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Requirements for

STOMP

Subsurface Transport Over Multiple Phases

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1.0 Introduction

This document serves as a requirement specification document for the subsurface simulator, STOMP (Subsurface Transport Over Multiple Phases). Although broadly termed a Requirements Document, this document only outlines user input requirements, since requirements on the subsurface flow and transport theory, and the mathematical representations of those theories, are specified in the STOMP Theory Guide and Addendums (e.g., White and Oostrom 2000; Ward et al. 2005; White and McGrail 2006). Hence, this document does not list the most important features and functional capabilities of the STOMP software, nor does it address objectives of any planned software upgrades. This document only addresses requirements as outlined in the STOMP User Guide (White and Oostrom 2006), with the primary purpose of guiding software testing.

As new capabilities and functionality are added to the STOMP software, those requirements will be added to this document for 1) guiding software development and 2) testing against the new requirements. Requirements for new capabilities will be identified in the Software Change Request (SCR) forms. These new requirements will be incorporated into this document and/or the STOMP theory documents (e.g., White and Oostrom 2000; Ward et al. 2005; White and McGrail 2006) once funding has been identified. This documentation will be maintained in Microsoft Word with manual versioning control and maintained by the CC. As new documentation is developed, all older versions of documents will be maintained electronically, as archival material. To create a new version, the latest version will be copied; all changes accepted using the “Track Changes” features of Word, and the version number incremented in the title page and the file name. Change tracking will be used to record changes since the last version. The older version will be moved into an archive subdirectory.

2.0 Operational Modes and General Requirements

2.1 STOMP Operational Modes

The STOMP simulator is designed with a variable source code, where source code configurations are referred to as operational modes. Operational modes are classified according to the solved governing flow and transport equations, constitutive relation extensions, and implementation type. The modes that allow for a scalable implementation contained the extension 'Sc' (e.g., STOMP-W-Sc). The names of the STOMP modes containing the ECKEChem modules have the extension 'R' attached (e.g., STOMP-W-R, STOMP-WCS-R-Sc). The extension '-B', as used in the STOMP-WAE-B mode, indicates that the evapotranspiration model is implemented as a boundary condition in the upper surface of the computational domain. The required operational modes with options in STOMP are summarized in Table 2.1.

2.2 STOMP Input File

The STOMP simulator is controlled through a text file, which must be titled *input* for proper execution. This input file has a structured format composed of cards, which contain associated groups of input data. Depending on the operational mode, input cards may be required and optional. The *input* file requirements are:

- Required cards must be present in an *input* file
- Optional cards may be required to execute a particular problem
- An error message will be generated and the code execution will stop if an attempt is made to execute the simulator on an *input* file with an incomplete set of required cards.
- Cards may appear in any order within the *input* file
- The input data are case insensitive
- Each card begins with a header, which must contain a tilde symbol in the first column followed by the card name
- Blank lines or additional comment lines may be included in the input file outside of the card structures
- Data are delimited by commas and a commas at the end of a card line is required
- The total length a single input line cannot exceed 132 characters
- Characters string data are limited to 64 characters unless otherwise noted
- Many input variables contain default values, which can be accessed by using null entry (no characters or only blank spaces between two the closing commas)
- User can declare units for both input and output data
- Unspecified units will be assumed to be in standard Systeme International (SI) units for the data item
- A unit character string comprises a combination of the recognized units delimited by spaces and/or a single divisor symbol (i.e., /). Only one divisor may appear in a unit character string. Space should not be used to separate the units immediately prior to or following the divisor symbol.

Table 2.1. STOMP Operational Mode Summary, where the abbreviations are represented by: W = Water, R = Reactions, A = Air, E = Energy, O = Oil, S = Salt, C = CO_2, M = Methane and Sc = Scalable.

NO.	Operational Mode Name	Operational Mode Identifier	Operational Mode Code
1	**STOMP-W**	**Water**	**1**
2	**STOMP-W-Sc**	**Water Scalable**	**1**
3	**STOMP-W-R**	**Water- Reactions**	**1**
4	**STOMP-WA**	**Water-Air**	**2**
5	STOMP-WA-R[(a)]	Water-Air-Reactions	2
6	**STOMP-WAE**	**Water-Air-Energy**	**3**
7	STOMP-WAE-Sc[(a)]	Water-Air-Energy Scalable	3
8	**STOMP-WAE-B**	**Water-Air-Energy-Barrier**	**3**
9	**STOMP-WO**	**Water-Oil**	**4**
10	STOMP-WO-R[(a)]	Water-Oil-Reactions	4
11	**STOMP-WOA**	**Water-Oil-Air**	**5**
12	**STOMP-WOA-Sc**	**Water-Oil-Air Scalable**	**5**
13	STOMP-WOA-R[(a)]	Water-Oil-Air-Reactions	5
14	STOMP-WOAE[(b)]	Water-Oil-Air-Energy	6
15	STOMP-WOD[(b)]	Water-Oil-Dissolved Oil	8
16	STOMP-WOM[(b)]	Water-Multicomponent Oil	4
17	STOMP-WS[(b)]	Water-Salt	11
18	STOMP-WS-Sc[(b)]	Water-Salt Scalable	11
19	STOMP-WAS[(b)]	Water-Air-Salt	12
20	STOMP-WAS-Sc[(b)]	Water-Air-Salt Scalable	12
21	STOMP-WASE[(b)]	Water-Air-Salt-Energy	13
22	STOMP-WCS[(b)]	Water-CO_2-Salt	32
23	STOMP-WCS-Sc[(b)]	Water-CO_2-Salt Scalable	32
24	STOMP-WCS-R[(b)]	Water-CO_2-Salt-Reactions	32
25	STOMP-WCS-R-Sc[(b)]	Water-CO_2-Salt-Reactions	32
26	STOMP-WCSE[(b)]	Water-CO_2-Salt-Energy	33
27	STOMP-WCMSE[(b)]	Water-CO_2-CH_4-Salt-Energy	36
28	STOMP-WCASE[(a)]	Water-CO_2-Air-Salt-Energy	–

[(a)] Mode was under development when this document was written

[(b)] Funding had not yet been identified for documented testing when this document was written

In the following sections, the requirements for each STOMP input card will be described. The cards are divided into four groups:

1. Common cards for all modes: generally, the requirement for these cards are similar for all operation modes with very few exceptions
2. Other Cards needed by STOMP-W and STOMP-W-Sc: some of these cards are needed by all the modes with water flow and the requirements are similar; others are for water mode only.
3. Cards needed by ECKEChem: These cards are needed for the modes with reactive transport only.
4. Other Cards: generally these are mode-specific cards

The four groups of cards are summarized in Table 2.2 and the requirements for them will be discussed in the following four sections.

