0.1 Introduction

This specification documents features required by PFLOTRAN to simulate physical and chemical processes within the subsurface environment. These required features are divided into functional and non-functional requirements. Functional requirements consist of physical or chemical processes, numerical methods, user interfaces, etc. Non-functional requirements include runtime performance metrics (e.g. scalability, performance), software maintenance and code availability. The specification maps these features to tests designed to verify their accuracy and robustness.

0.2 Functional Requirements

PFLOTRAN's functional requirements are divided into the following categories: constitutive relations, physics and chemistry, numerical methods, and user interaction.

0.2.1 Constitutive Relations

Constitutive relations employ mathematical equations to approximate the observed physical response of a material or fluid under conditions of interest. For instance, an equation of state calculates a fluid density as a function of input parameters pressure and temperature.

Equations of State

Equations of state calculate fluid density, enthalpy, and viscosity as a function of temperature and pressure. The following equations of state shall be implemented in the code:

CR 1. IFC67: PFLOTRAN shall implement the IFC67 (International Formulation Committee, 1967) equations of state for calculating the density, enthalpy, and viscosity of water as a function of pressure and temperature.

CR 2. IF97: PFLOTRAN shall implement the IF97 from the International Association for the Properties of Water and Steam (Wagner et al, 2000) equations of state for calculating the density and enthalpy of water and steam as a function of pressure and temperature.

Capillary Pressure/Saturation Functions

In variably saturated or multiphase flow in porous media it is essential to establish a relation between capillary pressure and saturation. This relation is set forth by several empirical models, and two of the more common are implemented in PFLOTRAN:

CR 3. van Genuchten: PFLOTRAN shall implement the van Genuchten function (van Genuchten, 1980) to calculate the saturation on a cell given its capillary pressure value.

CR 4. Brooks-Corey: The simulator may use the Brooks-Corey function (Brooks and Corey, 1964) to calculate the saturation on a cell given its capillary pressure value.

Relative Permeability Functions

Relative permeability functions establish a relationship between liquid relative permeability [-] (which varies from 0 to 1) and saturation. The simulator shall implement the following relative permeability functions:

CR 5. Mualem: The simulator calculates relative permeability as a function of saturation using either the Mualem-van Genuchten or the Mualem-Brooks-Corey functions (Chen et al. 1990).

CR 6. Burdine: The simulator calculates relative permeability as a function of saturation using either the Burdine-van Genuchten or the Burdine-Brooks-Corey functions (Chen et al. 1990).

Soil Compressibility Functions

The storage of fluids in porous media change according to compaction or expansion of fluids and porous media. While compaction (or expansion) of fluids is governed by the fluid compressibility, the changes in porous media volume is set forth by soil compressibility functions. These functions relate changes in porosity with changes in pressure. PFLOTRAN shall implement two soil compressibility functions:

CR 7. Leijnse: Leijnse function (Leijnse 1992) is the default soil compressibility function considered by the simulator. It calculates the current porosity as a function of pressure, given soil matrix compressibility coefficient, a reference pressure, and reference porosity.

CR 8. Exponential: An exponential soil compressibility function establishes an exponential relationship between changes in pressure and porosity, given a soil matrix compressibility coefficient, a reference pressure, and reference porosity. (Low - easy)

Constitutive Relation Coupling by Region

CR 9. PFLOTRAN shall allow for capillary pressure/saturation functions, relative permeability functions and soil compressibility functions to be specified by region. (HIGH - easy)

0.2.2 Physics and Chemistry

PFLOTRAN employs mathematical representations of physical and chemical process models to simulate phenomenon in the subsurface. These process models include:

Single phase variably saturated flow

PC 1. The governing mass balance equation that is used to model single phase variably saturated flow in PFLOTRAN is based on Richards' equation (see Richards 1931 and Freeze and Cherry 1979).

Should we add single phase fully saturated flow?

Multicomponent Solute Transport

Biogeochemical Reaction

0.2.3 Forcing Requirements (Boundary conditions, initial conditions and source/sinks)

PFLOTRAN shall allow the specification of the following flow boundary conditions:

Liquid Pressure

FR 1. Dirichlet: Pressure Dirichlet boundary conditions specify a particular pressure at the boundaries.

