Software Requirements Document for STOMP and eSTOMP, Rev. 3.2

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Approvals

This document is electronically approved and signed via the PNNL Electronic Records & Information Capture Architecture (ERICA) system.

Revision History

Revision	Date	Summary of Changes
1.0	2/5/2007	First draft of Requirements Document
1.1	2/25/2007	Review by QE; Completion of Sections 7 & 8
2.0	12/07/2012	Updated reqs with unique identifiers
2.1	6/14/2013	Added the requirement for STOMP-CO2e
3.0	02/2015	Added eSTOMP requirements
3.1	01/2016	Added additional requirements for benchmarking cement waste forms
3.2	05/2016	Added additional requirements for compressibility, bulk compressibility and pore compressibility options in Mechanical Properties card.

1.0 Introduction to STOMP/eSTOMP Requirements

This document serves as a requirements specification document for the subsurface simulators, STOMP (Subsurface Transport Over Multiple Phases) and eSTOMP, where the latter is the scalable implementation of STOMP. 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 eSTOMP software, nor does it address objectives of any planned software upgrades. This document only addresses requirements as outlined in the STOMP/eSTOMP User Guide (*in progress*), with the primary purpose of guiding software testing.

As new capabilities and functionality are added to STOMP/eSTOMP, those requirements will be added to this document for 1) guiding software development and 2) testing against the new requirements. Requirements for new capabilities may be identified in the Software Change Request (SCR) forms, and will be incorporated into this document. This documentation will be maintained in Confluence using the Confluence version control system.

2.0 Operational Modes and General Requirements

2.1 STOMP/eSTOMP Input File

Both the STOMP and eSTOMP simulators are 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.

STOMP Operational Mode Summary, where the abbreviations are represented by: W = Water, A = Air, E,e = Energy, O = Oil, CO2 = CO_2, R = Reactions, and EPMech = Geomechanics.

Operational Mode Name	Operational Mode Identifier	Operational Mode
STOMP-W[a]	Water	1
eSTOMP-W[a]	Water	1
STOMP-WAE[b]	Water-Air-Energy	3
eSTOMP-WAE[b]	Water-Air-Energy	3
STOMP-WO	Water-Oil	4
STOMP-WOA	Water-Oil-Air	5
STOMP-CO2[a,c]	Water-CO_2	32
STOMP-CO2e[a,c]	Water-CO_2-Energy	33

a Can also be executed with ECKEChem Reactive Transport Module (-R)
b Can also be executed with Barrier (Plant) Module (-B)
c Can also be executed with Geomechanics Module (-EPMech)

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

a. Common cards for all modes: generally, the requirements for these cards are similar but vary depending on the operational mode.
b. Common cards for all modes but unshared source code: these cards are needed by all the modes but the requirements generally differ among modes.
c. ECKEChem cards: these cards are needed for the modes using the reactive transport module, ECKEChem.
d. Inverse modeling cards: these cards are needed for modes interfacing with inverse codes such as UCODE or PEST.
e. Mode specific cards: these cards are specific to individual modes.

The five groups of cards are summarized in the Table below and the requirements for them are discussed in the sections that follow.

Five Groups of STOMP cards

Group 1: Common Cards for All Modes	**Group 2: Common Cards for All Modes But Unshared Source Code**	**Group 3: Cards Needed by ECKEChem (Reactive Geochemistry)**	**Group 4: Inverse Modeling Cards**	**Group 5: Mode Specific Cards**
Simulation Title	Saturation Function	Aqueous Species	UCODE Control	Gas Relative Permeability
Grid	Source	Gas Species	Observed Data	NAPL Relative Permeability
Rock/Soil Zonation	Well	Solid Species	Scaling Factor	Oil Properties
Inactive Nodes	Initial Conditions	Species Link		Dissolved-Oil Transport
Aqueous Relative Permeability	Boundary Conditions	Conservation Equations		Thermal Properties
Directional Aqueous Relative Permeability	Solution Control	Equilibrium Equations		Atmospheric Conditions
Mechanical Properties	Output Control	Equilibrium Reactions		Plant
Hydraulic Properties	Surface Flux	Kinetic Equations		Salt Transport
	Solute/Fluid Interactions	Kinetic Reactions		Coupled Well
	Solute/Porous Media Interactions	Lithology		Internal Boundary Conditions
				Vertical Equilibrium Card
				Geomechanics Link Card

				Geomechanics Boundary Conditions Card

2.2 STOMP/eSTOMP Operational Modes

The STOMP and eSTOMP 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 names of the STOMP modes containing the ECKEChem modules have the extension 'R' attached (e.g., STOMP-W-R, eSTOMP-W-R). The extension '-B', as used in the STOMP-WAE-B and eSTOMP-WAE-B, which indicates that the evapotranspiration model is implemented as a boundary condition in the upper surface of the computational domain.

3.0 Requirements for Group One - Common Cards for All Modes

These cards are needed in all modes of STOMP/eSTOMP, but requirements can vary depending on the selected operational mode.

3.1 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 aqueous phase for each defined rock/soil type. Aqueous relative permeability function types and required input items are dependent on the operational mode (Table ARP.1). 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 can be defaulted to 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: There is a minimum saturation for the porous medium.
- Mualem w/ Polmann: The Polmann anisotropy is used. This option is not available for the *Directional Aqueous Relative Permeability Cards*.
- Burdine: This function is applicable to the van Genuchten and Brooks and Corey Saturation functions. The Brooks and Corey '' 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. This option is not available for the *Directional Aqueous Relative Permeability Cards*.
- Corey
- Free Corey
- Haverkamp
- Tauma and Vaucline
- Tabular: Accepts tabulated relative permeability data; Interpolation type: linear or spline
- Constant
- Dual porosity/permeability models for fractured systems: These models require the assumption that fracture and matrix fluid pressures are in equilibrium, which inherently neglects transient fracture-matrix interactions. Fracture and matrix relative permeabilities are computed from either the Burdine or Mualem models using either the van Genuchten or Brooks and Corey soil moisture retention functions. In these functions the effective aqueous and gas saturations are replaced with the corresponding values for the fracture and matrix components of the soil.

The options for declaring the aqueous relative permeability parameters include:

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

Directional Aqueous Relative Permeability

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 *Aqu eous Relative Permeability Card* except that the Mualem Polmann and Fatt and Klickoff options are not allowed.

Table ARP.1. Aqueous Relative Permeability Options

Operational Mode Name	**STOMP-W**	**STOMP-WAE**	**STOMP-WO**	**STOMP-WOA**	**STOMP-CO2**	**STOMP-CO**
Operational Mode Code	**1**	**3**	**4**	**5**	**32**	**33**
Mualem	x	x	x	x	x	x
Mualem Modified	x					
Modified Mualem with Tensorial-Connectivity-Tortuosity	x					
Mualem Irreducible	x	x			x	x
Mualem with Polmann	x	x			x	x
Burdine	x	x	x	x	x	x
Fatt and Klikoff	x	x			x	x
Corey	x	x			x	x
Free Corey					x	x
Haverkamp	x	x			x	x
Tauma and Vauclin	x	x			x	x
Tabular	x	x			x	x
Constant	x	x	x	x	x	x

Specific Safety Software Requirements for Water in STOMP-W, STOMP-WO, and STOMP-W-R Include:

ARP.W.1. Aqueous Relative Permeability Function Type: Mualem (with Van Genuchten saturation function; default *m* parameter; default tortuosity-connectivity coefficient)

ARP.W.2. Aqueous Relative Permeability Function Type: Mualem (with Van Genuchten saturation function; specified *m* parameter; default tortuosity-connectivity coefficient)

ARP.W.3. Aqueous Relative Permeability Function Type: Modified Mualem (with Van Genuchten saturation function; default *m* parameter; default tortuosity-connectivity coefficient)

ARP.W.4. Aqueous Relative Permeability Function Type: Modified Mualem (with Van Genuchten saturation function; specified *m* parameter; prescribed directional tortuosity-connectivity

ARP.W.5. Aqueous Relative Permeability Function Type: Modified Mualem (with Van Genuchten saturation function; default *m* parameter; prescribed directional tortuosity-connectivity coefficient)

ARP.W.6. Aqueous Relative Permeability Function Type: Mualem with Polmann (with Van Genuchten saturation function)

ARP.W.7. Declaration of aqueous relative permeability options through Directional X-, Y-, and Z - Aqueous Relative Permeability Cards

ARP.W.8. Explicit Declaration of aqueous relative permeability options

ARP.W.9. Declaration of aqueous relative permeability options: IJK Indexing

ARP.W.10. Aqueous Relative Permeability Function Type: Burdine (with Van Genuchten saturation function; default *m* parameter; default tortuosity-connectivity coefficient)

Specific Safety Software Requirements for Water in eSTOMP-W and eSTOMP-W-R Include:

ARP.eW.1. Aqueous Relative Permeability Function Type: Mualem (with Van Genuchten saturation function; default *m* parameter; default tortuosity-connectivity coefficient)

ARP.eW.2. Aqueous Relative Permeability Function Type: Mualem (with Van Genuchten saturation function; specified *m* parameter; default tortuosity-connectivity coefficient)

ARP.eW.3. Aqueous Relative Permeability Function Type: Modified Mualem (with Van Genuchten saturation function; default *m* parameter; default tortuosity-connectivity coefficient)

ARP.eW.4. Aqueous Relative Permeability Function Type: Modified Mualem (with Van Genuchten saturation function; specified *m* parameter; prescribed directional tortuosity-connectivity

ARP.eW.5. Aqueous Relative Permeability Function Type: Modified Mualem (with Van Genuchten saturation function; default *m* parameter; prescribed directional tortuosity-connectivity coefficient)

ARP.eW.6. Aqueous Relative Permeability Function Type: Mualem with Polmann (with Van Genuchten saturation function)

ARP.eW.7. Declaration of aqueous relative permeability options through Directional X-, Y-, and Z - Aqueous Relative Permeability Cards

ARP.eW.8. Explicit Declaration of aqueous relative permeability options

ARP.eW.9. Declaration of aqueous relative permeability options: IJK Indexing

Specific Safety Software Requirements for STOMP-WAE Include:

ARP.WAE.1. Aqueous Relative Permeability Function Type: Mualem (with Van Genuchten saturation function; default *m* parameter; default tortuosity-connectivity coefficient)

ARP.WAE.2. Aqueous Relative Permeability Function Type: Constant (with Van Genuchten saturation function)

ARP.WAE.3. Aqueous Relative Permeability Function Type: Mualem (with Extended Van Genuchten saturation function; default m parameter; default tortuosity-connectivity coefficient)

ARP.WAE.4. Aqueous Relative Permeability Function Type: Fatt and Klikoff (with Rossi-Nimmo-Junction saturation function)

ARP.WAE.5. Aqueous Relative Permeability Function Type: Fatt and Klikoff (with Rossi-Nimmo-Sum saturation function)

ARP.WAE.6. Aqueous Relative Permeability Function Type: Modified Mualem (with Van Genuchten/Webb saturation function; specified m parameter; default tortuosity-connectivity coefficient)

ARP.WAE.7. Aqueous Relative Permeability Function Type: Constant (with Van Genuchten/Webb saturation function)

ARP.WAE.8. Aqueous Relative Permeability Function Type: Fatt and Klikoff (with Van Genuchten saturation function)

ARP.WAE.9. Explicit Declaration of aqueous relative permeability options

Specific Safety Software Requirements for STOMP-WAE-B Include:

ARP.WAE-B.1. Aqueous Relative Permeability Function Type: Mualem (with Extended Van Genuchten saturation function; default *m* parameter; default tortuosity-connectivity coefficient)

ARP.WAE-B.2. Aqueous Relative Permeability Function Type: Burdine (with Extended Brooks and Corey saturation function)

ARP.WAE-B.3. Explicit Declaration of aqueous relative permeability options

Specific Safety Software Requirements for STOMP-WO Include:

ARP.WO-O.1. Aqueous Relative Permeability Function Type: Mualem (with Van Genuchten saturation function; default *m* parameter; default tortuosity-connectivity coefficient)

ARP.WO-O.2. Aqueous Relative Permeability Function Type: Burdine (with Brooks and Corey With Residual saturation function)

ARP.WO-O.3. Explicit Declaration of aqueous relative permeability options

Specific Safety Software Requirements for STOMP-WO with Transport Include:

ARP.WO-T.1. Aqueous Relative Permeability Function Type: Mualem (with Van Genuchten saturation function; default *m* parameter; default tortuosity-connectivity coefficient)

ARP.WO-T.2. Aqueous Relative Permeability Function Type: Constant (with Entrapment Van Genuchten saturation function)

ARP.WO-T.3. Explicit Declaration of aqueous relative permeability options

Specific Safety Software Requirements for STOMP-WOA Include:

ARP.WOA.1. Aqueous Relative Permeability Function Type: Mualem (with Van Genuchten saturation function; default *m* parameter; default tortuosity-connectivity coefficient)

ARP.WOA.2. Explicit Declaration of aqueous relative permeability options

Specific Safety Software Requirements for STOMP-CO2 and STOMP-CO2e Include:

ARP.CO2(e).1. Mualem (with Brooks and Corey saturation function)

ARP.CO2(e).2. Mualem Irreducible (with Van Genuchten saturation function)

ARP.CO2(e).3. Burdine (with Brooks and Corey saturation function)

ARP.CO2(e).4. Tabular (with Brooks and Corey saturation function)

Specific Safety Software Requirements for STOMP-CO2e Include:

ARP.CO2e.1. Fatt and Klikoff

3.2 Grid Card Requirements

This card is used to specify the grid structure used with the STOMP simulator's integral finite difference formulation. All STOMP grids are structured and orthogonal to nearly orthogonal, with hexahedral grid cells. Grids can be specified with either relative or absolute coordinates. Grids may be specified as map projections (ie., UTM or State Plane) with their corresponding units (meters or feet). However, geographic coordinate systems (i.e., latitude-longitude) are not accepted. Vertical coordinates can be specified as elevation or as relative coordinates. The origin of STOMP grids is in the lower, left hand, front, corner. A number of different ways of specifying grids are available in STOMP.

- Cartesian: the Cartesian coordinate system has longitudinal axis (z-direction) aligned with the negative gravitational vector. Options include (Non-Uniform) Cartesian, Uniform Cartesian, and Tilted Cartesian.
- Cylindrical: The longitudinal axis (z-direction) is aligned with the negative gravitational vector and the radial (r–direction) and azimuthal (-direction) axes are constrained to a horizontal plane. The radial and azimuthal axes constrained in the horizontal plane. The azimuthal axes are restricted between zero and 360 degrees. Options include (Non-Uniform) Cylindrical and Uniform Cylindrical.
- Boundary fitted (or Curvilinear): This format allows for curvilinear boundaries and requires the vertices of each grid cell to be specified via an external grid file. This option assumes that adjacent grid cells have co-located vertices, requiring only ((nx+1)*(ny+1)*(nz+1)) vertex inputs. The number of grid cells in x, y and z, the filename, and the units are specified in the Grid Card.
- General Eclipse: This option reads a generic eclipse keyword (.grdecl) file, typically exported from Petrel™. This option allows for curvilinear boundaries. The number of grid cells in x, y and z, the file name, and the units are

specified in the Grid Card. The number of grid cells specified in the Grid Card must match what is specified in the generic eclipse file. The user also must specify a minimum z-direction spacing to avoid overlapping layers and negative cell volumes.

- Earthvision Sampled Input: This option reads a file generated from data exported from the EarthVision® geologic modeling software package. This option allows for curvilinear boundaries. The number of grid cells in x, y and z, the file name, and the units are specified in the Grid Card.
- Element and Vertices: This option requires the specification of eight vertices for every node, (i.e., (nx*ny*nz)*8) via an external grid file. The number of nodes in x, y and z, the filename and the units are specified in the Grid Card.

Two Grid Spacing Specification options are recognized for Non-Uniform Cartesian and Non-Uniform Cylindrical grid:

- Cell Surface Location: where the absolute locations of the cell edges are specified and there is one more value than the number of grid cells in the corresponding direction. Cell edge locations can be specified using either a local or global coordinate system. Therefore, the origin of the grid need not be 0,0,0.
- Count and Cell Size: where the first value must be the cell surface location at the origin, but after that, the number of cells and the cell size can be specified using the count@cell size syntax. The grid can be specified using either a local or global coordinate system. Therefore, the origin of the grid need not be 0,0,0.

The requirements for this card are the same for all operational modes except for eSTOMP, which allows the user to specify the processor distribution.

The following grid systems are recognized in eSTOMP.

- Cartesian: the Cartesian coordinate system has longitudinal axis (z-direction) aligned with the negative gravitational vector. Options include (Non-Uniform) Cartesian and Uniform Cartesian. Two Grid Spacing Specification options are recognized for the Non-Uniform Cartesian grid: Cell Surface Location and Count and Cell Size.
- Cartesian with processors: Options include (Non-Uniform) Cartesian with Processors and Uniform Cartesian with Processors. These two options are the same as the Uniform Cartesian and Non-uniform Cartesian options defined above, but allows the user to specify the processor distribution in the x-, y- and z-coordinate directions.

Specific Safety Software Requirements for All Modes in STOMP Include:

GC.A.1. Orthogonal grid system: Uniform Cartesian

GC.A.2. Orthogonal grid system: (Non-Uniform) Cartesian

with the Cell Surface Location grid spacing specification

GC.A.3. Orthogonal grid system: (Non-Uniform) Cartesian

with the Count and Cell Size grid spacing specification

GC.A.4. Orthogonal grid system: (Non-Uniform) Cartesian

with the Count and Cell Size grid spacing specification with Non-Zero Reference Point

GC.A.5. Orthogonal grid system: (Non-Uniform) Cylindrical

with the Count and Cell Size grid spacing specification

GC.A.6. Explicit Declaration of grid information

Specific Safety Software Requirements for All Modes in eSTOMP Include:

GC.eA.1. Orthogonal grid system: Uniform Cartesian

GC.eA.2. Orthogonal grid system: Uniform Cartesian with Processors

GC.eA.3. Orthogonal grid system: (Non-Uniform) Cartesian

with the Cell Surface Location grid spacing specification

GC.eA.4. Orthogonal grid system: (Non-Uniform) Cartesian

with the Cell Surface Location grid spacing specification with Processors

GC.eA.5. Orthogonal grid system: (Non-Uniform) Cartesian

with the Count and Cell Size grid spacing specification

GC.eA.6. Orthogonal grid system: (Non-Uniform) Cartesian

with the Count and Cell Size grid spacing specification with Non-Zero Reference Point

GC.eA.7. Explicit Declaration of grid information

GC.eA.8. Orthogonal grid system: (Non-Uniform) Cylindrical

with the Count and Cell Size grid spacing specification

3.3 Hydraulic Properties Card Requirements

The requirements for this card are the same for all modes in STOMP and eSTOMP, except for the modes STOMP-CO2 and STOMP-CO2e as indicated below.

This card allows users to assign values to the intrinsic permeability or hydraulic conductivity of each defined rock/soil type. Every rock/soil type defined on the *Rock/Soil Zonation Card* must be referenced. With the *IJK Indexing* option, node dependent parameters are entered via external files and node independent parameters are entered directly on the card. For fractured systems, if the dual porosity/permeability option is specified in the *Rock/Soil Zonation Card,* then hydraulic properties for both the matrix and fractures are specified.

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 string '*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 STOMP-CO2 and STOMP-CO2e modes.
- Kozeny-Carman Relatioship: permeability reduction model for reactive transport. The permeability or hydraulic conductivity can be increased or reduced due to mineral dissolution/precipitation.