Table 2.2. Four Groups of STOMP cards

Group 1: Common cards for all modes	**Group 2: Other Cards needed by STOMP-W and STOMP-Sc**	**Group 3: Cards needed by ECKEChem (reactive modes)**	**Group 4: Other Cards**
Simulation Title Card	Saturation Function Card	Aqueous Species Card	Gas Relative Permeability Card
Grid Card	Aqueous Relative Permeability Card	Gas Species Card	NAPL Relative Permeability Card
Rock/Soil Zonation Card	Directional Aqueous Relative Permeability Card	Solid Species Card	Oil Properties Card
Inactive Nodes Card	Solution Control Card	Species Link Card	Dissolved-Oil Transport Card
Mechanical Properties Card	Solute/Fluid Interactions Card	Conservation Equations Card	Well Card
Hydraulic Properties Card	Solute/Porous Media Interactions Card	Equilibrium Equations Card	Salt Transport Card
	Initial Conditions Card	Equilibrium Reactions Card	Thermal Properties Card
	Boundary Conditions Card	Kinetic Equations Card	Atmospheric Conditions Card
	Source Card	Kinetic Reactions Card	Plant Card
	Output Control Card	Lithology Card	
	Surface Flux Card		
	UCODE Control Card		
	Observed Data Card		
	Scaling Factor Card		

3.0 Requirements for Group One - Common Cards for All Modes

These cards are generally independent of the operational mode selected.

3.1.1 Simulation Title Card Requirements

This card provides a means to document a simulation. Information recorded in this card is rewritten on the *output* file. The requirements for this card are the same for all operation modes. This card includes the following lines sequentially:

- Input file version number
- Simulation title
- User name
- Company name
- Creation date
- Creation time
- Number of simulation note lines
- Simulation notes

3.1.2 Grid Card Requirements

The requirements for this card are the same for all operation modes except that, for the modes whose names contain a "-*Sc*", the number of processors need be specified.

The STOMP simulator's finite-difference formulation is based on orthogonal grid systems. Three orthogonal grid systems are recognized:

- Cartesian: the Cartesian coordinate system has longitudinal axis (z-direction) aligned with the negative gravitational vector. Options include Cartesian, Uniform Cartesian, Reference Point Cartesian, and Tilted Cartesian.
- Cylindrical: the cylindrical coordinate system has longitudinal axis (z-direction) aligned with the negative gravitational vector. The radial and azimuthal axes constrained in the horizontal plane. The azimuthal axes are restricted between zero and 360 degrees. Options include Cylindrical, Uniform Cylindrical, and Reference Point Cylindrical.
- Boundary fitted (orthogonal): Boundary fitted (orthogonal) allows for curvilinear boundaries. Options include Generalized, Boundary Fitted Orthogonal Generalized

The grid for both the Cartesian and cylindrical coordinate system can be either uniform or non-uniform. The origin of the coordinate system can be user-defined. The grid information can be contained either in the grid card or in an external file.

3.1.3 Rock/Soil Zonation Card Requirements

The requirements for this card are the same for all operation modes. The options for declaring the distribution of rock/soil types include:

- Explicit declaration: the rock/soil names are associated with portions of the computational domain. Rock/soil names must be unique and must contain no more than 64 characters. Rock/soil names can be repeatedly applied to a grid cells or domain of grid cells, with only the last definition being applied.
- External files: the file format can be either ASCII or binary
- IJK indexing: can be either IJK or JKI or KIJ indexing format

3.1.4 Inactive Nodes Card Requirements

The requirements for this card are the same for all operation modes. This card allows users to declare nodes, within the computational domain, as inactive or non-computational. Inactive nodes are those nodes that will remain permanently excluded from the computational domain.

The options for declaring the distribution of inactive nodes include:

- Explicit declaration
- External files
- IJK indexing

Boundary conditions may be applied to any surface between any active and inactive nodes.

3.1.5 Mechanical Properties Card Requirements

The requirements for this card are the same for all operation modes. This card allows users to assign values to particle density, total porosity, diffusive porosity and specific storativity for each defined rock/soil type. Compressibility and tortuosity function need to be assigned for the simulation involving solute transport or diffusion of components through phases (e.g., water vapor diffusing through the gas phase or dissolved oil diffusing through the aqueous phase). Every rock/soil type defined on the *Rock/Soil Zonation Card* must be referenced.

- Particle density represents the rock grain density. This value will be default to 2650 kg/m^3 by using a *null* entry for both the particle density and its associated units.
- Specific storativity will be the default value by using a *null* entry for both the variable value and its associated units.
- Default specific storativity is computed for from the diffusive porosity and a default value of 1.0×10^{-7} Pa^{-1} for the compressibility
- Tortuosities can be computed either as constants, which require input values, or as functions of the phase saturation and diffusive porosity through the Millington and Quirk function.
- The key words ‘dp’, ‘dual porosity’, or ‘fractured’ in the rock/soil name indicates a dual porosity medium, which triggers the reading of both matrix and fracture properties.

The options for declaring the mechanic properties include:

- Explicit declaration
- External files
- IJK indexing

3.1.6 Hydraulic Properties Card Requirements

The requirements for this card are the same for all operation modes except that, for the simulations salt is involved (e.g., STOMP-WCS and STOMP-WCSE), two additional parameters are required.

This card allows users to assign values to the intrinsic permeability of each defined rock/soil type. Every rock/soil type defined on the Rock/Soil Card must be referenced. Requirements:

- By default, the simulator reads the permeability values on this card as intrinsic permeabilities and the default units of m^2 are applied to null entries for the units associated with permeability vales.
- The simulator reads the saturated hydraulic conductivity values on this card if the character sting '*hc*' is included in the associated units.
- The key words 'dp', 'dual porosity', or 'fractured' in the rock/soil name indicates a dual porosity medium, which triggers the reading of both matrix and fracture properties.
- Reduction in intrinsic permeability with precipitation of salt requires two additional parameters, pore-body fractional length and fractional critical porosity, for the following operational modes: STOMP-WCS, STOMP-WCS-R, STOMP-WCS-R-Sc, STOMP-WCS-Sc, and STOMP-WCSE.

The options for declaring the hydraulic properties include:

- Explicit declaration
- External files
- IJK indexing

4.0 Requirements Group 2 Cards: Other Cards needed by STOMP-W and STOMP-W-Sc

This section describes the additional cards needed by STOMP-W and STOMP-W-Sc.

4.1 Saturation Function Card Requirements

This card allows users to declare and define a saturation-capillary pressure function for each defined rock/soil type. However, saturation function types and the required input items vary greatly among the operational modes (Table 4.1). Operational modes that consider NAPL flow require interfacial tension parameters. The description of these saturation function options are given below.

- For the operational mode that oil transport is involved, fluid pair interfacial tension are required before the saturation function is declared.
- The van Genuchten (VG) and Brook and Corey (BC) functions: These two fundamental saturation functions are available for all but one operation mode (i.e., STOMP-WOAE). For the VG function, the 'm' parameter ban be defaulted (with a *null* entry) or assigned a value. Default values will depend on which relative permeability model (Mualem or Burdine) is chosen on the Aqueous Relative Permeability Card.
- The entrapment VG and entrapment BC functions: These options are available for all but the STOMP-WAE, -WAE-B, and -WAE-B-Sc. Fluid entrapment functions consider the hysteresis between wetting and draining paths due only to entrapment of the non-wetting fluids by imbibing wetting fluids. Fluid entrapment functions allow the specification of initial trapped non-wetting fluid saturations without specifying detailed saturation path histories. These functions additionally allow dissolution of the non-wetting phase into the wetting phase (e.g., dissolution of air and oil into the aqueous phase).
- The extended VG and extended BC functions: These options are available for all the operational modes without oil flow.
- The fractured VG and fractured BC functions: These options are available for all the operational modes without oil flow for the porous media with dual porosity.
- The triple VG and triple BC functions: These options are available for the STOMP-W, -W-Sc, -W-R, and -WASE.
- The residual VG and residual BC functions: These options are available for the operational modes with oil flow but without energy transport.
- The nonhysteretic VG and nonhysteretic BC function: These functions are solely for the STOMP-WOAE operational mode.
- The Haverkamp function: This option is available for all operational modes except those with air-energy transport and those with oil flow.
- Tabular: This option available for all the operational modes without oil flow. There are two interpolation types – linear and spline and two options for the independent variable – water content and saturation.
- The Geel VG, Lenhard VG, Constant VG, Geel BC, Lenhard BC, and Constant BC functions: These options are available for the operational modes with oil flow but without energy transport.