FR 2. Pressure Hydrostatic: PFLOTRAN allows the specification of a pressure hydrostatic boundary or initial condition, where the pressure (p) is a function of the fluid density (ρ), the gravity (g), and the distance from a datum (h), that is $p = \rho g h$, where ρ may be a function of pressure and temperature. The hydrostatic pressure profile may also be assigned based on a gradient in the horizontal direction.

Liquid Flux

FR 3. Neumann: Flux Neumann boundary conditions specify a Darcy flux [m/s] across a boundary.

Liquid Source/Sink

FR 4. Mass rate: The mass rate shall be equally distributed across cells in the region where the source/sink term is applied.

FR 5. : Scaled mass rate by cell volume: The mass rate shall be distributed according to the ratio (r) of the cell volume (V_c) by the total volume of the region (V_t) where the source/sink term is applied to. The mass rate is scaled by the ratio $r = V_c/V_t$.

FR 6. Scaled mass rate by cell permeability: The mass rate shall be scaled according to the ratio (r) of cell volume (V_c) multiplied by the cell's intrinsic permeability (κ_c) and the sum of every cell volume in the region scaled by its permeability, that is $r = V_c \cdot \kappa_c \,/\, \sum_{n=1}^{n_r} V_n \cdot \kappa_n$, where n_r is the total number of cells in the region where the source/sink is applied.

FR 7. Volumetric rate: The volumetric rate shall be equally distributed across cells in the region where the source/sink term is applied.

FR 8. Scaled volumetric rate by cell volume: The volume rate shall be distributed according to the ratio (r) of the cell volume (V_c) by the total volume of the region (V_t) where the source/sink term is applied to, that is $r = V_c/V_t$.

FR 9. Scaled volumetric rate by cell permeability: The volumetric rate shall be scaled according to the ratio (r) of cell volume (V_c) multiplied by the cell's intrinsic permeability (κ_c) and the sum of every cell volume in the region scaled by its permeability, that is $r = V_c \cdot \kappa_c \,/\sum_{n=1}^{n_r} V_n \cdot \kappa_n$, where n_r is the total number of cells in the region where the source/sink is applied.

FR 10. The values applied to flow boundary conditions and source/sink terms may vary in time.

FR 11. If no boundary condition is specified, a no-flux condition is assumed.

0.2.4 Numerical Methods

Time Stepping

NM 1. Variable Time Stepping: PFLOTRAN shall have the ability to vary the time stepping. The time stepping will depend on the initial time step size, the minimal and maximum time step size, and the maximum growth and reduction factor. The maximum time step size may change during the simulation time. Time steps are increased or reduced according to growth and reduction factor as a function of the number of iterations needed for convergence. HIGH - medium

NM 2. Time Step Restriction by CFL: PFLOTRAN shall have the ability to restrict time steps as a function of the maximum flow velocity and grid discretization such that CFL (Courant–Friedrichs–Lewy) number is not exceeded. HIGH - easy

NM 3. Variable Time Step Size by Process Model: PFLOTRAN shall allow different process models, such as flow and transport, to comply with different time step settings. MEDIUM - easy

Nonlinear solvers

NM 4. PFLOTRAN shall implement a Newton-Raphson strategy to solve the set of nonlinear governing equations and iteratively drive the norm of the residual vector to below a desired convergence tolerance. LOW - easy

NM 5. The software shall report convergence failure and cut the timesetp size if the maximum number of Newton iterations is reached. LOW-easy

Convergence may be verified by five different convergence criteria, named as follows:

NM 6. ATOL: Convergence is met when the 2-norm of residual is less than ATOL.

NM 7. DTOL: DTOL establishes divergence when the 2-norm of the residual is greater than DTOL multiplied by the 2-norm of the initial residual (relative to the first Newton iteration).

NM 8. ITOL_UPDATE: Convergence is met when the infinity norm update (difference between the current and previous solution) is less than ITOL_UPDATE.

NM 9. RTOL: Convergence is met when the 2-norm of residual is less than RTOL multiplied by the 2-norm of the residual from the first Newton iteration.

NM 10. STOL: Convergence is met when the 2-norm of the update (difference between the current and the previous iteration solution) is less than STOL multiplied by the 2-norm of the previous iteration solution.