The options for declaring the hydraulic properties include:

- Explicit declaration
- IJK indexing (Formatted (ASCII) External Files or Binary External Files)

Specific Safety Software Requirements for Water in STOMP-W, STOMP-WO, and STOMP-W-R Include:

HP.W.1. Hydraulic Conductivity *"hc"* Specified

HP.W.2. Intrinsic Permeability Specified

HP.W.3. Heterogeneous Porous Media

HP.W.4. Anisotropic Porous Media

HP.W.5. Explicit Declaration of hydraulic properties

HP.W.6. Declaration of hydraulic properties: IJK Indexing

Specific Safety Software Requirements for Water in eSTOMP-W and eSTOMP-W-R Include:

HP.eW.1. Hydraulic Conductivity "hc" Specified

HP.eW.2. Intrinsic Permeability Specified

HP.eW.3. Heterogeneous Porous Media

HP.eW.4. Anisotropic Porous Media

HP.eW.5. Explicit Declaration of hydraulic properties

HP.eW.6. Declaration of hydraulic properties: IJK Indexing

HP.eW.7. Option for updating hydraulic conductivity: Kozeny

Specific Safety Software Requirements for STOMP-WAE Include:

HP.WAE.1. Hydraulic Conductivity *"hc"* Specified

HP.WAE.2. Permeability Specified

HP.WAE.3. Multilayered Porous Media

HP.WAE.4. Explicit Declaration of hydraulic properties

Specific Safety Software Requirements for STOMP-WAE-B Include:

HP.WAE-B.1. Hydraulic Conductivity *"hc"* Specified

HP.WAE-B.2. Multilayered Porous Media

HP.WAE-B.3. Explicit Declaration of hydraulic properties

Specific Safety Software Requirements for STOMP-WO Include:

HP.WO-O.1. Hydraulic Conductivity *"hc"* Specified

HP.WO-O.2. Permeability Specified

HP.WO-O.3. Explicit Declaration of hydraulic properties

Specific Safety Software Requirements for STOMP-WO with Transport Include:

HP.WO-T.1. Hydraulic Conductivity *"hc"* Specified

HP.WO-T.2. Explicit Declaration of hydraulic properties

Specific Safety Software Requirements for STOMP-WOA Include:

HP.WOA.1. Hydraulic Conductivity *"hc"* Specified

HP.WOA.2. Explicit Declaration of hydraulic properties

Specific Safety Software Requirements for STOMP-CO2 and *STOMP-CO2e Include:*

HP.CO2(e).1. Intrinsic permeability explicitly declared

HP.CO2(e).2. Pore-body fractional length explicitly declared

HP.CO2(e).3. Fractional critical porosity explicitly declared

Specific Safety Software Requirements for STOMP-CO2e Include:

HP.CO2e.1. Hydraulic conductivity explicitly declared

3.4 Inactive Nodes Card Requirements

The requirements for this card are the same for all operational modes in STOMP and eSTOMP. 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

Specific Safety Software Requirements for All Modes in STOMP *Include:*

IN.A.1. Declaration of distribution of inactive nodes: Explicit

IN.A.2. Declaration of distribution of inactive nodes: through External Files

Specific Safety Software Requirements for All Modes in eSTOMP *Include:*

IN.eA.1. Declaration of distribution of inactive nodes: Explicit

IN.eA.2. Declaration of distribution of inactive nodes: through External Files

3.5 Mechanical Properties Card Requirements

This card allows the user to assign values to the *particle density, porosity, specific storativity, compressibility,* and *tortuosity* fu nction 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 in 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.
- Total porosity refers to all the pores of the porous medium.
- Diffusive porosity refers to the connected pores for fluid flow.
- 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.
- Bulk or pore compressibility can be specified in the place of specific storativity, with or without a reference pressure.
- Tortuosity functions are required for simulations that involve solute transport or diffusion of components through phases.
  Tortuosity can be computed either as:
    - Constants (which require input values);
    - Millington and Quirk Model (specified using functions of the phase saturation and diffusive porosity);
    - Marshall Model (a non-linear relation for air-dry soils)
    - Archie's Law (implementaion of Archie's Law only applies to fully saturated systems)
- The key words 'dp', 'dual porosity', or 'fractured' in the *Rock/Soil Zonation Card* 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
- IJK indexing

Specific Safety Software Requirements for Water in STOMP-W, STOMP-WO, and STOMP-W-R Include:

MP.W.1. Particle Density Specified

MP.W.2. Total Porosity Specified

MP.W.3. Diffusive Porosity Specified

MP.W.4. Specific Storativity Specified

MP.W.5. Millington and Quirk tortuosity function

MP.W.6. Constant tortuosity

MP.W.7. Explicit Declaration of mechanical properties

MP.W.8. Declaration of mechanical properties: IJK Indexing

MP.W.9. Compressibility and Reference Pressure Specified

MP.W.10. Bulk Compressibility and Reference Pressure Specified

MP.W.11. Pore Compressibility and Reference Pressure Specified

Specific Safety Software Requirements for Water in eSTOMP-W and eSTOMP-W-R Include:

MP.eW.1. Particle Density Specified

MP.eW.2. Total Porosity Specified

MP.eW.3. Diffusive Porosity Specified

MP.eW.4. Specific Storativity Specified

MP.eW.5. Millington and Quirk tortuosity function

MP.eW.6. Constant tortuosity

MP.eW.7. Explicit Declaration of mechanical properties

MP.eW.8. Declaration of mechanical properties: IJK Indexing

MP.eW.9. Archie's Law tortuosity function

MP.eW.10. Initial Tortuosity Specified

MP.eW.11. Compressibility and Reference Pressure Specified

MP.eW.12. Bulk Compressibility and Reference Pressure Specified

MP.eW.13. Pore Compressibility and Reference Pressure Specified

Specific Safety Software Requirements for STOMP-WAE Include:

MP.WAE.1. Particle Density Specified

MP.WAE.2. Total Porosity Specified

MP.WAE.3. Diffusive Porosity Specified

MP.WAE.4. Millington and Quirk tortuosity function

MP.WAE.5. Constant tortuosity

MP.WAE.6. Explicit Declaration of mechanical properties

Specific Safety Software Requirements for STOMP-WAE-B Include:

MP.WAE-B.1. Particle Density Specified

MP.WAE-B.2. Total Porosity Specified

MP.WAE-B.3. Diffusive Porosity Specified

MP.WAE-B.4. Specific Storativity Specified

MP.WAE-B.5. Millington and Quirk tortuosity function

MP.WAE-B.6. Explicit Declaration of mechanical properties

Specific Safety Software Requirements for STOMP-WO Include:

MP.WO.1. Particle Density Specified

MP.WO.2. Total Porosity Specified

MP.WO.3. Diffusive Porosity Specified

MP.WO.4. Millington and Quirk tortuosity function

MP.WO.5. Explicit Declaration of mechanical properties

Specific Safety Software Requirements for STOMP-WO with Transport Include:

MP.WO-T.1. Particle Density Specified

MP.WO-T.2. Total Porosity Specified

MP.WO-T.3. Diffusive Porosity Specified

MP.WO-T.4. Millington and Quirk tortuosity function

MP.WO-T.5. Explicit Declaration of mechanical properties

Specific Safety Software Requirements for STOMP-WOA Include:

MP.WOA.1. Particle Density Specified

MP.WOA.2. Total Porosity Specified

MP.WOA.3. Diffusive Porosity Specified

MP.WOA.4. Millington and Quirk tortuosity function

MP.WOA.5. Explicit Declaration of mechanical properties

Specific Safety Software Requirements for STOMP-CO2 and STOMP-CO2e Include:

MP.CO2(e).1. Particle Density Specified

MP.CO2(e).2. Total Porosity Specified

MP.CO2(e).3. Diffusive Porosity Specified

MP.CO2(e).4. [Bulk] Compressibility Specified

MP.CO2(e).5. Pore Compressibility Specified

MP.CO2(e).6. Millington and Quirk tortuosity function

MP.CO2(e).7. Constant tortuosity

MP.CO2(e).8. Explicit Declaration of mechanical properties

3.6 Rock Soil Zonation Card Requirements

The *Rock/Soil Zonation Card* is used to associate rock/soil types with grid cells. There are three basic options for declaring the distribution of rock/soil types:

- Explicit Declaration
- External Files

- IJK Indexing

Explicit Declaration for eSTOMP and STOMP

The explicit zonation option is best suited for simulations with a limited number of rock/soil types. The approach is to define rock/soil names and then associate those names with a spatial zone across the computational domain. Rock/soil names are generally unrestricted, but need to be less than 64 characters in length. Intrinsic properties of the defined rock/soil types will then be associated with the grid cells within the spatial zone on other input cards (e.g., *Hydraulic Properties Card, Mechanical Properties Card*). Spatial zones are specified using ranges of indices in the three local grid directions.

External Files Options

for STOMP: Formatted (ASCII) files and Unformatted (binary) files

for eSTOMP: Formatted (ASCII) files, Unformatted (binary) files, and HDF5 Formatted files

The external file option is similar to the explicit zonation option, but the association of define rock/soil types with grid cells is via the external file. The external files contain one integer for every grid cell, using conventional i, j, k ordering. The integer corresponds with one of the defined rock/soil types.

IJK Indexing Options

for STOMP: IJK Indexing, JKI Indexing, and KIJ Indexing

for eSTOMP: IJK Indexing

The IJK Indexing option (IJK Indexing sub-option) assumes that every node will have a unique rock/soil type, with the rock/soil type number being determined by the i, j, k indexing of the grid cells. With this option the intrinsic properties of the rock/soil types can be specified uniquely for each grid cell via external file reads or uniformly via conventional inputs. Some operational modes additionally allow a hybrid IJK Indexing and Zonation specification of the saturation and relative permeability intrinsic parameters.

Specific Safety Software Requirements for All Modes in STOMP *Include:*

RSZ.A.1. Declaration of the distribution of rock/soil types: Explicit

RSZ.A.2. Declaration of the distribution of rock/soil types through External Files: Formatted Zonation File

RSZ.A.3. Declaration of the distribution of rock/soil types through External Files: Unformatted Zonation File

RSZ.A.4. Declaration of the distribution of rock/soil types: IJK Indexing Format

RSZ.A.5. Declaration of the distribution of rock/soil types: JKI Indexing Format

RSZ.A.6. Declaration of the distribution of rock/soil types: KIJ Indexing Format

Specific Safety Software Requirements for All Modes in eSTOMP *Include:*

RSZ.eA.1. Declaration of the distribution of rock/soil types: Explicit

RSZ.eA.2. Declaration of the distribution of rock/soil types through External Files: Formatted Zonation File

RSZ.eA.3. Declaration of the distribution of rock/soil types through External Files: Unformatted Zonation File

RSZ.eA.4. Declaration of the distribution of rock/soil types: IJK Indexing Format

3.7 Simulation Title Card Requirements

This card provides a means to document a simulation. Information recorded in this card is rewritten in the output file. The requirements for this card are the same for all operational modes in STOMP and eSTOMP. 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

Specific Safety Software Requirements for All Modes in STOMP Include:

ST.A.1. Input file version number

ST.A.2. Simulation title

ST.A.3. User name

ST.A.4. Company name

ST.A.5. Creation date

ST.A.6. Creation time

ST.A.7. Number of simulation note lines

ST.A.8. Simulation notes

Specific Safety Software Requirements for All Modes in eSTOMP Include:

ST.eA.1. Input file version number

ST.eA.2. Simulation title

ST.eA.3. User name

ST.eA.4. Company name

ST.eA.5. Creation date

ST.eA.6. Creation time

ST.eA.7. Number of simulation note lines

ST.eA.8. Simulation notes

4.0 Requirements Group 2 Cards_ Cards Common to All Modes But Source Code Is Not Shared

This section describes the cards used in all modes but the requirements differ among the different modes of STOMP and eSTOMP.

4.1 Boundary Conditions Card Requirements

Boundary Conditions card is used to impose state conditions or fluxes across grid-cell surfaces that are not coupled to an adjacent grid cell (e.g., external boundary surfaces).

This card is optional, but is generally necessary to simulate a particular problem. Requirements for all operational modes:

- Boundary conditions can only be applied to three types of grid cell surfaces: 1) surfaces on the boundary of the computational domain, 2) surfaces between active and inactive grid cells, and 3) surfaces along the boundary of an internal split in the computational domain.
- Boundary conditions are always applied to active grid cells and the grid-cell surface to which the boundary condition

is applied is in reference to the active grid cell.

- By default, all undeclared boundary surfaces have zero flux boundary conditions for both flow and transport
- The boundary surface direction is specified with respect to an active node adjacent to a boundary surface. 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.
- Generally, the number of boundary conditions 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 would 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
    - Hydraulic Gradient
    - Initial Conditions
- Boundary condition types required for all the components (i.e., solute, species, salt, dissolved oil):
    - Zero Flux
    - Initial Conditions
    - Outflow
    - Aqueous Concentration

All Boundary Condition types for all modes are listed in Table BC.1.

Options for declaring boundary indices and/or boundary conditions:

- Explicit declaration
- External files. These files contain one value for each grid cell being assigned the same boundary condition type and time series. Boundary direction indices: -3 for Bottom, -2 for South, -1 for West, 1 for East, 2 for North, and 3 for Top.

Table BC.1. Boundary Condition Types

Operational Mode Name	**STOMP-W**	**STOMP-WAE**	**STOMP-WO**	**STOMP-WOA**	**STOMP-CO2**	**STOMP-CO2e**
Operational Mode Code	**1**	**3**	**4**	**5**	**32**	**33**
Common aqueous phase BC types[(a)]	x	x	x	x	x	x
Common solute transport BC types[(b)]	x	x	x	x	x	x
Gas phase BC types[(a)]		x		x	x	x
Energy transport BC types[(c)]		x				x
Energy transport w/ barrier option BC types[(d)]		x				

NAPL phase BC types(e)			x	x		
Salt transport BC types(f)					x	x
Species transport BC types(g)	x					
[Aqueous] Saturated	x	x			x	x
[Aqueous] Unit Gradient	x	x	x	x		
[Aqueous] Free Gradient	x					
[Aqueous] Outflow	x	x	x			
[Aqueous] X-Y-Z Seepage Face	x					
[Aqueous] Seepage Face	x	x				
[Aqueous] Hydraulic Gradient	x	x	x	x	x	x
[Aqueous] X-Y-Z Hydraulic Gradient	x					
[Aqueous] Falling Head, Falling Pond	x					
[Aqueous] Fluctuating Water Table				x		
[Species] Inflow Aqueous	x					
[Species] Inflow-Outflow Aqueous	x					
[Solute] Inflow Volumetric, Inflow Aqueous	x		x	x		
[Solute] Inflow-Outflow Aqueous	x					
[Solute] Inflow-Outflow Volumetric	x					
[Solute] Gas Conc.		x		x	x	x
[Solute] NAPL Conc., Inflow NAPL			x	x		
[Gas] Inflow Gas, Unit Gradient, Dirichlet Outflow				x		

(a) Dirichlet, Neumann, Zero Flux, Hydraulic Gradient, Initial Condition
(b) Volumetric Concentration, Aqueous Concentration, Zero Flux, Outflow, Initial Condition
(c) Aqueous Concentration, Zero Flux, Outflow, Initial Condition
(d) Ground, Convective, Convective-Radioactive, Bare Shuttleworth-Walace, Shuttleworth-Walace
(e) Dirichlet, Neumann, Zero Flux, Outflow, Unit Gradient, Initial Condition, Hydraulic Gradient
(f) Volumetric Concentration, Aqueous Concentration, Zero Flux, Outflow, Initial Condition, Inflow Volumetric, Inflow Aqueous, [Inflow] Relative Saturation, Inflow Mass Fraction, Aqueous Relative Saturation, Aqueous Mass Fraction

(g) Aqueous Concentration, Zero Flux, Outflow, Initial Condition, Inflow Aqueous

Specific Safety Software Requirements for Water in STOMP-W and STOMP-WO Include:

BC.W.1. Boundary condition type: Dirichlet

BC.W.2. Boundary condition type: Neumann

BC.W.3. Boundary condition type: Hydraulic Gradient

BC.W.4. Boundary condition type: Saturated

BC.W.5. Boundary condition type: Zero Flux

BC.W.6. Boundary condition type: Initial Condition

BC.W.7. Boundary condition type: Unit Gradient

BC.W.8. Boundary condition type: Outflow

BC.W.9. Boundary condition type: Free Gradient

BC.W.10. Boundary condition type: Seepage face

BC.W.11. Boundary condition type: XYZ-Hydraulic Gradient

BC.W.12. Boundary condition type: XYZ-Seepage Face

BC.W.13. Boundary condition type: Not defined (No Flow by default)

BC.W.14. Time Varying Boundary Condition: Multiple Number of Boundary Times

BC.W.15. Declaration of boundary indices and/or boundary condition values: Explicit

BC.W.16. Declaration of boundary indices and/or boundary condition values: through External Files (data files)

BC.W.17. Declaration of boundary indices and/or boundary condition values: through External Files (Linked Lists of Boundary Cell Faces)

Specific Safety Software Requirements for Water in eSTOMP-W Include:

BC.eW.1. Boundary condition type: Dirichlet

BC.eW.2. Boundary condition type: Neumann

BC.eW.3. Boundary condition type: Hydraulic Gradient

BC.eW.4. Boundary condition type: Saturated

BC.eW.5. Boundary condition type: Zero Flux

BC.eW.6. Boundary condition type: Initial Condition

BC.eW.7. Boundary condition type: Unit Gradient

BC.eW.8. Boundary condition type: Outflow

BC.eW.9. Boundary condition type: Free Gradient

BC.eW.10. Boundary condition type: Seepage face

BC.eW.11. Boundary condition type: XYZ-Hydraulic Gradient

BC.eW.12. Boundary condition type: XYZ-Seepage Face

BC.eW.13. Boundary condition type: Not defined (No Flow by default)

BC.eW.14. Time Varying Boundary Condition: Multiple Number of Boundary Times

BC.eW.15. Declaration of boundary indices and/or boundary condition values: Explicit

BC.eW.16. Declaration of boundary indices and/or boundary condition values: through External Files (data files)

BC.eW.17. Declaration of boundary indices and/or boundary condition values: through External Files (Linked Lists of Boundary Cell Faces)

Specific Safety Software Requirements for Aqueous Transport in STOMP-W Include:

BC.W-T.1. Solute Boundary condition type: Aqueous Concentration

BC.W-T.2. Solute Boundary condition type: Volumetric Concentration

BC.W-T.3. Solute Boundary condition type: Outflow

BC.W-T.4. Solute Boundary condition type: Zero Flux

BC.W-T.5. Solute Boundary condition type: Initial Condition

BC.W-T.6. Solute Boundary condition type: Inflow Aqueous Concentration

BC.W-T.7. Solute Boundary condition type: Inflow Volumetric Concentration

BC.W-T.8. Solute Boundary condition type: Inflow-Outflow Aqueous Concentration

BC.W-T.9. Solute Boundary condition type: Inflow-Outflow Volumetric Concentration

Specific Safety Software Requirements for Aqueous Transport in eSTOMP-W Include:

BC.eW-T.1. Solute Boundary condition type: Aqueous Concentration

BC.eW-T.2. Solute Boundary condition type: Volumetric Concentration

BC.eW-T.3. Solute Boundary condition type: Outflow

BC.eW-T.4. Solute Boundary condition type: Zero Flux

BC.eW-T.5. Solute Boundary condition type: Initial Condition

BC.eW-T.6. Solute Boundary condition type: Inflow Aqueous Concentration

BC.eW-T.7. Solute Boundary condition type: Inflow Volumetric Concentration

BC.eW-T.8. Solute Boundary condition type: Inflow-Outflow Aqueous Concentration

BC.eW-T.9. Solute Boundary condition type: Inflow-Outflow Volumetric Concentration

Specific Safety Software Requirements for STOMP-W-R Include:

BC.W-R.1. Boundary condition type: Species Aqueous Concentration

BC.W-R.2. Boundary condition type: Species Outflow

BC.W-R.3. Boundary condition type: Species Aqueous Inflow

Specific Safety Software Requirements for eSTOMP-W-R Include:

BC.eW-R.1. Boundary condition type: Species Aqueous Concentration

BC.eW-R.2. Boundary condition type: Species Outflow

BC.eW-R.3. Boundary condition type: Species Aqueous Inflow

Specific Safety Software Requirements for STOMP-WAE Include:

BC.WAE.1. Boundary condition type: Dirichlet Energy

BC.WAE.2. Boundary condition type: Neumann Energy

BC.WAE.3. Boundary condition type: Outflow Energy

BC.WAE.4. Boundary condition type: Dirichlet Gas

BC.WAE.5. Boundary condition type: Zero Flux Gas

BC.WAE.6. Boundary condition type: Neumann Gas

Specific Safety Software Requirements for STOMP-WAE-B Include:

BC.WAE-B.1. Boundary condition type: Shuttleworth-Wallace

BC.WAE-B.2. Boundary condition type: Bare Shuttleworth-Wallace

BC.WAE-B.3. Boundary condition type: Dirichlet Energy

BC.WAE-B.4. Boundary condition type: Dirichlet Gas

BC.WAE-B.5. Boundary condition type: Zero Flux Gas

Specific Safety Software Requirements for STOMP-WOA Include:

BC.WOA.1. Boundary condition type: Dirichlet NAPL

BC.WOA.2. Boundary condition type: Zero Flux NAPL

BC.WOA.3. Boundary condition type: Neumann NAPL

BC.WOA.4. Boundary condition type: Dirichlet Gas

BC.WOA.5. Boundary condition type: Zero Flux Gas

BC.WOA.6. Boundary condition type: Hydraulic Gradient Gas

Specific Safety Software Requirements for Oil in STOMP-WO Include:

BC.WO-O.1. Oil Phase Boundary condition type: Dirichlet

BC.WO-O.2. Oil Phase Boundary condition type: Zero Flux

BC.WO-O.3. Oil Phase Boundary condition type: Neumann

BC.WO-O.4. Oil Phase Boundary condition type: Hydraulic Gradient

Specific Safety Software Requirements for STOMP-WO with Transport Include:

BC.WO-T.1. Solute Boundary condition type: Aqueous Concentration

BC.WO-T.2. Solute Boundary condition type: Outflow

BC.WO-T.3. Solute Boundary condition type: Inflow Aqueous

Specific Safety Software Requirements for STOMP-CO2 and *STOMP-CO2e Include:*

BC.CO2(e).1. Aqueous boundary condition type: Dirichlet

BC.CO2(e).2. Aqueous boundary condition type: Initial Condition

BC.CO2(e).3. Aqueous boundary condition type: Zero Flux

BC.CO2(e).4. Aqueous boundary condition type: Default

BC.CO2(e).5. CO2 boundary condition type: Dirichlet

BC.CO2(e).6. CO2 boundary condition type: Initial Condition

BC.CO2(e).7. CO2 boundary condition type: Default

BC.CO2(e).8. Salt boundary condition type: Aqueous Mass Fraction

BC.CO2(e).9. Salt boundary condition type: Initial Condition

BC.CO2(e).10. Salt boundary condition type: Default

BC.CO2(e).11. Aqueous species boundary condition type: Zero Flux

Specific Safety Software Requirements for STOMP-CO2e Include:

BC.CO2e.1. CO2 boundary condition type: Zero Flux

BC.CO2e.2. Energy boundary condition type: Dirichlet

BC.CO2e.3. Energy boundary condition type: Neumann

4.2 Initial Conditions Card Requirements

This card allows the user to assign starting values to both primary and secondary field variables (Table IC.1).

