IC-preconditioned conjugate gradient 'GMRES' = ILU-preconditioned generalized minimum residual 'ORTHOMIN' = ILU-preconditioned orthomin Mesh type and dimensionality do not constrain the choice of solver. However, if the DIRECT solver is used, it must be used for **both** the pressure and the transport solution; if either CSOLVP or CSOLVU (dataset 7C) is set to 'DIRECT', then the other must also be set to 'DIRECT'. Also, the CG solver may be used only in the absence of upstream weighting (UP=0. in dataset 5).
ITRMXP	Integer	Maximum number of solver iterations during pressure solution. May be omitted if the DIRECT solver is used.
TOLP	Real	Convergence tolerance for solver iterations during pressure solution. May be omitted if the DIRECT solver is used.

DATASET 7C: Matrix Equation Solver Controls for Transport Solution (one line)

Variable	Type	Description
CSOLVU	Character	Name of solver to be used to obtain the transport solution. Valid values are as follows: 'DIRECT' = Banded Gaussian elimination 'GMRES' = ILU-preconditioned generalized minimum residual 'ORTHOMIN' = ILU-preconditioned orthomin Mesh type and dimensionality do not constrain the choice of solver. However, if the DIRECT solver is used, it must be used for **both** the pressure and the transport solution; if either CSOLVU or CSOLVP (dataset 7B) is set to 'DIRECT', then the other must also be set to 'DIRECT'.
ITRMXU	Integer	Maximum number of solver iterations during transport solution. May be omitted if the DIRECT solver is used.
TOLU	Real	Convergence tolerance for solver iterations during transport solution. May be omitted if the DIRECT solver is used.

DATASET 8A: Output Controls and Options for "**.lst**" (Main Output) File and Screen Output (one line)

Variable	Type	Description
NPRINT	Integer	NPRINT is the main output cycle for transient simulation. Output is produced in the "**.lst**" file on time steps numbered n | NPRINT | (where n is a positive integer). Also for transient solutions, output is produced for initial conditions and on the first and last time steps. To cancel printed output for the first time step of a transient simulation, set NPRINT to a negative number (i.e., place a minus sign before the desired output cycle). For steady-state solutions, output is produced irrespective of the value of NPRINT.
CNODAL	Character	A value of 'N' cancels output of node coordinates, nodewise element thicknesses, and nodewise porosities. Set to 'Y' for full printout.
CELMNT	Character	A value of 'N' cancels output of elementwise permeabilities and elementwise dispersivities. Set to 'Y' for full output.

CINCID	Character	A value of 'N' cancels output of node incidences in elements. Set to 'Y' for full output.
CPANDS	Character	A value of 'N' cancels output of pressures and saturations computed at nodes. Set to 'Y' for full output.
CVEL	Character	Set to a value of 'Y' to calculate and output fluid velocities at element centroids each time output is produced. Note that for transient flow, velocities are based on results and pressures of the previous time step or iteration and not on the newest values. Set to 'N' to cancel option.
CCORT	Character	A value of 'N' cancels output of concentrations or temperatures computed at nodes. Set to 'Y' for full output.
CBUDG	Character	Set to a value of 'Y' to calculate and output a fluid mass budget and energy or solute mass budget each time output is produced. A value of 'N' cancels the option.
CSCRN	Character	Set to a value of 'Y' to write a summary of simulation progress to the screen during the simulation. A value of 'N' suppresses all output to the screen except for certain error messages.
CPAUSE	Character	Set to a value of 'Y' to have SUTRA pause for a user response at the end of the run so that simulation progress can be reviewed on the screen. A value of 'N' cancels the option except for certain error messages. Affects output only if CSCRN='Y'.

Note:

If a "**.smy**" file is assigned in the "**SUTRA.FIL**" input file, a summary of simulation progress may be reviewed after completion of the simulation in the "**.smy**" file (regardless of the value of CSCRN).

DATASET 8B: Output Controls and Options for "**.nod**" File
(Nodewise Results Listed in Columns) (one line)

Variable	Type	Description
NCOLPR	Integer	Nodewise output cycle for a transient simulation. Output is produced in the "**.nod**" file on time steps numbered n | NCOLPR | (where n is a positive integer). In addition, for transient solutions, output is produced for initial conditions and on the first and last time steps. To cancel printed output for the first time step of a transient simulation, make NCOLPR a negative number (i.e., place a minus sign before the desired output cycle). For steady-state solutions, output is produced irrespective of the value of NCOLPR.
NCOL	Character	List of names of variables to be printed in columns in the "**.nod**" file. Up to nine columns may be specified. The ordering of columns corresponds to the ordering of variable names in the list. Names may be repeated and may appear in any order, except as noted below. Valid names are as follows: 'N' = node number (if used, it must appear first in list) 'X' = x-coordinate of node 'Y' = y-coordinate of node 'Z' = z-coordinate of node (3D only) 'P' = pressure 'U' = concentration or temperature 'S' = total water saturation 'L' = liquid water saturation 'I' = ice saturation '-' = end of list (any names following '-' are ignored) The symbol '-' (a single dash) must be used at the end of the list.

Example:

To output the 3D node coordinates, pressure, and solute concentration in columns in the "**.nod**" file every 5 time steps, but not on the first time step, write the following:

-5 'X' 'Y' 'Z' 'P' 'U' '-'

DATASET 8C: Output Controls and Options for "**.ele**" File
(Velocities and Darcy Velocities at Element Centroids Listed in Columns) (one line)

Variable	Type	Description
LCOLPR	Integer	Elementwise output cycle for a transient simulation. Output is produced in the "**.ele**" file on time steps numbered n | LCOLPR | (where n is a positive integer). In addition, for transient solutions, output is produced for initial conditions and on the first and last time steps. For steady-state solutions, output is produced irrespective of the value of LCOLPR, and the velocities are reported only once (for time step 1). Velocities for time step 1 are always reported.
LCOL	Character	List of names of variables to be printed in columns in the "**.ele**" file. Up to ten columns may be specified. The ordering of columns corresponds to the ordering of variable names in the list. Names may be repeated and may appear in any order, except as noted below. Valid names are as follows: 'E' = element number (if used, it must appear first in list) 'X' = x-coordinate of element centroid 'Y' = y-coordinate of element centroid 'Z' = z-coordinate of element centroid (3D only) 'VX' = x-component of fluid (liquid water) velocity 'VY' = y-component of fluid (liquid water) velocity 'VZ' = z-component of fluid (liquid water) velocity (3D only) 'qX' = x-component of Darcy velocity 'qY' = y-component of Darcy velocity 'qZ' = z-component of Darcy velocity (3D only) '-' = end of list (any names following '-' are ignored) The symbol '-' (a single dash) must be used at the end of the list.

Note:
Reported velocities for time step 1 are based on initial or steady-state pressures. Reported velocities for subsequent time steps are based on pressures from the previous time step. Velocities used to formulate the transport equation within SUTRA are based on pressures from the previous nonlinearity iteration; thus, the updated velocities used internally may be different from the values reported for each time step in the "**.ele**" file.

Example:
To output the 3D element centroid coordinates and fluid (liquid water) velocity components in columns in the "**.ele**" file every 10 time steps, write the following:
10 'X' 'Y' 'Z' 'VX' 'VY' 'VZ' '-'

DATASET 8D: Output Controls and Options for "**.obs**" and "**.obc**" Files
(Observation Point Results Listed in Columns)
(one line for each observation point, plus one line)

<u>O M I T</u> when there are no observation points

Variable	Type	Description
<u>Line 1:</u>		
NOBLIN	Integer	NOBLIN is the maximum number of observations output to a single line in a "**.obs**" file. If the total number of observations exceeds NOBLIN, line wrapping will be used to limit the number of observations per line to NOBLIN. Has no effect on output to "**.obc**" files.
<u>Lines 2 to NOBS+1:</u>		
OBSNAM	Character	Observation point name. May be up to 40 characters long and may include spaces. The same observation name may be used more than once.
XOBS	Real	X coordinate of the observation point.
YOBS	Real	Y coordinate of the observation point.
ZOBS	Real	Z coordinate of the observation point. **<u>Omit for 2D problems.</u>**
OBSSCH	Character	Name of the schedule that controls output for this observation point. (Schedules are defined in dataset 6.) <u>For transient transport</u>: In addition to the scheduled output, observations are made automatically at time step "0", which represents initial and/or steady-state conditions, depending on the mode in which SUTRA is run. If flow is transient, time step "0" represents initial conditions. If flow is steady-state, time step "0" represents steady-state pressures and saturations and initial concentrations or temperatures. Observations are also made automatically at the end of the last time step. <u>For steady-state transport</u>: User-defined schedules are ignored, and observations are made at time step "1", which represents steady-state results.
OBSFMT	Character	Output format. Must be either 'OBS' or 'OBC'. See the note below for details.

Last line:

Character	A single dash, '-', must be placed on the line below the last observation point.

Notes:

The OBS and OBC output formats correspond to the "**.obs**" and "**.obc**" output files, respectively. Both formats present the same information.

The number of distinct "**.obs**" and "**.obc**" files generated by SUTRA depends on the combinations of output schedule and output format that appear in the list of observation points. All observations that are assigned the same schedule and format are written to the same file. The filename is generated by SUTRA using the corresponding base filename specified by the user in "**SUTRA.FIL**" and the output schedule.

Example:

The following defines five observation points in a 3D model:

```
2
'well_27'     1007.   1294.   -133.     'A'   'OBS'
'well_29'     1165.    980.   -142.     'A'   'OBS'
'well_30'     1102.    981.   -126.     'A'   'OBS'
'well_198'    2662.    703.   -289.     'B'   'OBS'
'well_344'     155.     49.    -90.     'A'   'OBC'
'-'
```

Assume the base filenames specified in "**SUTRA.FIL**" for "**.obs**" and "**.obc**" files are "project.obs" and "project.obc". Then observation data for the first three points listed above are written to the same file, "project_A.obs", in OBS format. Observation data for the fourth point listed are written to file "project_B.obs" in OBS format. In each "**.obs**" file, output is wrapped to the next line after the first two observations are written. Observation data for the last point listed are written to file "project_A.obc" in OBC format.

DATASET 8E: Output Controls and Options for "**.bcof**", "**.bcos**", "**.bcop**", "**.bcou**", "**.bcopg**", and "**.bcoug**" Files (Source and Boundary Condition Specifications and Results Listed in Columns) (one line)

Variable	Type	Description
NBCFPR	Integer	Fluid source node output cycle for transient simulation. Output is produced in the "**.bcof**" file on time steps numbered n | NBCFPR | (where n is a positive integer).
NBCSPR	Integer	Solute or energy source node output cycle for transient simulation. Output is produced in the "**.bcos**" file on time steps numbered n | NBCSPR | (where n is a positive integer).
NBCPPR	Integer	Specified pressure node output cycle for transient simulation. Output is produced in the "**.bcop**" file on time steps numbered n | NBCPPR | (where n is a positive integer).
NBCUPR	Integer	Specified concentration or temperature node output cycle for transient simulation. Output is produced in the "**.bcou**" file on time steps numbered n | NBCUPR | (where n is a positive integer).
NBGPPR	Integer	Generalized-flow node output cycle for transient simulation. Output is produced in the "**.bcopg**" file on time steps numbered n | NBGPPR | (where n is a positive integer).
NBGUPR	Integer	Generalized-transport node output cycle for transient simulation. Output is produced in the "**.bcoug**" file on time steps numbered n | NBGUPR | (where n is a positive integer).
CINACT	Character	Set to a value of 'Y' to list all sources and boundary conditions, including those that have been rendered inactive (using negative node numbers in a "**.bcs**" file; see the description of "**.bcs**" datasets 3 - 7). Set to 'N' to suppress output for inactive sources and boundary conditions.

Notes:

For transient simulations, output is also produced on the first and last time steps. For steady-state simulations, output is produced irrespective of the values of the output control variables.

The information that is output to the "**.bcof**", "**.bcos**", "**.bcop**", and "**.bcou**" files is described in section 5.9 of the main SUTRA documentation (Voss and Provost, 2002).

The information that is output to the "**.bcopg**" and "**.bcoug**" files is described in section 1.8, "Budget Output and Boundary-Condition Output Files," of the SUTRA version 3.0 documentation (Provost and Voss, 2019).