MEDIUM - easy

Linear solvers

The set of nonlinear governing equations is solved using Newton-Raphson's method, which uses a sequence of linearized problems to find the solution. To solve this system of linear equations, PFLOTRAN allows the use of two solvers: direct and iterative solvers. The direct solver uses an LU decomposition and iterative solver options are: Bi-CGStab (default), and GMRES. PFLOTRAN allows the specification of the maximum number iterations. For iterative solvers, three types of convergence criteria shall be implemented:

NM 11. ATOL: Convergence is met when the 2-norm of residual is less than ATOL.

NM 12. DTOL: DTOL establishes divergence when the 2-norm of the residual is greater than DTOL multiplied by the 2-norm of the initial residual (relative to the first linear iteration).

NM 13. RTOL: Convergence is met when the 2-norm of residual is less than RTOL multiplied by the 2-norm of the residual from the first linear iteration.

MEDIUM - easy

Finite volume implementation

NM 14. The governing equations are discretized in PFLOTRAN using a cell-centered finite volume approach, and a two-point flux approximation (TPFA) scheme is employed to discretize the mass flux between two grid cells.

Gridding

PFLOTRAN shall accept the following type of grids:

NM 15. Structured grids: PFLOTRAN has the capacity of creating structured cartesian grids of hexahedron cells with varying grid spacing.

NM 16. Implicit unstructured grids: An implicit unstructured grid allows the domain to be discretized with the following types of cells: tetrahedron (4 vertices), pyramid (5 vertices), wedge (6 vertices), and hexahedron (8 vertices). The implicit grid cells are defined by a list of vertices numbers and the vertices are defined by their coordinates.

NM 17. Explicitly unstructured grids: An explicit unstructured grid allows the domain to be discretized with all types of cells, including Voronoi cells. The grid is described by a list of cells and connectivity. Cells are defined by an id, the cell-center coordinates, and the cell volume. The connectivity between two cells is composed by the id for each cell, the area that connects the cells and the face-center coordinates.

We have a test that checks if structured irregular grids with a shifted origin is well built. Do we need a requirement for that?

0.2.5 Representation of Material Properties

PFLOTRAN easily handles highly heterogenous data. PFLOTRAN has the capability of assigining material properties such as permeability and porosity on a cell by cell basis.

RMP 1. PFLOTRAN has the capability of inactiving cells in a determined region.

RMP 2. Material properties are assembled within groups and an integer material ID is assigned to each group for identification. Material IDs can be non-contiguous integers numbers.

PFLOTRAN shall assign material properties and constitutive relationship on a heterogeneous domain using the following strategies:

RMP 3. By region: PFLOTRAN allows the definitions of different regions in the domain. Each region can be linked with a material property.

RMP 4. By location (x,y,z coodinates): PFLOTRAN allows the specification of different material properties based on the cells coordinates.

RMP 5. By cell IDs: PFLOTRAN allows the specification of different material properties based on the cells ID numbers.

0.2.6 Representation of Initial Conditions

PFLOTRAN has the capability of assigining different initial conditions on a cell by cell basis.

PFLOTRAN shall assign heterogeneous initial conditions across the domain using the following strategies:

RIC 1. By region: Several initial conditions are attributed based on the definition of different domain regions.

RIC 2. By location (x,y,z coodinates): Varying initial conditions are specified based on the location of the cells (and their coordinates).

RIC 3. By cell IDs: Initial conditions are set up based on cells IDs.

HIGH - easy

0.2.7 Representation of Boundary Conditions and Source/Sink terms

PFLOTRAN has the capability of assigining different boundary conditions and source-sink terms on a cell by cell basis.

PFLOTRAN shall allow the specification of various boundary conditions and source-sink terms using the following strategies:

RBC 1. By region: Boundary conditions may be linked with different domain regions.

RBC 2. By location (x,y,z coodinates): Boundary conditions may vary along the boundaries based on the cells coordinates.