Requirements for all operational modes include:

- 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. Default 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-Direction Gradient that is equal to the product of fluid's density times gravitational acceleration (-9793.5192 1/m for water at 20ºC).
- 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 = 20º C
    - Pressure of any phase = 101325 Pa
    - 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 (Table IC.1).
- 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.

Initial Conditions may be specified in a number of ways including external files:

- Direct Input (Parameters are read directly from the input file with an associated domain and directional gradients)
- Rock/Soil Zonation (Parameters are associated with a rock/soil type. All grid cells with the specified rock/soil type are assigned the specified parameter value)
- External Text (ASCII) File (Parameters are read from an external file in text format. This option requires one parameter be specified for every node, following the I-J-K indexing order)
- External Binary File (Parameters are read from an external file in binary format. This option requires one parameter be specified for every node, following the I-J-K indexing order)

Table IC.1. Initial Condition State Variable Options.

Operational Mode Name	**STOMP-W**	**STOMP-WAE**	**STOMP-WO**	**STOMP-WOA**	**STOMP-CO2**	**STOMP-CO2e**
Operational Mode Code	**1**	**3**	**4**	**5**	**32**	**33**
Initial Saturation Option	x	x			x	x
Common Var Option(a)	x	x	x	x	x	x
Air Var Options(b)				x		
Oil Var Options(c)			x	x		
Salt Var Options(d)					x	x
CO2 Var Options(e)					x	x
Species Var Options(g)	x					
Solute Var Options(h)	x		x			
Aqueous Saturation	x				x	x
Trapped Gas Saturation [Overwrite]			x		x	x
NAPL Pressure			x	x		
Residual NAPL Saturation [Overwrite]			x			
Solute Gas Volumetric Conc. [Overwrite]				x		

(a) Common State Variable Options: Temperature [Overwrite], Aqueous Pressure [Overwrite], Gas Pressure [Overwrite]
(b) Air Variable Options: Aqueous Dissolved Air Mole Fraction [Overwrite], Aqueous Dissolved Air Mass Fraction [Overwrite]
(c) Oil Variable Options: Aqueous Dissolved Oil Mole Fraction [Overwrite], Aqueous Dissolved Oil Mass Fraction [Overwrite]
(d) Salt Variable Options: Salt Mass Fraction [Overwrite], Salt Relative Saturation [Overwrite], Salt Aqueous Volumetric Conc. [Overwrite]
(e) CO2 Variable Options: CO2 Partial Pressure, Dissolved CO2 Relative Saturation [Overwrite], Dissolved CO2 Mass Fraction [Overwrite]
(f) CO2-CH4 Variable Options: CO2 Mass Fraction of Hydrate Formers [Overwrite], CO2 Mole Fraction of Hydrate Formers [Overwrite]
(g) Species Variable Options: Species Volumetric Conc. [Overwrite], Species Aqueous Volumetric Conc. [Overwrite], Species Aqueous Molal Conc. [Overwrite]

(h) Solute Variable Options: Solute Volumetric Conc. [Overwrite], Solute Aqueous Volumetric Conc. [Overwrite]

Specific Safety Software Requirements for Water in STOMP-W and STOMP-WO Include:

IC.W.1. Saturation-Pressure Variable Set Option: Gas Pressure - Aqueous Saturation

IC.W.2. Saturation-Pressure Variable Set Option: Gas Pressure - Moisture Content

IC.W.3. Saturation-Pressure Variable Set Option: Gas Pressure - Aqueous Pressure

IC.W.4. State Variable Option: Aqueous Pressure

IC.W.5. State Variable Option: Aqueous Saturation

IC.W.6. State Variable Option: Gas Pressure

IC.W.7. State Variable Option: Moisture Content

IC.W.8. Initial condition variables overwritten using *Overwrite* Option (Execution Mode: Restart)

IC.W.9. Initial condition gradient: Default X-direction Gradient

IC.W.10. Initial condition gradient: Default Y-direction Gradient

IC.W.11. Initial condition gradient: Default Z-direction Gradient

IC.W.12. Initial condition gradient: Prescribed Z-direction Gradient

IC.W.13. Direct Input of the Initial Condition parameters

Specific Safety Software Requirements for Water in eSTOMP-W Include:

IC.eW.1. Saturation-Pressure Variable Set Option: Gas Pressure - Aqueous Saturation

IC.eW.2. Saturation-Pressure Variable Set Option: Gas Pressure - Moisture Content

IC.eW.3. Saturation-Pressure Variable Set Option: Gas Pressure - Aqueous Pressure

IC.eW.4. State Variable Option: Aqueous Pressure

IC.eW.5. State Variable Option: Aqueous Saturation

IC.eW.6. State Variable Option: Gas Pressure

IC.eW.7. State Variable Option: Moisture Content

IC.eW.8. Initial condition variables overwritten using *Overwrite* Option (Execution Mode: Restart)

IC.eW.9. Initial condition gradient: Default X-direction Gradient

IC.eW.10. Initial condition gradient: Default Y-direction Gradient

IC.eW.11. Initial condition gradient: Default Z-direction Gradient

IC.eW.12. Initial condition gradient: Prescribed Z-direction Gradient

IC.eW.13. Direct Input of the Initial Condition parameters

Specific Safety Software Requirements for Aqueous Transport in STOMP-W Include:

IC.W-T.1. Solute Variable Option: Solute Aqueous Volumetric Concentration

IC.W-T.2. Solute Variable Option: Solute Volumetric Concentration

IC.W-T.3. Solute Variable Option: *Overwrite* Solute Aqueous Volumetric Concentration

Specific Safety Software Requirements for Aqueous Transport in eSTOMP-W Include:

IC.eW-T.1. Solute Variable Option: Solute Aqueous Volumetric Concentration

IC.eW-T.2. Solute Variable Option: Solute Volumetric Concentration

IC.eW-T.3. Solute Variable Option: *Overwrite* Solute Aqueous Volumetric Concentration

Specific Safety Software Requirements for STOMP-W-R Include:

IC.W-R.1. Species Variable Option: Species Aqueous Volumetric Concentration

IC.W-R.2. Species Variable Option: *Overwrite* Species Aqueous Volumetric Concentration

IC.W-R.3. State Variable Option: Temperature

Specific Safety Software Requirements for eSTOMP-W-R Include:

IC.eW-R.1. Species Variable Option: Species Aqueous Volumetric Concentration

IC.eW-R.2. Species Variable Option: *Overwrite* Species Aqueous Volumetric Concentration

IC.eW-R.3. State Variable Option: Temperature

Specific Safety Software Requirements for STOMP-WAE Include:

IC.WAE.1. Variable Name Option: Temperature

IC.WAE.2. Variable Name Option: Aqueous Dissolved Air Relative Saturation

Specific Safety Software Requirements for STOMP-WAE-B Include:

IC.WAE-B.1. Variable Name Option: Temperature Overwrite

IC.WAE-B.2. Variable Name Option: Temperature

Specific Safety Software Requirements for STOMP-WOA Include:

IC.WOA.1. Variable Name Option: NAPL Pressure

IC.WOA.2. Variable Name Option: Aqueous Dissolved Air Mass Fraction

IC.WOA.3. Variable Name Option: Aqueous Dissolved Oil Mass Fraction

IC.WOA.4. Variable Name Option : Solute Aqueous Concentration

Specific Safety Software Requirements for Oil in STOMP-WO Include:

IC.WO-O.1. Variable Name Option: NAPL Pressure

IC.WO-O.2. Variable Name Option: Trapped NAPL Saturation

Specific Safety Software Requirements for STOMP-WO with Transport Include:

IC.WO-T.1. Variable Name Option: Solute Aqueous Volumetric

Specific Safety Software Requirements for STOMP-CO2 and STOMP-CO2e Include:

IC.CO2(e).1. Variable Name Option: Gas Pressure

IC.CO2(e).2. Variable Name Option: Aqueous Pressure

IC.CO2(e).3. Variable Name Option: Temperature

IC.CO2(e).4. Variable Name Option: Salt Mass Fraction

IC.CO2(e).5. Variable Name Option: Species Aqueous Volumetric Concentration

4.3 Output Control Card Requirements

This card allows the user to control output written to the *output* file, *plot.n* file, and *screen* (i.e., standard input/output device (STDIO)). 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:
    - 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

Complete lists of requirements for the output variables are given in :

Table OC.1. for STOMP-W,

Table OC.2. for STOMP-WAE,

Table OC.3. for STOMP-WO,

Table OC.4. for STOMP-WOA,

Table OC.5. for STOMP-CO2,

Table OC.6. for STOMP-CO2e.

Table OC.1. STOMP-W Output Variables (* reference node variable only; ** plot file variable only)

Var No.	Var. Name
1	apparent aqueous saturation
2	aqueous courant [number]
3	aqueous density
4	aqueous fracture saturation
5	aqueous gauge pressure
6	aqueous hydraulic head
7	aqueous matrix saturation
8	aqueous moisture cont[ent]
9	aqueous pressure
10	aqueous relative perm[eability]
11	aqueous saturation
12	aqueous viscosity
13	aqueous well depth*
14	diffusive porosity
15	effective trapped gas saturation
16	gas gauge pressure
17	gas pressure
18	gas saturation
19	integrated water mass*
20	matric potential
21	matrix pressure
22	phase condition
23	rock/soil type
24	solute aqueous conc[entration]
25	solute aqueous mole frac[tion]
26	solute integrated mass
27	solute integrated aqueous
28	solute inventory
29	solute source int[egral]
30	solute volumetric conc[entration]
31	species aqueous conc[entration]
32	species volumetric conc[entration]

33	solid species aqueous concentration (T)
34	solid species volumetric concentration (T)
35	exchange species aqueous concentration (T)
36	exchange species volumetric concentration (T)
37	species source
38	species integrated mass
39	species mineral area
40	species mineral rate
41	temperature
42	total water mass
43	trapped gas saturation
44	well flow integral*
45	well flow rate*
46	water aqueous mass fraction
47	water mass source int[egral]
48	water mass source rate
49	x aqueous relative permeability
50	x aqueous vol[umetric flux]
51	x solute flux
52	xnc aqueous vol[umetric flux (node centered)]
53	y aqueous relative permeability
54	y aqueous vol[umetric flux]
55	y solute flux
56	ync aqueous vol[umetric flux (node centered)]
57	y aqueous relative permeability
58	z aqueous vol[umetric flux]
59	z solute flux
60	znc aqueous vol[umetric flux (node centered)]

(T) Indicates a total concentration on either an aqueous or volumetric basis, and can only be used with species listed in the Conservation Equation Card that are preceded by 'total_'.

Table OC.2. STOMP-WAE Output Variables (* reference node variable only; ** plot file variable only)

Var No.	Var. Name
1	actual evaporation rate*

2	actual transpiration rate*
3	air aqueous conc[entration]
4	air aqueous mass frac[tion]
5	air gas conc[entration]
6	air gas mass frac[tion]
7	air gas mole frac[tion]
8	air mass source int[egral]
9	air mass source rate
10	air partial pressure
11	apparent aqueous saturation
12	aqueous courant [number]
13	aqueous density
14	aqueous fracture saturation
15	aqueous gauge pressure
16	aqueous hydraulic head
17	aqueous matric potential
18	aqueous moisture cont[ent]
19	aqueous pressure
20	aqueous relative perm[eability]
21	aqueous saturation
22	aqueous viscosity
23	atmospheric pressure*
24	atmospheric relative humidity*
25	atmospheric solar radiation*
26	atmospheric temperature*
27	atmospheric wind speed*
28	axial aqueous flux*
29	axial gas flux*
30	bare-soil aero[dynamic resistance] *
31	bare-surface aero[dynamic resistance] *
32	diffusive porosity
33	dissolved air saturation
34	effective trapped air

35	energy source int[egral]
36	energy source rate
37	gas courant [number]
38	gas density
39	gas fracture saturation
40	gas gauge pressure
41	gas hydraulic head
42	gas matrix saturation
43	gas pressure
44	gas relative perm[eability]
45	gas saturation
46	integrated air mass*
47	integrated aqueous air [mass]*
48	integrated aqueous water [mass] *
49	integrated gas air [mass]*
50	integrated gas water [mass] *
51	integrated trapped gas air*
52	integrated water mass*
53	phase condition
54	plant temperature
55	potential evaporation rate*
56	potential transpiration rate*
57	rainfall interception mass*
58	rock/soil type
59	solute aqueous conc[entration]
60	solute aqueous mole fra[ction]
61	solute gas conc[entration]
62	solute gas mole fra[ction]
63	solute source int[egral]
64	solute volumetric conc[entration]
65	stomatal resistance*
66	surface aqueous pressure*
67	surface aqueous saturation*

68	surface gas pressure*
69	surface ground heat flux*
70	surface latent heat flux*
71	surface mass precipitation*
72	surface net long-wave rad[iation] *
73	surface net-short wave rad[iation] *
74	surface net total rad[iation] *
75	surface sensible heat flux*
76	surface volumetric precipitation*
77	surface temperature*
78	surface vapor pressure*
79	surface water mass bal[ance] *
80	temperature
81	total air mass frac[tion]
82	total water mass frac[tion]
83	vertical aqueous flux
84	vertical gas flux
85	water aqueous conc[entration]
86	water aqueous mass frac[tion]
87	water gas conc[entration]
88	water gas mass frac[tion]
89	water gas mole frac[tion]
90	water mass source int[egral]
91	water mass source rate
92	water vapor partial pressure
93	x aqueous vol[umetric flux]
94	x gas vol[umetric flux]
95	x heat flux
96	x solute flux
97	x thermal cond[uctivity]
98	xnc aqueous vol[umetric flux (node centered)]
99	xnc gas vol[umetric flux (node centered)]
100	xnc heat flux (node centered)

101	y aqueous vol[umetric flux]
102	y gas vol[umetric flux]
103	y heat fluxy solute flux
104	y thermal cond[uctivity]
105	ync aqueous vol[umetric flux (node centered)]
106	ync gas vol[umetric flux (node centered)]
107	ync heat flux (node centered)
108	z aqueous vol[umetric flux]
109	z gas vol[umetric flux]
110	z heat fluxz solute flux
111	z thermal cond[uctivity]
112	znc aqueous vol[umetric flux (node centered)]
113	znc gas vol[umetric flux (node centered)]
114	znc heat flux (node centered)

Table OC.3. STOMP-WO Output Variables (* reference node variable only; ** plot file variable only)

Var No.	Var. Name
1	apparent aqueous saturation
2	apparent total saturation
3	apparent aqueous saturation
4	aqueous courant [number]
5	aqueous density
6	aqueous gauge pressure
7	aqueous hydraulic head
8	aqueous moisture cont[ent]
9	aqueous pressure
10	aqueous relative perm[eability]
11	aqueous saturation
12	aqueous viscosity
13	aqueous trapped gas saturation
14	diffusive porosity
15	entrapped napl-water interfacial area
16	effective trapped gas saturation

17	effective trapped napl saturation
18	free napl saturation
19	free napl-water interfacial area
20	gas-free napl interfacial area
21	gas-water interfacial area
22	integrated aqueous water [mass]*
23	integrated aqueous oil [mass]*
24	integrated oil mass*
25	integrated water mass*
26	mobile napl saturation
27	napl courant [number]
28	napl density
29	napl gauge pressure
30	napl hydraulic head
31	napl moisture cont[ent]
32	napl pressure
33	napl relative perm[eability]
34	napl saturation
35	napl trapped gas saturation
36	oil aqueous conc[entration]
37	oil aqueous mass frac[tion]
38	oil gas conc[entration]
39	oil gas mass frac[tion]
40	oil gas mole frac[tion]
41	oil mass source int[egral]
42	oil mass source rate
43	phase condition
44	residual napl saturation
45	rock/soil type
46	solute aqueous conc[entration]
47	solute aqueous mole frac[tion]
48	solute napl conc[entration]
49	solute napl mole frac[tion]

50	solute source int[egral]
51	solute volumetric conc[entration]
52	temperature
53	total moisture cont[ent]
54	total oil mass
55	total saturation
56	total water mass
57	total well flow rate*
58	trapped gas saturation
59	trapped napl saturation
60	water aqueous conc[entration]
61	water aqueous mass frac[tion]
62	water gas conc[entration]
63	water gas mass frac[tion]
64	water gas mole frac[tion]
65	water mass source int[egral]
66	water mass source rate
67	well depth*
68	x aqueous vol[umetric flux]
69	x napl vol[umetric flux]
70	x solute flux
71	xnc aqueous vol[umetric flux (node centered)]
72	xnc napl vol[umetric flux (node centered)]
73	y aqueous vol[umetric flux]
74	y napl vol[umetric flux]
75	y solute flux
76	ync aqueous vol[umetric flux (node centered)]
77	ync napl vol[umetric flux (node centered)]
78	z aqueous vol[umetric flux]
79	z napl vol[umetric flux]
80	z solute flux
81	znc aqueous vol[umetric flux (node centered)]
82	znc napl vol[umetric flux (node centered)]

Table OC.4. STOMP-WOA Output Variables (* reference node variable only; ** plot file variable only)