Example:

To output source and boundary condition information to the "**.bcof**", "**.bcos**", "**.bcop**", "**.bcou**", "**.bcopg**", and"**.bcoug**" files every 10 time steps, suppressing output for inactive sources and boundary conditions, write the following:

```
10  10  10  10  10  10   'N'
```

DATASET 9: Liquid Water and Ice Properties (one line)

Variable	Type	Description
COMPL	Real	Liquid water compressibility, $\beta_L = (1/\rho_L)(\partial\rho_L/\partial p)$. $[M/(L\cdot s^2)]^{-1}$.
CL	Real	Liquid water specific heat, c_L. [E/(M·ºC)] Set to any arbitrary number (for example, zero) for a solute-transport simulation.
SIGMAL	Real	Liquid-water diffusivity, σ_L. For energy transport, represents liquid-water thermal conductivity, λ_L. [E/(L·ºC·s)]. For solute transport, represents molecular diffusivity of solute in pure liquid water, D_m [L^2/s]. May be decreased from value in pure water to account for tortuosity of fluid paths. (User-specified constant value for the entire model.)
RHOLØ	Real	For solute transport: Density of liquid water at base concentration for linear liquid density function. [M/L^3]. (User-specified constant value for the entire model.) ρ_L = RHOLØ + DRLDU (U - URHOWØ) For energy transport: either – Density of liquid water at base temperature for linear liquid density function. [M/L^3], ρ_L = RHOLØ + DRLDU (U - URHOWØ), or – Set to a negative number for SUTRA to use the nonlinear liquid density function. The nonlinear liquid density function is available only for an energy transport simulation. The function calculates liquid density in units of [kg/m^3] as a function of temperature in [ºC]. The absolute value of RHOLØ can be used to convert units of [kg/m^3] to desired units of density: [desired units] = −RHOLØ * [kg/(m^3)] To have SUTRA use density units of [kg/m^3], set RHOLØ = −1.0
URHOLØ	Real	For linear liquid density function, represents base value of solute concentration (as mass fraction) or temperature of liquid water at which base liquid density, RHOWØ, is specified. [M_s/M] or [ºC]. (User-specified constant value for the entire model.) ρ_L = RHOLØ + DRLDU (U - URHOWØ)

		For nonlinear liquid density function, an arbitrary value (usually set to 0).
DRLDU	Real	For linear liquid density function, represents coefficient of liquid water density change with concentration (fraction) or temperature. $[M^2/(L^3 \cdot M_s)]$ or $[M/(L^3 \cdot {}^oC)]$ (User-specified constant value for the entire model.) ρ_L = RHOLØ + DRLDU (U - URHOWØ). For nonlinear liquid density function, an arbitrary value (usually set to 0).
VISCØ	Real	For solute transport: Liquid water viscosity, μ, $[M/(L \cdot s)]$. (User-specified constant value for the entire model.) For energy transport: This value is a scale factor. (User-specified constant value for the entire model.) It multiplies the viscosity, which is calculated as a function of temperature in [ºC] in units of [kg/(m·s)]. VISCØ may be used for energy transport to convert units of [kg/(m·s)] to desired units of viscosity. [desired units] = VISCØ * [kg/(m·s)] To have SUTRA use viscosity units of [kg/(m·s)], set VISCØ = 1.0
COMPI	Real	Ice compressibility, $\beta_I = (1/\rho_I)(\partial\rho_I/p)$. $[M/(L \cdot s^2)]^{-1}$ **May be omitted for simulations that do not involve FREEZING.**
CI	Real	Ice specific heat, c_I. $[E/(M \cdot {}^oC)]$ **May be omitted for simulations that do not involve FREEZING.**
SIGMAI	Real	Ice thermal conductivity, $\sigma_I \equiv \lambda_I$. $[E/(L \cdot {}^oC \cdot s)]$ **May be omitted for simulations that do not involve FREEZING.**
RHOI	Real	Ice density, ρ_I. $[M/L^3]$ **May be omitted for simulations that do not involve FREEZING.**

DATASET 10: *no longer used; solid matrix properties are spatially variable and are input in datasets 14 and 15*

DATASET 11: Regionwise Parameters (1 line, plus 2 – 6 lines per parameter region, depending on the type of simulation). This dataset includes all input parameters that are specified region-wise. These include parameters for adsorption or thermal conductivity, total water saturation, relative permeability, and liquid water saturation, and the freezing temperature and latent heat.

Variable	Type	Description
Line 1:		
NPMREG	Integer	Number of parameter regions, which must be greater than or equal to 1.

For each of the NPMREG parameter regions, include datasets 11A-E as necessary, depending on the type of simulation. In other words, all the required datasets for region 1 are listed first, followed by all the required datasets for region 2, etc. Region numbers must appear in numerical order starting with 1.

For each of the NPMREG regions:

NR	Integer	Region number. (Region numbers must appear in numerical order starting with 1.)

DATASET 11A: Adsorption Parameters for Solute Transport Simulations (1 line per region)

NOTE: This form of dataset 11A involves adsorption parameters and is used for solute transport simulations only. The form used for energy transport simulations is described further below.

Variable	Type	Description
ADSMOD(NR)	Character	Name of the adsorption model for region NR (for solute transport only). For no sorption, set to 'NONE'. Otherwise, set to 'LINEAR', 'FREUNDLICH', or 'LANGMUIR': For linear sorption model, set to 'LINEAR'. For Freundlich sorption model, set to 'FREUNDLICH'. For Langmuir sorption model, set to 'LANGMUIR'.

If ADSMOD(NR) = 'NONE': **Omit the rest of the line.**

If ADSMOD(NR) = 'LINEAR', 'FREUNDLICH', or 'LANGMUIR':

(line continued):

CHI1(NR)	Real	Value of linear, Freundlich or Langmuir distribution coefficient for region NR, depending on sorption model chosen in ADSMOD(NR). χ_1. [L_f^3/M_G].
CHI2(NR)	Real	Value of Freundlich or Langmuir coefficient for region (NR), depending on sorption model chosen in ADSMOD(NR). Set to any real value for linear sorption. χ_2. [1] for Freundlich. [L_f^3/M_s] for Langmuir.

DATASET 11A: Thermal Conductivity Model for Energy Transport Simulations (one line per region)

NOTE: This form of dataset 11A involves the thermal conductivity model and is used for energy transport simulations (with or without freezing) only. The form used for solute transport simulations is described above.

Variable	Type	Description
TCMOD(NR)	Character	Name of the thermal conductivity model for region NR (for energy transport only). Set to 'ARITHM', 'GEOMET, or 'HARMON': For arithmetic-mean bulk thermal conductivity, set to 'ARITHM'. For geometric-mean bulk thermal conductivity, set to 'GEOMET'. For harmonic-mean bulk thermal conductivity, set to 'HARMON'.

DATASET 11B: Total Water Saturation Parameters (1 line per region)

This dataset is required only if the simulation is UNSATURATED and (or) involves FREEZING. Omit otherwise.

Variable	Type	Description
For no specified total water saturation function (simulated total water saturation will always have a value of 1):		
SWMOD(NR)	Character	Set to 'NONE'.
For the van Genuchten total water saturation function:		
SWMOD(NR)	Character	Set to 'VGEN'.
SWRES(NR)	Real	Value of the residual total water saturation in the van Genuchten function for region NR, S_{Wres}. [1].

AA(NR)	Real	van Genuchten function parameter a_{VG} for region NR. [(L·s^2)/M]
VN(NR)	Real	van Genuchten function parameter n_{VG} for region NR. [1]

For the Brooks-Corey total water saturation function:

SWMOD(NR)	Character	Set to 'BCOR'.
SWRES(NR)	Real	Value of the residual total water saturation in the Brooks-Corey function for region NR, S_{Wres}. [1].
PENT(NR)	Real	Value of the air-entry pressure (usually has value of zero or is a negative number) in the Brooks-Corey function for region NR, p_{ent}. [M/(L·s^2)]
RLAMB(NR)	Real	Value of the pore size distribution index in the Brooks-Corey function for region NR, λ. [1]

For the piecewise-linear total water saturation function:

SWMOD(NR)	Character	Set to 'PLIN'.
SWRES(NR)	Real	Value of the residual total water saturation in the piecewise-linear function for region NR, S_{Wres}. [1].
PENT(NR)	Real	Value of the air-entry pressure (usually has value of zero or is a negative number) in the piecewise-linear function for region NR, p_{ent}. [M/(L·s^2)]
PSWRES(NR)	Real	Value of the pressure (usually is a negative number) below which $S_{\mathrm{W}} = S_{\mathrm{Wres}}$ in the piecewise-linear function for region NR, p_{Swres}. [M/(L·s^2)]

For a user-defined total water saturation function:

SWMOD(NR)	Character	Set to 'UDEF'. **If the user-defined function is used, it must be programmed by the user in the designated section of subroutine UNSAT.**
NSWPAR(NR)	Integer	The number of user-defined function parameters specified for region NR, which must be less than or equal to 10.
SWPAR(NR)	Real	List of function parameter values for the user-defined function for region NR. [user-specified units].

DATASET 11C: Relative Permeability Parameters (1 line per region)

This dataset is required only if the simulation is UNSATURATED and (or) involves FREEZING. Omit otherwise.

Variable	Type	Description
For no specified relative permeability function (simulated relative permeability will always have a value of 1):		
RKMOD(NR)	Character	Set to 'NONE'.
For the van Genuchten relative permeability function:		
RKMOD(NR)	Character	Set to 'VGEN'.
VN(NR)	Real	van Genuchten function parameter n_{VG} for region NR. [1]
RKMIN(NR)	Real	Value of the minimum relative permeability, k_{rmin}, allowed a for region NR. [1] Setting RKMIN(NR)=0 allows the relative permeability in region NR to approach zero asymptotically as determined by the van Genuchten function.
For the Brooks-Corey relative permeability function:		
RKMOD(NR)	Character	Set to 'BCOR'.
RLAMB(NR)	Real	Value of the pore size distribution index in the Brooks-Corey function for region NR, λ. [1]
RKMIN(NR)	Real	Value of the minimum relative permeability, k_{rmin}, allowed a for region NR. [1] Setting RKMIN(NR)=0 allows the relative permeability in region NR to approach zero asymptotically as determined by the Brooks-Corey function.
For the piecewise-linear relative permeability function:		
RKMOD(NR)	Character	Set to 'PLIN'.
SLRKMIN(NR)	Real	Value of the liquid-water saturation in the piecewise-linear function at which relative permeability reaches its minimum value for region NR, $S_{\mathrm{L_{krmin}}}$. [1].
RKMIN(NR)	Real	Value of the minimum relative permeability, k_{rmin}, allowed a for region NR. [1]

For a user-defined relative permeability function:

RKMOD(NR)	Character	Set to 'UDEF'. **If the user-defined function is used, it must be programmed by the user in the designated section of subroutine RELPERM.**
NRKPAR(NR)	Integer	The number of user-defined function parameters specified for region NR, which must be less than or equal to 10.
RKPAR(NR)	Real	List of function parameter values for the user-defined function for region NR. [user-specified units].

DATASET 11D: Liquid Water Saturation Parameters (1 line per region)

This dataset is required only if the simulation involves FREEZING. <u>Omit</u> otherwise.

Variable	Type	Description

For no specified liquid water saturation function
(simulated liquid water saturation at full saturation will always have a value of 1):

SLMOD(NR)	Character	Set to 'NONE'.

For the exponential liquid water saturation function:

SLMOD(NR)	Character	Set to 'EXPO'.
SLSATRES(NR)	Real	Value of the residual liquid water saturation in the exponential function for region NR, $S_{\mathrm{Lres}}^{\mathrm{sat}}$. [1].
W (NR)	Real	exponential parameter w_{EXP} for region NR. [°C]

For the modified power-law liquid water saturation function:

SLMOD(NR)	Character	Set to 'POWR'.
SLSATRES(NR)	Real	Value of the residual liquid water saturation in the modified power law function for region NR, $S_{\mathrm{Lres}}^{\mathrm{sat}}$. [1].
ALPHA (NR)	Real	Modified power law model parameter, α_{POW}. $[(℃)^{-\beta_{\mathrm{POW}}}]$
BETA (NR)	Real	Modified power law model parameter, β_{POW}. [1]

For the piecewise-linear liquid water saturation function:

SWMOD(NR)	Character	Set to 'PLIN'.
SLSATRES(NR)	Real	Value of the residual liquid water saturation in the piecewise-linear function for region NR, $S_{\mathrm{Lres}}^{\mathrm{sat}}$. [1].
TLRES(NR)	Real	Value of the relative temperature, $T - T_{\mathrm{f}}$, below which $S_{\mathrm{L}}^{\mathrm{sat}} = S_{\mathrm{Lres}}^{\mathrm{sat}}$ in the piecewise-linear function for region NR, T_{Lres}. [M/(L·s^2)]

For a user-defined liquid water saturation function:

SLMOD(NR)	Character	Set to 'UDEF'. **If the user-defined function is used, it must be programmed by the user in the designated section of subroutine LIQSAT.**
NSLPAR(NR)	Integer	The number of user-defined function parameters specified for region NR, which must be less than or equal to 10.
SLPAR(NR)	Real	List of function parameter values for the user-defined function for region NR. [user-specified units].

DATASET 11E: Freezing Temperature and Latent Heat (1 line per region)

This dataset is required only if the simulation involves FREEZING. <u>Omit</u> otherwise.