The options for declaring the parameters of saturation properties include:

- Explicit declaration
- IJK indexing: node dependent parameters are entered via external files and node independent parameters are entered directly on the card

4.2 Aqueous Relative Permeability Cards Requirements and Directional Aqueous Relative Permeability Cards Requirements

This card allows the user to declare and define a relative permeability-saturation function for the aqueous phase for each defined rock/soil type. Aqueous relative permeability function types and required input items are dependent on the operational mode (Table 4.2). Required aqueous relative permeability options:

- Mualem: this function is applicable to the van Genuchten and Brooks and Corey Saturation functions. The van Genuchten 'm' parameter or the Brooks and Corey 'λ' parameter can the values entered or defaulted with the saturation function. The tortuosity-connectivity coefficient is defaulted as 0.5.
- Mualem modified: The tortuosity-connectivity coefficient is user-defined.
- Mualem irreducible
- Muale w/ Polmann: the Polmann anisotropy is used
- Burdine: this function is applicable to the van Genuchten and Brooks and Corey Saturation functions. The van Genuchten 'm' parameter or the Brooks and Corey 'λ' parameter can be defaulted to the values entered or defaulted with the saturation function. The tortuosity-connectivity coefficient is defaulted as 2.
- Fatt and Klikoff
- Corey
- Free Corey
- Haverkamp
- Tauma and Vaucline
- Tabular
    - Interpolation type: linear or spline
    - Variable option: water content or saturation
- Constant

The options for declaring the parameters of saturation properties include:

- Explicit declaration
- IJK indexing: node dependent parameters are entered via external files and node independent parameters are entered directly on the card

For rock/soil types with saturation-dependent anisotropy, aqueous relative permeability functions are specified as diagonal tensor, i.e., unique aqueous relative permeability functions are declared for the principal grid-coordinate directions. A maximum of three directional aqueous relative permeability cards, respectively named as X-, Y-, and Z-Aqueous Relative Permeability Card, can be included in an input file. The requirements for these three cards are the same as those for the Aqueous Relative Permeability Card except that the Mualem Polmann option is not allowed.

4.3 Solution Control Card Requirements

This card controls many general operational aspects of a simulation. It first declares the execution mode, which varies among operational modes (Table 4.3a). Execution modes options recognized in all operational modes include

- Normal: The simulator executes using an initial state declared through the Initial Conditions Card. The default Euler time differencing (i.e., first order backward) is used.
- Restart: The simulator executes using an initial state defined by a previous execution
- Normal second order, Restart second order: Second order time differencing is used.
- Initial condition: The simulator reads the input files checking for formatting errors and stops; no time steps are executed.

Other execution modes are dependent on operational modes and include (similar options are placed together and separated by a comma):

- Normal no flow, Restart no flow: These options are for STOMP-W with transport mode only and used for transporting solutes though a steady-state flow field. The flow field is computed once during the initial time step and then remains unaltered.
- Normal dynamic domain, Restart dynamic domain: These options are for STOMP-W only. It conserves computation by temporarily removing nodes from the computational domain where changes in the flow field are insignificant. The active computational domain is updated every time step.
- Normal inverse, Restart inverse: These options will trigger the capability for inverse simulations.
- Normal scaling, Restart scaling
- Normal PETSc, Restart PETSc: the PETSc solver is used.

The line following the execution modes declares the operational mode with options. The identifiers of the operational modes are listed in Table 2.1. Only water flow will be simulated when there are no other options after the operational mode identifier. Other options that follow the operational mode identifier vary among the operational modes and are summarized in Table 4.3b. Operational modes options recognized in all operational modes include

- Transport: Solute transport is solved using the Patankar method
- Leonard-TVD Transport: Solute transport is solved using the TVD method
- Roe's Superbee Transport
- No Aqueous Advection Transport
- No Vapor Pressure Lowering Transport
- Courant: The Courant limit is applied to the transport simulation
- Vadose Courant: The Courant limit is applied to the vadose zone transport simulation only

The following options are dependent on the operational modes:

- No Gas Advection Transport (for operational modes that involve gas transport)
- No NAPL Advection Transport (for the operational modes that involve NAPL transport)
- Electrolyte Transport (for STOMP-W, -W-Sc and -W-R)
- Partitioning Transport, Kinetic Transport (for STOMP-WO, -WO-R, and -WOM)
- LFL Transport, Osmotic Surface Tension Transport, Surface Tension Transport (for operational modes that salt transport is involved)

- Poynting Transport (for operational modes that CO_2 transport is involved)
- EckeChem Transport, Globally EckeChem Transport, Guess EckeChem Transport (for operational modes with reactive transport)
- Dissolution Transport, Dissolved Oil Transport (for STOMP-WOD only)
- Isobrine Transport (for STOMP-WCMSE only)

Simulation periods and options. The simulator allows the user to specify a single or multiple execution periods. For each execution period, the user can control the initial time step, maximum time step, time step acceleration factor, maximum number of Newton-Raphson iterations, and convergence criterion.

For operational modes that two or more fluid flow is involved, the diffusion of the advective fluids and dissolved fluids are required (Table 4.3c). Other special transport-related options (e.g., Clay Mass Fraction, Electrolyte Density Function) are also specified here.

Interfacial averaging schemes can be either defaulted or declared individually for each field variable through the interfacial averaging variables input. The default averaging scheme is either harmonic or upwind. The harmonic averaging scheme is defaulted for viscosity and diffusion, while the upwind averaging scheme is defaulted for density and relative permeability.

4.4 Solute/Fluid Interactions Card Requirements

This card allows the user to define solutes, solute-fluid interactions, and solute radioactive decay paths. This card is required only for simulations involving transport of solutes. The simulator is capable of simulating any number of solutes with the assumption that solute concentrations remain dilute (solute concentrations do not vary the physical properties of the transporting fluid phases). Solutes are defined by a unique solute name, which must contain no more than 64 characters. The transport related options vary among operational modes (Table 4.4). Requirements:

- Solute aqueous effective diffusion options:
    - Constant
    - Conventional
    - Empirical
    - Time-dependent
- Solute-Aqueous partition options:
    - Continuous
    - Noncontinuous
- Gas-Aqueous partition options:
    - Constant
    - Temperature Dependent
- Aqueous-NAPL Adsorption Options include Linear, Freundlich, and Langmuir
- Radioactive decay: Required for all operational modes involving radioactive decay. An addition option is the chain radioactive decay.
- First-order reaction

4.5 Solute/Porous Media Interactions Card Requirements

This card allows the user to define solid-aqueous phase partition coefficients and porous media dependent hydraulic dispersivities. This card is required only for simulations involving transport of solutes.
Requirements for all operational modes:

- For every solute defined on the *Solute/Fluid Interaction Card*, every rock/soil type defined on the *Rock/Soil Zonation Card* must be referenced.
- Longitudinal and transverse hydraulic dispersion are properties only of the rock/soil type. Longitudinal dispersivity is defined with respect to dispersion along the flow path and is assumed to be independent of the flow direction. Likewise, transverse dispersivity is defined with respect to dispersion transverse to the flow path, independent of the flow direction.
- The solid-aqueous partition coefficient is required for each solute and each rock/soil type.
- With IJK Indexing option, node dependent parameters are entered via external files, and node independent parameters are entered directly on the card.