Var No.	Var. Name
1	air aqueous conc[entration]
2	air aqueous mass frac[tion]
3	air gas conc[entration]
4	air gas mass frac[tion]
5	air gas mole frac[tion]
6	air mass source int[egral]
7	air mass source rate
8	air partial pressure
9	apparent total saturation
10	apparent aqueous saturation
11	aqueous courant [number]
12	aqueous density
13	aqueous gauge pressure
14	aqueous hydraulic head
15	aqueous moisture cont[ent]
16	aqueous pressure
17	aqueous relative perm[eability]
18	aqueous saturation
19	aqueous viscosity
20	diffusive porosity
21	effective trapped gas saturation
22	effective trapped napl saturation
23	free napl saturation
24	gas courant [number]
25	gas density
26	gas gauge pressure
27	gas hydraulic head
28	gas pressure
29	gas relative perm[eability]
30	integrated air mass*
31	integrated aqueous air [mass]*
32	integrated aqueous oil [mass]*

33	integrated aqueous water [mass]*
34	integrated gas air [mass]*
35	integrated gas oil [mass]*
36	integrated gas water [mass]*
37	integrated oil mass*
38	integrated water mass*
39	gas saturation
40	mobile napl saturation
41	napl courant [number]
42	napl density
43	napl gauge pressure
44	napl hydraulic head
45	napl moisture cont[ent]
46	napl pressure
47	napl relative perm[eability]
48	napl saturation
49	napl vapor partial pressure
50	oil aqueous conc[entration]
51	oil aqueous mass frac[tion]
52	oil gas conc[entration]
53	oil gas mass frac[tion]
54	oil gas mole frac[tion]
55	oil mass source int[egral]
56	oil mass source rate
57	phase condition
58	residual napl saturation
59	rock/soil type
60	solute aqueous conc[entration]
61	solute aqueous mole frac[tion]
62	solute gas conc[entration]
63	solute gas mole frac[tion]
64	solute napl conc[entration]
65	solute napl mole frac[tion]

66	solute source int[egral]
67	solute volumetric conc[entration]
68	temperature
69	total air mass
70	total moisture cont[ent]
71	total oil mass
72	total saturation
73	total water mass
74	trapped gas saturation
75	trapped napl saturation
76	water aqueous conc[entration]
77	water aqueous mass frac[tion]
78	water gas conc[entration]
79	water gas mass frac[tion]
80	water gas mole frac[tion]
81	water mass source int[egral]
82	water mass source rate
83	water vapor partial pressure
84	x aqueous vol[umetric flux]
85	x gas vol[umetric flux]
86	x napl vol[umetric flux]
87	x solute flux
88	xnc aqueous vol[umetric flux (node centered)]
89	xnc gas vol[umetric flux (node centered)]
90	xnc napl vol[umetric flux (node centered)]
91	y aqueous vol[umetric flux]
92	y gas vol[umetric flux]
93	y napl vol[umetric flux]
94	y solute flux
95	ync aqueous vol[umetric flux (node centered)]
96	ync gas vol[umetric flux (node centered)]
97	ync napl vol[umetric flux (node centered)]
98	z aqueous vol[umetric flux]

99	z gas vol[umetric flux]
100	z napl vol[umetric flux]
101	z solute flux
102	znc aqueous vol[umetric flux (node centered)]
103	znc gas vol[umetric flux (node centered)]
104	znc napl vol[umetric flux (node centered)]

Table OC.5. STOMP-CO2 Output Variables (* reference node variable only; ** plot file variable only)

Var No.	Var. Name
1	apparent aqueous saturation
2	aqueous courant [number]
3	aqueous density
4	aqueous fracture
5	aqueous gauge pressure
6	aqueous hydraulic head
7	aqueous matrix
8	aqueous moisture cont
9	aqueous pressure
10	aqueous relative perm[eability]
11	aqueous salt conc[entration]
12	aqueous salt mass frac[tion]
13	aqueous saturation
14	aqueous viscosity
15	CO2 Aqueous Diff[usion coefficient]
16	CO2 aqueous conc[entration]
17	CO2 aqueous mass frac[tion]
18	CO2 aqueous mole frac[tion]
19	CO2 gas conc[entration]
20	CO2 gas mass frac[tion]
21	CO2 gas mole frac[tion]
22	CO2 mass source int[egral]*
23	CO2 mass source rate
24	coupled well mass nodal CO2 rate

25	coupled well mass nodal water rate
26	coupled well press[ure]
27	coupled-well CO2 mass rate
28	coupled-well CO2 mass int[egral]
29	coupled-well water mass rate
30	coupled-well water mass integral
31	apparent aqueous saturation
32	diffusive porosity
33	effective trapped gas saturation
34	final restart**
35	gas courant [number]
36	gas density
37	gas fracture saturation
38	gas gauge pressure
39	gas hydraulic head
40	gas matrix saturation
41	gas pressure
42	gas relative perm[eability]
43	gas saturation
44	gas viscosity
45	gas-aqueous scaling [factor]
46	integrated CO2 mass*
47	integrated precipitated salt mass *
48	mean eff[ective] stress
49	no restart**
50	node number
51	osmotic eff
52	osmotic pressure
53	phase condition
54	rock/soil type
55	salt aqueous conc[entration]
56	salt aqueous mass fraction
57	salt aqueous mole frac[tion]

58	salt conc[entration]
59	salt mass source int[egral]
60	salt mass source rate *
61	salt saturation
62	similitude variable
64	solute aqueous mole frac[tion]
65	[solute species] gas conc[entration]
66	solute [solute species] integrated mass *
67	solute gas mole frac[tion]
68	[solute species] source int[egral]
69	[solute species] volumetric conc[entration]
70	source-well pres[sure]
71	temperature
72	total CO2 mass
73	total salt mass
74	total water mass
75	trapped gas sat[uration]
76	vert[ical-]equil[ibrium gas-aqueous] inter[face] eleva[tion]
77	vert[ical-]equil[ibrium] gas press[ure]
78	ver[tical-]equil[ibrium] aqu[eous] press[ure]
79	vert[ical-]equil[ibrium] gas sat[uration]
80	vert[ical-]equil[ibrium] trap[ped] gas sat[uration]
81	vert[ical-]equil[ibrium] aqu[eous] sat[uration]
82	vert[ical-]equil[ibrium] gas rel[ative] perm[eability]
83	vert[ical-]equili[brium] aqu[eous] rel[ative] perm[eability]
84	vert[ically-]int[egrated] aqu[eous] CO2 mass
85	vert[ically-]int[egrated] aqu[eous] CO2 mass [per] area
86	vert[ically-]int[egrated] CO2 mass
87	vert[ically-]int[egrated] CO2 mass [per] area
88	verti[cally-]int[egrated] gas CO2 mass
89	vert[ically-]int[egrated] gas CO2 mass [per] area
90	water aqueous conc[entration]
91	water gas conc[entration]

92	water aqueous mass frac[tion]
93	water gas diff[usion coefficient]
94	water gas mass frac[tion]
95	water gas mole frac[tion]
96	water mass source int[egral*
97	water mass source rate
98	water vapor part[ial] press[ure]
99	well-node pres[sure] *
100	x aqueous vol[umetric flux]
101	x displ[acement]
102	x gas vol[umetric flux]
103	x intrinsic perm[eability]
104	x normal strain
105	x salt flux
106	x solute flux
107	xnc aqueous vol[umetric flux (node centered)]
108	xnc gas vol[umetric flux (node centered)]
109	xnc salt flux (node centered)
110	y aqueous vol[umetric flux]
111	y displ[acement]
112	y gas vol[umetric flux]
113	y intrinsic perm[eability]
114	y normal strain
115	y salt flux
116	y solute flux
117	ync aqueous vol[umetric flux (node centered)]
118	ync gas vol[umetric flux (node centered)]
119	ync salt flux (node centered)
120	z aqueous vol[umetric flux]
121	z displ[acement]
122	z gas vol[umetric flux]
123	z intrinsic perm[eability]
124	z normal strain

125	z salt fluxz solute flux
126	znc aqueous vol[umetric flux (node centered)]
127	znc gas vol[umetric flux (node centered)]
128	znc salt flux (node centered)

Table OC.6. STOMP-CO2e Output Variables (* reference node variable only; ** plot file variable only)

Var No.	Var. Name
1	aqueous fracture
2	aqueous gauge pressure
3	aqueous hydraulic head
4	aqueous internal energy
5	aqueous matrix
6	aqueous moisture cont
7	aqueous pressure
8	aqueous relative perm[eability]
9	aqueous salt conc[entration]
10	aqueous salt mass frac[tion]
11	aqueous saturation
12	aqueous thermal
13	conduc[tivity]
14	aqueous viscosity
15	CO2 aqueous diff[usion coefficient]
16	CO2 aqueous conc[entration]
17	CO2 aqueous mass frac[tion]
18	CO2 aqueous mole frac[tion]
19	CO2 gas conc[entration]
20	CO2 gas mass frac[tion]
21	CO2 gas mole frac[tion]
22	CO2 mass source int[egral]
23	CO2 mass source rate
24	coupled well mass nodal CO2 rate
25	coupled well mass nodal water rate
26	coupled well press[ure]

27	coupled-well CO2 mass rate
28	coupled-well CO2 mass int[egral]
29	coupled-well water mass rate
30	coupled-well water mass integral
31	diffusive porosity
32	mean eff[ective] stress
33	effective trapped gas saturation
34	final restart**
35	gas courant [number]
36	gas density
37	gas enthalpy
38	gas fracture saturation
39	gas gauge pressure
40	gas hydraulic head
41	gas internal energy
42	gas matrix saturation
43	gas pressure
44	gas relative perm[eability]
45	gas saturation
46	gas thermal conduc[tivity]
47	gas viscosity
48	gas-aqueous scaling [factor]
49	integrated CO2 mass*
50	integrated aqueous CO2 [mass] *
51	integrated aqueous water [mass] *
52	integrated CO2 mass sour[ce] *
53	integrated gas CO2 [mass] *
54	integrated gas water [mass] *
55	integrated water mass sour[ce] *
56	integrated water mass*
57	integrated precipitated salt mass *
58	no restart**
59	node number

60	osmotic eff
61	osmotic pressure
62	phase condition
63	saturated CO2 aqueous mass fraction
64	rock/soil type
65	salt aqueous conc[entration]
66	salt aqueous mass fraction
67	salt aqueous mole frac[tion]
68	salt conc[entration]
69	salt mass source int[egral]
70	salt mass source rate *
71	salt saturation
72	similitude variable
73	[solute species] aqueous conc[entration]
74	solute aqueous mole frac[tion]
75	[solute species] gas conc[entration]
76	[solute species] integrated mass *
77	solute gas mole frac[tion]
78	[solute species] source int[egral]
79	[solute species] volumetric conc[entration]
80	source-well pres[sure]
81	temperature
82	total CO2 mass
83	total salt mass
84	total water mass
85	trapped gas sat[uration]
86	vert[ical-]equil[ibrium gas-aqueous] inter[face] eleva[tion]
87	vert[ical-]equil[ibrium] gas press[ure]
88	ver[tical-]equil[ibrium] aqu[eous] press[ure]
89	vert[ical-]equil[ibrium] gas sat[uration]
90	vert[ical-]equil[ibrium] trap[ped] gas sat[uration]
91	vert[ical-]equil[ibrium] aqu[eous] sat[uration]
92	vert[ical-]equil[ibrium] gas rel[ative] perm[eability]

93	vert[ical-]equili[brium] aqu[eous] rel[ative] perm[eability]
94	vert[ically-]int[egrated] aqu[eous] CO2 mass
95	vert[ically-]int[egrated] aqu[eous] CO2 mass [per] area
96	vert[ically-]int[egrated] CO2 mass
97	vert[ically-]int[egrated] CO2 mass [per] area
98	verti[cally-]int[egrated] gas CO2 mass
99	vert[ically-]int[egrated] gas CO2 mass [per] area
100	water aqueous conc[entration]
101	water aqueous mass frac[tion]
102	water gas conc[entration]
103	water gas diff[usion coefficient]
104	water gas mass frac[tion]
105	water gas mole frac[tion]
106	water mass source int[egral
107	water mass source rate
108	water vapor part[ial] press[ure]
109	well-node pres[sure] *
110	x aqueous vol[umetric flux]
111	x displ[acement]
112	x gas vol[umetric flux]
113	x intrinsic perm[eability]
114	x normal strain
115	x salt flux
116	x solute flux
117	x thermal cond[uctivity]
118	xnc aqueous vol[umetric flux (node centered)]
119	xnc gas vol[umetric flux (node centered)]
120	xnc salt flux (node centered)
121	y aqueous vol[umetric flux]
122	y displ[acement]
123	y gas vol[umetric flux]
124	y intrinsic perm[eability]
125	y normal strain

126	y salt flux
127	y solute flux
128	y thermal cond[uctivity]
129	ync aqueous vol[umetric flux (node centered)]
130	ync gas vol[umetric flux (node centered)]
131	ync salt flux (node centered)
132	z aqueous vol[umetric flux]
133	z displ[acement]
134	z gas vol[umetric flux]
135	z intrinsic perm[eability]
136	z normal strain
137	z salt flux
138	z solute flux
139	z thermal cond[uctivity]
140	znc aqueous vol[umetric flux (node centered)]
141	znc gas vol[umetric flux (node centered)]
142	znc salt flux (node centered)

Specific Safety Software Requirements for STOMP-W Include:
Reference Node and Plot File Variable Options (* reference node variable only):

OC.W.1. Apparent Aqueous Saturation

OC.W.2. Aqueous Courant

OC.W.3. Aqueous Density

OC.W.4. Aqueous Fracture Saturation

OC.W.5. Aqueous Gauge Pressure

OC.W.6. Aqueous Hydraulic Head

OC.W.7. Aqueous Matrix Saturation

OC.W.8. Aqueous Moisture Content

OC.W.9. Aqueous Pressure

OC.W.10. Aqueous Relative Permeability

OC.W.11. Aqueous Saturation

OC.W.12. Aqueous Viscosity

OC.W.13. Diffusive Porosity

OC.W.14. Effective Trapped Gas Saturation

OC.W.15. Gas Gauge Pressure

OC.W.16. Gas Pressure

OC.W.17. Gas Saturation

OC.W.18. Matric Potential

OC.W.19. Matrix Pressure

OC.W.20. Phase Condition

OC.W.21. Rock/Soil Type

OC.W.22. Temperature

OC.W.23. Total Water Mass

OC.W.24. Trapped Gas Saturation

OC.W.25. Water Mass Source Rate

OC.W.26. X Aqueous Relative Permeability

OC.W.27. Y Aqueous Relative Permeability

OC.W.28. Z Aqueous Relative Permeability

OC.W.29. X Aqueous Volumetric Flux

OC.W.30. Y Aqueous Volumetric Flux

OC.W.31. Z Aqueous Volumetric Flux

OC.W.32. XNC Aqueous Volumetric Flux (node centered)

OC.W.33. YNC Aqueous Volumetric Flux (node centered)

OC.W.34. ZNC Aqueous Volumetric Flux (node centered)

OC.W.35. Integrated Water Mass *

Specific Safety Software Requirements for eSTOMP-W Include:
Reference Node and Plot File Variable Options (* reference node variable only):

OC.eW.1. Apparent Aqueous Saturation

OC.eW.2. Aqueous Courant

OC.eW.3. Aqueous Density

OC.eW.4. Aqueous Fracture Saturation

OC.eW.5. Aqueous Gauge Pressure

OC.eW.6. Aqueous Hydraulic Head

OC.eW.7. Aqueous Matrix Saturation

OC.eW.8. Aqueous Moisture Content

OC.eW.9. Aqueous Pressure

OC.eW.10. Aqueous Relative Permeability

OC.eW.11. Aqueous Saturation

OC.eW.12. Aqueous Viscosity

OC.eW.13. Diffusive Porosity

OC.eW.14. Effective Trapped Gas Saturation

OC.eW.15. Gas Gauge Pressure

OC.eW.16. Gas Pressure

OC.eW.17. Gas Saturation

OC.eW.18. Matric Potential

OC.eW.19. Matrix Pressure

OC.eW.20. Phase Condition

OC.eW.21. Rock/Soil Type

OC.eW.22. Temperature

OC.eW.23. Total Water Mass

OC.eW.24. Trapped Gas Saturation

OC.eW.25. Water Mass Source Rate

OC.eW.26. X Aqueous Relative Permeability

OC.eW.27. Y Aqueous Relative Permeability

OC.eW.28. Z Aqueous Relative Permeability

OC.eW.29. XNC Aqueous Volumetric Flux (node centered)

OC.eW.30. YNC Aqueous Volumetric Flux (node centered)

OC.eW.31. ZNC Aqueous Volumetric Flux (node centered)

OC.eW.32. Integrated Water Mass *

Specific Safety Software Requirements for Aqueous Transport in STOMP-W Include:
Reference Node and Plot File Variable Options (* reference node variable only):

OC.W-T.1. Solute Volumetric Concentration

OC.W-T.2. Solute Aqueous Concentration

OC.W-T.3. Solute Aqueous Mole Fraction

OC.W-T.4. Solute Inventory

OC.W-T.5. Solute Source Integral

OC.W-T.6. X- Solute Flux

OC.W-T.7. Y- Solute Flux

OC.W-T.8. Z- Solute Flux

OC.W-T.9. Solute Integrated Mass*

OC.W-T.10. Solute Integrated Aqueous*

Specific Safety Software Requirements for Aqueous Transport in eSTOMP-W Include:
Reference Node and Plot File Variable Options (* reference node variable only):

OC.eW-T.1. Solute Volumetric Concentration

OC.eW-T.2. Solute Aqueous Concentration

OC.eW-T.3. Solute Aqueous Mole Fraction

OC.eW-T.4. Solute Inventory

OC.eW-T.5. Solute Source Integral

OC.eW-T.6. Solute Integrated Mass *

OC.eW-T.7. Solute Integrated Aqueous *

OC.eW-T.8. X- Solute Flux *

OC.eW-T.9. Y- Solute Flux *

OC.eW-T.10. Z- Solute Flux *

Specific Safety Software Requirements for STOMP-W-R Include:
Reference Node and Plot File Variable Options:

OC.W-R.1. Species Aqueous Concentration

OC.W-R.2. Species Volumetric Concentration

OC.W-R.3. Solid Species Aqueous Concentration (T)

OC.W-R.4. Solid Species Volumetric Concentration (T)

OC.W-R.5. Exchange Species Aqueous Concentration (T)

OC.W-R.6. Exchange Species Volumetric Concentration (T)

OC.W-R.7. Species Integrated Mass

OC.W-R.8. Species Mineral Area

OC.W-R.9. Species Mineral Rate

(T) Indicates a total concentration on either an aqueous or volumetric basis, and can only be used with species listed in the Conservation Equation Card that are preceded by 'total_'.

Specific Safety Software Requirements for eSTOMP-W-R Include:
Reference Node and Plot File Variable Options:

OC.eW-R.1. Species Aqueous Concentration

OC.eW-R.2. Species Volumetric Concentration

OC.eW-R.3. Solid Species Aqueous Concentration (T)

OC.eW-R.4. Solid Species Volumetric Concentration (T)

OC.eW-R.5. Exchange Species Aqueous Concentration (T)

OC.eW-R.6. Exchange Species Volumetric Concentration (T)

OC.eW-R.7. Species Integrated Mass

OC.eW-R.8. Species Mineral Area

OC.eW-R.9. Species Mineral Rate

(T) Indicates a total concentration on either an aqueous or volumetric basis, and can only be used with species listed in the Conservation Equation Card that are preceded by 'total_'.