<u>Variable</u>	<u>Type</u>	<u>Description</u>
TFREEZ(NR)	Real	Maximum freezing temperature of pore water, T_{f}. Typically 0 °C, but may be set to, for example, a negative value that is representative of the freezing-point depression caused by solutes dissolved in the groundwater. [°C]
HTLAT(NR)	Real	Latent heat of fusion, ΔH. [E/M]

DATASET 12: *no longer used; production parameters are spatially variable and are input in dataset 14*

DATASET 13: Orientation of Gravity Vector (one line)

Variable	Type	Description
GRAVX	Real	Component of gravity vector in +x direction. [L/s^2] GRAVX = $-\left\|\underline{g}\right\| (\partial$ ELEVATION$/\partial$ x), where $\left\|\underline{g}\right\|$ is the total acceleration due to gravity in [L/s^2].
GRAVY	Real	Component of gravity vector in +y direction. [L/s^2] GRAVY= $-\left\|\underline{g}\right\| (\partial$ ELEVATION$/\partial$ y), where $\left\|\underline{g}\right\|$ is the total acceleration due to gravity in [L/s^2].
GRAVZ	Real	Component of gravity vector in +z direction. [L/s^2] GRAVZ= $-\left\|\underline{g}\right\| (\partial$ ELEVATION$/\partial$ z), where $\left\|\underline{g}\right\|$ is the total acceleration due to gravity in [L/s^2]. Set to any arbitrary number (e.g., zero) for 2D problems.

DATASET 14A: Scale Factor for Nodewise Data (one line)

Variable	Type	Description
	Character	Line must begin with the word 'NODE'.
SCALX	Real	The scaled x-coordinates of nodes in dataset 14B are multiplied by SCALX in SUTRA. May be used to change from map to field scales, or from English to SI units. A value of 1.0 gives no scaling.
SCALY	Real	The scaled y-coordinates of nodes in dataset 14B are multiplied by SCALY in SUTRA. May be used to change from map to field scales or from English to SI units. A value of 1.0 gives no scaling.
SCALZ	Real	For 3D problems, the scaled z-coordinates of nodes in dataset 14B are multiplied by SCALZ in SUTRA. May be used to change from map to field scales or from English to SI units. A value of 1.0 gives no scaling. For 2D problems, the scaled element (mesh) thicknesses at nodes in dataset 14B are multiplied by SCALZ in SUTRA. May be used to easily change entire mesh thickness or to convert English to SI units. A value of 1.0 gives no scaling.
PORFAC	Real	The scaled nodewise porosities of dataset 14B are multiplied by PORFAC in SUTRA. May be used to easily assign a constant porosity value to all nodes by setting PORFAC=porosity, and all POR(II)=1.0 in dataset 14B.
COMPMAF	Real	The scaled nodewise solid matrix compressibilities of dataset 14B are multiplied by COMPMAF in SUTRA. May be used to easily assign a constant solid matrix compressibility value to all nodes by setting COMPMAF= solid matrix compressibility, and all COMPMA(II)=1.0 in dataset 14B.
CSF	Real	The scaled nodewise solid grain specific heats of dataset 14B are multiplied by CSF in SUTRA. May be used to easily assign a constant solid grain specific heat value to all nodes by setting CSF= solid grain specific heat, and all CS(II)=1.0 in dataset 14B. Set to any arbitrary number (for example, zero) for a solute-transport simulation.
RHOSF	Real	The scaled nodewise densities of a solid grain of dataset 14B are multiplied by RHOSF in SUTRA. May be used to easily assign a constant density of a solid grain value to all

		nodes by setting RHOSF= density of a solid grain, and all RHOS(II)=1.0 in dataset 14B.
PRODIN	Character	Set to 'PROD' if parameters for production or decay of solute or energy are specified; otherwise, set to 'NOPROD' to indicate that there is no production or decay.
PRODLØF	Real	The scaled nodewise values of zero-order rate of production in the liquid water (dataset 14B) are multiplied by PRODL0F in SUTRA. May be used to easily assign a constant zero-order rate of production in the liquid water value to all nodes by setting PRODL0F= zero-order rate of production in the liquid water, and all PRODL0(II)=1.0 in dataset 14B. **May be omitted if there is no production or decay (PRODIN ='NOPROD').**
PRODSØF	Real	The scaled nodewise values of zero-order rate of production in the immobile phase (dataset 14B) are multiplied by PRODS0F in SUTRA. May be used to easily assign a constant zero-order rate of production in the immobile phase value to all nodes by setting PRODS0F= zero-order rate of production in the immobile phase, and all PRODS0(II)=1.0 in dataset 14B. **May be omitted if there is no production or decay (PRODIN ='NOPROD').**
PRODL1F	Real	The scaled nodewise values of first-order rate of solute mass production in the liquid water (dataset 14B) are multiplied by PRODL1F in SUTRA. May be used to easily assign a constant first-order rate of solute mass production in the liquid water value to all nodes by setting PROLF1F= first-order rate of solute mass production in the liquid water, and all PRODL1(II)=1.0 in dataset 14B. **Omit for energy transport simulations with or without freezing**. **May be omitted if there is no production or decay (PRODIN ='NOPROD').**
PRODS1F	Real	The scaled nodewise values of first-order rate of adsorbate mass production in the immobile phase (dataset 14B) are multiplied by PRODS1F in SUTRA. May be used to easily assign a constant first-order rate of adsorbate mass production in the immobile phase value to all nodes by setting PRODS1F= first-order rate of adsorbate mass production in the immobile phase, and all PRODS1(II)=1.0 in dataset 14B. **Omit for energy transport simulations with or without freezing**. **May be omitted if there is no production or decay (PRODIN ='NOPROD').**
PRODIØF	Real	For energy transport simulations with FREEZING, the scaled nodewise values of zero-order rate of production in

		the ice (dataset 14B) are multiplied by PRODI0F in SUTRA. May be used to easily assign a constant zero-order rate of production in the ice value to all nodes by setting PRODI0F= zero-order rate of production in the ice, and all PRODI0(II)=1.0 in dataset 14B. **May be omitted for simulations that do not involve FREEZING**. **May be omitted if there is no production or decay (PRODIN ='NOPROD').**

DATASET 14B: Nodewise Data (one line for each of NN nodes)

Variable	Type	Description
II	Integer	Number of node, i, to which data on this line refers.
NREG (II)	Integer	Region number to which node II belongs. (Minimum of 1 and maximum of 10 regions allowed; see NPMREG in dataset 11.) The node region number is usually the same as the region number of the elements in which it appears. When the node is at the boundary of two regions, it may be assigned to either region.
X(II)	Real	Scaled x-coordinate of node II, x_{i}. [L]
Y(II)	Real	Scaled y-coordinate of node II, y_{i}. [L]
Z(II)	Real	For 3D problems, scaled z-coordinate of node II, z_{i}. [L] For 2D problems, scaled thickness of mesh at node II. [L] To simulate radial cross sections, set Z(II) = (2π)(radius$_{\mathrm{i}}$), where radius$_{\mathrm{i}}$ is the radial distance from the vertical center axis (axis of radial symmetry) to node i.
POR(II)	Real	Scaled porosity value at node II, ε_{i}. [1]
COMPMA(II)	Real	Solid matrix compressibility at node II, $\alpha_{\mathrm{S_i}} = (1 - \varepsilon_{\mathrm{i}})^{-1}(\partial\varepsilon_{\mathrm{i}}/\partial p)$. $[\mathrm{M/(L{\cdot}s^2)}]^{-1}$.
CS(II)	Real	Solid grain specific heat value at node II, $c_{\mathrm{S_i}}$. [E/(M·ºC)] Set to any arbitrary number (for example, zero) for a solute-transport simulation.
RHOS(II)	Real	Density of a solid grain value at node II, $\rho_{\mathrm{S_i}}$. [M/L^3].

		Value used only for energy-transport simulations or solute-transport simulations with sorption; may otherwise be set to any arbitrary number (for example, zero).
PRODLØ(II)	Real	Zero-order rate of production in the liquid water at node II, $\gamma_{0_i}^{L}$. [(E/M)/s] for energy production, [(M_s/M)/s] for solute mass production. **May be omitted if there is no production or decay (PRODIN ='NOPROD' in dataset 14A).**
PRODSØ(II)	Real	Zero-order rate of production in the immobile phase at node II, $\gamma_{0_i}^{S}$. [(E/M_G)/s] for energy production, [(M_s/M_G)/s] for adsorbate mass production. **May be omitted if there is no production or decay (PRODIN ='NOPROD' in dataset 14A).**
PRODL1(II)	Real	First-order rate of solute mass production in the liquid water at node II, $\gamma_{1_i}^{L}$. [s^{-1}]. **Omit for energy transport simulations with or without freezing. May be omitted if there is no production or decay (PRODIN ='NOPROD' in dataset 14A).**
PRODS1(II)	Real	First-order rate of adsorbate mass production in the immobile phase at node II, $\gamma_{1_i}^{S}$. [s^{-1}]. **Omit for energy transport simulations with or without freezing. May be omitted if there is no production or decay (PRODIN ='NOPROD' in dataset 14A).**
PRODIØ(II)	Real	Zero-order rate of production in the ice at node II, $\gamma_{0_i}^{I}$. [(E/M)/s]. **May be omitted for simulations that do not involve FREEZING. May be omitted if there is no production or decay (PRODIN ='NOPROD' in dataset 14A).**

NOTE: When the DIRECT solver is used, the order in which the nodes are numbered affects the bandwidth of the global banded matrix, NBI, which in turn affects computational and storage efficiency. In this case, **the user should take care to number the nodes to minimize NBI**. SUTRA sets NBI equal to one plus twice the maximum difference in node numbers in the element containing the largest node number difference in the mesh. See figure 7.1 of Voss and Provost (2002) for an example. When an iterative solver is used, it is still advantageous to minimize NBI, although not as critical as in the case of the DIRECT solver.

DATASET 15A: Scale Factors for Elementwise Data (one line)

Variable	Type	Description
	Character	Line must begin with the word 'ELEMENT'.
PMAXFA	Real	The scaled maximum permeability values, PMAX, in dataset 15B are multiplied by PMAXFA in SUTRA. May be used to convert units or to aid in assignment of maximum permeability values in elements.
PMIDFA	Real	The scaled middle permeability values, PMID, in dataset 15B are multiplied by PMIDFA in SUTRA. May be used to convert units or to aid in assignment of maximum permeability values in elements. **Omit for 2D problems.**
PMINFA	Real	The scaled minimum permeability values, PMIN, in dataset 15B are multiplied by PMINFA in SUTRA. May be used to convert units or to aid assignment of minimum permeability values in elements.
ANG1FA	Real	The scaled angles ANGLE1 in dataset 15B are multiplied by ANG1FA in SUTRA. For 2D problems, may be used to easily assign a uniform direction of anisotropy by setting ANG1FA=angle, and all ANGLE1(L)=1.0 in dataset 15B.
ANG2FA	Real	The scaled angles ANGLE2 in dataset 15B are multiplied by ANG2FA in SUTRA. **Omit for 2D problems.**
ANG3FA	Real	The scaled angles ANGLE3 in dataset 15B are multiplied by ANG3FA in SUTRA. **Omit for 2D problems.**
ALMAXF	Real	The scaled longitudinal dispersivities ALMAX in dataset 15B are multiplied by ALMAXF in SUTRA. May be used to convert units or to aid in assignment of dispersivities.
ALMIDF	Real	The scaled longitudinal dispersivities ALMID in dataset 15B are multiplied by ALMIDF in SUTRA. May be used to convert units or to aid in assignment of dispersivities. **Omit for 2D problems.**
ALMINF	Real	The scaled longitudinal dispersivities ALMIN in dataset 15B are multiplied by ALMINF in SUTRA. May be used to convert units or to aid in assignment of dispersivities.
ATMAXF	Real	The scaled transverse dispersivities ATMAX in dataset 15B are multiplied by ATMAXF in SUTRA. May be used to convert units or to aid in assignment of dispersivity.

ATMIDF	Real	The scaled transverse dispersivities ATMID in dataset 15B are multiplied by ATMIDF in SUTRA. May be used to convert units or to aid in assignment of dispersivity. **Omit for 2D problems.**
ATMINF	Real	The scaled transverse dispersivities ATMIN in dataset 15B are multiplied by ATMINF in SUTRA. May be used to convert units or to aid in assignment of dispersivity.
SIGMASF	Real	The scaled solid grain thermal conductivity values, SIGMAS, in dataset 15B are multiplied by SIGMASF in SUTRA. May be used to convert units or to aid in assignment of solid grain thermal conductivity values in elements. **May be omitted for solute transport simulations.**
SIGMAAF	Real	The scaled effective air thermal conductivity values, SIGMAA, in dataset 15B are multiplied by SIGMAAF in SUTRA. May be used to convert units or to aid in assignment of effective air thermal conductivity values in elements. **May be omitted for solute transport simulations.**

DATASET 15B: Elementwise Data (one line for each of NE elements)

Variable	Type	Description
L	Integer	Number of element to which data on this line refers.
LREG(L)	Integer	Region number to which this element belongs. (Minimum of 1 and maximum of 10 regions allowed; see NPMREG in dataset 11.)
PMAX(L)	Real	Scaled maximum permeability value, $k_{\max}$, of element L. [L^2]
PMID(L)	Real	Scaled middle permeability value, k_{mid}, of element L. [L^2] Isotropic permeability requires: PMID(L)=PMAX(L). **Omit for 2D problems.**
PMIN(L)	Real	Scaled minimum permeability value, $k_{\min}$, of element L. [L^2] Isotropic permeability requires: PMIN(L)=PMAX(L).
ANGLE1(L)	Real	Scaled first angle, θ_1 [°], used to define the directions of maximum, middle, and minimum permeability in element L.