Other mode-dependent requirements (Table 4.5):

- For the operational modes STOMP-W, -W-R, and -W-Sc, the macrodispersivity enhancement factor is optional.
- For the operational modes STOMP-W, -W-R, -W-Sc, and -WS, additional parameters are required if the effective diffusion in the *Solute/Fluid Card* is *Empirical*

4.6 Initial Conditions Card Requirements

This card allows the user to assign starting values to both primary and secondary field variables.
Requirements for all operational modes:

- For *restart* simulations, initial conditions are obtained from the restart file, unless the word "*overwrite*" appears with the initial condition variable name. Not all initial condition variables can be overwritten.
- Initial condition can be declared repeatedly for a node with the last definition being applied
- The initial condition variable assigned to an initial condition domain applies to the node with the lowest x-, y-, and z-direction indices.
- Gradients to the initial conditions allow the user to specify that the initial values of field variables vary along one or more directions in the physical domain. Defaults values for the initial condition gradients are zero, indicating no variation.
- For problems that start with hydrostatic conditions, the pressure at the lowest z-direction node positions would be entered with a Z-Dir. Gradient that is equal to the product of the fluid's density times gravitational acceleration. (-9793.5192 1/m for water at 20℃).
- Solute units are undefined and can be expressed as the user chooses (e.g., Ci, pCi, kg, mol) but must be consistent for a single solute among all input data entries.
- Transport problem simulations with the simulator require the solution of the flow fields.
- Initial conditions for solutes are expressed in terms of solute per unit volume, where the volume can refer to the total node volume (*Volumetric*), the aqueous-phase volume (*Aqueous Volumetric*), the gas-phase volume (*Gas Volumetric*), or the NAPL volume (*NAPL Volumetric*).
- Default variables:
    - Temperature = 20.D+0°C

    - Pressure of any phase = 101325.D+0
    - Saturation of any phase, mole fraction of any component in any phase, and salt concentration in any phase are assigned as double-precision zero.

Mode-dependent requirements:

- The variables that may be initialized depend on the operational mode (Tables 4.6).
- For two-phase aqueous-gas operational modes (e.g., STOMP-WA, -WCS), STOMP allows the user to specify the initial aqueous saturation by assigning initial conditions for any two of the following three variables and the unassigned variable will be computed:
    - gas pressure
    - aqueous pressure
    - aqueous saturation
- For three-phase aqueous-NAPL-gas operational modes (e.g., STOMP-WO, -WOA), initial condition must be declared by specifying initial aqueous, NAPL, and gas pressures. If the initial NAPL pressure is assigned a value below the critical point, which signifies no NAPL, then the initial NAPL pressure is reset within the simulator to the critical pressure. Therefore, conditions without NAPL can be specified by initializing the NAPL pressure to any value below the aqueous pressure.

4.7 Boundary Conditions Card Requirements

This card allows the user to control the simulation by defining time varying boundary conditions. This card is optional, but is generally necessary to simulate a particular problem. Requirements for all operational modes:

- Boundary conditions may be applied to any boundary surface or surface dividing active and inactive nodes. By default, all undeclared boundary surfaces have zero flux boundary conditions for both flow and transport
- To apply a boundary condition to a boundary surface, the surface is referenced by the adjacent active node and a direction with respect to the adjacent node. To apply a boundary condition to a surface dividing an active and inactive node, the surface is referenced by the active node
- The boundary surface direction is specified with respect to the active node adjacent to a boundary surface.
    - For the Cartesian coordinate system, the terms *west, south,* and *bottom* refer to the negative x-, y-, and z-directions; and the terms *east, north,* and *top,* refer to the positive x-, y-, and z-directions, respectively.
    - For the cylindrical coordinate system, the terms *west, south,* and *bottom* refer to the negative r-, θ-, and z-directions; and the terms *east, north,* and *top,* refer to the positive r-, θ-, and z-directions, respectively.
- Files can be used to boundary condition nodes and surfaces. The files contains x, y, z node indices and surface indicator (-3 for bottom, -2 for south, -1 for west, 1 for east, 2 for north, and 3 for top)
- Generally, the number of boundary types that must be declared for each boundary equals the number of solved equations governing flow and transport (e.g., water, gas, NAPL, liquid CO_2,; solute, energy, species, salt, dissolved oil).

- All boundary time inputs are referenced against the *Initial Time* specified in the *Solution Control* card or obtained from a restart file.
- Boundary conditions are time varying. The user is not allowed to assign multiple boundary conditions to a boundary surface during the same time period, multiple boundary conditions can be applied to a boundary surface over different time periods. The simulator controls time steps to agree with time transitions in boundary conditions.
- A boundary condition declared with a single *Boundary Time* implies that the boundary condition is time invariant and the specified boundary time represents the start time for the boundary condition. The specified boundary condition will remain in effect from the start time until the execution is completed. Prior to the start time the boundary surface will be assumed to be of type *Zero Flux*.
- If a boundary condition is declared with multiple boundary times, then the first time listed equals the start time, the last time listed equals the stop time, and the intermediate times are transition points. For simulation times between two boundary times, linear interpolation of the boundary conditions is applied. For simulation times outside of the start and stop time limits, *Zero Flux* boundary conditions apply.
- Step boundary condition changes can be simulated by defining duplicate boundary times. The first time would indicate the completion of the previous boundary condition and the second time could indicate the start of the new boundary condition.
- Boundary condition types required for all fluids (i.e., water, gas, NAPL, energy, liquid CO_2):
    - Dirichlet
    - Neumann
    - Zero flux
    - Initial conditions
- Boundary condition types required for all the components (i.e., solute, species, salt, dissolved oil):
    - Zero flux
    - Initial conditions
    - Outflow
    - Aqueous Concentration

Mode-dependent Requirements:

- Other boundary condition types for different types of fluid and components:
    - Aqueous phase boundary condition types (Table 4.7a)
    - Solute transport boundary condition types (Table 4.7b)
    - Gas phase boundary condition types (Table 4.7c)
    - Energy boundary condition types (Table 4.7d)
    - NAPL phase boundary condition types (Table 4.7e)
    - Dissolved oil boundary condition types (Table 4.7f)
    - Salt transport boundary condition types (Table 4.7g)
    - Species boundary condition types (Table 4.7h)
    - Liquid CO_2 boundary condition types (Table 4.7i)

Options for declaring boundary indices and/or boundary condition values:

- Explicit declaration
- External files

4.8 Source Card Requirements

This card allows the user to control sources and/or sinks of mass, energy, and solutes. Requirements for all operational modes:

- By definition, sinks are negative sources, and sources refer to an influx of mass, energy, or solute into a node.
- Sources can be specified for interior or boundary nodes and are functionally analogous to Neumann type boundary conditions. Sources applied to inactive nodes are not recognized.
- Sources are time varying and STOMP control time steps to agree with time transitions in sources.
- Multiple sources may be applied to a node

