Demonstrating Integration of CBP and ASCEM Simulation Tools – 15627

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ABSTRACT

DOE-EM is supporting two crosscutting projects to develop software and conduct targeted experiments to enhance performance and risk assessment capabilities: the Cementitious Barriers Partnership (CBP) and the Advanced Simulation Capability for Environmental Management (ASCEM). The CBP is a smaller-scale project of coordinated software development and experimentation focused on cementitious materials. ASCEM is a larger-scale project aimed at developing next-generation, science-based, reactive flow and transport simulation capabilities and supporting modeling toolsets within a high-performance computing framework to address DOE-EM's waste management and environmental cleanup challenges. Complementary integration of CBP and ASCEM software toolsets has been demonstrated through a joint simulation of radionuclide release and transport in a representative tank closure scenario. Specialized CBP capabilities for simulating reactive transport in cementitious materials were utilized in a near-field simulation of radionuclide leaching from the engineered system. The high-performance computing (HPC) capabilities of the ASCEM Amanzi simulator were utilized to simulate far-field flow and transport in the natural environment outside the closed tank. The ASCEM flow simulation provided boundary conditions to the CBP near-field model, which in turn provided radionuclide source terms to the ASCEM far-field transport simulation. The joint demonstration illustrates how the two crosscutting projects can be used in a complementary manner to enhance DOE performance and risk assessment.

INTRODUCTION

The United States Department of Energy, Office of Environmental Management (DOE-EM) uses fate and transport modeling as an input to support decision-making for a variety of applications in site restoration, tank closure, and waste management. Waste disposal facilities and tank closure efforts must include site specific Performance Assessments (PAs) to demonstrate compliance with DOE Order 435.1, Radioactive Waste Management and, as applicable, other Federal and/or State requirements. Risk assessments are also conducted to support decision making for environmental restoration activities. A large focus of such modeling efforts is on processes occurring in the natural environment, which are often supplemented by engineered solutions. Engineered barriers involving cementitious materials and waste forms are commonly used to enhance the performance for tank closure and waste disposal facilities. Such assessments require site-specific data for precipitation, cap, soil and waste properties, engineered barrier properties and ground water which are used in models to consider water balance, contaminant transport in the disposal facility (near field), flow and transport through the vadose zone and groundwater (far field) and dose calculations for exposure to the public.

Recognizing the importance of modeling and the prominent role of cementitious materials in many activities, DOE-EM is supporting two crosscutting projects to develop software and conduct targeted experiments to enhance PA and risk assessment capabilities: the Cementitious Barriers Partnership (CBP) and the Advanced Simulation Capability for Environmental Management (ASCEM). The two projects are being developed in a complementary manner, including efforts to demonstrate how they can be used in an integrated approach to support improved decision-making.

The CBP project is a coordinated software development and experimentation focused on cementitious materials (http://cementbarriers.org) [1–4]. The CBP works to improve understanding and prediction of the long-term structural, hydraulic, and chemical performance of cementitious materials and waste forms used primarily in nuclear waste disposal. The CBP released its CBP Software Toolbox version 1.0 in December 2012 and version 2.0 in May 2014 [5, 6]. The Toolbox is currently composed of LeachXS/Orchestra [7] (http://cementbarriers.org/partner-codes/leachxs-orchestra/), Stadium [8] (http://www.stadium-software.com/), and a GoldSim (www.goldsim.com) graphical user interface and uncertainty framework. The CBP is distinguished by its focus on processes occurring in cementitious materials and consideration of material damage / material property alteration using primarily one-dimensional flow and reactive transport and simulation on Windows OS computers.

The ASCEM project is aimed at developing next-generation, science-based, reactive flow and transport simulation capabilities and supporting modeling workflow within a high-performance computing framework to address DOE-EM's waste management and environmental cleanup challenges (http://ascemdoe.org) [9,10]. ASCEM accomplished its first Research code release in January 2014 and a Community code release is planned for fiscal year 2015. The major components of ASCEM are a flow and transport simulator named Amanzi, a job control and sensitivity analysis/uncertainty analysis driver named Agni, and a graphical user interface and integrating platform for modeling workflow named Akuna. The ASCEM project is distinguished by its comprehensive scope and emphasis on high-performance computing capabilities.