ANGLE2(L)	Real	Scaled second angle, θ_2 [°], used to define the directions of maximum, middle, and minimum permeability in element L. **Omit for 2D problems.**
ANGLE3(L)	Real	Scaled third angle, θ_3 [°], used to define the directions of maximum, middle, and minimum permeability in element L. **Omit for 2D problems.**
ALMAX(L)	Real	Scaled longitudinal dispersivity value, α_{Lmax}, of element L that controls longitudinal dispersion along the maximum permeability direction when the flow direction is in the maximum permeability direction. [L]
ALMID(L)	Real	Scaled longitudinal dispersivity value, α_{Lmid}, of element L that controls longitudinal dispersion along the middle permeability direction when the flow direction is in the middle permeability direction. [L] **Omit for 2D problems.**
ALMIN(L)	Real	Scaled longitudinal dispersivity value, α_{Lmin}, of element L that controls longitudinal dispersion along the minimum permeability direction when the flow direction is in the minimum permeability direction. [L]
ATMAX(L)	Real	Scaled transverse dispersivity value, α_{Tmax}, of element L that controls transverse dispersion in the maximum permeability direction when the flow direction is perpendicular to the maximum permeability direction. [L]
ATMID(L)	Real	Scaled transverse dispersivity value, α_{Tmid}, of element L that controls transverse dispersion in the middle permeability direction when the flow direction is perpendicular to the middle permeability direction. [L] **Omit for 2D problems.**
ATMIN(L)	Real	Scaled transverse dispersivity value, α_{Tmin}, of element L that controls transverse dispersion in the minimum permeability direction when the flow direction is perpendicular to the minimum permeability direction. [L]
SIGMAS(L)	Real	Scaled solid grain thermal conductivity value, $\sigma_S \equiv \lambda_S$, of element L. [E/(L·°C·s)] **May be omitted for solute transport simulations.**

SIGMAA(L) Real — Scaled effective air thermal conductivity value, $\sigma_A \equiv \lambda_A$, of element L. [E/(L·°C·s)] **<u>May be omitted</u> for solute transport simulations.**

<u>Notes:</u>

The SUTRA permeability model is described in detail in section 2.2, "Saturated-Unsaturated Ground-Water Flow," of the main SUTRA documentation (Voss and Provost, 2002). The SUTRA dispersion model is described in detail in section 2.5, "Dispersion." The notes that follow are included to further assist the user in specifying the input parameters for permeability and dispersion in SUTRA models, particularly in 3D.

Permeability

The "permeability ellipse" and "permeability ellipsoid" that form the basis of the SUTRA permeability model in 2D and 3D, respectively, are described in section 2.2 and pictured in Figure 2.2 of the main SUTRA documentation (Voss and Provost, 2002).

In 3D, the principal axes of the permeability ellipsoid are, by definition, mutually perpendicular and aligned with the directions of maximum, middle, and minimum permeability. SUTRA requires that the orientation of this ellipsoid relative to the x-, y-, and z-coordinate axes be defined for each element in the mesh by specifying three parameters -- ANGLE1, ANGLE2, and ANGLE3 – in each element. These three angles may be thought of, in aeronautical terms, as the "yaw," "pitch," and "roll" of the permeability ellipsoid with respect to a reference orientation, which is described below.

In defining ANGLE1, ANGLE2, and ANGLE3, we make the following assumptions and definitions:

- The Cartesian (x, y, z) coordinate system is right-handed: it can be viewed such that the +x-axis points forward, the +y-axis points to the left, and the +z-axis points upward.
- The maximum, middle, and minimum permeability axes are the principal axes of the permeability ellipsoid. Initially, before the three rotations defined by ANGLE1, ANGLE2, and ANGLE3 have been performed, let these three principal axes be aligned with the x-, y-, and z-coordinate axes, respectively; this is the reference orientation. After the three rotations are completed, the maximum, middle, and minimum permeability axes will be aligned with the directions of maximum, middle, and minimum permeability, respectively.
- The *positive* maximum, middle, and minimum permeability axes (which will be called the "+max," "+mid," and "+min" axes below) are the semi-axes that are initially aligned with the +x-, +y-, and +z-axes, respectively.

The rotations and corresponding angles are then defined as follows:

- The first rotation of the permeability ellipse is about the z-axis. After this rotation has been performed, ANGLE1 is the angle between the +max axis and the +x-axis. It is measured within the x,y-plane, with a positive angle denoting *counterclockwise*

rotation when viewed from positive z, looking toward the origin. It represents the azimuth of the +max axis.

- The second rotation of the permeability ellipse is upward or downward from the x,y-plane. After this rotation has been performed, ANGLE2 is the angle between the +max axis and the x,y-plane. It is measured perpendicularly from the x,y-plane, with a positive angle denoting upward rotation (toward the +z-axis). It represents the angular elevation or declination of the +max axis.
- The third rotation of the permeability ellipse is about the +max axis. After this rotation has been performed, ANGLE3 is the angle between the +mid axis and the x,y-plane. It is measured within the plane perpendicular to the +max axis, with a positive angle denoting *clockwise* rotation when viewed from the origin, looking along the +max axis.

In 3D simulations, ANGLE3 is arbitrary if the permeability and dispersion tensors are isotropic within the (MID,MIN)-plane, that is, if, after the application of scale factors, PMIN=PMID, ALMIN=ALMID, and ATMIN=ATMID. All three angles, ANGLE1, ANGLE2, and ANGLE3, are arbitrary if the permeability and dispersion tensors are completely isotropic, that is, if, after the application of scale factors, PMIN=PMID=PMAX, ALMIN=ALMID=ALMAX, and ATMIN=ATMID=ATMAX.

In 2D simulations, ANGLE1 is arbitrary if the permeability and dispersion tensors are isotropic, that is, if, after application of scale factors, PMIN=PMAX, ALMIN=ALMAX, and ATMIN=ATMAX.

Dispersivity

The convention for determining the 2D transverse dispersivity, α_T, differs from the one used in versions of SUTRA (Voss, 1984) prior to version 2.0 (2D3D.1), as described in section 2.5 of the main SUTRA documentation (Voss and Provost, 2002).

In the SUTRA dispersion model in 3D, the effective longitudinal dispersivity is computed as the squared radius of a "longitudinal dispersivity ellipsoid" (pictured in Figure 2.4b) in the direction of ground-water flow, as described in section 2.5. For simplicity, the principal axes of this ellipsoid are assumed to be aligned with the directions of maximum, middle, and minimum permeability, which are mutually perpendicular and are specified by parameters ANGLE1, ANGLE2, and ANGLE3 for each element.

The dispersivities ALMAX(L), ALMID(L), and ALMIN(L) represent the squared radii of the longitudinal dispersivity ellipsoid in the maximum, middle, and minimum permeability directions, respectively, for element L. Thus, ALMAX, ALMID, and ALMIN are the effective longitudinal dispersivities for flow in the maximum, middle, and minimum permeability directions, respectively. Note that "MAX," "MID," and "MIN" do not refer to the relative magnitudes of the dispersivities, but rather to the direction in which they apply.

Use of different longitudinal dispersivities for various flow directions may be justified in a few ways. Differences in longitudinal dispersivity in various flow directions may either be due to a local anisotropy in porous medium or aquifer structure, or to the different sizes of heterogeneities experienced by flows along vertical and horizontal transport reaches in an aquifer system. Regional horizontal flows typically encounter much larger heterogeneities than flows occurring vertically through an aquifer, causing higher longitudinal dispersion for horizontal flows than for vertical flows.

The effective transverse dispersivities in 3D may be computed as the squares of two radii of a "transverse dispersivity ellipsoid" (pictured in Figure 2.4c) measured perpendicular to the direction of ground-water flow, as described in section 2.5. For simplicity, the principal axes of this ellipsoid are also assumed to be aligned with the directions of maximum, middle, and minimum permeability.

The dispersivities ATMAX(L), ATMID(L), and ATMIN(L) represent the squared radii of the transverse dispersivity ellipsoid in the maximum, middle, and minimum permeability directions, respectively, for element L. Note that:

- For all flow directions within the (MAX,MID)-plane, ATMIN is the effective dispersivity that controls transverse dispersion in the MIN direction.
- For all flow directions within the (MAX,MIN)-plane, ATMID is the effective dispersivity that controls transverse dispersion in the MID direction.
- For all flow directions within the (MID,MIN)-plane, ATMAX is the effective dispersivity that controls transverse dispersion in the MAX direction.

It follows that when the flow direction coincides with one of the principal permeability directions, the effective transverse dispersivities are those corresponding to the remaining two principal permeability directions:

- For flow in the MAX permeability direction, the effective transverse dispersivities are ATMID and ATMIN.
- For flow in the MID permeability direction, the effective transverse dispersivities are ATMAX and ATMIN.
- For flow in the MIN permeability direction, the effective transverse dispersivities are ATMAX and ATMID.

For any given flow direction in 3D, there are two transverse dispersivities. Thus, for flow in the maximum, middle, and minimum permeability directions, there would be a maximum of six different transverse dispersivity values (two for each of the three directions, assuming that flow in exactly opposite directions have the same transverse dispersivities). However, the SUTRA model assumes that transverse dispersivity in a given direction is the same irrespective of in which perpendicular direction the flow occurs, and thus allows only three different values to be specified for each element: ATMAX, ATMID, and ATMIN. The user must decide, based on the description of the dispersion model in section 2.5 and the information outlined above, which values best describe the behavior of the system being simulated.

Use of different transverse dispersivities for various flow directions is not as easily justified as flow-direction-dependent longitudinal dispersivities. Normally, the flow-

direction-dependent transverse dispersivities should be set to the same value (unless the user has a specific dispersion behavior in mind). This results in the same effective transverse dispersion in all directions for all flow directions just as given by the classical model.

DATASET 16: *no longer used*

DATASET 17: Constant Values for Fluid Sources and Sinks (one line for each of NSOP fluid source nodes as specified in dataset 3, plus one line)

O M I T when there are no fluid source/sink nodes (NSOP=0).

Specifications made in this dataset are constant values that are used by SUTRA unless/until they are superseded by time-dependent specifications in dataset 3 of an optional ".bcs" file.

Variable	Type	Description
Lines 1 to NSOP:		
IQCP	Integer	Number of node to which source/sink data on this line refers. Specifying the node number with a negative sign indicates to SUTRA that the manner in which the source flow rate, concentration, or temperature of the source fluid varies with time has been programmed by the user in subroutine BCTIME.
QINC	Real	Fluid source (or sink) which is a specified constant value at node IQCP, Q_{IN}. [M/s]. A positive value is a source of fluid to the aquifer. May be omitted if this value is specified as time-dependent in subroutine BCTIME (IQCP<0). Sources are allocated by cell as shown in Figure B.1 for equal-sized elements. For unequal-sized elements, sources are allocated in proportion to the cell length, area or volume over which the source fluid enters the system.
UINC	Real	Temperature or solute concentration (mass fraction) of fluid entering the aquifer, which is a specified constant value for a fluid source at node IQCP, U_{IN}. [°C] or [M_s/M] May be omitted if this value is specified as time-dependent in subroutine BCTIME (IQCP<0) or if QINC≤0.
Last line:		
	Integer	Placed immediately following all NSOP fluid source node lines. Line must begin with the integer 0.