Inputs Option Requirements (Tables 4.8)

4.9 Output Control Card Requirements

This file allows the user to control output written to the output file, plot file, and screen (i.e., standard input/out device). Requirements for all operational modes:

- The output file contains an interpreted and reformatted version of the input file and simulation results for selected variables at selected reference nodes over the simulation period
- The output to the screen comprises the reference node variable results versus simulation time and/or time step
- The plot.n (where n is an integer to denote simulation time step number) file contains values of geometric parameters and selected variables for the entire computational domain (both active and inactive nodes) at selected simulation times. A plot.n file will always be generated at the conclusion of an execution.
- A restart.n file is generated with every plot.n file.
- Reference node output is generated by selecting reference nodes and output variables. The user may request any number of reference nodes. Reference nodes are defined with three indices, which indicate the x-, y-, and z-direction coordinates of the node.
- Reference node screen output frequency and reference node output file frequency are parameters that indicate how often, with respect to time step reference node, output will be written to STDIO and the output file, respectively.
- The user has control over the output time and length units and the number of significant digits reported to the various output media. Unless declared through the output time units or output length units input items, values for time and lengths recorded to the output media will be expressed in units of seconds and meters, respectively.
- Output units for all variables can be specified immediately following the variable name. Variable without units require a null entry for the variable units. Null entries for variables with units yield default output units, which are expressed in SI units.
- Common output variables for all operational modes (Table 4.9a):
    - apparent aqueous saturation
    - aqueous courant [number]

- aqueous density
- aqueous gauge pressure
- aqueous hydraulic head
- aqueous pressure
- aqueous relative perm[eability]
- diffusive porosity
- effective trapped gas saturation
- integrated water mass
- phase condition
- rock/soil type
- solute aqueous conc[entration]
- solute source[integral]
- solute volumetric conc[entration]
- temperature
- water mass source int[egral]
- water mass source rate
- x aqueous vol[umetric flux]
- x solute flux
- xnc aqueous vol[umetric flux (node centered)]
- y aqueous vol[umetric flux]
- y solute flux
- ync aqueous vol[umetric flux (node centered)]
- z aqueous vol[umetric flux]
- znc aqueous vol[umetric flux (node centered)]
- z solute flux

Mode-dependent requirements:

- Additional output variable options related to the aqueous phase (Table 4.9b)
- Additional output variable options related to solute/species transport (Table 4.9c)
- Additional output variable options related to the gas phase and/or air transport (Table 4.9d)
- Common Output Variable Options Related to the NAPL Phase/Transport (Table 4.9e)
- Additional output variable options related to the NAPL phase/transport (Table 4.9f)
- Additional output variable options related to salt transport (Table 4.9g)
- Additional output variable options related to energy transport (Table 4.9h)
- Output variable options Related to CO2 transport (Table 4.9i)
- Output variable options only for STOMP-WCMSE (Table 4.9j)
- Output variable options related only for STOMP-WAE-B (Table 4.9k)

4.10 Surface Flux Card Requirements

This card allows the user to define surfaces to track fluxes of fluid mass, fluid volume, heat, and/or solutes. Requirements for all operational modes:

- A surface is composed of rectangular areas of coplanar surfaces on exterior boundaries or between interior nodes

- Output contains flux rate and integral data for each defined surface at every time step. One surface flux rate and integral value is computed for each computed surface and represents the summation of surface flux contributions from the individual surfaces in the coplanar group of surfaces
- Surfaces are defined by referencing a group of coplanar nodes and a surface direction with respect to the nodes For the Cartesian coordinate system, the terms *west, south,* and *bottom* refer to the negative x-, y-, and z-directions; and the terms *east, north,* and *top,* refer to the positive x-, y-, and z-directions, respectively.
- For the cylindrical coordinate system, the terms *west, south,* and *bottom* refer to the negative r-, θ-, and z-directions; and the terms *east, north,* and *top,* refer to the positive r-, θ-, and z-directions, respectively.
- Common output variables
    - Aqueous volumetric
    - Aqueous mass
    - Solute

Mode-dependent output requirement: variables that are dependent on operational mode are listed in Table 4.10

4.11 UCODE Control Card Requirements

This card allows users to specify the control information in a UCODE universal file. This card is an option only for operation modes STOMP-W and STOMP-WAE. Parameters and options read from this card are written to an external file *out_uc.uni* that are then read and used by UCODE.

4.12 Observed Data Card Requirements

This card allows the user to define observed data parameters and observation data. This card is an option only for operation modes STOMP-W and STOMP-WAE. Data type options:

- Field, reference: variables include aqueous pressure, aqueous hydraulic head, matric potential, aqueous saturation, aqueous moisture content, solute aqueous concentration, solute volumetric concentration, solute aqueous mole fraction
- Surface flux: variables include aqueous volumetric flux, aqueous mass flux, solute flux
- Surface rate
- Surface integral: variables include aqueous volumetric flux integral, aqueous mass flux integral, solute flux integral
- Options for inputting data:
    - Explicit declaration
    - External files
    - IJK indexing

4.13 Scaling Factor Card Requirements

This card declares the scaling factors for a group of soils. Requirements:

- Only the hydraulic parameters for the scaling group (not the individual rock/soil types) need to be declared
- Scaling functions are either linear or logarithmic

5.0 STOMP Reactive Modes Requirements

The cards in this section are options for the operational mode with reactive transport by including the module ECKEChem.

5.1 Aqueous Species Card Requirements

This card defines the aqueous species to be considered in the simulation. Required inputs:

- species name
- aqueous molecular diffusion coefficient
- activity coefficient option: Davies, B-Dot, Pitzer, constant
- for non-constant activity coefficient options, addition required inputs: species charge, species diameter, species molecular weight

5.2 Gas Species Card Requirements

This card defines the gas species to be considered in the simulation. Requirements:

- Required inputs:
    - species name
    - gas molecular diffusion coefficient
    - associate aqueous species name
    - gas-aqueous partitioning parameter
- The species name must be unique and distinct from aqueous and solid species names
- All gas species must be associated with an aqueous species, with which it is in equilibrium
- Equilibrium partitioning between the gas and aqueous species is specified via a temperature-dependent function.

5.3 Solid Species Card Requirements

This card defines the solid species to be considered in the simulation. Requirements:

- Required inputs
    - species name
    - species mass density
    - species molecular weight
- Species name must be unique and distinct from aqueous and gas species names

5.4 Species Link Card Requirements

This card associates reactive species with components in the coupled flow and transport equations and defines which species name defines the system pH. Requirements

- components that can be associated
    - aqueous water

    - gas water
    - aqueous air
    - gas air
    - aqueous CO_2
    - gas CO_2
    - aqueous CH_4
    - gas CH_4
    - aqueous salt
    - solid salt
- Required inputs
    - number of species links
    - species names
    - linked components

5.5 Conservation Equations Card Requirements

This card specifies the conservation equations to be considered in the simulation. Requirements:

- Required equation form: $d\sum(a_i C_i)/dt = 0$, where C_i is the aqueous molar concentration of species i, a_i is the stoichiometric coefficient of species i.
- Required inputs:
    - component species name. The component species name must begin with 'Total_' followed by the species name of a reactive species in the conservation equation
    - number of species in the conservation equation
    - species names
    - species stoichiometric coefficients

5.6 Equilibrium Equations Card Requirements

This card specifies the equilibrium equations to be considered in the simulation. Requirements:

- Required equation form: $(C_i) = K_{eq}\prod_{j\neq i}(C_j)^{e_j}$, where K_{eq} is the equilibrium reaction constant specified via the Equilibrium Reactions Card, (C_i) is the activity of the equilibrium species i, e_j is species exponents, which can be positive or negative.
- Required inputs
    - number of species in the equilibrium equation
    - species names
    - equilibrium reaction name
    - species exponents
- The equilibrium species (indicated with the subscript i) is distinguished from the other species in the equilibrium equation (indicated with the subscript j) by being the first species listed for the equilibrium equation

5.7 Kinetic Equations Card Requirements

This card specifies the kinetic equations to be considered in the simulation. Requirements:

- Required equation form: $d\sum(b_i C_i)/dt = \sum(c_j R_j)$, where C_i is the aqueous molar concentration of species i, b_i is the stoichiometric coefficient of species i, R_j is the kinetic reaction rate, and c_j is the kinetic reaction rate coefficient.
- Required inputs:
    - number of species in the kinetic equation
    - species names
    - species stoichiometric coefficients
    - number of kinetic reaction rates
    - kinetic reaction names
    - kinetic reaction rate coefficients

5.8 Equilibrium Reactions Card Requirements

This card specifies the equilibrium reaction constants to be considered in the simulation. Requirements:

- Species are associated with the defined equilibrium reaction constants via the *Equilibrium Equation Card*.
- Required inputs
    - equilibrium reaction name
    - equation coefficients for the temperature dependent equilibrium constant
- The equilibrium reaction name must be unique and distinct from kinetic reaction names

5.9 Kinetic Reactions Card Requirements

This card specifies the kinetic reactions to be considered in the simulation. Requirements:

- Required inputs
    - kinetic reaction name
    - kinetic reaction type
    - number of reactant species
    - reactant species names
    - reactant species stoichiometric coefficients
    - number of product species
    - product species names
    - products species stoichiometric coefficients
    - kinetic reaction parameters
- The kinetic reaction name must be unique and distinct from equilibrium reaction names
- *Kinetic Reaction Type* options
    - Precipitation-dissolution
    - Forward-backward
    - Valocchi-monod
    - Valocchi-sorption

5.10 Lithology Card Requirements

This card specifies the mineral specific areas and species volume fractions for every rock/soil type defined on the *Rock/Soil Zonation Card*. This card is only required when the *Precipitation-Dissolution* kinetic reaction type is specified for the *Kinetic Reaction Type* option. Required inputs:

- primary and secondary mineral specific area
- species volume fractions

6.0 Additional STOMP Requirements

This section describe the requirements for the for additional STOMP input cards needed in the transport simulation of gas, oil/NAPL, energy, CO_2, and CH_4.

6.1 Gas Relative Permeability Card Requirements

This card is used to declare and define a relative permeability-saturation function for the gas phase for each defined rock/soil type. Requirements:

- This card is required only for simulations involving flow and/or transport through the gas phase.
- Common gas relative permeability options
    - Constant
    - Mualem
    - Burdine
    - Any one of the above three options with Klinkenberg extension
- Other mode-specific gas relative permeability options (Table 5.1)
    - Fatt and Klikoff
    - Corey
    - Free Corey
    - Tabular water content
    - Any one of the above four options with Klinkenberg extension
    - Tabular saturation
- Options for declaring parameters:
    - Explicit declaration
    - External files
    - IJK indexing

6.2 NAPL Relative Permeability Card Requirements

This card allows the user to declare and define a relative permeability-saturation function for the NAPL for each defined rock/soil type. Requirements:

- The card is required only for simulations involving flow and/or transport through the NAPL phase
- NAPL relative permeability-saturation function options
    - Constant
    - Mualem
    - Burdine
- The Mualem and Burdine relative permeability functions for the NAPL phase are applicable to the van Genuchten and Brooks Corey functions. Either the van Genuchten ‘m’ parameter or the Brooks and Corey ‘λ’ parameter can be defaulted to the values entered or defaulted with the saturation function.
- Options for declaring parameters:
    - Explicit declaration
    - External files

- IJK indexing

6.3 Oil Properties Card Requirements

This card allows the user to declare functions and assign values required to compute the physical properties for an oil or dissolved oil. Requirements:

- This card is required only for simulations involving flow and/or transport of an oil or dissolved oil (STOMP-WO, STOMP-WO-Sc, STOMP-WOD, STOMP-WOA, STOMP-WOA-Sc, STOMP-WOD)
- Properties for oils are computed from critical properties and functional parameters following the corresponding states method as presented by Reid et al. (1987)
- Card name options
  - ~Volatile organic compound properties Card
  - ~Organic compound properties Card
  - ~VOC Properties Card
  - ~Oil Properties Card
- Required inputs
  - Number of NAPL components (for STOMP-WOD only)
  - oil name
  - molecular weight with units, freezing point temperature with units, normal boiling point with units, critical temperature with units
  - Critical pressure with units, critical molar volume with units, critical compressibility, Pitzner Acentric factor, dipole moment with units
  - Isobaric molar specific heat constants a, b, c, d: $\bar{c}_{Pn}^{o} = a + bT + cT^2 + dT^3$ in J/mol K
  - Saturated vapor pressure function options
    - Equation 1: $\ln(P_g^o / P_c^o) = (ax + bx^{1.5} + cx^3 + dx^6)/(1-x)$, where x = 1-T/$T_c^o$
    - Equation 2: $\ln(P_g^o) = a - b/T + c\ln(T) + d(P_g^o / T^2)$
    - Equation 3: $\ln(P_g^o) = a - b/(c+T)$
    - Constant: $P_g^o = \bar{P}_g^o$
  - Liquid density options
    - HBT Technique: Reid et al. 1987, pp55-56
    - Modified Rackett w/ reference: Reid et al. 1987, p67
    - Modified Rackett: Reid et al. 1987, p67
    - Constant: $\rho_g^o = \bar{\rho}_g^o$
  - Liquid viscosity function options (in cP and K for viscosity and temperature, respectively):
    - Reference: $\mu_n^o = \left[(\bar{\mu}_n^o)^{-0.2661} + (T - \bar{T}_n^o)/233.0\right]^{-3.758}$
    - Equation 1: $\mu_n^o = aT^b$
    - Equation 2: $\mu_n^o = \exp(a + b/T)$
    - Equation 3: $\mu_n^o = \exp(a + b/T + cT + dT^2)$

        - Constant: $\mu_n^o = \overline{\mu}_n^o$
    - Henry's constant for aqueous solubility (1.E+20) with units

6.4 Dissolved-Oil Transport Card Requirements

This card allows the user to declare functions and assign values required for dissolved oil transport. Requirements:

- This card is required only for simulations involving transport of dissolved oil (STOMP-WO, STOMP-WOD, STOMP-WOA, STOMP-WOA-Sc)
- Card name options
    - ~Dissolved oil transport Card
    - ~Dissolved VOC transport Card
    - ~Dissolved organic transport Card
- Required inputs
    - Interphase mass transfer function options (for STOMP-WOD only)
        - Welty: $Sh = k_{nl}^o d_p / D_l^o = a + b\,\mathrm{Re}^m\, Sc^n$
        - Parker: $Sh = k_{nl}^o d_p / D_l^o = a + b\,\mathrm{Re}^m (s_n n_D)^n$
    - Rock/soil name, longitudinal dispersivity with units, transverse dispersivity with units,
    - Dissolved-oil adsorption function options
        - Linear: $R_D = 1 + k / s_l n_D$
        - Linear Kd: $R_D = 1 + K_d \rho_b / s_l n_D$
        - Freundlich: $R_D = 1 + nkC_l^{n-1} / s_l n_D$
        - Langmuir: $R_D = 1 + a / s_l n_D (1 + bC_l)^2$
    - Nominal particle diameter with units (for STOMP-WOD only)

