Advanced Simulation Capability for Environmental Management

ASCEM Software Capabilities and Performance Assessment Deployments

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Performance & Risk Assessment Community of Practice
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Why ASCEM?

- **Standardized and consistent** modeling approaches across DOE Complex
- Tools that help explain complex information in an understandable way to all constituents (e.g., public, regulators)
- **Capability to explore problems in greater detail**
  - Manage uncertainty and reduce reliance on over-conservatism that can lead to costly decisions
  - Scientist determines desired complexity

![Active DOE-EM Sites](image-url)
Advanced Simulation Capability for Environmental Management (ASCEM)

- **HPC (Amanzi) Thrust**
  - State-of-the-art subsurface flow and reactive transport simulator
  - Designed to take advantage of modern computing architectures (e.g., multiple cores)

- **Platform (Akuna / Agni / Velo) Thrust**
  - Integrated toolset to address entire modeling workflow:
    - Amanzi simulation, visualization, UQ, SA, PE, data management, and more

- **Site Applications Thrust**
  - ASCEM testing, demonstration and deployment
Amanzi Multi-Process Flow and Reactive Transport Simulator

Salient Features

- Selection of governing equation
  - Transient unsaturated flow with Richards equation
  - Transient single-phase flow with specific storage/yield
- Uniform interface to access existing biogeochemistry codes thru Alquimia
  - PFLOTRAN
  - CRUNCHFLOW
- Meshing
  - Internal mesh generation for rectangular domains
  - Unstructured with polyhedral cells
  - Block-structured adaptive mesh refinement
- Tight integration with Platform Software
  - Parallel computing accessible
ASCEM Platform and Integrated Toolsets

- **Akuna**
  - Mesh generation
  - Input file generation
    - Multiple simulations (e.g., sensitivity analysis [SA], uncertainty quantification [UQ], parameter estimation [PE])
  - Results visualization
    - VisIt integration for spatial viz

- **Velo**
  - Workflow
  - Job launching and monitoring
  - Data and simulation provenance and management

- **Agni**
  - Simulation controller
  - Analysis tool for SA, UQ, PE
ASCEM Platform and Integrated Toolsets

- **Velo**
  - Collaboration
  - Provenance
  - Tool Integration
  - Job Control
  - Data Storage
  - Remote Data

- **Akuna Customized User Environment**
  - Desktop Tools
    - Model Setup
    - Toolset UIs
    - Viz
  - WW
  - L/G

- **HPC Computing Environment**
  - Simulation Controller
  - Agni
  - Model Analysis
  - SR
  - SA
  - PE
  - UQ

- **Simulator Amanzi**

ASCEM Platform and Integrated Toolsets
ASCEM Strengths

- **High Performance Computing (HPC)**
  - Computational algorithms that take advantage of modern computing hardware (multiple cores)

- **Toolset integration**
  - More efficient workflows
  - Automated execution of multiple simulations
    - SA, PE, UQ
  - Data and simulation provenance

- **Cloud computing**
  - Enhanced collaboration
  - Ready access to high-performance computing resources
Site Applications Thrust

- Guide software development
- Assist with testing and QA
- Provide site data for model testing and validation
- Conduct demonstrations of Platform and HPC capabilities
- **Facilitate ASCEM deployments, for example,**
  - Hanford Waste Management Area (WMA) C
  - Savannah River H-Area Tank Farm (HTF)
  - Collaboration with Cementitious Barriers Partnership (CBP)
  - Savannah River F-Area Seepage Basins Plume
Waste Management Area C (WMA C)

- WMA C is located in the 200 East Area of the Hanford Central Plateau
- Tank farm consists of
  - 16 tanks
  - Waste transfer pipelines
  - Tank ancillary equipment (e.g. diversion boxes, valve boxes)
- Tanks in WMA C have stored high-level waste from defense-related nuclear research, development, and weapons production since the late 1940s
- Multiple unplanned releases have occurred
Modeling WMA C Closure

- Preparations for final closure of WMA C is underway
  - Closure follows retrieval of as much tank waste that is technically and economically practical
    - Tanks will be backfilled with grout
    - Will be closed on site as a landfill
- The WMA C Performance Assessment will be used to evaluate risks from landfill closure (i.e., waste left in place at WMA-C)
  - To obtain a ROD, risks from wastes left in place need to be assessed
ASCEM investigating impacts of

- Small-scale heterogeneities on flow and transport under closure and past leak conditions
- Generate multiple realizations of lithofacies distribution using indicator simulation methods
  - Each realization honors borehole data, then reproduces spatial model of lithofacies continuity between boreholes
  - Incorporates heterogeneity of lithofacies, rather than treating stratigraphic units as homogeneous layers
- ASCEM investigating impacts of
  - Use of orthogonal grids in representing the geologic conceptual model
Several SRS waste tanks are fully or partially submerged below water table aquifer.