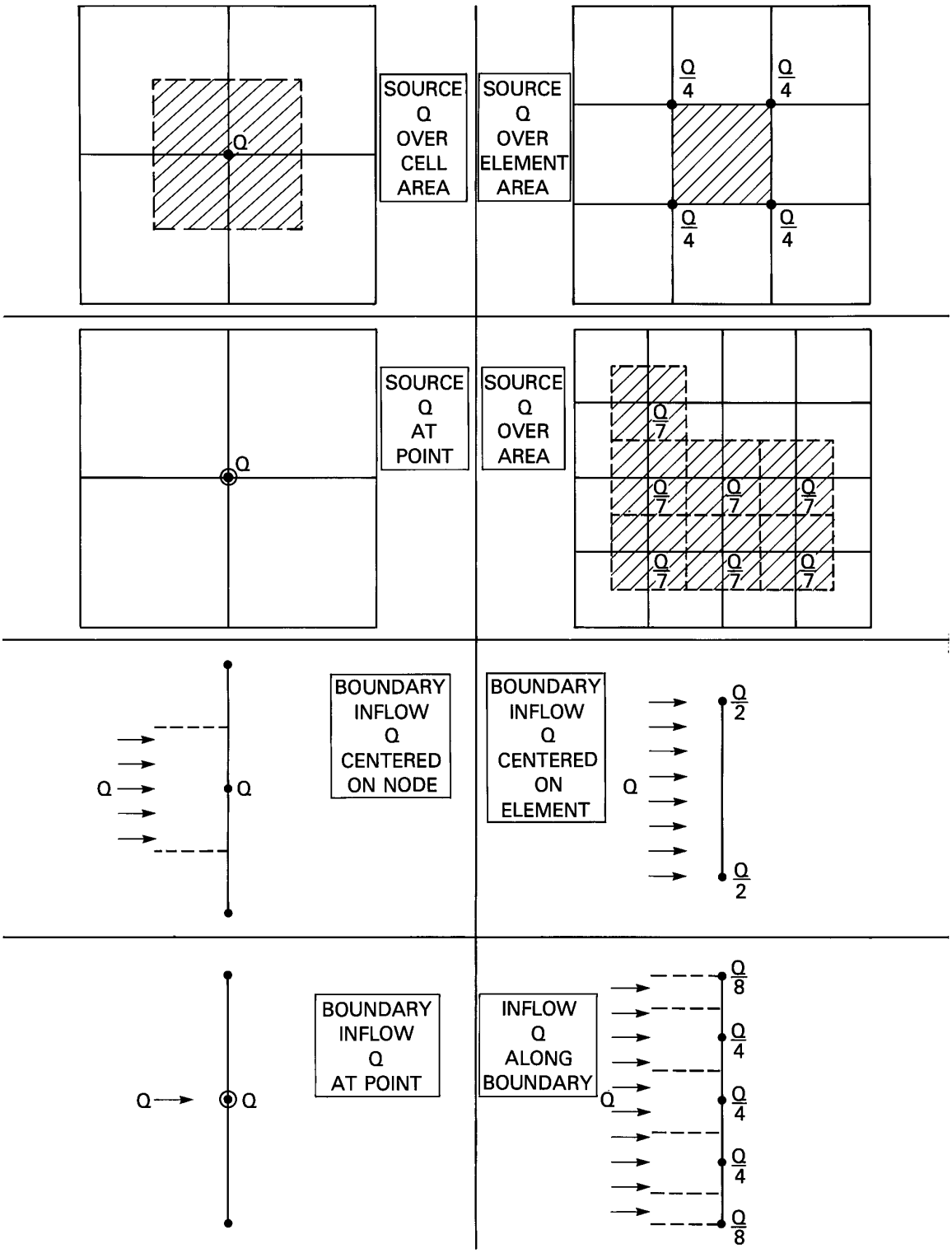

Figure B.1. Allocation of sources and boundary fluxes in equal-sized elements. The top four panels pertain to 2D areal and 3D meshes. The bottom four panels pertain to 2D cross-sectional meshes. Though sources are always specified at nodes, a variety of spatial source distributions may be obtained by appropriate specification of nodal source values. From Voss and Provost (2002).

DATASET 18: Constant Values for Energy or Solute Mass Sources and Sinks
(one line for each NSOU energy or solute source nodes as specified in dataset 3, plus one line)

O M I T when there are no energy or solute source/sink nodes (NSOU=0).

Specifications made in this dataset are constant values that are used by SUTRA unless/until they are superseded by time-dependent specifications in dataset 4 of an optional ".bcs" file.

Variable	Type	Description
Lines 1 to NSOU:		
IQCU	Integer	Number of node to which source/sink data on this line refers. Specifying the node number with a *negative sign* indicates to SUTRA that the manner in which the source rate varies with time has been programmed by the user in subroutine BCTIME.
QUINC	Real	Source (or sink) that is a specified constant value at node IQCU, ψ_{IN}. [E/s] for energy transport, [M_s/s] for solute transport. A positive value is a source to the aquifer. May be omitted if this value is specified as time-dependent in subroutine BCTIME (IQCU <0). Sources are allocated by cell as shown in Figure B.1 for equal-sized elements. For unequal-sized elements, sources are allocated in proportion to the cell length, area or volume over which the source energy or solute mass enters the system.
Last line:		
	Integer	Placed immediately following all NSOU energy or solute mass source node lines. Line must begin with the integer 0.

DATASET 19: Constant Values for Specified Pressure Nodes (one line for each of NPBC specified pressure nodes as indicated in dataset 3, plus one line)

O M I T when there are no specified pressure nodes (NPBC=0).

Specifications made in this dataset are constant values that are used by SUTRA unless/until they are superseded by time-dependent specifications in dataset 5 of an optional ".bcs" file.

Variable	Type	Description
Lines 1 to NPBC:		
IPBC	Integer	Number of node to which specified pressure data on this line refers. Specifying the node number with a negative sign indicates to SUTRA that the manner in which the specified pressure value or inflow concentration or temperature at this node varies with time has been programmed by the user in subroutine BCTIME.
PBC	Real	Pressure value which is a specified constant at node IPBC. $[M/(L \cdot s^2)]$. May be omitted if this value is specified as time-dependent in subroutine BCTIME.
UBC	Real	Temperature or solute concentration of any external fluid that enters the aquifer at node IPBC. UBC is a specified constant value. [°C] or $[M_s/M]$. May be omitted if this value is specified as time-dependent in subroutine BCTIME.
Last line:		
	Integer	Placed immediately following all NPBC specified pressure lines. Line must begin with the integer 0.

DATASET 20: Constant Values for Specified Concentration or Temperature Nodes
(one line for each of NUBC specified concentration or temperature nodes indicated in dataset 3, plus one line)

O M I T when there are no specified concentration or temperature nodes (NUBC=0).

Specifications made in this dataset are constant values that are used by SUTRA unless/until they are superseded by time-dependent specifications in dataset 6 of an optional ".bcs" file.

Variable	Type	Description
Lines 1 to NUBC:		
IUBC	Integer	Number of node to which specified concentration or temperature data on this line refers. Specifying the node number with a negative sign indicates to SUTRA that the manner in which the specified value at this node varies with time has been programmed by the user in subroutine BCTIME.
UBC	Real	Temperature or solute concentration value which is a specified constant at node IUBC. [°C] or [M_s/M]. May be omitted if IUBC is negative and this value is specified as time-dependent in subroutine BCTIME.
Last line:		
	Integer	Placed immediately following all NUBC specified temperature or concentration lines. Line must begin with the integer 0.

DATASET 21A: Constant Values for Generalized-Flow Nodes (one line for each of NPBG generalized pressure nodes as indicated in dataset 3, *plus* one line)

O M I T when there are no generalized-flow nodes (NPBG = 0).

Specifications made in this dataset are constant values that are used by SUTRA unless/until they are superseded by time-dependent specifications in dataset 7A of an optional ".bcs" file.

Variable	Type	Description
Lines 1 to NPBG:		
IPBG	Integer	Number of node to which generalized-flow data on this line refers. Specifying the node number with a *negative sign* indicates to SUTRA that the manner in which the input variable values at this node vary with time has been *programmed by the user* in subroutine BCTIME.
PBG1	Real	Pressure value at the first of two points that define the linear relation between fluid inflow/outflow and pressure at node IPBG. [M/(L·s^2)]. May be omitted if IPBG<0.
QPBG1	Real	Rate of inflow/outflow of fluid mass when the computed pressure equals PBG1 at node IPBG. [M/s]. May be omitted if IPBG < 0.
PBG2	Real	Pressure value at the second of two points that define the linear relation between fluid inflow/outflow and pressure at node IPBG. [M/(L·s^2)]. May be omitted if IPBG < 0.
QPBG2	Real	Rate of inflow/outflow of fluid mass when the computed pressure equals PBG2 at node IPBG. [M/s]. May be omitted if IPBG < 0.
CPQL1	Character	Determines whether a limit is set on fluid inflow/outflow, pressure, or neither at the first of two points that define the linear relation between fluid inflow/outflow and pressure at node IPBC. [M/(L·s^2)]. Valid values are as follows: 'Q' = set limit of Q ≤ QPBG1 'P' = set limit of p ≥ PBG1 'N' = set no limit at point 1 May be omitted if IPBG < 0.
CPQL2	Character	Determines whether a limit is set on fluid inflow/outflow, pressure, or neither at the second of two points that define the linear relation between fluid inflow/outflow and

		pressure at node IPBC. [M/(L·s^2)]. Valid values are as follows: 'Q' = set limit of Q ≥ QPBG2 'P' = set limit of p ≤ PBG2 'N' = set no limit at point 2 May be omitted if IPBG < 0.
UPBGI	Real	Temperature or solute concentration of any external fluid that enters the model at node IPBC. UPBGI is a specified constant value. [°C] or [M_s/M]. May be omitted if IPBG < 0.
CUPBGO	Character	One word. Must be either ’DIR‘ or ’REL‘. Indicates whether the temperature or solute concentration, UPBGO, of any fluid that exits the model at node IPBG is being specified directly (‘DIR’) or relative to the computed concentration or temperature at the node (‘REL’). May be omitted if IPBG < 0.
UPBGO	Real	Temperature or solute concentration of any fluid that exits the model at node IPBG. If CUPBGO = ’DIR’, the exit temperature or concentration is set directly to the value UPBGO. If CUPBGO = ’REL’, the exit temperature or concentration is set to the value U+UBPGO, where U is the temperature or concentration computed at the node. [°C] or [M_s/M]. May be omitted if IPBG < 0.
<u>Last line</u>:		
	Integer	Placed immediately following all NPBG generalized-flow lines. Line must begin with the integer 0.

DATASET 21B: Constant Values for Generalized-Transport Nodes
(one line for each of NUBG generalized-transport nodes indicated in dataset 3, *plus* one line)

O M I T when there are no generalized-transport nodes (NUBG=0).

Specifications made in this dataset are constant values that are used by SUTRA unless/until they are superseded by time-dependent specifications in dataset 7B of an optional ".bcs" file.

Variable	Type	Description
Lines 1 to NUBG:		
IUBG	Integer	Number of node to which generalized-transport data on this line refers. Specifying the node number with a *negative sign* indicates to SUTRA that the manner in which the input variable values at this node vary with time has been *programmed by the user* in subroutine BCTIME.
UBG1	Real	Concentration or temperature value at the first of two points that define the linear relation between solute mass or energy inflow/outflow and concentration or temperature at node IUBG. [M_s/M or C°]. May be omitted if IPBG < 0.
QUBG1	Real	Rate of inflow/outflow of solute mass or energy when the computed concentration or temperature equals UBG1 at node IUBG. [M_s/s or E/s]. May be omitted if IPBG < 0.
UBG2	Real	Concentration or temperature value at the second of two points that define the linear relation between solute mass or energy inflow/outflow and concentration or temperature at node IUBG. [M_s/M or C°]. May be omitted if IPBG < 0.
QUBG2	Real	Rate of inflow/outflow of solute mass or energy when the computed concentration or temperature equals UBG2 at node IUBG. [M_s/s or E/s]. May be omitted if IPBG < 0.
Last line:		
	Integer	Placed immediately following all NUBG specified temperature or concentration lines. Line must begin with the integer 0.

DATASET 22: Element Incidence Data (one line, plus one line for each of NE elements)

Variable	Type	Description
Line 1:		
	Character	Line must begin with the word 'INCIDENCE'.
Lines 2 to NE+1:		
LL	Integer	Number of element to which data on this line refers.
IIN	Integer	Node incidence list; list of corner node numbers in element LL, beginning at any node. For 2D problems, the four nodes are listed in an order counterclockwise about the element. For 3D problems, the eight nodes are listed as follows. Approach the element from any of its six sides. On the face farthest away (the "back" face, viewed looking through the element), list the four nodes in an order counterclockwise about the face. Then, on the closest face (the "front" face), again list the four nodes counterclockwise, starting with the node directly in front of the node that was listed first. (This convention assumes a right-handed coordinate system.)

List of Input Data for the Time-Dependent Sources and Boundary Conditions Files (**.bcs**)

Model Version: ***SUTRA 4.0***

Optional **".bcs"** input files provide a way to specify time-dependent sources and boundary conditions without programming subroutine BCTIME. They may be omitted if there are no time-dependent sources or boundary conditions other than those specified in subroutine BCTIME.