6.5 Well Card Requirements

This card allows users to specify monitoring and pumping wells for the STOMP-WO operational mode. Input variable requirements:

- well type
- well radius
- well aqueous depth
- well NAPL depth
- well head pressure
- dissolved oil saturation
- number of screen intervals
- well times

6.6 Salt Transport Card Requirements

This card allows the user to define porous media dependent dispersivities for salt. Requirements:

- This card is required only for simulations involving salt transport (STOMP-WS, STOMP-WS-Sc, STOMP-WAS, STOMP-WASE, STOMP-WCS, STOMP-WCS-R, STOMP-WCS-R-Sc, STOMP-WCS-Sc, STOMP-WCSE, STOMP-WCMSE)
- Required inputs only for operational modes STOMP-WS, STOMP-WS-Sc, STOMP-WAS, STOMP-WASE
    - Salt name options
        - Sodium chloride
        - Sodium nitrate
        - Sodium Thiosulfate
        - Sodium chloride Henry
        - Sodium chloride Elder
    - Number of anions, number of cations, number of positive charges, number of negative charges, Pitzer pairwise ion-interaction parameters B0, B1, B2, Pitzer triplet ion-interaction parameter, surface to bulk molality ratio
    - Effective diffusion options
        - Constant: $D_{le}^{s} = D_{l}^{s}$
        - Conventional: $D_{le}^{s} = \tau_l s_l n_D D_l^s$
        - Empirical [Kemper and van Schaik]: $D_{le}^{s} = aD_l^s \exp(bn_D s_l)$
    - Rock/soil name, longitudinal dispersivity with units, transverse dispersivity with units
    - Aqueous molecular diffusion coefficient with units, constants a, b (for empirical effective diffusion only)
- Required inputs only for operational modes STOMP-WCS, STOMP-WCS-R, STOMP-WCS-R-Sc, STOMP-WCS-Sc, STOMP-WCSE, STOMP-WCMSE
    - Rock/soil name, longitudinal dispersivity with units, transverse dispersivity with units
- Options for declaring parameters for all applicable operational modes:
    - Explicit declaration
    - External files
    - IJK indexing

6.7 Thermal Properties Card Requirements

This card allows the user to assign values to the thermal conductivity, specific heat, and short-wave albedo for each defined rock/soil type. Requirements:

- This card is required only for simulations involving the solution of the energy conservation equation (STOMP-WAE-B, STOMP-WOAE, STOMP-WASE, STOMP-WCSE, STOMP-WCMSE)
- Requirements of all applicable modes
    - Thermal conductivity options and inputs
        - Constant: X-, Y-, and Z-direction thermal conductivity with units (W/m K)
        - Parallel: X-, Y-, and Z-direction thermal conductivity with units, specific heat with units (W/m K)

        - Linear: X-, Y-, and Z-direction unsaturated thermal conductivity with units, X-, Y-, and Z-direction water saturated thermal conductivity with units, specific heat with units (W/m K)
        - Somerton: X-, Y-, and Z-direction unsaturated thermal conductivity with units, X-, Y-, and Z-direction water saturated thermal conductivity with units (W/m K), specific heat with units (J/kg K)
        - Campbell: parameters a (0.734, W/m K), b (1.45, W/m K), c (2.01, W/m K), (0.204, W/m K), e (4.0), specific heat with units (J/kg K)
        - Cass: parameters a, b, c, d with units (W/m K), parameter e, specific heat with units (J/kg K)
- Requirements for STOMP-WAE-B
    - Operational mode options
        - with water-vapor enhanced diffusion, without ground-surface albedo
        - without water-vapor enhanced diffusion, with ground-surface albedo
        - with water-vapor enhanced diffusion, with ground-surface albedo
    - Ground-Surface albedo options and inputs
        - Pleim and Xiu Albedo: dry-soil albedo, wet-soil albedo, albedo attenuation factor
        - Wang Albedo: dry-soil albedo, wet-soil albedo, albedo attenuation factor, reference albedo at solar zenith = 60 deg
        - Briegleb Albedo: dry-soil albedo, wet-soil albedo, albedo attenuation factor, reference albedo at solar zenith = 60 deg, parameter C
        - Constant Albedo: mean soil albedo (0.20)
    - Water vapor diffusion options
        - Water vapor diffusion, Enhanced

6.8 Atmospheric Conditions Card Requirements

This card allows the user to specify time-varying atmospheric conditions for air temperature, pressure, relative humidity, net solar radiation, and wind speed. Requirements:

- This card is required only for the operational mode STOMP-WAE-B
- Required general inputs: atmospheric start month, day, year, time (in military format), wind speed measurement height with units, local longitude and meridian with units (deg)
- Required data inputs: atmospheric condition time, temperature, pressure, water-vapor relative humidity, net solar radiation, and wind speed, all followed by appropriate units
- Options for declaring parameters for all applicable operational modes:
    - Explicit declaration
    - External files

6.9 Plant Card Requirements

This card is used to specify plant varietals and characteristics growing on the ground surface, their time-invariant characteristics, and how the canopy microclimate is handles. Requirements:

- This card is required only for the operational mode STOMP-WAE-B
- Plant temperature option: Single plant temperature

- Rainfall interception options
    - Rainfall interception
    - No rainfall interception
- Plant stress options and required inputs
    - Vrugt Root Stress Model, Jarvis Root Stress Model: water stress points 1, 2, 3, and 4, each followed by units (m)
    - No Root Stress: root uptake reduced 50% with units (m)
- Stomatal resistance options
    - Hicks Stomatal Resistance Model
    - No Stomatal Resistance Model
- Plant albedo options and required inputs:
    - Temporal: Plant albedo initial stage start, plant albedo crop development start, plant albedo mid-season start, plant albedo late-season start, plant albedo late-season stop, plant canopy height with units
    - Not temporal: plant albedo, plant canopy height with units
- Required inputs
    - Number of plant species, plant temperature option, rainfall interception option
    - Plant name, plant stress option, stomatal resistance
    - Max. root depth with units, null root depth with units, root depth fit parameter
    - Plant albedo option with inputs
    - Plant stress option with inputs
    - Crop coefficient start, crop coefficient day of year (start) with units, crop coefficient (mature stage 1), crop coefficient day of year (mature stage 1) with units, crop coefficient (mature stage 2), crop coefficient day of year (mature stage 2) with units, crop coefficient (die-off), crop coefficient day of year (die-off) with units

7.0 STOMP Documentation Requirements

7.1 User's Guide (White and Oostrom, 2006)

The STOMP User Guide describes the general use and input file formatting for the simulator. The input file is organized by input cards with formatting specifications, which must be followed to create an input file readable by the simulator. This manual provides a detailed guide for formatting the required input. Beyond providing formatting and operational type instructions, this document also contains useful information for executing the simulator with a debug utility or making modifications to the source code. To assist the user in performing debug executions or in making modifications to the code, critical information about the operational flow path, subroutine functions, and variable descriptions have been provided in this guide. A description of the indexing patterns developed for the simulator is also provided in this guide.