Specific Safety Software Requirements for STOMP-WAE Include:
Output Variable Options:

OC.WAE.1. Total Water Mass Fraction

OC.WAE.2. Water Aqueous Concentration

OC.WAE.3. Water Gas Concentration

OC.WAE.4. Water Gas Mass Fraction

OC.WAE.5. Water Gas Mole Fraction

OC.WAE.6. Energy Source Integral

OC.WAE.7. Energy Source Rate

OC.WAE.8. X Thermal Conductivity

OC.WAE.9. Y Thermal Conductivity

OC.WAE.10. Z Thermal Conductivity

OC.WAE.11. X Heat Flux

OC.WAE.12. XNC Heat Flux (node centered)

OC.WAE.13. Y Heat Flux

OC.WAE.14. YNC Heat Flux (node centered)

OC.WAE.15. Z Heat Flux

OC.WAE.16. ZNC Heat Flux (node centered)

OC.WAE.17. Air Aqueous Concentration

OC.WAE.18. Air Aqueous Mass Fraction

OC.WAE.19. Air Gas Concentration

OC.WAE.20. Air Gas Mass Fraction

OC.WAE.21. Air Gas Mole Fraction

OC.WAE.22. Air Mass Source Integral

OC.WAE.23. Air Mass Source Rate

OC.WAE.24. Gas Courant Number

OC.WAE.25. Gas Density

OC.WAE.26. Gas Fracture Saturation

OC.WAE.27. Gas Hydraulic Head

OC.WAE.28. Gas Matrix Saturation

OC.WAE.29. Gas Relative Permeability

OC.WAE.30. Integrated Air Mass

OC.WAE.31. Integrated Aqueous Air Mass

OC.WAE.32. Integrated Gas Air Mass

OC.WAE.33. Integrated Gas Water Mass

OC.WAE.34. Total Air Mass Fraction

OC.WAE.35. X Gas Volumetric Flux

OC.WAE.36. XNC Gas Volumetric Flux (node centered)

OC.WAE.37. Y Gas Volumetric Flux

OC.WAE.38. YNC Gas Volumetric Flux (node centered)

OC.WAE.39. Z Gas Volumetric Flux

OC.WAE.40. ZNC Gas Volumetric Flux (node centered)

OC.WAE.41. Water Vapor Partial Pressure

OC.WAE.42. Water Relative Humidity

Specific Safety Software Requirements for STOMP-WAE-B Include:
Output Variable Options:

OC.WAE-B.1. Atmospheric Solar Radiation

OC.WAE-B.2. Surface Net Long-Wave Radiation

OC.WAE-B.3. Surface Net Short-Wave Radiation

OC.WAE-B.4. Surface Sensible Heat Flux

OC.WAE-B.5. Surface Latent Heat Flux

OC.WAE-B.6. Surface Ground Heat Flux

OC.WAE-B.7. Atmospheric Temperature

OC.WAE-B.8. Surface Temperature

OC.WAE-B.9. Surface Volumetric Precipitation

OC.WAE-B.10. Potential Evaporation

OC.WAE-B.11. Actual Evaporation

OC.WAE-B.12. Potential Transpiration

OC.WAE-B.13. Actual Transpiration

Specific Safety Software Requirements for STOMP-WOA Include:
Output Variable Options:

OC.WOA.1. Apparent Total Saturation

OC.WOA.2. Aqueous Trapped Gas Saturation

OC.WOA.3. Water Aqueous Concentration

OC.WOA.4. Water Gas Concentration

OC.WOA.5. Water Gas Mass Fraction

OC.WOA.6. Water Gas Mole Fraction

OC.WOA.7. NAPL Courant Number

OC.WOA.8. NAPL Density

OC.WOA.9. NAPL Gauge Pressure

OC.WOA.10. NAPL Hydraulic Head

OC.WOA.11. NAPL Moisture Content

OC.WOA.12. NAPL Pressure

OC.WOA.13. NAPL Relative Permeability

OC.WOA.14. NAPL Saturation

OC.WOA.15. Oil Aqueous Concentration

OC.WOA.16. Oil Aqueous Mass Fraction

OC.WOA.17. Oil Gas Concentration

OC.WOA.18. Oil Gas Mass Fraction

OC.WOA.19. Oil Gas Mole Fraction

OC.WOA.20. Oil Mass Source Integral

OC.WOA.21. Oil Mass Source Rate

OC.WOA.22. Total Moisture Content

OC.WOA.23. Total Oil Mass

OC.WOA.24. Total Saturation

OC.WOA.25. Trapped NAPL Saturation

OC.WOA.26. X NAPL Volumetric Flux

OC.WOA.27. XNC NAPL Volumetric Flux (node centered)

OC.WOA.28. Y NAPL Volumetric Flux

OC.WOA.29. YNC NAPL Volumetric Flux (node centered)

OC.WOA.30. Z NAPL Volumetric Flux

OC.WOA.31. ZNC NAPL Volumetric Flux (node centered)

OC.WOA.32. Effective Trapped NAPL Saturation

OC.WOA.33. Free NAPL Saturation

OC.WOA.34. Integrated Aqueous Oil Mass

OC.WOA.35. Integrated Oil Mass

OC.WOA.36. Mobile NAPL Saturation

OC.WOA.37. Residual NAPL Saturation

OC.WOA.38. Air Aqueous Concentration

OC.WOA.39. Air Aqueous Mass Fraction

OC.WOA.40. Air Gas Concentration

OC.WOA.41. Air Gas Mass Fraction

OC.WOA.42. Air Gas Mole Fraction

OC.WOA.43. Air Mass Source Integral

OC.WOA.44. Air Mass Source Rate

OC.WOA.45. Gas Courant Number

OC.WOA.46. Gas Density

OC.WOA.47. Gas Hydraulic Head

OC.WOA.48. Gas Relative Permeability

OC.WOA.49. Integrated Air Mass

OC.WOA.50. Integrated Aqueous Air Mass

OC.WOA.51. Integrated Gas Air Mass

OC.WOA.52. Integrated Gas Oil Mass

OC.WOA.53. Total Air Mass

OC.WOA.54. X Gas Volumetric Flux

OC.WOA.55. XNC Gas Volumetric Flux (node centered)

OC.WOA.56. Y Gas Volumetric Flux

OC.WOA.57. YNC Gas Volumetric Flux (node centered)

OC.WOA.58. Z Gas Volumetric Flux

OC.WOA.59. ZNC Gas Volumetric Flux (node centered)

Specific Safety Software Requirements for STOMP-WO Include:
Output Variable Options:

OC.WO.1. Water Aqueous Concentration

OC.WO.2. Water Gas Concentration

OC.WO.3. Water Gas Mass Fraction

OC.WO.4. Water Gas Mole Fraction

OC.WO.5. Well Depth

OC.WO.6. Apparent Total Saturation

OC.WO.7. NAPL Courant Number

OC.WO.8. NAPL Density

OC.WO.9. NAPL Gauge Pressure

OC.WO.10. NAPL Hydraulic Head

OC.WO.11. NAPL Moisture Content

OC.WO.12. NAPL Pressure

OC.WO.13. NAPL Relative Permeability

OC.WO.14. NAPL Saturation

OC.WO.15. Oil Aqueous Concentration

OC.WO.16. Oil Aqueous Mass Fraction

OC.WO.17. Oil Gas Concentration

OC.WO.18. Oil Gas Mass Fraction

OC.WO.19. Oil Gas Mole Fraction

OC.WO.20. Oil Mass Source Integral

OC.WO.21. Oil Mass Source Rate

OC.WO.22. Total Moisture Content

OC.WO.23. Total Oil Mass

OC.WO.24. Total Saturation

OC.WO.25. Trapped NAPL Saturation

OC.WO.26. X NAPL Volumetric Flux

OC.WO.27. XNC NAPL Volumetric Flux (node centered)

OC.WO.28. Y NAPL Volumetric Flux

OC.WO.29. YNC NAPL Volumetric Flux (node centered)

OC.WO.30. Z NAPL Volumetric Flux

OC.WO.31. ZNC NAPL Volumetric Flux (node centered)

OC.WO.32. Effective Trapped NAPL Saturation

OC.WO.33. Free NAPL Saturation

OC.WO.34. Integrated Aqueous Oil Mass

OC.WO.35. Integrated Oil Mass

OC.WO.36. Mobile NAPL Saturation

OC.WO.37. Residual NAPL Saturation

Specific Safety Software Requirements for STOMP-WO with Transport Include:
Output Variable Options:

OC.WO-T.1. Solute Volumetric Concentration

OC.WO-T.2. Solute Aqueous Concentration

OC.WO-T.3. Solute Aqueous Mole Fraction

OC.WO-T.4. Solute Integrated Mass

OC.WO-T.5. Solute Source Integral

OC.WO-T.6. X Solute Flux

OC.WO-T.7. Y Solute Flux

OC.WO-T.8. Z Solute Flux

Specific Safety Software Requirements for STOMP-CO2 and STOMP-CO2e Include:
Output Variable Options:

OC.CO2(e).1. Aqueous Density

OC.CO2(e).2. Aqueous Pressure

OC.CO2(e).3. Aqueous Relative Permeability

OC.CO2(e).4. Aqueous Saturation

OC.CO2(e).5. Aqueous Viscosity

OC.CO2(e).6. CO2 Aqueous Concentration

OC.CO2(e).7. CO2 Aqueous Mass Fraction

OC.CO2(e).8. CO2 Gas Mass Fraction

OC.CO2(e).9. Diffusive Porosity

OC.CO2(e).10. Gas Density

OC.CO2(e).11. Gas Pressure

OC.CO2(e).12. Gas Relative Permeability

OC.CO2(e).13. Gas Saturation

OC.CO2(e).14. Gas Viscosity

OC.CO2(e).15. Integrated Aqueous CO2 Mass

OC.CO2(e).16. Integrated CO2 Mass

OC.CO2(e).17. Integrated Gas CO2 Mass

OC.CO2(e).18. Integrated CO2 Trapped-Gas Mass

OC.CO2(e).19. Phase Condition

OC.CO2(e).20. Rock/Soil Type

OC.CO2(e).21. Salt Aqueous Mass Fraction

OC.CO2(e).22. Salt Saturation

OC.CO2(e).23. Similitude Variable

OC.CO2(e).24. Species Aqueous Concentration

OC.CO2(e).25. Trapped Gas Saturation

OC.CO2(e).26. Water Gas Mass Fraction

Specific Safety Software Requirements for STOMP-CO2e Include:

OC.CO2e.1. Temperature

OC.CO2e.2. X Thermal Cond[uctivity]

OC.CO2e.3. Y Thermal Cond[uctivity]

OC.CO2e.4. Z Thermal Cond[uctivity]

OC.CO2e.5. XNC Heat Flux (node centered)

OC.CO2e.6. ZNC Heat Flux (node centered)

4.4 Saturation Function Card Requirements

This card allows users to declare and define a saturation-capillary pressure function for each defined rock/soil type (Table S.F.1). However, saturation function types and the required input items vary greatly among the operational modes. Operational modes that consider NAPL flow require interfacial tension parameters. The saturation function models, model options and model parameters are given below.

- For the operational mode where oil transport is involved, fluid pair interfacial tension is required before the saturation function is declared.
- The van Genuchten (VG) and Brook and Corey (BC) function are available for all operational modes. For the VG function, the 'm' parameter can be defaulted (with a *null* entry) or assigned a value. Default values will depend on which relative permeability model (Mualem or Burdine) is chosen in the Aqueous Relative Permeability Card.
- The entrapment VG and entrapment BC functions are available in all modes except -WAE. 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 fractured VG and fractured BC functions: These options are used for a fractured medium. The retention properties for both the fracture and the matrix are needed. Dual porosity functions or equivalent continuum models for aqueous-gas systems relate the gas-aqueous capillary pressure to the bulk aqueous saturation for fractured geologic media through two functions [Klavetter and Peters 1986; Nitao 1988].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 consider the hysteresis of the saturation curve for the Van Genuchten or Brooks Corey model and are available in -W.
- The residual VG and residual BC functions: These options are available for the operational modes with oil flow but without energy transport.

- The Extended VG and Extended BC functions.
- 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 is available for all the operational modes without oil flow. This option accepts the tabulated retention data. The default is the data of pressure head and saturation data pairs and linear interpolation is used between data points. Alternately, water content vs capillary head can be provided using the keyword "water content." Other interpolation schemes that can be specified are linear-log, cubic spline, or cubic-spline-log.
- The van Geel VG, Lenhard VG, Constant VG, van 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 - capillary pressure function properties include:

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

Table SF.1. Saturation Function Options

Operational Mode Name	**STOMP-W**	**STOMP-WAE**	**STOMP-WO**	**STOMP-WOA**	**STOMP-CO2**	**STOMP-CO2e**
Operational Mode Code	**1**	**3**	**4**	**5**	**32**	**33**
VG, BC	x	x	x	x	x	x
Entrapment VG, Entrapment BC	x		x	x	x	x
Fractured VG, Fractured BC	x	x			x	x
Triple VG, Triple BC	x					
Extended VG, Extended BC		x			x	x
Haverkamp	x				x	x
Tabular	x	x			x	x
Residual VG, Residual BC			x	x		
van Geel VG, Lenhard VG, Constant VG van Geel BC, Lenhard BC, Constant BC			x	x		

Specific Safety Software Requirements for Water in STOMP-W, STOMP-WO, and STOMP-W-R Include:

SF.W.1. Van Genuchten Saturation-Capillary Pressure Function

SF.W.2. Brooks and Corey Saturation-Capillary Pressure Function

SF.W.3. Explicit declaration of saturation properties

SF.W.4. Declaration of saturation properties: IJK Indexing

Specific Safety Software Requirements for Water in eSTOMP-W and eSTOMP-W-R Include:

SF.eW.1. Van Genuchten Saturation-Capillary Pressure Function

SF.eW.2. Brooks and Corey Saturation-Capillary Pressure Function

SF.eW.3. Explicit declaration of saturation properties

SF.eW.4. Declaration of saturation properties: IJK Indexing

Specific Safety Software Requirements for STOMP-WAE Include:

SF.WAE.1. Van Genuchten Saturation-Capillary Pressure Function

SF.WAE.2. Van Genuchten/Webb Saturation-Capillary Pressure Function

SF.WAE.3. Rossi-Nimmo-Junction Saturation-Capillary Pressure Function

SF.WAE.4. Rossi-Nimmo-Sum Saturation-Capillary Pressure Function

SF.WAE.5. Explicit declaration of saturation properties

Specific Safety Software Requirements for STOMP-WAE-B Include:

SF.WAE-B.1. Extended van Genuchten Saturation-Capillary Function Pressure Function

SF.WAE-B.2. Extended Brooks and Corey Saturation-Capillary Function Pressure Function

SF.WAE-B.3. Explicit declaration of saturation properties

Specific Safety Software Requirements for STOMP-WO Include:

SF.WO-O.1. Van Genuchten Saturation-Capillary Pressure Function

SF.WO-O.2. Brooks and Corey with Residual Saturation-Capillary Pressure Function

SF.WO-O.3. Explicit declaration of saturation properties

Specific Safety Software Requirements for STOMP-WO with Transport Include:

SF.WO-T.1. Van Genuchten Saturation-Capillary Pressure Function

SF.WO-T.2. Entrapment Van Genuchten Saturation-Capillary Pressure Function

SF.WO-T.3. Explicit declaration of saturation properties

Specific Safety Software Requirements for STOMP-WOA Include:

SF.WOA.1. Van Genuchten Saturation-Capillary Pressure Function

SF.WOA.2. Explicit declaration of saturation properties

Specific Safety Software Requirements for STOMP-CO2 and STOMP-CO2e Include:

SF.CO2(e).1. Van Genuchten Saturation-Capillary Pressure Function

SF.CO2(e).2. Brooks and Corey Saturation-Capillary Pressure Function

SF.CO2(e).3. Extended Brooks and Corey Saturation-Capillary Pressure Function

SF.CO2(e).4. Explicit Declaration of saturation properties

4.5 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.

Requirements include:

- Solute aqueous effective diffusion options:
    - Constant

    - Conventional
    - Empirical (Kemper and van Schaik)
    - Power Function

- Solid Aqueous partition options:
    - Continuous
    - Noncontinuous

- Gas-Aqueous partition options:
    - Constant
    - Temperature Dependent

- Reaction options:
    - No reaction: no reaction occurs
    - Radioactive decay: decay or generation of solutes occurs in the STOMP simulator through an Arrhenius type kinetic reaction. Required for all operational modes involving radioactive decay.
    - First-order reaction: decay is simulated based on the first-order and Monod chemical reactions.

- Aqueous-NAPL adsorption options:
    - Linear Isotherm
    - Freundlich
    - Langmuir

Specific Safety Software Requirements for Aqueous Transport in STOMP-W Include:

SFI.W-T.1. Solute Aqueous Effective Diffusion Option: Conventional

SFI.W-T.2. Solute Aqueous Effective Diffusion Option: Constant

SFI.W-T.3. Solute-Aqueous Partition Option: Continuous

SFI.W-T.4. Solute-Aqueous Partition Option: Noncontinuous

SFI.W-T.5. Reaction Option: No reaction

SFI.W-T.6. Reaction Option: Radioactive Decay

Specific Safety Software Requirements for Aqueous Transport in eSTOMP-W Include:

SFI.eW-T.1. Solute Aqueous Effective Diffusion Option: Conventional

SFI.eW-T.2. Solute Aqueous Effective Diffusion Option: Constant

SFI.eW-T.3. Solute-Aqueous Partition Option: Continuous

SFI.eW-T.4. Solute-Aqueous Partition Option: Noncontinuous

SFI.eW-T.5. Reaction Option: No reaction

SFI.eW-T.6. Reaction Option: Radioactive Decay

Specific Safety Software Requirements for STOMP-WOA Include:

SFI.WOA.1. Gas-Aqueous Partition Option: Constant

Specific Safety Software Requirements for STOMP-WO with Transport Include:

SFI.WO-T.1. Aqueous-NAPL Adsorption Option: Linear Isotherm

4.6 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. This card differs from the *Solute/Fluid Interaction Card* because the input parameters declared are dependent on both the solute and rock/soil type. For every solute defined on the *Solute/Fluid Interaction Card*, every rock/soil type defined on the *Rock/Soil Zonation Card* must be referenced.

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 dispersivities 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.
- Solid-Aqueous partition coefficient defines the interface equilibrium of a solute adsorbed on the solid and dissolved in the aqueous phase, and refers to the concentration of solute adsorbed on the solid phase (per unit mass of solid phase) over the concentration of solute dissolved in the aqueous phase (per unit mass aqueous phase).
- With IJK Indexing option, node dependent parameters are entered via external files, and node independent parameters are entered directly on the card.

- For the operational mode STOMP-W, the macrodispersivity enhancement factor is optional.
- For the operational mode STOMP-W, additional parameters are required if the effective diffusion in the *Solute/Fluid Card* is *Empirical or Power. Power* Option *is not currently implemented in eSTOMP).*

Specific Safety Software Requirements for Aqueous Transport in STOMP-W Include:

SPM.W-T.1. Longitudinal Dispersivity specified

SPM.W-T.2. Transverse Dispersivity specified

SPM.W-T.3. Solid-Aqueous Partition Coefficient specified (non-zero value)

SPM.W-T.4. Macrodispersivity Enhancement Factor specified (non-zero value)

SPM.W-T.5. Explicit Declaration

Specific Safety Software Requirements for Aqueous Transport in eSTOMP-W Include:

SPM.eW-T.1. Longitudinal Dispersivity specified

SPM.eW-T.2. Transverse Dispersivity specified

SPM.eW-T.3. Solid-Aqueous Partition Coefficient specified (non-zero value)

SPM.eW-T.4. Macrodispersivity Enhancement Factor specified (non-zero value)

SPM.eW-T.5. Explicit Declaration

4.7 Solution Control Card Requirements

This card controls many of the general operational aspects of a simulation. The execution mode (*Normal* or *Restart)* and execution parameters such as time stepping and convergence criterion can be specified. Keywords can be included to indicate that solute transport or reactive transport are to be solved. In addition, when solving for solute or reactive transport, the user may choose to compute the coupled flow and transport equations only once, eliminating the flow calculations at each time step for a transport problem with a steady flow field. This card also allows the user to specify certain solution schemes if the default approach is not appropriate for a particular problem.

Two *Execution Mode* options are recognized: *Normal*, and *Restart*. In the *Normal* mode, initial state conditions are declared through the *Initial Conditions Card*. In the *Restart* mode, initial state conditions are assigned via a restart file from a previous execution or declared through the *Initial Conditions Card*, using the special *Overwrite* option for selected parameters.

Execution Mode 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 until the declared stop time, the declared number of time steps, an execution error, or a sequence of convergence failures; requires a file named '*rest art*' in the working directory.
- Restart file: This option triggers STOMP to read an additional character string, which is the name of the restart file.