In addition to changing the values of the input variables associated with sources and boundary conditions, **".bcs"** files allow any source or boundary condition to be inactivated ("turned off") and reactivated ("turned on") during a simulation. For specified-pressure and specified-concentration or temperature conditions, this capability is unique to **".bcs"** files; it cannot be accomplished via the **".inp"** input file or subroutine BCTIME. (Sources and sinks can be effectively turned off by setting their associated rates to zero in the **".inp"** file, subroutine BCTIME, or a **".bcs"** file.)

The user may assign as many **".bcs"** files as desired, which allows considerable flexibility in organizing time-dependent sources and boundary conditions. At the beginning of each time step, SUTRA checks all of the **".bcs"** files (in the order in which they are listed in the "**SUTRA.FIL**" file) and reads in any source and boundary condition specifications that pertain to that time step.

General rules

The general rules for specifying sources and boundary conditions using **".bcs"** files are as follows:

- Any node at which a **".bcs"** specification is made must also be listed in datasets 17 – 20 of the **".inp"** file. (For example, a node that is specified as a fluid source node on any time step of any **".bcs"** file must also be listed in dataset 17 of the **".inp"** file.) Doing so "registers" the node as a source or boundary condition node and provides "default" values that remain in force unless/until overridden by a **".bcs"** specification.
- Datasets 3, 4, 5, and 6 of a **".bcs"** file correspond to datasets 17, 18, 19, and 20, respectively, of the **".inp"** file. (For example, **".bcs"** dataset 5 and **".inp"** dataset 19 both define specified-pressure nodes.) The formats of these four **".bcs"** datasets parallel those of the corresponding **".inp"** datasets.
- Specifications made in "**.bcs**" files take precedence over those made in the **".inp"** file and (on the same or earlier time step) in subroutine BCTIME, and they are persistent – they remain in force until overridden by a subsequent specification in a **".bcs"** file or subroutine BCTIME.
- Multiple **".bcs"** specifications of the same kind at the same node on the same time step are resolved in favor of the specification that is read in last. On each time step, the **".bcs"** files are processed in the order in which they are listed in the **"SUTRA.FIL"** file.

- Each **".bcs"** file may contain specifications for a series of time steps. The time steps on which the specifications are applied are determined by a schedule. Each **".bcs"** file may be controlled by a different schedule if desired.
- The **".bcs"** files need contain only those specifications that change on each time step – it is not necessary to provide a **".bcs"** specification for every source and boundary condition node on every time step.

Use in steady-state and transient simulations

Although **".bcs"** files are intended primarily for time-dependent sources and boundary conditions, they can also be used in steady-state simulations (in which case they override corresponding specifications made in the **".inp"** file and subroutine BCTIME):

- For steady-state flow, flow-related sources and boundary conditions (**".bcs"** datasets 3 and 5) may be specified on time step 0. This is consistent with the SUTRA convention of solving for steady-state flow on time step 0. Flow-related specifications made after time step 0 will not affect the solution.
- For transient flow, flow-related sources and boundary conditions (**".bcs"** datasets 3 and 5) may be specified beginning with time step 1. Flow-related specifications made on time step 0 will not affect the solution.
- For steady-state transport, transport-related sources and boundary conditions (**".bcs"** datasets 4 and 6) may be specified on time step 1. This is consistent with the SUTRA convention of solving for steady-state transport on time step 1. Transport-related specifications made after time step 1 will not affect the solution. Transport-related specifications are never needed, and are therefore not permitted, on time step 0.
- For transient transport, transport-related sources and boundary conditions (**".bcs"** datasets 4 and 6) may be specified beginning with time step 1. Transport-related specifications are never needed, and are therefore not permitted, on time step 0.

It is usually simplest to specify steady-state sources and boundary conditions in datasets 17 – 20 of the **".inp"** file. However, **".bcs"** files can be convenient for inactivating ("turning off") selected steady-state specifications, which would otherwise have to be deleted or commented out of the **".inp"** file, or for efficiently implementing alternative sets of steady-state specifications simply by swapping out the names of **".bcs"** files in "**SUTRA.FIL**".

Automatic solution sequencing

SUTRA requires that a flow solution and/or a transport solution be generated on time steps on which the relevant sources or boundary conditions change. For time-dependent sources and boundary conditions programmed in subroutine BCTIME, the user is responsible for ensuring that flow and transport solutions are generated on the appropriate time steps (by setting NPCYC and NUCYC to appropriate values in dataset 6 of the **".inp"** file). However, SUTRA automatically ensures that flow and/or transport solutions are generated whenever relevant sources or boundary conditions are specified in a **".bcs"** file.

Example

An example of a simple **".bcs"** file is provided after the description of dataset 6 below.

Each ".bcs" file consists of dataset 1, which specifies a schedule of time steps, followed by one repetition of datasets 2 – 6 for each time step in the schedule.

DATASET 1: Schedule name (one line)

Variable	Type	Description
BCSSCH	Character	Name of the schedule that controls input of sources and boundary conditions in the **".bcs"** file. The schedule may contain only whole-numbered time steps (0, 1, 2, 3, etc.). Fractional time step numbers (e.g., 1.5) are not allowed.

Notes:

This dataset specifies the schedule that controls input of sources and boundary conditions in the **".bcs"** file. Each **".bcs"** file may be controlled by a different schedule. (Schedules are defined in dataset 6 of the **".inp"** file.)

The **".bcs"** file must include a set of source and/or boundary condition specifications (datasets 2 - 6) for every time step listed in the schedule. The first set of specifications encountered is applied to the first time step listed in the schedule, the second set of specifications encountered is applied to the second time step listed, etc. If the schedule includes time step 0, then a set of specifications must be given for time step 0, even if it does not affect the solution (as is the case in a transient-flow, transient-transport simulation).

For convenience, SUTRA automatically defines three schedules:

- "STEP_0", which consists only of time step 0,
- "STEP_1", which consists only of time step 1, and
- "STEPS_1&UP", which consists of all time steps after time step 0.

Schedules "STEP_0" and "STEP_1" can be useful for specifying steady-state sources and boundary conditions. Schedule "STEPS_1&UP" can be useful for specifying time-dependent sources and boundary conditions in transient-flow, transient-transport simulations, which do not require a specification on time step 0.

When transport is steady-state, user-defined schedules are disabled, and the only schedules available are "STEP_0", "STEP_1", "STEPS_1&UP" (which then consists only of time step 1), and "TIME_STEPS" (which SUTRA automatically defines as consisting only of time steps 0 and 1).

DATASET 2: Identifier and Time-Dependent Source and Boundary Condition Counts (one line)

Required for each time step on which there is a source or boundary condition specification in the ".bcs" file (that is, for each time step in the controlling schedule specified in dataset 1).

Variable	Type	Description
BCSID	Character	Name that identifies the set of sources and (or) boundary conditions that follows in datasets 3– 7. May be up to 40 characters long and may include spaces.
NSOP1	Integer	Exact number of nodes at which a fluid source/sink is specified for the current time step.
NSOU1	Integer	Exact number of nodes at which an energy or solute mass source/sink is specified for the current time step.
NPBC1	Integer	Exact number of nodes at which pressure is specified for the current time step.
NUBC1	Integer	Exact number of nodes at which temperature or concentration is specified constant for the current time step.
NPBG1	Integer	Exact number of nodes at which a generalized-flow condition is specified for the current time step.
NUBG1	Integer	Exact number of nodes at which a generalized-transport is specified constant for the current time step.

Note:

The source and boundary condition counts NSOP1, NSOU1, NPBC1, NUBC1, NPBG1, and NUBG1 correspond to **".bcs"** datasets 3, 4, 5, 6, 7A, and 7B, respectively, and must be listed in that order. The counts refer to specifications made on the current time step in the current **".bcs"** file; specifications made on other time steps and (or) in other files are not included in the counts.

Specifications need be included in **".bcs"** files only when they are changing on a given time step. Specifications are persistent – once set, they remain in force unless/until superseded by another specification.

If the controlling schedule includes time steps for which no **".bcs"** specification is desired, one can simply set NSOP1=NSOU1=NPBC1=NUBC1=NPBG1=NUBG1=0 on those time steps.

To assist the user in keeping track of where various boundary conditions are set, SUTRA includes the identifier BCSID with each source or boundary condition listed in the "**.bcof**", "**.bcos**", "**.bcop**", "**.bcou**", "**.bcopg**", and "**.bcoug**" output files.

DATASET 3: Time-Dependent Fluid Sources and Sinks (one line for each of NSOP1 fluid source nodes as specified in "**.bcs**" dataset 2, plus one line)

O M I T when there are no fluid sources/sinks to be specified for the current time step (NSOP1=0 in dataset 2).

Specifications made in this dataset take precedence over those made in ".inp" dataset 17 (and subroutine BCTIME). A specification remains in force unless/until superseded by a corresponding specification on a later time step (or in another ".bcs" file read later on the same time step).

Variable	Type	Description
Lines 1 to NSOP1:		
IQCP1	Integer	Number of node to which source/sink data on this line refers. Specifying the node number with a negative sign renders the fluid-source/sink condition inactive at node IQCP1, which effectively sets the source/sink rate to zero and gives the user the option of suppressing output for the inactive source node by setting CINACT='N' in "**.inp**" dataset 8E. Any node listed in this dataset must also be listed in "**.inp**" dataset 17.
QINC1	Real	Fluid source (or sink) at node IQCP1, Q_{IN}. [M/s]. A positive value is a source of fluid to the aquifer. May be omitted if the source node is inactive (IQCP1<0). Sources are allocated by cell as shown in Figure B.1 for equal-sized elements. For unequal-sized elements, sources are allocated in proportion to the cell length, area or volume over which the source fluid enters the system.

UINC1	Real	Temperature or solute concentration (mass fraction) of fluid entering the aquifer at node IQCP1, U_{IN}. [°C] or [M_s/M]. May be omitted if if the source node is inactive (IQCP1<0) or if QINC1≤0.

Last line:

	Integer	Placed immediately following all NSOP1 fluid source node lines. Line must begin with the integer 0.

Note:

It is not sufficient to specify only the input variable that is changing on the current time step. For example, if QINC1 is changing but UINC1 is not, one must still provide a value for UINC1 as well as QINC1.

DATASET 4: Time-Dependent Energy or Solute Mass Sources and Sinks
(one line for each NSOU1 energy or solute source nodes as specified in "**.bcs**" dataset 2, plus one line)

O M I T when there are no energy or solute sources/sinks to be specified for the current time step (NSOU1=0 in dataset 2).

Specifications made in this dataset take precedence over those made in ".inp" dataset 18 (and subroutine BCTIME). A specification remains in force unless/until superseded by a corresponding specification on a later time step (or in another ".bcs" file read later on the same time step).

Variable	Type	Description
Lines 1 to NSOU1:		
IQCU1	Integer	Number of node to which source/sink data on this line refers. Specifying the node number with a negative sign renders the solute/energy-source/sink condition inactive at node IQCU1, which effectively sets the source/sink rate to zero and gives the user the option of suppressing output for the inactive source node by setting CINACT='N' in "**.inp**" dataset 8E. Any node listed in this dataset must also be listed in "**.inp**" dataset 18.

QUINC1	Real	Source (or sink) of solute or energy at node IQCU1, ψ_{IN}. [E/s] for energy transport, [M_s/s] for solute transport. A positive value is a source to the aquifer. May be omitted if the source node is inactive (IQCU1<0). Sources are allocated by cell as shown in Figure B.1 for equal-sized elements. For unequal-sized elements, sources are allocated in proportion to the cell length, area or volume over which the source energy or solute mass enters the system.
Last line:		
	Integer	Placed immediately following all NSOU1 energy or solute mass source node lines. Line must begin with the integer 0.

DATASET 5: Time-Dependent Specified Pressures (one line for each of NPBC1 specified pressure nodes as indicated in "**.bcs**" dataset 2, plus one line)

O M I T when there are no pressures to be specified for the current time step (NPBC1=0 in dataset 2).

Specifications made in this dataset take precedence over those made in ".inp" dataset 19 (and subroutine BCTIME). A specification remains in force unless/until superseded by a corresponding specification on a later time step (or in another ".bcs" file read later on the same time step).

Variable	Type	Description
Lines 1 to NPBC1:		
IPBC1	Integer	Number of node to which specified pressure data on this line refers. Specifying the node number with a negative sign renders the specified-pressure condition inactive (it is not applied) at node IPBC1, which gives the user the option of suppressing output for the inactive boundary condition by setting CINACT='N' in "**.inp**" dataset 8E. Any node listed in this dataset must also be listed in "**.inp**" dataset 19.
PBC1	Real	Pressure value specified at node IPBC1. [$M/(L \cdot s^2)$]. May be omitted if the boundary condition is inactive (IPBC1<0).
UBC1	Real	Temperature or solute concentration of any external fluid that enters the aquifer at node IPBC1. [°C] or [M_s/M]. May be omitted if the boundary condition is inactive (IPBC1<0).
Last line:		
	Integer	Placed immediately following all NPBC1 specified pressure lines. Line must begin with the integer 0.