0.2.8 User Interaction

Input format

UI 1. PFLOTRAN reads an ASCII file as input. The input file is divided into blocks and sub-blocks. The block that specifies the type of simulation to run (e.g.: subsurface) and the process model to use (e.g.: subsurface flow or subsurface transport) is called the simulation block. The simulation block is required in every input file. The remaining blocks define numerical methods, solver options, domain discretization, material properties, constitutive relations, time step options, output options, initial and boundary conditions and regions within the domain. LOW - easy

UI 2. PFLOTRAN allows the definition of regions within the domain, which can be cuboids, rectangles or points. These regions may be linked with different material properties, initial and boundary conditions, allowing those to be linked on a cell by cell basis. HIGH - easy

UI 3. Except for temperature (C), default units and values shall be assumed when no specification is inserted in the input file. LOW - hard

UI 4. If any required keyword, block, sub-block, or property is missing, the simulation will throw an error message informing the user about their mistake. LOW - hard

Output format

UI 5. Output files may be generated for specific moments in time or for periodic times or time steps. HIGH - easy

UI 6. Output results are printed in screen for specified periodic time steps. Screen output may show the 2-norm of the residual, solution, update, and the infinity norm of the residual and update for every Newton iteration. It also shows the number of linear and non-linear iterations needed to reach convergence. LOW - easy

UI 7. The screen output is saved in an ASCII file, which also contains a summary of all parameters and problem setup inputs. HIGH - easy

PFLOTRAN outputs the following results:

UI 8. Snapshot file: A snapshot file outputs the value of specified variables over the entire domain at a specific time. Tecplot block, and HDF5 (default) formats shall serve as snapshot files.

UI 9. Observation file: An observation file outputs the values of specified variables at a determined point over prescribed times. The observation file format in ASCII columns.HIGH - easy

UI 10. Mass balance file: A mass balance output file returns the global mass balance and the fluxes at all boundaries for water at specified times using an ASCII file.HIGH - easy

VTK output files do not output the specific time of the results. I am not including it in the requirements.

In the Tecplot manual, Tecplot block is recommended as the default format. I will only include Tecplot block in

0.3 Non-Functional Requirements

0.3.1 Runtime Performance

NFR 1. The code shall report the total run time at the end of simulation and record the number of processes employed to run the problem. LOW - easy

0.3.2 Software Maintenance

NFR 2. PFLOTRAN shall use a distributed version control to promote a collaborative environment for software development. The collaborative environment is facilitated by the possibility to have remote repositories, which encourages developers to work using several workflow configurations. Distributed version control tracks changes in the code and allows developers to have the full history record.

NFR 3. All code shall meet the standards provided in the Developer's guide.

NFR 4. PFLOTRAN developers' guide shall provide instructions for reporting bugs.

NFR 5. Automated testing shall be implemented for any new capability added.

NFR 6. Any user may contribute to PFLOTRAN code. Changes to the code must undergo peer review before being accepted and must pass all unit and regression tests.

0.3.3 User support

NFR 7. PFLOTRAN shall provide a channel to support to users. This channel may be used for reporting bugs, asking and answering questions, as well as creating a connected community.

0.3.4 Code Availability

NFR 8. PFLOTRAN is a free software and available in an open access repository.

0.4 Tests

Test a. Source/sink test: Mass rate
Test b. Source/sink test: Scaled mass rate by volume
Test c. Source/sink test: Scaled mass rate by permeability
Test d. Source/sink test: Volume rate
Test e. Source/sink test: Scaled volume rate by volume
Test f. Source/sink test: Scaled volume rate by permeability
Test g. 1D fully saturated hydrostatic initial condition: Problem 2.2.6 from Kolditz et al. 2015
Test h. 1D fully saturated Dirichlet BC: Problem 2.2.7 from Kolditz et al. 2015
Test i. 1D fully saturated Neumann BC: Problem 2.2.8 from Kolditz et al. 2015
Test j. 2D fully saturated Dirichlet and Neumann BC:Problem 2.2.10 from Kolditz et al. 2015
Test k. 1D variably saturated from Celia et al. 1990
Test l. 2D variably saturated: Infiltration in a large caisson: problem 10.13.3 from Feflow's manual
Test m. EOS test for IFC67: compare density calculations between PFLOTRAN and python script from STOMP documentation
Test n. EOS test for IF97: compare density calculations between PFLOTRAN and online calculator
Test o. Representation of material properties by cell ID on structured grid (with a 2x2x2 cube)
Test p. Representation of material properties by cell ID on structured grid using random correlated fields of porosity and permeability
Test q. Representation of material properties by cell ID on unstructured grid (with a 2x2x2 cube)
Test r. Representation of material properties by location using gridded datasets on structured grid
Test s. Representation of material properties by location using gridded datasets on unstructured grid
Test t. Representation of material properties by location using regions on structured grid
Test u. Representation of material properties by location using regions on unstructured grid
Test v. Representation of material properties with IJK indices on structured grid
Test w. Test capability of inactivating cells
Test x. Test non-contiguous material IDs
Test y. Test the ability to create structured grids with irregular spacing.
Test z. Representation of initial conditions by cell ID on structured grid (with a 2x2x2 cube)
Test α. Representation of initial conditions by cell ID on unstructured grid (with a 2x2x2 cube)
Test β. Representation of initial conditions by cell ID on structured grid using random correlated fields of porosity, permeability, and initial pressure.
Test γ. Representation of initial conditions by location using regions on structured

grid

Test δ. Representation of initial conditions by location using regions on unstructured grid