Other *Execution Mode* options are dependent on operational modes and include:

- 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 inverse, Restart inverse: These options will trigger the capability for inverse simulations.
- Normal PETSc, Restart PETSc: the PETSc solver is used.

The line following the execution modes declares the *Operational Mode* with modifiers. Only water flow will be simulated when there are no other modifier options after the operational mode identifier. The options that follow the operational mode identifier vary among the operational modes and are summarized in Table SC.1.

Operational Mode Modifier options recognized in all operational modes include:

- Transport (or Patankar Transport): Solute transport is solved using the Patankar method
- Leonard-TVD Transport: Solute transport is solved using the TVD method
- Roe's Superbee Transport
- First Order Upwind
- 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 Operational Mode Modifier options are dependent on the operational modes:

- No Gas Advection Transport (for operational modes that involve gas transport)
- No NAPL Advection Transport (for operational modes that involve NAPL transport)
- Electrolyte Transport (for STOMP-W and -W-R)
- Partitioning Transport, Kinetic Transport (for STOMP-WO)
- LFL Transport, Osmotic Surface Tension Transport, Surface Tension Transport (for operational modes that involve salt transport)
- Poynting Transport (for operational modes that involve CO_2 transport)
- EckeChem, EckeChem Transport, EckeChem Equilibrium Reduced, EckeChem Minimum Concentration, EckeChem Log, EckeChem Guess, EckeChem Flow Velocity Hydraulic Dispersion Coefficient, EckeChem Flux Velocity Hydraulic Dispersion Coefficient, EckeChem Porosity Alteration with Precipitation, EckeChem Effective Reaction Area, EckeChem Constant Surface Area (for STOMP-W-R)
- Isobrine Transport (for STOMP-CO2e only)

Table SC.1. Operational Mode Modifier Options in the Solution Control Card

Operational Mode Name	**STOMP-W**	**STOMP-WAE**	**STOMP-WO**	**STOMP-WOA**	**STOMP-CO2**	**STOMP-CO2e**
Operational Mode Code	**1**	**3**	**4**	**5**	**32**	**33**
Transport (Patankar)	x	x	x	x	x	x
Courant Transport	x	x	x	x	x	x
Vadose Courant Transport	x	x	x	x	x	x
TVD Transport	x	x	x	x	x	x
Roe Superbee Transport	x	x	x	x	x	x
First Order Upwind Transport	x	x	x	x	x	x

No Vapor Transport		x	x	x	x	x
No Gas Advection Transport		x		x		
No NAPL Advection Transport			x	x		
Electrolyte Transport	x					
[Partitioning] [Kinetic]			x			
LFL Transport					x	x
Osmotic Surface Tension Transport					x	x
Surface Tension Transport					x	x
Poynting Transport					x	x
Time Lag		x				
[Globally][Guess] EckeChem	x					
Equilibrium Reduced EckeChem	x					
Minimum Concentration EckeChem	x					
Log EckeChem	x					
Porosity Alteration with Precipitation EckeChem	x					
Effective Reaction Area EckeChem	x					
Constant Surface Area EckeChem	x					

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 the operational modes with the multifluid flow simulation, specifying the diffusion of the advective and dissolved fluids is required (Table SC.2). Other special transport-related options (e.g., Clay Mass Fraction, Electrolyte Density Function) are also specified here.

Table SC.2. Diffusion Options and Their Transport Options in the Solution Control Card

Operational Mode Name	**STOMP-W**	**STOMP-WAE**	**STOMP-WO**	**STOMP-WOA**	**STOMP-CO2**	**STOMP-CO2e**
Operational Mode Code	**1**	**3**	**4**	**5**	**32**	**33**
Zero Aqueous Diffusion		x	x	x		
Constant Aqueous Diffusion		x	x	x		
Variable Aqueous Diffusion		x	x	x		
Zero Gas Diffusion		x	x	x		
Constant Gas Diffusion		x	x	x		
Variable Gas Diffusion		x	x	x		

Enhanced Gas Diffusion				x	x	x
Water Vapor Diffusion Coeff				x	x	x
Dissolved Air diffusion Coeff		x		x		
Dissolved Oil diffusion Coeff				x		
Dissolved CO2 Diffusion Coeff					x	x
Oil Vapor diffusion Coeff				x		
Clay Mass Fraction				x		
Electrolyte Density Function(d)	x					

State variables at the centroids of grid-cell surfaces are required to compute fluxes between grid-cell centroids. Models for computing the state variables on grid-cell surfaces are referred to as *Interfacial Averaging Schemes* and use the state variables at adjacent grid-cells to compute the surface variables.

Field variables, which include physical, thermodynamic, and hydrologic properties, are defined in the finite-difference formulation at the node centers. Conversely, flux variables are defined at node interfaces. Computation of flux variables requires knowledge of field variables at node interfaces. Values of flux variables at node interfaces are evaluated by averaging the field values for the two nodes adjoining an interfacial surface. Interfacial averaging schemes may be declared individually for each field variable through the *Interfacial Averaging Variables* input.

The default interfacial averaging schemes for the simulator are shown in the Table SC.3.

Table SC.3. Default Interfacial Averaging Schemes.

Field Variable	***Default Interfacial Averaging Scheme***
Aqueous Density	Upwind
Aqueous Relative Permeability	Upwind
Aqueous Viscosity	Harmonic
Hydraulic Dispersion	Harmonic
Intrinsic Permeability	Harmonic
Solute Diffusion	Harmonic

Specific Safety Software Requirements for Water in STOMP-W, and STOMP-WO Include:

SC.W.1. Execution Mode: Normal

SC.W.2. Execution Mode: Restart (with *Default* Restart Name)

SC.W.3. Execution Mode: Restart File (with *Specified* Restart File Name)

SC.W.4. Single Execution Time Period

SC.W.5. Multiple Execution Time Periods

SC.W.6. Default Interfacial Averaging Schemes

Specific Safety Software Requirements for Water in eSTOMP-W Include:

SC.eW.1. Execution Mode: Normal

SC.eW.2. Execution Mode: Restart (with *Default* Restart Name)

SC.eW.3. Execution Mode: Restart File (with *Specified* Restart File Name)

SC.eW.4. Single Execution Time Period

SC.eW.5. Multiple Execution Time Periods

SC.eW.6. Default Interfacial Averaging Schemes

Specific Safety Software Requirements for Aqueous Transport in STOMP-W Include:

SC.W-T.1. Execution Mode: Normal No Flow

SC.W-T.2. Operational Mode Option: Transport (or Patankar Transport)

SC.W-T.3. Operational Mode Option: TVD Transport

SC.W-T.4. Operational Mode Option: Roe Superbee Transport

SC.W-T.5. Operational Mode Option: Transport with Courant

SC.W-T.6. Operational Mode Option: Transport with Vadose Courant

Specific Safety Software Requirements for Aqueous Transport in eSTOMP-W Include:

SC.eW-T.1. Execution Mode: Normal No Flow

SC.eW-T.2. Operational Mode Option: Transport (or Patankar Transport)

SC.eW-T.3. Operational Mode Option: TVD Transport

SC.eW-T.4. Operational Mode Option: Roe Superbee Transport

SC.eW-T.5. Operational Mode Option: Transport with Courant

SC.eW-T.6. Operational Mode Option: Transport with Vadose Courant

Specific Safety Software Requirements for STOMP-W-R Include:

SC.W-R.1. Operational Mode Option: Eckechem

SC.W-R.2. Operational Mode Option: Eckechem Transport (or Patankar Transport)

SC.W-R.3. Operational Mode Option: Eckechem with Guess

SC.W-R.4. Operational Mode Option: Eckechem with Reduced (Chemistry)

SC.W-R.5. Operational Mode Option: Eckechem with Minimum Concentration

SC.W-T.6. Operational Mode Option: Transport with Upwind

Specific Safety Software Requirements for eSTOMP-W-R Include:

SC.eW-R.1. Operational Mode Option: Eckechem

SC.eW-R.2. Operational Mode Option: Eckechem Transport (or Patankar Transport)

SC.eW-R.3. Operational Mode Option: Eckechem with Guess

SC.eW-R.4. Operational Mode Option: Eckechem with Reduced (Chemistry)

SC.eW-R.5. Operational Mode Option: Eckechem with Minimum Concentration

SC.eW-T.6. Operational Mode Option: Transport with Upwind

SC.eW-R.7. Operational Mode Option: Eckechem with Update Porosity

Specific Safety Software Requirements for STOMP-WAE Include:

SC.WAE.1. Aqueous Diffusion Option: Variable

SC.WAE.2. Gas Diffusion Option: Variable

Specific Safety Software Requirements for STOMP-WO Include:

SC.WO-O.1. Aqueous Diffusion Option: Variable

Specific Safety Software Requirements for STOMP-WO with Transport Include:

SC.WO-T.1. Operational Mode Option: Transport

SC.WO-T.2. Aqueous Diffusion Option: Variable

Specific Safety Software Requirements for STOMP-WOA Include:

SC.WOA.1. Operational Mode Option: TVD transport with Courant

SC.WOA.2. Aqueous Diffusion Option: Variable

SC.WOA.3. Gas Diffusion Option: Constant

SC.WOA.4. Water-Vapor Diffusion Coefficient Specified

SC.WOA.5. Oil-Vapor Diffusion Coefficient Specified

Specific Safety Software Requirements for STOMP-CO2 and *STOMP-CO2e Include:*

SC.CO2(e).1. Execution Mode: Normal

SC.CO2(e).2. Execution Mode: Restart with *Specified* Restart Name

SC.CO2(e).3. Single Execution Time Period

SC.CO2(e).4. Default Interfacial Averaging Schemes

SC.CO2(e).5. With ECKEChem

SC.CO2(e).6. With Invariant Fluid Density and Viscosity

SC.CO2(e).7. With Fractional CO2 Solubility

Specific Safety Software Requirements for STOMP-CO2e Include:

SC.CO2e.1. Variable Aqueous Diffusion

SC.CO2e.2. Variable Gas Diffusion

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 controls time steps to agree with time transitions in sources.
- Multiple sources may be applied to a node during the same time period.

Input requirements for all modes are shown in Table SRC.1.

Table SRC.1. Source options

Operational Mode Name	**STOMP-W**	**STOMP-WAE**	**STOMP-WO**	**STOMP-WOA**	**STOMP-CO2**	**STOMP-CO2e**
Operational Mode Code	**1**	**3**	**4**	**5**	**32**	**33**
Aqueous Volumetric	x	x	x	x	x	x
Aqueous Mass	x	x	x	x	x	x
Aqueous Volumetric Density	x					
Aqueous Mass Density	x					
Flow Well*****	x		x			
[Elevation] [Depth] [Head] Well			x			
Other Well Options(a)*****	x					
Solute	x	x	x	x	x	x
Other Solute Options(b)	x					
Gas Volumetric		x		x	x	x
Gas Mass		x		x	x	x
Others Gas Source Options(c)		x		x		
Power [Density], Condensate		x				
NAPL Volumetric			x	x		
NAPL Mass			x	x		
Salt [Density]					x	x
Dissolved Salt Options(d)					x	x
Dissolved CO2 Options(e)					x	x
Water Vapor Options (f)					x	x

(a) Well options: Flow Well Packer [no volume], Flow Well [no volume], Slug Well [no volume], Pulse Well [no volume], Pressure Well [no volume]
(b) Other Solute Options: Solute Density, Solute Inventory, Solubility Controlled Solute, Solubility-Controlled Salt Cake, Solute Advection Dominated, Solute Diffusion Dominated, Solute Variable Diffusion Dominated
(c) Others Gas Source Options: Gas Volumetric Mass Fraction, Gas Volumetric Relative Humidity, Gas Mass Fraction, Gas Mass Relative Humidity
(d) Dissolved Salt Options: Dissolved Salt Aqueous Concentration, Dissolved Salt Mass Fraction
(e) Dissolved CO2 Options: Dissolved CO2 Aqueous Concentration, Dissolved CO2 Mass Fraction

(f) Water Vapor Options: Water Vapor Gas Relative Humidity, Water Vapor Gas Mass Fraction
***** The Well Options are for internal PNNL use only and were not released to the users outside of PNNL.

Specific Safety Software Requirements for Water in STOMP-W and STOMP-WO Include:

SRC.W.1. Source Option: Aqueous Volumetric

SRC.W.2. Source Option: Aqueous Volumetric Density

SRC.W.3. Source Option: Aqueous Mass

SRC.W.4. Source Option: Aqueous Mass Density

SRC.W.5. Source Type: Influx

SRC.W.6. Single Source applied

SRC.W.7. Source specified for Interior Nodes

SRC.W.8. Source specified for Boundary Nodes

Specific Safety Software Requirements for Water in eSTOMP-W Include:

SRC.eW.1. Source Option: Aqueous Volumetric

SRC.eW.2. Source Option: Aqueous Volumetric Density

SRC.eW.3. Source Option: Aqueous Mass

SRC.eW.4. Source Option: Aqueous Mass Density

SRC.eW.5. Source Type: Influx

SRC.eW.6. Single Source applied

SRC.eW.7. Source specified for Interior Nodes

SRC.eW.8. Source specified for Boundary Nodes

Specific Safety Software Requirements for Aqueous Transport in STOMP-W Include:

SRC.W-T.1. Source Option: Solute

SRC.W-T.2. Source Option: Solute Density

SRC.W-T.3. Source Option: Solute Inventory

SRC.W-T.4. Source Option: Solute Solubility

SRC.W-T.5. Source Option: Solute Salt Cake Solubility

Specific Safety Software Requirements for Aqueous Transport in eSTOMP-W Include:

SRC.eW-T.1. Source Option: Solute

SRC.eW-T.2. Source Option: Solute Density

SRC.eW-T.3. Source Option: Solute Inventory

SRC.eW-T.4. Source Option: Solute Solubility

SRC.eW-T.5. Source Option: Solute Salt Cake Solubility

Specific Safety Software Requirements for STOMP-WAE Include:

SRC.WAE.1. Source Option: Gas Volumetric with Relative Humidity

SRC.WAE.2. Source Option: Gas Mass with Relative Humidity

Specific Safety Software Requirements for STOMP-CO2 and STOMP-CO2e Include:

SRC.CO2(e).1. Gas Mass Rate

4.9 Surface Flux Card Requirements

This card allows the user to specify the output of rates and integrals of fluxes of fluid mass, fluid volume, heat, component mass, solutes, and reactive species crossing grid-cell surfaces. Requirements for all operational modes:

- A surface is composed of rectangular areas of coplanar surfaces on exterior boundaries or between interior nodes. A surface can be a single surface of a grid cell, or a collection of grid-cell surfaces. Collections of grid-cell surfaces are created defining a span of surfaces or by linking surfaces together.
- 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. Surface fluxes are positive in sign when the flux is into the grid-cell volume. It allows the user to directly compute the total flux entering or exiting the grid volume from the surface fluxes. Table SFL.1 shows the convention used for grid cell surfaces in STOMP. Individual grid-cell surfaces can be combined via the *Surface Flux Card* so that total flux rates and integrals are reported for the grouped surfaces. The *Surface Flux Card* even allows for all of the surfaces surrounding a grid-cell to be grouped into one surface.
- The types of fluxes that can be tracked depend on the operational mode (Table SFL.2). To aid in the organization of surface flux data, surface fluxes can be output to multiple files. The default output file is named *surface*.

Table SFL.1. Grid-Cell Surface Conventions with respect to the computational coordinate system (CCS).

Grid-Cell Surface Name	Positive Surface Flux Direction	GCS Orientation	GCS Position	GCS Surface Normal
Bottom	Positive Z-Direction	X-Y Trending	Lower Surface	Negative Z-Direction
South	Positive Y-Direction	X-Z Trending	Lower Surface	Negative Y-Direction
West	Positive X-Direction	Y-Z Trending	Lower Surface	Negative X-Direction
East	Negative X-Direction	Y-Z Trending	Upper Surface	Positive X-Direction
North	Negative Y-Direction	X-Z Trending	Upper Surface	Positive Y-Direction
Top	Negative Z-Direction	X-Y Trending	Upper Surface	Positive Z-Direction

Table SFL.2. Surface Flux options

Operational Mode Name	STOMP-W	STOMP-WAE	STOMP-WO	STOMP-WOA	STOMP-CO2	STOMP-CO2e
Operational Mode Code	**1**	**3**	**4**	**5**	**32**	**33**
Aqueous Volumetric	x	x	x	x	x	x
Aqueous Mass	x	x	x	x	x	x
Solute Flux	x	x	x	x	x	x
Conservation Component Flux (Species)	x					

Kinetic Component Flux (Species)	x					
Gas Mass				x	x	x
Gas Volumetric				x	x	x
Gas-Phase CO2 Mass, Gas-Phase CO2e Mass					x	x
NAPL Volumetric, NAPL Mass, Dossolved Oil, Water Mass			x	x		
Gas-Advective Oil Mass, Gas-Diffusive Oil Mass, Gas-Total Oil Mass				x		
Salt Mass					x	x
Energy Transport variables(a)		x				

(a) Heat, Condensate Water Mass, Gas Advective Heat, Gas Advective Water Mass, Gas Advective Air Mass, Gas Diffusive Heat, Gas Diffusive Water Mass, Gas Diffusive Air Mass, Actual Evaporation, Potential Evaporation, Actual Transpiration, Potential Transpiration, Net Long-Wave Radiation, Net Short-Wave Radiation, Net Total Radiation, Water-Mass Balance

Specific Safety Software Requirements for Water in STOMP-W and STOMP-WO Include:

SFL.W.1. Surface Flux Type Option: Aqueous Volumetric Flux

SFL.W.2. Surface Flux Type Option: Aqueous Mass Flux

SFL.W.3. Surface Direction: Top

SFL.W.4. Surface Direction: Bottom

SFL.W.5. Surface Direction: North

SFL.W.6. Surface Direction: South

SFL.W.7. Surface Direction: East

SFL.W.8. Surface Direction: West

SFL.W.9. Single Surface File Output

SFL.W.10. Multiple Surface Files Outputs

SFL.W.11. Surface Definition: through Files

SFL.W.12. Surface Definition: by Nodes

Specific Safety Software Requirements for Water in eSTOMP-W Include:

SFL.eW.1. Surface Flux Type Option: Aqueous Volumetric Flux

SFL.eW.2. Surface Flux Type Option: Aqueous Mass Flux

SFL.eW.3. Surface Direction: Top

SFL.eW.4. Surface Direction: Bottom

SFL.eW.5. Surface Direction: North

SFL.eW.6. Surface Direction: South

SFL.eW.7. Surface Direction: East

SFL.eW.8. Surface Direction: West

SFL.eW.9. Single Surface File Output

SFL.eW.10. Multiple Surface Files Outputs

SFL.eW.11. Surface Definition: through Files

SFL.eW.12. Surface Definition: by Nodes

Specific Safety Software Requirements for Aqueous Transport in STOMP-W Include:

SFL.W-T.1. Surface Flux Type Option: Solute Flux

SFL.W-T.2. Surface Direction: East

SFL.W-T.3. Single Surface File Output

SFL.W-T.4. Surface Definition: by Nodes

Specific Safety Software Requirements for Aqueous Transport in eSTOMP-W Include:

SFL.eW-T.1. Surface Flux Type Option: Solute Flux

SFL.eW-T.2. Surface Direction: East

SFL.eW-T.3. Single Surface File Output

SFL.eW-T.4. Surface Definition: by Nodes

Specific Safety Software Requirements for STOMP-W-R Include:

SFL.W-R.1. Surface Flux Type Option: Conservation Component Flux

SFL.W-R.2. Surface Direction: Bottom

SFL.W-R.3. Single Surface File Output

SFL.W-R.4. Surface Definition: by Nodes

Specific Safety Software Requirements for eSTOMP-W-R Include:

SFL.eW-R.1. Surface Flux Type Option: Conservation Component Flux

SFL.eW-R.2. Surface Direction: Bottom

SFL.eW-R.3. Single Surface File Output

SFL.eW-R.4. Surface Definition: by Nodes

Specific Safety Software Requirements for STOMP-WAE Include:

SFL.WAE.1. Surface Flux Type Option: Gas Volumetric Flux

SFL.WAE.2. Surface Flux Type Option: Heat Flux

SFL.WAE.3. Surface Flux Type Option: Gas Mass Flux

Specific Safety Software Requirements for STOMP-WAE-B Include:

SFL.WAE-B.1. Surface Flux Type Option: Heat Flux

SFL.WAE-B.2. Surface Flux Type Option: Potential Evaporation

SFL.WAE-B.3. Surface Flux Type Option: Actual Evaporation

SFL.WAE-B.4. Surface Flux Type Option: Potential Transpiration

SFL.WAE-B.5. Surface Flux Type Option: Actual Transpiration

Specific Safety Software Requirements for STOMP-WOA Include:

SFL.WOA.1. Surface Flux Type Option: NAPL Volumetric Flux

SFL.WOA.2. Surface Flux Type Option: Gas Mass Flux

Specific Safety Software Requirements for Oil in STOMP-WO Include:

SFL.WO-O.1. Surface Flux Type Option: NAPL Volumetric Flux

Specific Safety Software Requirements for STOMP-WO with Transport Include:

SFL.WO-T.1. Surface Flux Type Option: Solute Flux

Specific Safety Software Requirements for STOMP-CO2 and STOMP-CO2e Include:

SFL.CO2(e).1. Surface Flux Type Option: Total CO2 Flux

SFL.CO2(e).2. Surface Flux Type Option: Aqueous Mass Flux

Specific Safety Software Requirements for STOMP-CO2e Include:

SFL.CO2e.1. Heat Flux

4.10 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

There are no specific safety software requirements.