Note:

It is not sufficient to specify only the input variable that is changing on the current time step. For example, if PBC1 is changing but UBC1 is not, one must still provide a value for UBC1 as well as PBC1.

DATASET 6: Time-Dependent Specified Concentrations or Temperatures

(one line for each of NUBC1 specified concentration or temperature nodes indicated in "**.bcs**" dataset 2, plus one line)

O M I T when there are no concentrations or temperatures to be specified for the current time step (NUBC1=0 in dataset 2).

Specifications made in this dataset take precedence over those made in ".inp" dataset 20 (and subroutine BCTIME). A specification remains in force unless/until superseded by a corresponding specification on a later time step (or in another ".bcs" file read later on the same time step).

Variable	Type	Description
Lines 1 to NUBC1:		
IUBC1	Integer	Number of node to which specified concentration or temperature data on this line refers. Specifying the node number with a negative sign renders the specified-concentration/temperature condition inactive (it is not applied) at node IUBC1, which gives the user the option of suppressing output for the inactive boundary condition by setting CINACT='N' in "**.inp**" dataset 8E. Any node listed in this dataset must also be listed in "**.inp**" dataset 20.
UBC1	Real	Temperature or solute concentration value specified at node IUBC1. [°C] or [M_s/M]. May be omitted if the boundary condition is inactive (IUBC1<0).
Last line:		
	Integer	Placed immediately following all NUBC1 specified temperature or concentration lines. Line must begin with the integer 0.

Example:

Suppose that the specification

#	IQCP	QINC	UINC
	100	0.1	0.

is given for node 100 in dataset 17 (fluid sources and sinks) of the **".inp"** file and that the specification

```
#        IUBC          UBC
           500            0.
```

is given for node 500 in dataset 20 (specified concentrations) of the **".inp"** file. Thus, node 100 is a fluid source/sink node initially set to inject 0.1 [M/s] of fresh water, and node 500 is a specified-concentration node initially set to a concentration of 0. [M_s/M].

The following **".bcs"** file modifies the specifications at nodes 100 and/or 500 according to schedule "STEPS_2&4", which consists of time steps 2 and 4 and is assumed to have been defined in **".inp"** dataset 6:

```
#  Schedule name
'STEPS_2&4'
#
#  TIME STEP 2
#  Dataset 2: identifier and counts
#       BCSID        NSOP1        NSOU1        NPBC1          NUBC1
          'ts02'             1              0              0          1
#  Dataset 3: fluid sources/sinks
#       IQCP1        QINC1          UINC1
            100          -0.3
              0
#  Dataset 6: specified concentrations
#       IUBC1          UBC1
            500          0.02
              0
#
#  TIME STEP 4
#  Dataset 2: identifier and counts
#       BCSID        NSOP1        NSOU1        NPBC1          NUBC1
          'ts04'             0              0              0          1
#  Dataset 6: specified concentrations
#       IUBC1          UBC1
           -500
              0
```

Note that specifications are given for each of the two time steps in the controlling schedule. At a minimum, ".bcs" dataset 2 must be provided for each time step in the controlling schedule. If there are no specifications to be made for a given time step in the controlling schedule, one should set NSOP1=NSOU1=NPBC1=NUBC1=0 for that time step.

If flow and transport are transient and there are no other specifications for nodes 100 and 500 other than those described above, then those two nodes will exhibit the following time dependence over the first five time steps of the simulation:

Time step	Node 100 (fluid source/sink)		Node 500 (specified concentration)
	QINC	UINC	UBC
1	0.1	0.	0.
2	-0.3	n/a	0.02
3	-0.3	n/a	0.02
4	-0.3	n/a	inactive
5	-0.3	n/a	inactive

By virtue of the specification in **".inp"** dataset 17, node 100 starts out as a fluid source of 0.1 [M/s]. The **".bcs"** specification on time step 2 (dataset 3) then changes node 100 to a fluid sink of 0.3 [M/s], which it remains thereafter. (UINC is not applicable when the node is a fluid sink because fluid leaves the model at whatever concentration is computed at node 100).

By virtue of the specification in **".inp"** dataset 20, node 500 starts out at a specified concentration of 0. [M_s/M]. The **".bcs"** specification on time step 2 (dataset 6) then changes the specified concentration to 0.02 [M_s/M], where it remains until the specification is rendered inactive through the use of a negative node number on time step 4.

DATASET 7A: Time-Dependent Generalized Flows (one line for each of NPBG1 generalized-flow nodes as indicated in "**.bcs**" dataset 2, plus one line)

O M I T when there are no generalized flows to be specified for the current time step (NPBG1 = 0 in dataset 2).

Specifications made in this dataset take precedence over those made in ".inp" dataset 21A (and subroutine BCTIME). A specification remains in force unless/until superseded by a corresponding specification on a later time step (or in another ".bcs" file read later on the same time step).

Variable	Type	Description
Lines 1 to NPBG1:		
IPBG1	Integer	Number of node to which generalized-flow data on this line refers. Specifying the node number with a negative sign renders the generalized-flow condition inactive (it is not applied) at node IPBG1, which gives the user the option of suppressing output for the inactive boundary condition by setting CINACT = 'N' in "**.inp**" dataset 8E.

PBG11	Real	Pressure value at the first of two points that define the linear relation between fluid inflow/outflow and pressure at node IPBG1. [M/(L·s^2)]. May be omitted if the boundary condition is inactive (IPBG1 < 0).
QPBG11	Real	Rate of inflow/outflow of fluid mass when the computed pressure equals PBG11 at node IPBG1. [M/s]. May be omitted if the boundary condition is inactive (IPBG1 < 0).
PBG21	Real	Pressure value at the second of two points that define the linear relation between fluid inflow/outflow and pressure at node IPBG1. [M/(L·s^2)]. May be omitted if the boundary condition is inactive (IPBG1 < 0).
QPBG21	Real	Rate of inflow/outflow of fluid mass when the computed pressure equals PBG21 at node IPBG1. [M/s]. May be omitted if the boundary condition is inactive (IPBG1 < 0).
CPQL11	Character	Determines whether a limit is set on fluid inflow/outflow, pressure, or neither at the first of two points that define the linear relation between fluid inflow/outflow and pressure at node IPBG1. [M/(L·s^2)]. Valid values are as follows: 'Q' = set limit of Q ≤ QPBG11 'P' = set limit of p ≥ PBG11 'N' = set no limit at point 1 May be omitted if the boundary condition is inactive (IPBG1 < 0).
CPQL21	Character	Determines whether a limit is set on fluid inflow/outflow, pressure, or neither at the second of two points that define the linear relation between fluid inflow/outflow and pressure at node IPBG1. [M/(L·s^2)]. Valid values are as follows: 'Q' = set limit of Q ≥ QPBG21 'P' = set limit of p ≤ PBG21 'N' = set no limit at point 2 May be omitted if the boundary condition is inactive (IPBG1 < 0).
UPBGI1	Real	Temperature or solute concentration of any external fluid that enters the model at node IPBG1. UPBGI1 is a specified constant value. [°C] or [M_s/M].

		May be omitted if the boundary condition is inactive (IPBG1 < 0).
CUPBGO1	Character	One word. Must be either 'DIR' or 'REL'. Indicates whether the temperature or solute concentration, UPBGO1, of any fluid that exits the model at node IPBG1 is being specified directly ('DIR') or relative to the computed concentration or temperature at the node ('REL'). May be omitted if the boundary condition is inactive (IPBG1 < 0).
UPBGO1	Real	Temperature or solute concentration of any fluid that exits the model at node IPBG1. If CUPBGO1 = 'DIR', the exit temperature or concentration is set directly to the value UPBGO1. If CUPBGO1 = 'REL', the exit temperature or concentration is set to the value U+UBPGO1, where U is the temperature or concentration computed at the node. [°C] or [M_s/M]. May be omitted if the boundary condition is inactive (IPBG1 < 0).

Last line:

	Integer	Placed immediately following all NPBG1 specified pressure lines. Line must begin with the integer 0.

Note:
It is not sufficient to specify only the input variable that is changing on the current time step. For example, if PBG11 is changing but the other input variables (for example, QPBG11) are not, one must still provide a value for each input variable.

DATASET 7B: Time-Dependent Generalized Transport

(one line for each of NUBG1 generalized-transport nodes indicated in "**.bcs**" dataset 2, plus one line)

O M I T when there are no generalized-transport nodes to be specified for the current time step (NUBG1 = 0 in dataset 2).

Specifications made in this dataset take precedence over those made in ".inp" dataset 21B (and subroutine BCTIME). A specification remains in force unless/until superseded by a corresponding specification on a later time step (or in another ".bcs" file read later on the same time step).

Variable	Type	Description

Lines 1 to NUBG1:

IUBG1	Integer	Number of node to which generalized-transport data on this line refers. Specifying the node number with a *negative sign* renders the generalized-transport condition *inactive* (it is not applied) at node IUBG1, which gives the user the option of suppressing output for the inactive boundary condition by setting CINACT = 'N' in "**.inp**" dataset 8E. Any node listed in this dataset must also be listed in "**.inp**" dataset 21B.
UBG11	Real	Concentration or temperature value at the first of two points that define the linear relation between solute mass or energy inflow/outflow and concentration or temperature at node IUBG1. [M_s/M or C°]. May be omitted if the boundary condition is inactive (IUBG1 < 0).
QUBG11	Real	Rate of inflow/outflow of solute mass or energy when the computed concentration or temperature equals UBG11 at node IUBG1. [M_s/s or E/s]. May be omitted if the boundary condition is inactive (IUBG1 < 0).
UBG21	Real	Concentration or temperature value at the second of two points that define the linear relation between solute mass or energy inflow/outflow and concentration or temperature at node IUBG1. [M_s/M or C°]. May be omitted if the boundary condition is inactive (IUBG1 < 0).
QUBG21	Real	Rate of inflow/outflow of solute mass or energy when the computed concentration or temperature equals UBG21 at node IUBG1. [M_s/s or E/s]. May be omitted if the boundary condition is inactive (IUBG1 < 0).
Last line:		
	Integer	Placed immediately following all NUBG1 specified temperature or concentration lines. Line must begin with the integer 0.

Note:
It is not sufficient to specify only the input variable that is changing on the current time step. For example, if UBG11 is changing but the other input variables (for example, QUBG11) are not, one must still provide a value for each input variable.

Input Data for the Main Input File for the Lake Capability (**.lkin**)

Model Version: ***SUTRA 4.0***

The .lkin input file is optional in general but is required for the lake capability. If this input file is omitted, the lake capability is not used.

DATASET 1: Lake Output Control (one line)

Variable	Type	Description
NLAKPR	Integer	Output cycle for lake information during a transient simulation. Output is produced in the lake output files on time steps numbered n │ NLAKPR │ (where n is a positive integer). Also, for transient solutions, output is produced for initial conditions and on the first and last time steps. To cancel printed output for the first time step of a transient simulation, set NLAKPR to a negative number (that is, place a minus sign before the desired output cycle). For steady-state solutions, output is produced irrespective of the value of NLAKPR.

DATASET 2: Number of lake specifications and default values (one line)

Variable	Type	Description
NLSPEC	Integer	Number of lake specifications. Set NLSPEC = 0 if there are no lake specifications.
FRROD	Real	Default value of the fraction of groundwater recharge diverted as runoff from generalized-flow nodes. (See section 3.2.3.4, “Runoff to Lakes,” of the SUTRA version 3.0 documentation (Provost and Voss, 2019.)) This default value is applied to the basins of all lakes not identified in the lake specifications in DATASET 3 below.
FDROD	Real	Default value of the fraction of groundwater discharge diverted as runoff from generalized-flow nodes. (See section 3.2.3.4, “Runoff to Lakes,” of the SUTRA version 3.0 documentation (Provost and Voss, 2019).) This default

		value is applied to the basins of all lakes not identified in the lake specifications in DATASET 3 below.
RNOLK	Real	Value output (in place of lake stage) to the "**.lkst**" output file at nodes not submerged by lake water. May be set to any real value.

DATASET 3: Lake specifications (one line for each of NLSPEC optional lake specifications)

Variable	Type	Description
CTYPE	Character	One word. Must be either 'LAKE' or 'NODE'.
ILON	Integer	Number of the lake or node to which the specification applies. If CTYPE = 'LAKE', ILON is the number of the lake to which the specification applies. If CTYPE = 'NODE', ILON is the number of a node within the basin of the lake to which the specification applies. Node ILON must be on the top surface of the model.
STGI	Real	Initial stage in the lake to which the specification applies. If STGI is below the lowest point in the lake bathymetry, the lake is initially dry. SUTRA resolves any conflicting initial stage specifications in favor of the highest stage specified.
UWI	Real	Initial lake-water concentration or temperature in the lake to which the specification applies. [Ms/M or C°]
FRRO	Real	Value of the fraction of groundwater recharge diverted as runoff from generalized-flow nodes within the basin of the lake to which the specification applies. (See section 3.2.3.4, "Runoff to Lakes," of the SUTRA version 3.0 documentation (Provost and Voss, 2019).)
FDRO	Real	Value of the fraction of groundwater discharge diverted as runoff from generalized-flow nodes within the basin of the lake to which the specification applies. (See section 3.2.3.4, "Runoff to Lakes," of the SUTRA version 3.0 documentation (Provost and Voss, 2019).)