Test ε. Representation of initial conditions with IJK indices on structured grid

Test ζ. Representation of initial conditions by location using gridded datasets on structured grid

Test η. Representation of boundary conditions by location using gridded datasets on structured grid (shortcourse example and comparison available at www.pflotran.org/qa)

Test θ. Test time step variablity following the growth factor until it reaches the maximum time step size.

Test ι. Test time step variablity following the reduction factor until it reaches the maximum number of consecutive cuts.

Test κ. Test time step variablity following the reduction factor until it reaches the minimum time step size.

0.4.1 Test matrix for Constitutive Relations

Requirement	Tests that use capability	Tests that verify capability
CR 1	Test m	Yes
CR 2	Test n	Yes
CR 3	Test k, Test l, Test o, doc-dev	Yes
CR 4	doc-dev	Yes
CR 5	Test k, Test l, Test o, doc-dev	Yes
CR 6	doc-dev	Yes
CR 7	Test l, Test o	No
CR 8	**??**	No
CR 9	**??**	No

0.4.2 Test matrix for Physics and Chemistry

Requirement	Tests that use capability	Tests that verify capability
PC 1	Test a to Test x	Yes

0.4.3 Test matrix for Forcing Requirements

Requirement	Tests that use capability	Tests that verify capability
FR 1	Test h, Test j, Test k	Yes
FR 2	Test g, Test w	Yes
FR 3	Test i, Test l	Yes
FR 4	Test a	Yes
FR 5	Test b	Yes
FR 6	Test c	Yes
FR 7	Test d	Yes
FR 8	Test e	Yes
FR 9	Test f	Yes
FR 10	Test i	Yes
FR 11	Test l, Test o	Yes

0.4.4 Test matrix for Numerical Methods

Requirement	Tests that use capability	Tests that verify capability
NM 1	Test θ, Test ι, Test κ	Yes
NM 2	**??**	
NM 3	**??**	
NM 4	**??**	
NM 5	**??**	
NM 6	**??**	
NM 7	**??**	
NM 8	**??**	
NM 9	**??**	
NM 10	**??**	
NM 11	**??**	
NM 12	**??**	
NM 13	**??**	
NM 14	**??**	
NM 15	Test g to Test l, Test y	Yes
NM 16	Test q, Test s	Yes
NM 17	Test b, Test c, Test e, Test f	Yes

0.4.5 Test matrix for Representation of Material Properties

Requirement	Tests that use capability	Tests that verify capability
RMP 3	Test t, Test u, Test v	Yes
RMP 4	Test r, Test s	Yes
RMP 5	Test o, Test q	Yes

0.4.6 Test matrix for Representation of Initial Conditions

Requirement	Tests that use capability	Tests that verify capability
RIC 1	Test γ, Test δ, Test ε	Yes
RIC 2	Test ζ	Yes
RIC 3	Test z, Test β, Test α,	Yes

0.4.7 Test matrix for Representation of Boundary Conditions and Source/Sink terms

Requirement	Tests that use capability	Tests that verify capability
RBC 1	Test b, Test c, Test e, Test f	Yes
RBC 2	Test η	Yes

0.4.8 Test matrix for User Interaction

Requirement	Tests that use capability	Tests that verify capability
UI 1	??	
UI 2	??	
UI 3	??	
UI 4	??	
UI 5	??	
UI 6	??	
UI 7	??	
UI 8	??	
UI 9	??	
UI 10	??	

0.4.9 Test matrix for Non-Functional Requirements

Requirement	Tests that use capability	Tests that verify capability
NFR 2	??	
NFR 3	??	
NFR 4	??	
NFR 5	??	
NFR 6	??	
NFR 7	??	
NFR 8	??	