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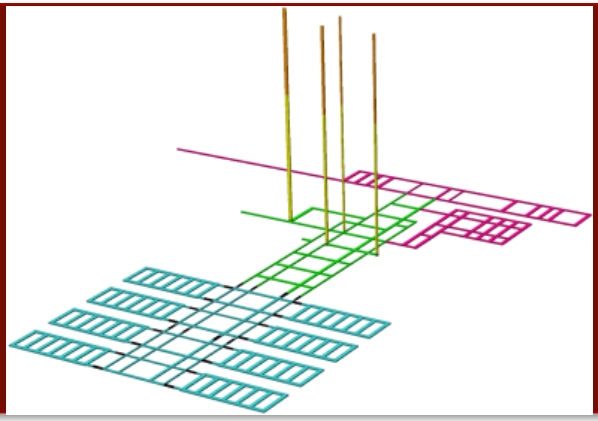

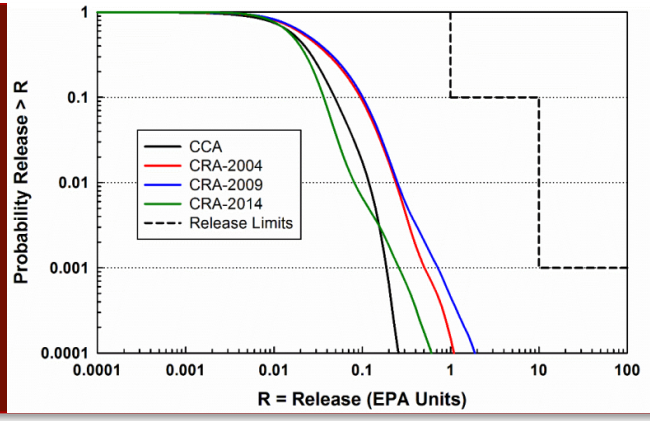

PFLOTRAN QA update

Feb, 11, 2021

Cliff Hansen, Michael Nole, Heeho Park, Jennifer Frederick, Emily Stein

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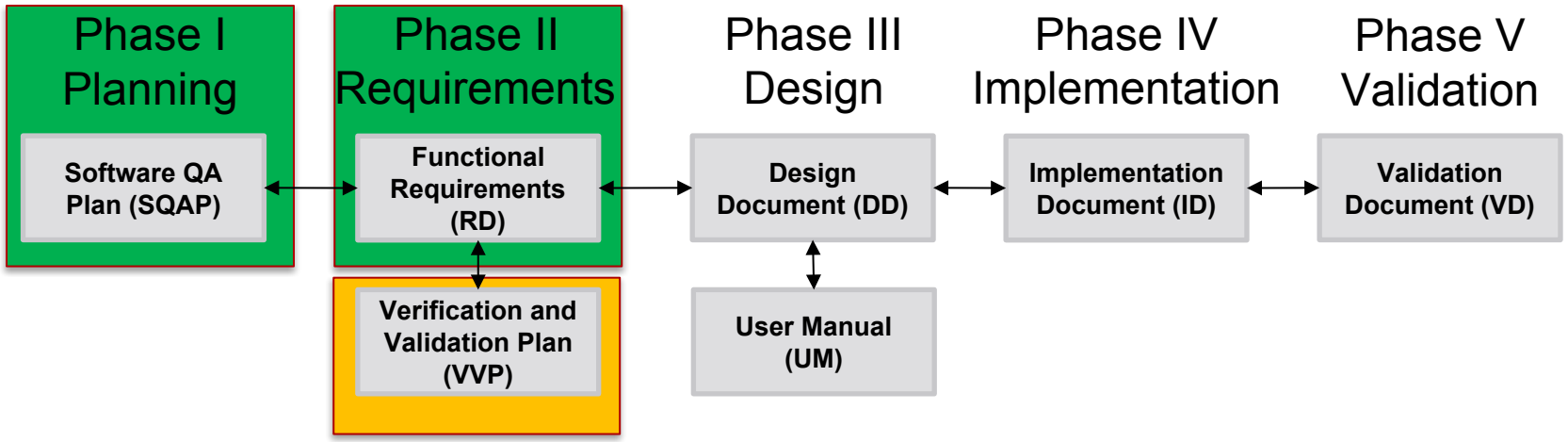
U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Objectives

- FY21: Support the Additional Panels PA (APPA):
  - Qualify PFLOTRAN v3.01 for use in WIPP PA for Salado flow
  - APPA will use existing WIPP models (2D) to support the Planned Change Request (PCR)
  - We will corroborate the 2D flow solution using PFLOTRAN and a 3D model of a 19-panel repository
- PFLOTRAN ready for use in CRA-2024:
  - For both Salado flow and Salado transport
  - Transport capabilities are in development
  - QA of transport capabilities in FY22/23
  - Not planning to use PFLOTRAN for Direct Brine Release

PFLOTRAN v3.01 QA Status



SQAP completed: Feb 2021
RD completed: Feb 2021
VVP draft complete: Feb 2021

- In technical review and editing
- Anticipated published March 2021

Remaining documents planned for June 2021

PFLOTRAN v3.01 requirements

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- Requirements are equivalent to requirements for BRAGFLO as currently used in WIPP PA
  - Two-phase, immiscible, isothermal flow and liquid and gas driven by pressure, capillary and gravity forces in a heterogenous porous medium
  - Gas generation by iron corrosion, microbial degradation of CPR, and radiolysis
  - Chemical reactions involving sulfidation of iron and iron hydroxide, hydration and carbonation of MgO
  - During-simulation material changes
  - Notable change:
    - BRAGFLO "finite difference grid for the problem to be run, including values of Δx, Δy, and Δz"
    - PFLOTRAN "constructs a finite volume three-dimensional grid"

PFLOTRAN vs. BRAGFLO requirements

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- "reset" vs. "restart" capability
  - BRAGFLO "BRAGFLO allows for the change of pressure and saturation values, as well as the capability to turn off the chemistry reactions when materials change"
  - PFLOTRAN "outputs and reads back in a binary-format file containing values necessary to restart a simulation"
- PFLOTRAN v3.01 does not have two BRAGFLO v7.01 capabilities that are tested:
  - For DBR modeling
    - R.16 Well models in BRAGFLO allow simulation of wells that are completed within the formations or porous media being modeled
  - Not used in PA currently
    - R.24 BRAGFLO allows for the smooth change in permeability of materials in time

PFLOTRAN Test Summary

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- Six unit tests – verify lower-level functions
  1. Capillary pressure and relative permeability characteristics (9 total)
  2. Liquid water equation of state
  3. Gas equation of state
  4. Pore compressibility
  5. Fracture initiation and change in porosity
  6. Klinkenberg effect (gas permeability as a function of gas pressure)
- 16 functional tests – verify pressure and saturation solutions
  1. 1D, 2D and 3D grids (simplified) using no-flow, Dirichlet and Neumann boundary conditions
  2. Single phase steady-state and transient flows
  3. Two-phase transient flows
  4. Process models: gas generation, decay and ingrowth, iron and MgO chemistry
  5. Mini-repository test – synthesis of models produces reasonable results