Note:
Lakes are identified and numbered automatically by SUTRA. Therefore, the user generally will not know the lake numbering scheme until a preliminary run is performed. Once the lake numbering is known, CTYPE = 'LAKE' can be used to allow lake specifications to be made conveniently using lake numbers. Until then, the user has the

option to make specifications using node numbers by setting CTYPE = ‘NODE’. Setting the desired specifications can involve trial and error, especially for complex lake systems.

Input Data for the Boundary-Condition Interaction Input File for the Lake Capability (**.lkbc**)

Model Version: ***SUTRA 4.0***

DATASET 1: Boundary-condition interaction specification counts (one line)

Variable	Type	Description
NBCIF	Integer	Number of interaction specifications for fluid sources/sinks.
NBCIS	Integer	Number of interaction specifications for sources/sinks of solute mass or energy.
NBCIP	Integer	Number of interaction specifications for specified pressures.
NBCIU	Integer	Number of interaction specifications for specified concentrations or temperatures.
NBCIPG	Integer	Number of interaction specifications for generalized-flow conditions.
NBCIUG	Integer	Number of interaction specifications for generalized-transport conditions.

DATASET 2: Boundary-condition interaction specifications for fluid sources/sinks (one line for each of NBCIF nodes)

Variable	Type	Description
BCSFNM	Character	On the first line, set BCSFNM = 'DEFAULT'. SUTRA applies DEFAULT specifications to all fluid-source/sink nodes that can form lakes but are not identified as fluid sources/sinks in the optional list of "**.bcs**" files that follows. On each subsequent line (optional), set BCSFNM to the name of a "**.bcs**" file that contains fluid sources/sinks with which lakes will interact.

ILKF	Integer	Effect that the presence or absence of lake water has on the pplication of fluid sources/sinks identified by BCSFNM. When ILKF = -1, a fluid source/sink is applied to a node only when lake water is absent at that node. When ILKF=0, a fluid source/sink is a applied to a node whether lake water is present or absent at that node. When ILKF=1, a fluid source/sink is applied to a node only when lake water is present at that node.

DATASET 3: Boundary-condition interaction specifications for sources/sinks of solute mass or energy

(one line for each of NBCIS nodes)

Variable	Type	Description
BCSFNM	Character	On the first line, set BCSFNM = 'DEFAULT'. SUTRA applies DEFAULT specifications to all solute mass or energy-source/sink nodes that can form lakes but are not identified as sources/sinks of solute mass or energy in the optional list of "**.bcs**" files that follows. On each subsequent line (optional), set BCSFNM to the name of a "**.bcs**" file that contains sources/sinks of solute mass or energy with which lakes will interact.
ILKS	Integer	Effect that the presence or absence of lake water has on the application of sources/sinks of solute mass or energy identified by BCSFNM. When ILKS = -1, a source/sink of solute or energy is applied to a node only when lake water is absent at that node. When ILKS = 0, a source/sink of solute or energy is applied to a node whether lake water is present or absent at that node. When ILKS = 1, a source/sink of solute or energy is applied to a node only when lake water is present at that node.

DATASET 4: Boundary-condition interaction specifications for specified pressures

(one line for each of NBCIP nodes)

Variable	Type	Description
BCSFNM	Character	On the first line, set BCSFNM = 'DEFAULT'. SUTRA applies DEFAULT specifications to all specified-pressure nodes that can form lakes but are not identified as

		specified-pressure nodes in the optional list of "**.bcs**" files that follows. On each subsequent line (optional), set BCSFNM to the name of a "**.bcs**" file that contains specified pressures with which lakes will interact.
ILKP	Integer	Effect that the presence or absence of lake water has on the application of specified pressures identified by BCSFNM. When ILKP = -1, a specified pressure is applied to a node only when lake water is absent at that node. When ILKP = 0, a specified pressure is applied to a node whether lake water is present or absent at that node. When ILKP = 1, a specified pressure is applied to a node only when lake water is present at that node.

DATASET 5: Boundary-condition interaction specifications for specified concentrations/temperatures
(one line for each of NBCIU nodes)

Variable	Type	Description
BCSFNM	Character	On the first line, set BCSFNM = 'DEFAULT'. SUTRA applies DEFAULT specifications to all specified-concentration/temperature nodes that can form lakes but are not identified as specified-concentration/temperature nodes in the optional list of "**.bcs**" files that follows. On each subsequent line (optional), set BCSFNM to the name of a "**.bcs**" file that contains specified concentrations/temperatures with which lakes will interact.
ILKU	Integer	Effect that the presence or absence of lake water has on the application of specified concentrations or temperatures identified by BCSFNM. When ILKU = -1, a specified concentration or temperature is applied to a node only when lake water is absent at that node. When ILKU = 0, a specified concentration or temperature is applied to a node whether lake water is present or absent at that node. When ILKU = 1, a specified concentration or temperature is applied to a node only when lake water is present at that node.

DATASET 6A: Boundary-condition interaction specifications for generalized-flow conditions (one line for each of NBCIPG nodes)

Variable	Type	Description
BCSFNM	Character	On the first line, set BCSFNM = 'DEFAULT'. SUTRA applies DEFAULT specifications to all generalized-flow nodes that can form lakes but are not identified as generalized-flow nodes in the optional list of "**.bcs**" files that follows. On each subsequent line (optional), set BCSFNM to the name of a "**.bcs**" file that contains generalized-flow conditions with which lakes will interact.
ILKPG	Integer	Effect that the presence or absence of lake water has on the application of generalized-flow conditions identified by BCSFNM. When ILKPG = -1, a generalized-flow condition is applied to a node only when lake water is absent at that node. When ILKPG = 0, a generalized-flow condition is applied to a node whether lake water is present or absent at that node. When ILKPG = 1, a generalized-flow condition is applied to a node only when lake water is present at that node.
CTIPG	Character	Type of interaction between the generalized-flow condition and lakes. Select one of the following: 'F' = Interaction analogous to that between a fluid source/sink node and a lake 'P' = Interaction analogous to that between a specified-pressure node and a lake (See section 3.2.3.3, "Interaction with Generalized-Flow Conditions," of the SUTRA version 3.0 documentation (Provost and Voss, 2019).)

DATASET 6B: Boundary-condition interaction specifications for generalized-transport conditions (one line for each of NBCIUG nodes)

Variable	Type	Description
BCSFNM	Character	On the first line, set BCSFNM = 'DEFAULT'. SUTRA applies DEFAULT specifications to all generalized-transport nodes that can form lakes but are not identified as generalized-transport nodes in the optional list of "**.bcs**" files that follows. On each subsequent line (optional), set BCSFNM to the name of a "**.bcs**" file that contains generalized-transport conditions with which lakes will interact.
ILKUG	Integer	Effect that the presence or absence of lake water has on the application of generalized-transport conditions identified by BCSFNM. When ILKUG = -1, a generalized-transport condition is applied to a node only when lake water is absent at that node. When ILKUG = 0, a generalized-transport condition is applied to a node whether lake water is present or absent at that node. When ILKUG = 1, a generalized-transport condition is applied to a node only when lake water is present at that node.
CTIUG	Character	Type of interaction between the generalized-flow condition and lakes. Select one of the following: 'S' = Interaction analogous to that between a solute or energy source/sink node and a lake 'U' = Interaction analogous to that between a specified-concentration or specified-temperature node and a lake (See section 3.2.3.7, "Interaction with Generalized-Transport Conditions," of the SUTRA version 3.0 documentation (Provost and Voss, 2019).)

Input Data for the Lake-Area Input File for the Lake Capability (**.lkar**)

Model Version: ***SUTRA 4.0***

This input file is optional. If the lake capability is used and this input file is omitted, all nodes on the top surface of the model are eligible to form lakes.

DATASET 1A: Number of lake nodes (one line)

Variable	Type	Description
	Character	Line must begin with the word 'LAKE'.
NLAN	Integer	Exact number of nodes on the top surface of the model that are eligible to form lakes.
CBOT	Character	One word. Set to 'DEFAULT' to have SUTRA use the top of the groundwater model to set lake-bottom elevations. Set to 'SPECIFIED' to have lake-bottom elevations be user-specified in dataset 1B.

DATASET 1B: List of lake nodes (one line for each of NNLK nodes, *plus* one line)

Variable	Type	Description
Lines 1 to NNLK:		
IL	Integer	Number of node that is eligible to form lakes. Node IL must be on the top surface of the model.
ELVLB	Real	User-specified lake-bottom elevation at node IL. May be omitted if lake-bottom elevations are set by default (CBOT = 'DEFAULT').
Last line:		
	Integer	Placed immediately following all NLAN lake-node lines. Line must begin with the integer 0.

List of Input Data for the Initial Conditions File (**.ics**)

Model Version: ***SUTRA 4.0***

The data in the "**.ics**" file need be created by the user only for the very first time step of a given simulation or series of restarted simulations. Thereafter, if the user has chosen to optionally store the final results of the simulation in a "**.rst**" file, this "**.rst**" file may be used directly as the "**.ics**" file for later restarts. The restart options are controlled by CREAD and ISTORE in dataset 4 of the "**.inp**" file.

DATASET 1: Simulation Starting Time (one line)

Variable	Type	Description
TICS	Real	Time (in seconds) to which the initial conditions specified in the "**.ics**" file correspond. [s]. TICS can be used as the starting time of the simulation by defining schedule "TIME_STEPS" in terms of ELAPSED times – see description of dataset 6 in the main input ("**.inp**") file. Usually set to a value of zero for a "cold start".

Example:

If the initial conditions correpsond to time 1990 years on the simulation clock, set TICS=(1990 yrs)(3.15576x10^7 s/yr)= 6.2799624x10^{10} s as follows:

```
6.2799624d+10
```

See the description of "**.inp**" dataset 6 for conversion factors between various time units.

DATASET 2: Initial Pressure Values at Nodes (two lines; second line can be broken up over multiple lines)

Variable	Type	Description
Line 1:		
CPUNI	Character	One word. Set to 'UNIFORM' to specify a uniform pressure for all nodes. Set to 'NONUNIFORM' to specify a separate pressure for each node.
Line 2:		
PVEC	Real	For UNIFORM pressure specification, a single value of initial (starting) pressure to be applied at all NN nodes at the start of the simulation. [$M/(L \cdot s^2)$] For NONUNIFORM pressure specification, a list of values of initial (starting) pressures at the start of the simulation, one value for each of NN nodes, in exact order of node numbers. [$M/(L \cdot s^2)$]. List can be broken up over multiple lines, and any number of values may be placed on each line (as long as no line contains more than 1000 characters). If the STEADY (steady-state) flow option in dataset 4 of the "**.inp**" file has been chosen, PVEC serves as an initial guess for the pressure solution when an ITERATIVE solver is used, and is ignored when the DIRECT solver is used. Initial hydrostatic or natural pressures in a cross-sectional or 3D model may be obtained by running a single steady-flow time step with the store option. Then the natural pressures are calculated and stored in the "**.rst**" file, and may be copied to the corresponding section of the "cold start" "**.ics**" file without change in format, to be used as initial conditions for a transient run.

DATASET 3: Initial Temperature or Concentration Values at Nodes (two lines; second line can be broken up over multiple lines)

Variable	Type	Description
Line 1:		
CUUNI	Character	One word. Set to 'UNIFORM' to specify a uniform temperature to solute concentration for all nodes. Set to 'NONUNIFORM' to specify a separate value for each node.
Line 2:		
UVEC	Real	For UNIFORM temperature or solute concentration specification, a single initial (starting) value to be applied at all NN nodes at the start of the simulation. [°C] or [M_S/M] For NONUNIFORM temperature or solute concentration specification, a list of initial (starting) values at the start of the simulation, one value for each of NN nodes, in exact order of node numbers. [°C] or [M_S/M]. List can be broken up over multiple lines, and any number of values may be placed on each line (as long as no line contains more than 1000 characters).

End of Input Data List

References

Version 2.2 (main SUTRA documentation):
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:
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.

Version 4.0:
Voss, C.I., Provost, A.M., McKenzie, J.M. and Kurylyk, B.L., 2024, SUTRA—A code for simulation of saturated-unsaturated, variable-density groundwater flow with solute or energy transport—Documentation of the version 4.0 enhancements—freeze-thaw capability, saturation and relative-permeability relations, spatially varying properties, and enhanced budget and velocity outputs: U.S. Geological Survey Techniques and Methods, book 6, chap. A63, 91 p., https://doi.org/10.3133/tm6A63.