Closure requires isolation from subsurface flow. A low-permeability cover will not isolate these tanks from subsurface flow, unlike tanks above the water table.

The NRC has expressed the following concern:

*The HTF Performance Assessment does not adequately assess waste release from the submerged and partially submerged tanks via a preferential pathway*  
(NRC Staff Request for Additional Information 31 July 2013)
ASCEM Support for SRS H-Tank Farm Performance Assessment (PA)

- **Current base case modeling approach**
  - Two-dimensional axi-symmetric simulation models
  - Approach suited to tanks in the unsaturated zone
  - Grid sizes are limited to 10,000s nodes to achieve reasonable computational times

- **Challenge for Submerged Tanks**
  - Three-dimensional geometry required because of lateral flow
  - Thin features (e.g. preferential pathway) require fine-scale mesh resolution
  - Millions of nodes required
  - Not feasible with current approach

- **ASCEM deployed to addresses challenges**
ASCEM Deployment

- Use HPC software and hardware to achieve feasible computational runtimes

FY14 ASCEM Deployment

- Collaboration with PA Contractor to define scenario of interest to address NRC concern
- 3D mesh with local resolution of steel liners and fast-flow pathways
- Scale up of problem to millions of nodes with Adaptive Mesh Refinement

Cylindrical tank

Degraded tank configuration w/exaggerated thicknesses for thin features

Physical dimensions for numerical simulation
Unstructured Grid Capability
Unstructured Grid Capability
Unstructured Grid Capability
Structured Grid AMR Capability
Hydraulic Head Simulation
Streamtraces
Velocity Field
Anticipated Next Steps

- Transport simulations for Sr-90 and Cs-137
- Scenario refinements
  - More realistic fast-flow path configurations
  - Patch corrosion of steel liners
  - Time-dependent material degradation
Collaborate with DOE-EM Cementitious Barriers Partnership (CBP) for interface of processes within a cement barrier

Use ASCEM HPC processes outside the cement barrier
Interfaces (Information handoffs)

ASCEM far-field flow simulation

Flow field (CBP boundary condition)

CBP near-field simulation

Contaminant leach rate (ASCEM source term)

ASCEM far-field transport simulation

Contaminant flux to water table
Savannah River F-Area: Controls on Plume migration at geochemically complex

- Savannah River F-Area; Disposal of low-level radioactive, acid waste solutions (1955–1989) created groundwater plume (pH 3–3.5, NO₃, U, ⁹⁰Sr, ¹²⁹I, ⁹⁹Tc, tritium)
- Ongoing remediation includes capping (1989), active pump and treat (1997-2003), and pH manipulation since 2004
- Natural attenuation is desired as a long-term remediation strategy but technical underpinning is lacking.
  - U sorption as function of pH variability
  - Uncertainty: Role of heterogeneity on long term plume tails, source/recharge characteristics on plume longevity, etc.
Visualization Communicates the Results of F-Area Uranium Reactive Transport

Geology and Water table

- TCCZ
- LUTRA
- UUTRA

Total U(VI)

- 3.0e-05
- 2.4e-05
- 1.8e-05
- 1.2e-05
- 6.0e-06
- 0.0

Max: 1.2e-10
Min: 1.2e-10

Distance km

X (m) (x10^3)

Year = 1954

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Environmental Management

safety  performance  cleanup  closure

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Summary

- ASCEM represents the next-generation **agile, open source, and modular computing framework** that has utility for multiple DOE missions
  - ASCEM facilitates model setup, execution, analysis, and visualization
  - High performance computing enables multiple simulations of complex models with reduced computational times
  - Multiple simulation launching capability for UQ, SA, PE

- **ASCEM capabilities are being deployed** to support DOE-EM Performance Assessments

- **ASCEM v2.0 Community Code release anticipated in 2015**
Questions?

http://ascemdoe.org/