The STOMP User Guide is updated frequently, although no specific requirement exists for addressing the frequency of those updates. In general, a new User Guide is published when additional user documentation is warranted, which in the past, has occurred every two to three years.

7.2 Theory Guide (White and Oostrom, 2000)

The Theory Guide describes the governing equations and constitutive relations and their numerical solution as formulated in the STOMP simulator. This guide traces the solution of subsurface flow and transport problems from theory to numerical implementation. The theory discussions begin with descriptions of the basal governing equations, which are conservation equations for component mass (i.e., water, air, oil, and salt), thermal energy, and solute mass. These equations that describe flow and transport through multiple-phase subsurface environments are presented in their partial differential form. The constitutive relations describe the dependence of secondary variables to the primary unknowns and complete the specification of the thermodynamic and hydrological states of the subsurface system. Primary variables (primary unknowns) for the governing equations of the STOMP simulator are selected dynamically and are dependent on the hydrologic phase condition of the local subsurface environment. Numerical solution includes the discretization of the governing conservation equations and constitutive relations to a system of nonlinear algebraic equations, and the transformation of these equations into a linear system using Newton-Raphson iteration. Also included are the details of implementing the various types of boundary conditions and an overview of two linear system solvers incorporated into the STOMP simulator. This guide concludes with a synopsis of the source code architecture, thus providing the final link between numerical theory and practical implementation of the solution scheme.

Since changes to the constitutive relations are unlikely, the STOMP Theory Guide will not be updated. Instead, both published and unpublished addendums will be used to describe the theory associated with any new functionality implemented in the STOMP simulator.

7.3 Design Document (Nichols and White, 2007)

This document describes the STOMP software design in sufficient detail to address how the system implements the requirements. The information provided in this document also includes the analysis or

rationale for the design chosen, as well as any assumptions. In addition to describing how the software satisfies the requirements, this document addresses how the software functions internally, and how the operating system, structure, interfaces, design inputs and sources, design constraints, timing between components, and data structures are considered and integrated into the code. Methods to mitigate the consequences of software failure are also addressed in this document.

The Design Document will be updated as new requirements are defined and design specifications are required to support the new requirements. However, frequent updates to the design document are not anticipated, and will only be performed as funding is identified to support this documentation.

7.4 Application Guide (Nichols et al. 1997)

The Application Guide is organized into several sections that group similar classical groundwater problems and presents their solution using the STOMP simulator. The examples in this guide were selected to demonstrate the application of the simulator to a variety of thermal and hydrogeologic flow and transport problems while illustrating a range of features available in the simulator. Simultaneously, the application examples serve as verification and benchmark cases wherever possible through comparison to analytic solutions or results reported elsewhere in the literature for similar problems solved using other computer codes.

The Application Guide is not expected to be updated. Software test problems that compare analytical solutions to STOMP numerical solutions will provide the necessary documentation for demonstration (and verification) of any new capabilities.

7.5 Short Course Guide (Oostrom et al. 2003)

The STOMP Short Course Guide contains a collection of small problems designed to introduce the user to the development of STOMP input files. The 10 problems are of increasing complexity, ranging from simple one-dimensional saturated flow of a single phase, to problems describing flow and transport of several phases. Each problem consists of the following sections: Problem Description, Exercises, Input File, and Solutions to Selected Exercises.

As the STOMP Short Course evolves, additional problems may be added to the Short Course Guide. However, no specific requirements exist for updating this documentation, and shall be performed on an as needed basis when funding has been identified.

7.6 ECKEChem Module Addendum (White and McGrail 2005)

This addendum to the STOMP guides describes the theory, use, and application of the ECKEChem (Equilibrium- Conservation-Kinetic Equation Chemistry) reactive transport package for the STOMP simulator. This document describes the methods that the STOMP ECKEChem module uses; a reaction-based model where equilibrium reactions are modeled with an infinite reaction rate via equilibrium equations, and kinetic reactions are modeled using finite reaction rates. Currently there are four reaction rate models available with the STOMP simulator, though it is anticipated that the number of kinetic

reaction rate models will quickly expand. Any additional models or capabilities to the ECKEChem module will be documented in separate addendums.

7.7 STOMP-WAE-R Addendum (Ward et al. 2005)

This addendum describes the theory, input file formatting, and application of a sparse vegetation evapotranspiration model for the Water-Air-Energy Operational Mode of the Subsurface Transport Over Multiple Phases (STOMP) numerical simulator. The Water-Air-Energy Operational Mode (STOMP-WAE) solves the coupled conservation equations for water mass, air mass, and thermal energy transported over three phases: aqueous, gas, and soil matrix. The evapotranspiration model is implemented as a boundary condition on the upper surface of the computational domain and has capabilities for modeling evaporation from bare surfaces as well as evapotranspiration from sparsely vegetated surfaces populated with multiple plant species. This mode is the barrier extension of the WAE mode and is designated as STOMP-WAE-B. This document is not expected to be updated, but any additional functionality that may be implemented in the WAE-B mode will be documented in an additional addendum.

8.0 STOMP Execution Requirements

This section briefly describes the system, compilation and execution requirements for the STOMP simulator. Specific details of compilation and execution can be found in the STOMP User Guide (White and Oostrom 2006).

8.1 System Requirements

The STOMP simulator is written in the FORTRAN 77 language, following American National Standards Institute (ANSI 1978) standards, and was designed primarily for execution on computers with UNIX operating systems. An assembled source code, however, can be compiled and executed on any computer with an ANSI FORTRAN compiler, provided that the machine has sufficient memory. Although there is a general correspondence in computer design between memory size and execution speed, sufficient memory to compile and execute is not an assurance that the machine will have sufficient execution speeds to complete a simulation within a reasonable time period.

8.2 Compilation Requirements

Compiling the source code into an executable differs between operating systems, compilers, and memory options. Currently, all testing and development of the STOMP simulator is performed using the Portland Group International compiler (www.pgroup.com) in UNIX based environments. The normal procedure for building an executable version for a particular operational mode involves compiling the required group of library source codes, using the declared and computed parameters in the "parameters" file to define memory requirements, and linking the compiled object files to create an executable. An alternative would be to assemble or concatenate all of the source code libraries required for a particular operational mode into a single file and then subsequently compile the assembled source code. Either procedure can be performed manually or automatically. The "make" utility, which generates a sequence of commands for execution by the UNIX shell, can be used to automatically compile and link the required source code libraries for a particular operational mode. A "makefile," which contains a "make" utility instruction set, has been built to generate an executable or assembly source code for the simulator.

8.3 Execution Requirements

Executing the simulator is a straight forward and only requires that the executable version of the code and an input file named input reside in the current directory. For restart simulations a restart file named restart must also reside in the current directory. For a UNIX operating system, execution is started by typing in the name of the executable file. Execution will be indicated by the printing of a STOMP title banner and program disclaimer to the standard input/output device (e.g., screen). Two types of error messages may be generated, during an STOMP execution. The first type is a system generated message that typically indicates a memory, FORTRAN, or other system error identified by the system. The second type of error messages refer to those generated by the STOMP code, which typically refer to input, parameter, or convergence failure type messages.

9.0 Literature Cited

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