5.0 ECKEChem 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 include:

- species name
- effective diffusion function options: Constant, Conventional (default), Empirical, Power
- aqueous molecular diffusion coefficient
- activity coefficient options: Davies, B-Dot, Pitzer, Constant
- additional inputs are required for Davies, B-Dot, and Pitzer activity coefficient options: species charge, species

diameter, species molecular weight

Specific Safety Software Requirements for STOMP-W-R Include:

AS.W-R.1. Species Name Specified

AS.W-R.2. Effective Diffusion Function Option: Conventional (default)

AS.W-R.3. Effective Diffusion Function Option: Power

AS.W-R.4. Aqueous Molecular Diffusion Coefficient Specified

AS.W-R.5. Activity Coefficient Option: Davies

AS.W-R.6. Activity Coefficient Option: B-Dot

AS.W-R.7. Activity Coefficient Option: Pitzer

AS.W-R.8. Activity Coefficient Option: Constant

AS.W-R.9. Species Charge Specified

AS.W-R.10. Species Diameter Specified

AS.W-R.11. Species Molecular Weight Specified

Specific Safety Software Requirements for eSTOMP-W-R Include:

AS.eW-R.1. Species Name Specified

AS.eW-R.2. Effective Diffusion Function Option: Conventional (default)

AS.eW-R.3. Effective Diffusion Function Option: Power

AS.eW-R.4. Aqueous Molecular Diffusion Coefficient Specified

AS.eW-R.5. Activity Coefficient Option: Davies

AS.eW-R.6. Activity Coefficient Option: B-Dot

AS.eW-R.7. Activity Coefficient Option: Pitzer

AS.eW-R.8. Activity Coefficient Option: Constant

AS.eW-R.9. Species Charge Specified

AS.eW-R.10. Species Diameter Specified

AS.eW-R.11. Species Molecular Weight Specified

5.2 Conservation Equations Card Requirements

This card specifies the conservation equations to be considered in the simulation. The requirements include:

- Equations of the form:

$$\frac{\mathrm{d}\sum_{N^s_{tc\,j}}(a_i C_i)}{\mathrm{d}t} = 0 \qquad for \quad j = 1, N^{eq}_{cn}$$

Symbols	
C_i	concentration of species *i*, mol/m^3 aqu.

a_i	conservation equation stoichiometric coefficient of species *i*
$\sum (a_i C_i)$	component species concentration, mol/m^3 aqu.
N_{cn}^{eq}	number of conservation equations
$N_{tc\,j}^{s}$	number of species in total-component species *j*

- Inputs that specify
  - 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

Specific Safety Software Requirements for STOMP-W-R Include:

CE.W-R.1. Component Species Name Specified

CE.W-R.2. Number of Species Specified

CE.W-R.3. Species Names Specified

CE.W-R.4. Species Stoichiometric Coefficients Specified

Specific Safety Software Requirements for eSTOMP-W-R Include:

CE.eW-R.1. Component Species Name Specified

CE.eW-R.2. Number of Species Specified

CE.eW-R.3. Species Names Specified

CE.eW-R.4. Species Stoichiometric Coefficients Specified

5.3 Equilibrium Equations Card Requirements

This card specifies the equilibrium equations to be considered in the simulation. The requirements include:

- Equations of the form:

$$(C_j) = K_{eq\,j} \prod_{N_{eq\,j}^{s}} (C_i)^{e_i} \qquad (i \neq j) \qquad for \quad j = 1, N_{eq}^{eq}$$

Symbols	
C_i	concentration of species *i*, mol/m^3 aqu.
C_j	aqueous activity of species *j*, mol/m^3 aqu.

e_i	stoichiometric exponent of species *i*
N_{eq}^{eq}	number of equilibrium equations
$N_{eq\,j}^{s}$	number of equilibrium species in equilibrium equation *j*
$K_{eq\,j}$	equilibrium constant of equilibrium equation *j*

- Inputs that specify:
  - 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

Specific Safety Software Requirements for STOMP-W-R Include:

EE.W-R.1. Specification of the Number of Species in the Equilibrium Equation

EE.W-R.2. Species Name Specified

EE.W-R.3. Equilibrium Reaction Name Specified

EE.W-R.4. Species Exponents Specified

Specific Safety Software Requirements for eSTOMP-W-R Include:

EE.eW-R.1. Specification of the Number of Species in the Equilibrium Equation

EE.eW-R.2. Species Name Specified

EE.eW-R.3. Equilibrium Reaction Name Specified

EE.eW-R.4. Species Exponents Specified

5.4 Equilibrium Reactions Card Requirements

This card specifies the parameters used in the temperature dependent equations for the equilibrium reaction constant:

$$\log(K_{eq}) = a_{eqC}\ln(T) + b_{eqC} + c_{eqC}T + \frac{d_{eqC}}{T} + \frac{e_{eqC}}{T^2}$$

Symbols	
K_{eq}	equilibrium constant
T	temperature, K
a_{eqC}	equilibrium constant coefficient
b_{eqC}	equilibrium constant coefficient

c_{eqC}	equilibrium constant coefficient
d_{eqC}	equilibrium constant coefficient
e_{eqC}	equilibrium constant coefficient

The requirements include:

- Species are associated with the defined equilibrium reaction constants via the *Equilibrium Equation Card*.
- Inputs that specify
    - equilibrium reaction name (must be unique and distinct from kinetic reaction names)
    - equation coefficients for the temperature dependent equilibrium constant

Specific Safety Software Requirements for STOMP-W-R Include:

ER.W-R.1. Equilibrium Reaction Name Specified

ER.W-R.2. Equation Coefficients for Equilibrium Constant Specified

Specific Safety Software Requirements for eSTOMP-W-R Include:

ER.eW-R.1. Equilibrium Reaction Name Specified

ER.eW-R.2. Equation Coefficients for Equilibrium Constant Specified

5.5 Gas Species Card Requirements

This card defines the gas species to be considered in the simulation. The requirements include:

- Inputs that specify
    - 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.

There are no specific safety software requirements.

5.6 Kinetic Equations Card Requirements

This card specifies the kinetic equations to be considered in the simulation. The requirements include:

- Equations of the form:

$$\frac{\mathrm{d}\sum_{N^s_{tk\,j}}(b_i C_i)}{\mathrm{d}t} = \sum_{N^r_{tk\,j}}(c_k R_k) \quad for \quad k = 1, N^{eq}_{kn}$$

Symbols

C_i	concentration of species *i*, mol/m^3 aqu.
b_i	kinetic-equation stoichiometric coefficient of species *i*
$\sum (b_i C_i)$	kinetic species concentration, mol/m^3 aqu.
c_k	kinetic-equation reaction-rate coefficient of reaction *k*
R_k	kinetic rate of reaction *k*, mol/s m^3 aqu.
$N^r_{tk\,j}$	number of kinetic reactions associated with total-kinetic species *j*
$N^s_{tk\,j}$	number of species in total-kinetic species *j*
N^{eq}_{kn}	number of kinetic equations

- Inputs that specify
  - number of kinetic equations
  - kinetic component species name
  - number of species in the kinetic equation
  - species names
  - species stoichiometric coefficients
  - number of kinetic reactions
  - kinetic reaction names
  - kinetic reaction stoichiometric coefficients

Specific Safety Software Requirements for STOMP-W-R Include:

KE.W-R.1. Number of Kinetic Equations Specified

KE.W-R.2. Kinetic Component Species Name Specified

KE.W-R.3. Number of Species in the Kinetic Equation Specified

KE.W-R.4. Species Name Specified

KE.W-R.5. Species Stoichiometric Coefficients Specified

KE.W-R.6. Number of Kinetic Reactions Specified

KE.W-R.7. Kinetic Reaction Names Specified

KE.W-R.8. Kinetic Reaction Stoichiometric Coefficients Specified

Specific Safety Software Requirements for eSTOMP-W-R Include:

KE.eW-R.1. Number of Kinetic Equations Specified

KE.eW-R.2. Kinetic Component Species Name Specified

KE.eW-R.3. Number of Species in the Kinetic Equation Specified

KE.eW-R.4. Species Name Specified

KE.eW-R.5. Species Stoichiometric Coefficients Specified

KE.eW-R.6. Number of Kinetic Reactions Specified

KE.eW-R.7. Kinetic Reaction Names Specified

KE.eW-R.8. Kinetic Reaction Stoichiometric Coefficients Specified

5.7 Kinetic Reactions Card Requirements

This card is required when a reaction system has kinetic/slow reactions and specifies the kinetic reaction formulations to be considered in the simulation. The required kinetic reaction parameters depend on the specified *Kinetic Reaction Type* option. The requirements include:

- Inputs that specify
  - kinetic reaction name
  - kinetic reaction type
  - kinetic reaction parameters
- The kinetic reaction name must be unique and distinct from equilibrium reaction names
- *Kinetic Reaction Type* options
  - Steefel-Lasaga Dissolution-Precipitation or TST model
  - Steefel-Lasaga Dissolution-Precipitation or TST model Toward Reactants
  - Steefel-Lasaga Dissolution-Precipitation or TST model Toward Products
  - Steefel-Lasaga Dissolution-Precipitation or TST with pH
  - Dissolution-Precipitation or TST with pH Toward Reactants model
  - Dissolution-Precipitation or TST with pH Toward Products model
  - Schaef Dissolution-Precipitation or TST with pH Toward Reactants model
  - Schaef Dissolution-Precipitation or TST with pH Toward Products model
  - Dissolution-Precipitation or TST with Glass Toward Reactants model
  - Steefel-Lasaga Dissolution-Precipitation or TST w/Coefficient Matrix model
  - Constant Rate TST
  - Smith-Atkins Forward-Backward model
  - Valocchi-Monod model
  - Valocchi-Monod w/Biomass model
  - Valocchi-Sorption model
  - Langmuir Sorption model
  - Dual Monod model
  - Single Monod model
  - Monod model
  - Biomass model
  - Liu Lognormal model
  - Liu DualDomain model

Specific Safety Software Requirements for STOMP-W-R Include:

KR.W-R.1. Kinetic Reaction Name Specified

KR.W-R.2. Kinetic Reaction Parameters Specified

KR.W-R.3. Kinetic Reaction Type Option : Valocchi-Sorption

KR.W-R.4. Kinetic Reaction Type Option : Valocchi-Monod

KR.W-R.5. Kinetic Reaction Type Option : Valocchi w/Biomass

KR.W-R.6. Kinetic Reaction Type Option : Steefel-Lasaga Dissolution-Precipitation or TST model

KR.W-R.7. Kinetic Reaction Type Option : Steefel-Lasaga Dissolution-Precipitation or TST model Toward Reactants

KR.W-R.8. Kinetic Reaction Type Option : Dissolution-Precipitation or TST with Glass Toward Reactants model

KR.W-R.9. Kinetic Reaction Type Option : Dissolution-Precipitation or TST with pH

Specific Safety Software Requirements for eSTOMP-W-R Include:

KR.eW-R.1. Kinetic Reaction Name Specified

KR.eW-R.2. Kinetic Reaction Parameters Specified

KR.eW-R.3. Kinetic Reaction Type Option : Valocchi-Sorption

KR.eW-R.4. Kinetic Reaction Type Option : Valocchi-Monod

KR.eW-R.5. Kinetic Reaction Type Option : Valocchi w/Biomass

KR.eW-R.6. Kinetic Reaction Type Option : Steefel-Lasaga Dissolution-Precipitation or TST model

KR.eW-R.7. Kinetic Reaction Type Option : Steefel-Lasaga Dissolution-Precipitation or TST model Toward Reactants

KR.eW-R.8. Kinetic Reaction Type Option : Dissolution-Precipitation or TST with Glass Toward Reactants model

KR.eW-R.9. Kinetic Reaction Type Option : Dissolution-Precipitation or TST with pH

KR.eW-R.10. Kinetic Reaction Type Option : Constant Rate TST

5.8 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. The required inputs include:

- primary and secondary mineral specific area
- initial and current species volume fractions (for every solid species defined on the *Solid Species Card*)
- inert mineral volume fraction (for each Rock/Soil Name, optional)
- parameter specification option: Rock/Soil Zonation; IJK -Indexing
- parameter specification sub-option: Overwrite

Specific Safety Software Requirements for STOMP-W-R Include:

LC.W-R.1. Primary and Secondary Mineral Specific Area Specified

LC.W-R.2. Species Volume Fractions Specified

LC.W-R.3. Parameter Specification Option: Rock/Soil Zonation

LC.W-R.4. Parameter Specification Sub-Option: Overwrite

Specific Safety Software Requirements for eSTOMP-W-R Include:

LC.eW-R.1. Primary and Secondary Mineral Specific Area Specified

LC.eW-R.2. Species Volume Fractions Specified

LC.eW-R.3. Parameter Specification Option: Rock/Soil Zonation

LC.eW-R.4. Parameter Specification Sub-Option: Overwrite

LC.eW-R.5. Inert Mineral Volume Fraction Specified

5.9 Solid Species Card Requirements

This card is required when there are immobile species present in the reaction system and defines the solid species to be considered in the simulation. The immobile species include sorbed species, mineral species etc. Requirements include:

- Inputs that specify
    - species name
    - species mass density
    - species molecular weight

- Species name must be unique and distinct from aqueous and gas species names

Specific Safety Software Requirements for STOMP-W-R Include:

SS.W-R.1. Species Name Specified

SS.W-R.2. Species Mass Density Specified

SS.W-R.3. Species Molecular Weight Specified

Specific Safety Software Requirements for eSTOMP-W-R Include:

SS.eW-R.1. Species Name Specified

SS.eW-R.2. Species Mass Density Specified

SS.eW-R.3. Species Molecular Weight Specified

5.10 Species Link Card Requirements

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

- The following are components that can be linked in this card:
  - aqueous water
  - gas water
  - aqueous air
  - gas air
  - aqueous CO_2
  - gas CO_2
  - aqueous CH_4
  - gas CH_4
  - aqueous salt
  - solid salt
- Inputs that specify
  - number of reactive species links
  - reactive species names
  - linked components

This card is required when pH is defined in the initial condition card, or when the mode is for multiphase simulation, such as STOMP-CO2.

Specific Safety Software Requirements for STOMP-W-R Include:

SL.W-R.1. Number of reactive Species Links

SL.W-R.2. Reactive Species Name Specified

SL.W-R.3. Linked Components Specified: pH

Specific Safety Software Requirements for eSTOMP-W-R Include:

SL.eW-R.1. Number of Reactive Species Links

SL.eW-R.2. Reactive Species Name Specified

SL.eW-R.3. Linked Components Specified: pH

6.0 Requirements Group 5 Cards_ Inverse Modeling

This section describes the additional cards needed for performing inverse modeling using off-the-shelf inverse codes such as UCODE and PEST.

6.1 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 include:

- 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

There are no specific safety software requirements.

6.2 Scaling Factor Card Requirements

This card declares the scaling factors for a group of soils. The requirements include:

- 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

There are no specific safety software requirements.

6.3 UCODE Control Card Requirements

This card allows users to specify the control information in a UCODE universal file. This card can only be used in 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.

7.0 Additional STOMP/eSTOMP Requirements

This section describes the requirements for input cards specific to a particular mode of STOMP, which includes the simulation of gas, oil/NAPL, energy and CO_2.

7.1 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. This card is required only for simulations involving flow and/or transport through the gas phase. The requirements include:

- 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
    - 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

Specific Safety Software Requirements for STOMP-WAE Include:

GRP.WAE.1. Gas Relative Permeability Option: Mualem

GRP.WAE.2. Gas Relative Permeability Option: Fatt and Klikoff

GRP.WAE.3. Declaration of Gas permeability Options: Explicit

Specific Safety Software Requirements for STOMP-WAE-B Include:

GRP.WAE-B.1. Gas Relative Permeability Option: Corey

GRP.WAE-B.2. Gas Relative Permeability Option: Burdine

GRP.WAE-B.3. Declaration of Gas permeability Options: Explicit

Specific Safety Software Requirements for STOMP-WOA Include:

GRP.WOA.1. Gas Relative Permeability Option: Mualem

GRP.WOA.2. Declaration of Gas permeability Options: Explicit

Specific Safety Software for STOMP-CO2 and *STOMP-CO2e Include:*

GRP.CO2(e).1. Mualem (with Brooks and Corey saturation function)

GRP.CO2(e).2. Corey (with Van Genuchten saturation function)

GRP.CO2(e).3. van Genuchten (with Van Genuchten saturation function)

GRP.CO2(e).4. Burdine (with Brooks and Corey saturation function)

GRP.CO2(e).5. Tabular (with Brooks and Corey saturation function)

Specific Safety Software Requirements for STOMP-CO2e Include:

GRP.CO2e.1. Fatt and Klikoff

7.2 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. The card is required only for simulations involving flow and/or transport through the NAPL phase. The requirements include:

- 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 '' parameter can be defaulted to the values entered or defaulted with the saturation function.
- Options for declaring parameters:
    - Explicit declaration
    - External files
    - IJK indexing

Specific Safety Software Requirements for STOMP-WOA Include:

NAPLRP.WOA.1. NAPL Relative Permeability-Saturation Function Option: Mualem

NAPLRP.WOA.2. NAPL Relative Permeability-Saturation Function Option: Constant

NAPLRP.WOA.3. Declaration of NAPL Relative Permeability Options: Explicit

Specific Safety Software Requirements for STOMP-WO Include:

NAPLRP.WO.1. NAPL Relative Permeability-Saturation Function Option: Mualem

NAPLRP.WO.2. NAPL Relative Permeability-Saturation Function Option: Burdine

NAPLRP.WO.3. Declaration of NAPL Relative Permeability Options: Explicit

7.3 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. This card is required only for simulations involving flow and/or transport of an oil or dissolved oil (e.g., STOMP-WO and STOMP-WOA). The requirements include:

- 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
- Inputs that specify
    - Number of NAPL components
    - 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:

      $$\bar{c}^o_{p_n} = a + bT + cT^2 + dT^3$$

      in J/mol K
    - Saturated vapor pressure function options
        - Equation 1:

          $$ln\left(\frac{P^o_g}{P^o_c}\right) = \frac{ax + bx^{1.5} + cx^3 + dx^6}{(1-x)}$$

          where $$x = 1 - \frac{T}{T^o_c}$$
        - Equation 2:

          $$ln\left(P^o_g\right) = a - \frac{b}{T} + c\ln(T) + d\left(\frac{P^o_g}{T^2}\right)$$
        - Equation 3:

$$ln\left(P_g^o\right) = a - \frac{b}{(c+T)}$$

- Constant:

$$P_g^o = \overline{P}_g^o$$

- Liquid density options
  - HBT Technique: Reid et al. 1987, pp. 55-56
  - Modified Rackett w/ reference: Reid et al. 1987, p. 67
  - Modified Rackett: Reid et al. 1987, p. 67
  - Constant:

$$\rho_g^o = \overline{\rho}_g^o$$

- Liquid viscosity function options (in cP and K for viscosity and temperature, respectively):
  - Reference:

$$\mu_n^o = \left[\left(\overline{\mu}_n^o\right)^{-0.2661} + \frac{\left(T - \overline{T}_n^o\right)}{233}\right]^{-3.758}$$

  - Equation 1:

$$\mu_n^o = aT^b$$

  - Equation 2:

$$\mu_n^o = \exp\left(a + \frac{b}{T}\right)$$

  - Equation 3:

$$\mu_n^o = \exp\left(a + \frac{b}{T} + cT + dT^2\right)$$

  - Constant:

$$\mu_n^o = \overline{\mu}_n^o$$

- Henry's constant for aqueous solubility (1.E+20) with units

Specific Safety Software Requirements for STOMP-WOA Include:
Inputs that specify

OP.WOA.1. Oil Name

OP.WOA.2. Molecular Weight

OP.WOA.3. Freezing Point Temperature

OP.WOA.4. Normal Boiling Point

OP.WOA.5. Critical Temperature

OP.WOA.6. Critical Pressure

OP.WOA.7. Critical Molar Volume

OP.WOA.8. Critical Compressibility

OP.WOA.9. Pitzer Acentric Factor

OP.WOA.10. Dipole Moment

OP.WOA.11. Isobaric Molar Specific Heat Constants: a, b, c, d

OP.WOA.12. Henry's Constant for Aqueous Solubility

OP.WOA.13. Saturated Vapor Pressure Function Option: Constant

OP.WOA.14. Liquid Density Option: Constant

OP.WOA.15. Liquid Viscosity Function Option: Constant

Specific Safety Software Requirements for STOMP-WO Include:
Inputs that specify:

OP.WO.1. Oil Name

OP.WO.2. Molecular Weight

OP.WO.3. Freezing Point Temperature

OP.WO.4. Normal Boiling Point

OP.WO.5. Critical Temperature

OP.WO.6. Critical Pressure

OP.WO.7. Critical Molar Volume

OP.WO.8. Critical Compressibility

OP.WO.9. Pitzner Acentric Factor

OP.WO.10. Dipole Moment

OP.WO.11. Isobaric Molar Specific Heat Constants: a, b, c, d

OP.WO.12. Henry's Constant for Aqueous Solubility

OP.WO.13. Saturated Vapor Pressure Function Option: Constant

OP.WO.14. Saturated Vapor Pressure Function Option: Equation 1

OP.WO.15. Liquid Density Option: Constant

OP.WO.16. Liquid Viscosity Function Option: Constant

7.4 Dissolved-Oil Transport Card Requirements

This card allows the user to declare functions and assign values required for dissolved oil transport. This card is required only for simulations involving transport of dissolved oil (e.g., STOMP-WO and STOMP-WOA) The requirements include:

- Card name options
    - ~Dissolved oil transport Card
    - ~Dissolved VOC transport Card
    - ~Dissolved organic transport Card
- Inputs that specify
    - Rock/soil name, longitudinal dispersivity with units, transverse dispersivity with units,
    - Dissolved-oil adsorption function options
        - Linear:

$$R_D = 1 + \frac{k}{s_l n_D}$$

- Linear Kd:

$$R_D = 1 + \frac{K_d \rho_b}{s_l n_D}$$

- Freundlich:

$$R_D = 1 + \frac{nkC_l^{(n-1)}}{s_l n_D}$$

- Langmuir:

$$R_D = 1 + \frac{a}{s_l n_D (1 + bC_l)^2}$$

- Nominal particle diameter with units

Specific Safety Software Requirements for STOMP-WOA Include:
Inputs that specify

DOT.WOA.1. Rock-Soil Name

DOT.WOA.2. Longitudinal Dispersivity

DOT.WOA.3. Transverse Dispersivity

DOT.WOA.4. Dissolved-Oil Adsorption Function Option: Linear Kd

DOT.WOA.5. Nominal Particle Diameter (Default Value)

7.5 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. This card is only required for simulations involving the solution of the energy conservation equation (e.g., STOMP-WAE and STOMP-WAE-B). The requirements for STOMP-WAE include:

- 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)

The requirements for STOMP-WAE-B include:

- 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

The requirements for STOMP-CO2e include:

- Assign values of thermal conductivity and specific heat for each defined rock/soil type
- Thermal conductivity function options
    - Constant
    - Parallel (DeVries 1966)
    - Linear
    - Somerton (1973, 1974)

Specific Safety Software Requirements for STOMP-WAE Include:

TP.WAE.1. Thermal Conductivity Option: Constant

TP.WAE.2. Thermal Conductivity Option: Somerton

Specific Safety Software Requirements for STOMP-WAE-B Include:

TP.WAE-B.1.Thermal Conductivity Option: Cass

TP.WAE-B.2. Thermal Conductivity Option: Somerton

TP.WAE-B.3. Ground-Surface Albedo Option: Wang Albedo

TP.WAE-B.4. Water-vapor Diffusion Option: Enhanced

Specific Safety Software Requirements for STOMP-CO2e Include:

TP.CO2e.1. Thermal Conductivity Function Option: Parallel

7.6 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 for STOMP-WAE-B include:

- General input requirements
- General inputs
    - Atmospheric start month, day, year, time (in military format)
    - ind speed measurement height with units
    - Local longitude and meridian with units (deg)
- Data inputs
    - Atmospheric condition time with units
    - Temperature with units
    - Pressure with units
    - Water-vapor relative humidity
    - Net solar radiation with units
    - Wind speed with units
- Options for declaring parameters:
    - Explicit declaration
    - External files

Specific Safety Software Requirements for STOMP-WAE-B Include:
General Input Requirements:

AC.WAE-B(G).1. Declaration of Atmospheric Conditions parameters: Explicit

AC.WAE-B(G).2. Atmospheric Start Month Specified

AC.WAE-B(G).3. Atmospheric Start Day Specified

AC.WAE-B(G).4. Atmospheric Start Year Specified

AC.WAE-B(G).5. Atmospheric Start Time Specified

AC.WAE-B(G).6. Wind Speed Measurement Height Specified

AC.WAE-B(G).7. Local Longitude Specified

AC.WAE-B(G).8. Meridian Specified

Data Input Requirements:

AC.WAE-B(D).1. Atmospheric Condition Time Specified

AC.WAE-B(D).2. Temperature Specified

AC.WAE-B(D).3. Pressure Specified

AC.WAE-B(D).4. Water-Vapor Relative Humidity Specified

AC.WAE-B(D).5. Net Solar Radiation Specified

AC.WAE-B(D).6. Wind Speed Specified

7.7 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 handle. Requirements for operational mode STOMP-WAE-B include:

- Plant temperature option: Single plant temperature and units
- Rainfall interception options
  - Rainfall interception
  - No rainfall interception
- Plant stress options
  - 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
- Inputs that specify
  - 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

Specific Safety Software Requirements for STOMP-WAE-B Include:

PC.WAE-B.1. Plant Temperature Option: Single Plant Temperature

PC.WAE-B.2. Rainfall Interception Option: Rainfall Interception

PC.WAE-B.3. Plant Stress Option: Vrugt Root Stress Model

PC.WAE-B.4. Plant Albedo Option: Temporal Albedo

PC.WAE-B.5. Stomatal Resistance Option: Hicks Stomatal Resistance Model

Inputs that specify:

PC.WAE-B(I).1. Number of Plant Species

PC.WAE-B(I).2. Plant Name

PC.WAE-B(I).3. Maximum Root Depth

PC.WAE-B(I).4. Null Root Depth

PC.WAE-B(I).5. Root Depth Fit Parameter

PC.WAE-B(I).6. Crop Coefficient Start

PC.WAE-B(I).7. Crop Coefficient Day of Year (Start)

PC.WAE-B(I).8. Crop Coefficient (Mature Stage 1)

PC.WAE-B(I).9. Crop Coefficient Day of Year (Mature Stage 1)

PC.WAE-B(I).10. Crop Coefficient (Mature Stage 2)

PC.WAE-B(I).11. Crop Coefficient Day of Year (Mature Stage 2)

PC.WAE-B(I).12. Crop Coefficient (Die-off)

PC.WAE-B(I).13. Crop Coefficient Day of Year (Die-off)

7.8 Salt Transport Card Requirements

This card allows the user to define porous media dependent dispersivities for salt. This card is required for simulations involving salt transport (STOMP-CO2 and STOMP-CO2e). The CO2 modes of STOMP can also be used to simulate water with salt transport only, without CO2 in the domain. The requirements include:

- 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:

      $$D_{le}^{s} = D_{l}^{e}$$

    - Conventional:

      $$D_{le}^{s} = \tau_l s_l n_D D_{l}^{e}$$

    - Empirical [Kemper and van Schaik]:

$$D_{le}^{s} = aD_{l}^{e} \exp\left(bn_{D}s_{l}\right)$$

- 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)
    - 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

Specific Safety Software Requirements for STOMP-CO2 and STOMP-CO2e Include:

SaT.CO2(e).1. Direct declaration of longitudinal dispersivity and transverse dispersivity

7.9 Coupled Well Card Requirements

This card allows users to specify injection wells for the STOMP-CO2 and –CO2e operational modes. Requirements:

- The well under a specified mass rate is subject to a pressure limit. When the injection rate can be met, the well is considered to be flow-controlled. Otherwise, the well is pressured-controlled and the injection rate becomes unknown.
- Well segments are specified using straight-line well intervals
- Well specification is independent of grid
- Points defining a well interval can be located inside or outside the computational domain
- Each well interval can have a unique radius and skin factor
- The injection schedule can vary over time. Linear interpolation is used between the injection schedule times

Inputs requirements

- Well type options:
    - CO2 injection well
    - aqueous injection well
    - volumetric well
    - mass well
- Water vapor options
    - relative humidity
    - mass fraction
    - null
- Dissolved CO_2 options
    - relative humidity
    - mass fraction
    - null
- Dissolved salt options
    - relative humidity
    - mass fraction
    - null
- Well fraction factors
- Total injection limit
- Total production limit
- Number of well intervals
- 1st x, y, z coordinate with units
- 2nd x, y, z coordinate with units
- Well bore radius with units
- Well interval skin factor
- Well interval screen options
    - screened
    - null
- CO2 injection rate and limiting pressure
- Water vapor humidity or mass fraction
- Aqueous injection rate and limiting pressure
- Dissolved CO2 relative saturation or mass fraction
- Injection temperature (for STOMP-CO2e only)

- Dissolved salt relative saturation or mas fraction

Specific Safety Software Requirements for STOMP-CO2 and STOMP-CO2e Include:

CW.CO2(e).1. CO2 Injection Well

7.10 Internal Boundary Surfaces Card Requirements

The requirements for this card are the same for all operation modes. Internal boundary surfaces serve the internal connections between adjacent nodes, making the fluxes between these nodes controlled by the applied boundary conditions.

- By default, internal boundary surfaces have a Zero Flux type boundary.
- If a split, or discontinuity in the interior of the grid occurs, then internal boundary surfaces are implicitly defined and do not need to be explicitly defined.
- The format of input that specifies the boundary nodes with a list or a file is the same as that for the Boundary Surfaces Card
- The boundary surface direction specification is the same as that for the Boundary Surfaces Card

Requirement for all the operational modes:

- The zero flux type boundary by default

7.11 Vertical Equilibrium Card

This card, by assuming the static equilibrium of the gas and aqueous phases in the vertical direction, converts 3-D domains into 2-D domains, or 2-D into 1-D domains. The vertical equilibrium assumption can be applied to the entire computational domain or portions of the domain. For STOMP-CO2e, the vertical equilibrium assumptions further assumes a single temperature in the vertical direction. This card is used to define regions of the computational domain.

- This card is required only for the operational mode STOMP-CO2 and –CO2e
- Required general inputs: number of vertical equilibrium domains
- Required general inputs: indices for the vertical equilibrium domains

7.12 Geomechanics Link Card

This card allows users to assign function forms and functional parameters that define the linkage between the geomechanical simulation and the coupled flow and transport simulation. Requirements:

- This card is only required for simulations that include geomechanical calculations using the EPMech (Elastic-Plastic Geomechanics) module
- Porosity-Mean stress Function options
    - Davis-Davis
    - null, or n/a, or none, or zero
- Intrinsic Permeability-Porosity Function options
    - Davis-Davis
    - null, or n/a, or none, or zero
- Capillary Pressure-Permeability/Porosity Function options
    - Leverett
    - null, or n/a, or none, or zero

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

There are no specific safety software requirements.

7.13 Geomechanics Boundary Conditions Card

This card defines the boundary conditions for the geomechanical simulation. Requirements:

- This card is only required for simulations that include geomechanical calculations using the EPMech (Elastic-Plastic Geomechanics) module
- The nodes that accepts this condition follows the same convention as that for the boundary conditions card
- Definition of boundary surface direction follows the same convention as that for the boundary conditions card
- Every geomechanical boundary condition requires the specification of five geomechanical boundary types
    - X-direction traction boundary type
    - Y-direction traction boundary type
    - Z-direction traction boundary type
    - Normal displacement boundary type
    - Shear displacement boundary type
- The X-. Y-, or Z-direction traction boundary type options
    - zero
    - no
    - Traction
    - prescribed
- The normal or shear displacement boundary condition type options
    - zero
    - no
    - fixed
    - free
    - yes

8.0 Documentation Requirements

8.1 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, although any of the problems could also be applied to eSTOMP. 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.

8.2 ECKEChem Module Addendum (White and McGrail 2005)

This addendum to the STOMP/eSTOMP guides describes the theory, use, and application of the ECKEChem (Equilibrium-Conservation-Kinetic Equation Chemistry) reactive transport package for the STOMP and eSTOMP simulators. This document describes the methods that the 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. Any additional models or capabilities to the ECKEChem module will be documented in separate addendum's, and/or the STOMP/eSTOMP online User Guide.

8.3 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. These problems range in complexity, 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.

8.4 STOMP-CO2 and STOMP-CO2e Guide (White et al. 2012)

This guide describes the theory, input file formatting, and benchmark problems of geologic sequestration of CO_2 in saline reservoirs model for the Water-Salt-CO_2 Operational Mode (STOMP-CO2) and the Water-Salt-CO_2-Energy Operational Mode (STOMP-CO2e) of the STOMP simulator. STOMP-CO2 and –CO2e simulators solve conservation equations for component mass (i.e., water, CO_2, and salt) and energy on a structured orthogonal grid. The STOMP-CO_2 simulator has three primary variables and the STOMP-CO2e has an extra fourth primary variable for energy conservation equation. The core modeling capabilities include the structural, dissolution, and hydraulic (capillary) trapping. The ECKEChem module allows for mineralization trapping. This guide includes a series of benchmark problems for the STOMP-CO2 and –CO2e simulators.

8.5 STOMP-WAE-B 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 (WAE-B) Operational Mode of STOMP and eSTOMP. 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 either an additional addendum, or on the online User Guide.

8.6 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 STOMP (and eSTOMP) 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. Theoretical information will also be published on the online STOMP/eSTOMP User Guide.

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

The STOMP User Guide published in 2006 (White and Oostrom) describes the general use and input file formatting for both the STOMP and eSTOMP simulators. In this document, pseudo-code was used to describe the different input options. In 2015, an online User Guide was published that replaced the pseudo-code with clickable dialogues that allow the user to identify the required input structure for the user's particular problem.

The online User Guide provides guidance on the input file structure and its formatting specifications. Several example inputs are also provided. 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. A description of the indexing patterns developed for the simulator is also provided in both the 2006 and online guides.

The online User Guide does not contain guidance on all modes. Modes will be added to the online guide as funding permits.

The online STOMP/eSTOMP User Guide will be updated on an as needed basis. It is anticipated that the online accessibility of this document will facilitate frequent updating of the document.

9.0 STOMP Execution Requirements

This section briefly describes the system, compilation and execution requirements for both the STOMP and eSTOMP simulators. Specific details of compilation and execution can be found in the online User Guide:

STOMP: http://stomp.pnnl.gov/user_guide/STOMP_guide.stm

eSTOMP: http://stomp.pnnl.gov/estomp_user_guide/eSTOMP_guide.stm

9.1 Compilation Requirements

STOMP Compilation

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.

eSTOMP Compilation

Each mode eSTOMP contains a unique set of FORTRAN files and modules. The eSTOMP simulator is distributed as source code for a particular operational mode, with the source code required for external packages (e.g., PETSc and GA Toolkit libraries).   Assembly of the executable occurs through the make utility (Talbott 1988) which is also distributed with the source code. Except for external packages, the eSTOMP simulator is coded in FORTRAN.

Distributing an open source allows users to read and modify the simulator, which will hopefully result in an open exchange of scientific ideas. A drawback of an open source is that the user is responsible for compiling and linking the source code to generate an executable. Users will also need to compile the external libraries independently of eSTOMP. This inherently assumes that the user has a FORTRAN 90 compiler and is familiar with its use for generating code. The unassembled eSTOMP source is coded in a combination of FORTRAN 77 and FORTRAN 90.

9.1 Execution Requirements

STOMP

Executing the STOMP 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 (default name *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.

eSTOMP

Executing eSTOMP requires that the MPI, GA and PETSc libraries be linked to the executable, either dynamically at run time, or statically at compile time. Execution is usually accomplished via the *mpirun* command (from the MPI library), where the number of processors and executable location is specified. Like STOMP, an input file named *input* must reside in the run directory. For restart simulations a restart file (default name *restart*) must also reside in the current directory. Two types of error messages may be generated during runtime: 1) a system generated message that typically indicates a memory, FORTRAN, or other system error identified by the system; or 2) an eSTOMP generated message that indicates a problem with the input file read, or convergence failure. A successful execution will result in input information sent to both the screen and *output file*, as well as the time steps and reference node information requested within the *input* file.

9.3 System Requirements

STOMP

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.

eSTOMP

The eSTOMP simulator is written in FORTRAN following both the 77 and 90 language standards. A FORTRAN 90 compiler is required to compile eSTOMP. eSTOMP must be executed on computers with UNIX operating systems, and is designed to take advantage of multiple processor cores, whether if be on a Linux workstation, a small cluster, or a supercomputer with thousands of cores.

10.0 Literature Cited

Nichols WE, NJ Aimo, M Oostrom, and MD White. 1997. STOMP Subsurface Transport Over Multiple Phases Application Guide. PNNL-11216 UC-2010, Pacific Northwest National Laboratory, Richland, Washington.

Oostrom M, DH Meck, and MD White. 2003. STOMP Subsurface Transport Over Multiple Phases Version 3.0 An Introductory Short Course. PNNL-14440, Pacific Northwest National Laboratory, Richland, Washington.

Reid RC, JM Prausnitz, and BE Poling. 1987. The Properties of Gases and Liquids. McGraw-Hill, New York.

Ward AL, MD White, EJ Freeman, and ZF Zhang. 2005. STOMP Subsurface Transport Over Multiple Phases Version 1.0 Addendum: Sparse Vegetation Evapotranspiration Model for the Water-Air-Energy Operational Mode. PNNL-15465, Pacific Northwest National Laboratory, Richland, Washington.

White MD and BP McGrail. 2005. STOMP Subsurface Transport Over Multiple Phases Version 1.0 Addendum: ECKEChem Equilibrium-Conservation-Kinetic Equation Chemistry and Reactive Transport. PNNL-15482, Pacific Northwest National Laboratory, Richland, Washington.

White MD and M Oostrom. 2006. STOMP Subsurface Transport Over Multiple Phases Version 4.0 User's Guide. PNNL-15782, Pacific Northwest National Laboratory, Richland, Washington.

White MD and M Oostrom. 2006. STOMP Subsurface Transport Over Multiple Phases Version 2.0 Theory Guide. PNNL-12030 UC-2010, Pacific Northwest National Laboratory, Richland, Washington.

White MD, DJ Watson, DH Bacon, SK White, BP McGrail, and ZF Zhang. 2012. STOMP Subsurface Transport Over Multiple Phases STOMP-CO2 and –CO2e Guide. PNNL-21268, Pacific Northwest National Laboratory, Richland, Washington.