The two software packages can be jointly applied to DOE-EM needs in a complementary manner. Specifically, the ASCEM toolset can provide the overall project framework and system model. The CBP toolset can provide specialized information supporting the ASCEM system model in two broad areas: 1) physical and/or chemical degradation of cementitious materials, and 2) species leaching from cementitious materials as a near-field source term. To illustrate how the two tools can be leveraged to address modeling challenges for waste tank closure, the CBP and ASCEM projects are pursuing the joint demonstration described below. This initial demonstration highlights one manner in which the strengths of the two toolsets can be combined in a complementary manner.

DEMONSTRATION CONCEPT

Figure 1 illustrates a waste tank closure scenario that is representative of the DOE-EM Hanford and Savannah River Sites [11]. Following waste removal, a residual waste layer rests on the bottom of the steel-lined, concrete tank, and the remaining void space has been filled with a reducing grout. The concrete shell surrounding the primary steel liner provides an additional barrier between the waste and natural environment. A post-closure, engineered, low-infiltration cover system is assumed to be in place in a humid climate as a bounding case.

During Performance Assessment analysis timescales extending potentially to many thousands of years, engineered barriers can be expected to degrade physically and chemically. The steel liner will be subject to general and/or pitting corrosion making the component increasingly permeable over time. Of particular interest is movement of a carbonation front through the adjoining concrete barrier, which will lead to loss of passivated steel conditions (including rebar) and accelerated corrosion. Depending on the exposure environment, concrete barrier properties may evolve through a number of processes including decalcification (primary constituent leaching), carbonation, oxidation, and sulfate attack. Radionuclide contaminant transport through cementitious materials will be affected by evolving cement chemistry, for example Eh and pH changes, as well as advection and diffusion influenced by changing physical properties (e.g. cracking) and infiltration.

ASCEM includes capabilities for modeling workflow and general multi-dimensional flow and reactive transport modeling designed to take advantage of high-performance computing resources. CBP software provides specialized capabilities for simulating cementitious material evolution and multiphase reactive transport in cementitious materials, but is typically used to evaluate one-dimensional scenarios using desktop computing resources. To leverage these respective strengths, ASCEM and CBP software can be utilized in the manner depicted in Figure 2. In this configuration, the Amanzi simulator from ASCEM is used to simulate far-field flow conditions around the closed waste tank. The ASCEM Amanzi flow field becomes a boundary condition for a near-field CBP simulation of contaminant leaching through cementitious materials (tank-fill grout and concrete barriers). The leach rate from the CBP near-field model becomes the source term for an ASCEM Amanzi simulation of far-field contaminant transport to the water table.

From a practical perspective, this initial demonstration is also being used to identify the information content and format that need to be exchanged between the two toolsets and to identify ways to facilitate efficient inter-code communication, and to enhance each code along its development path.

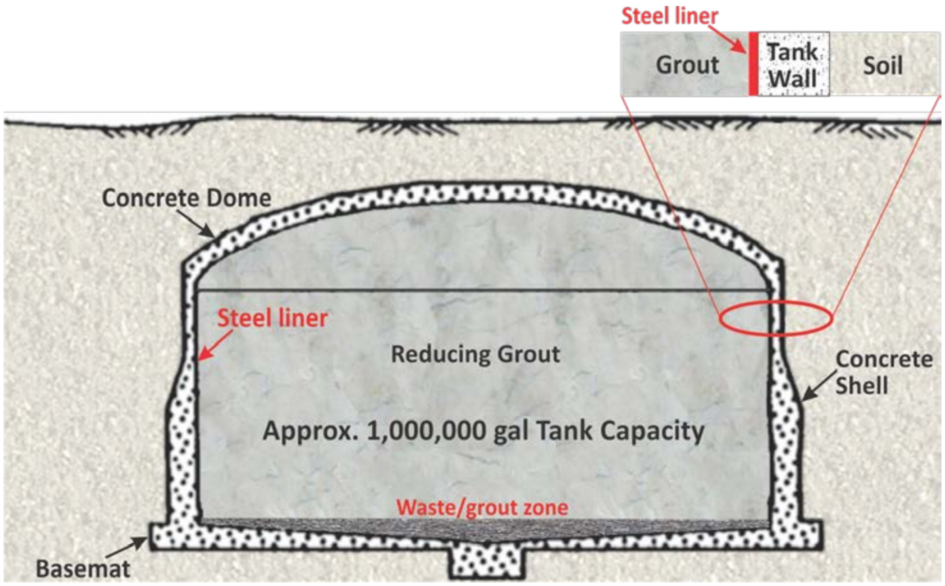

Fig. 1. Representative DOE-EM Waste Tank Closure Scenario.

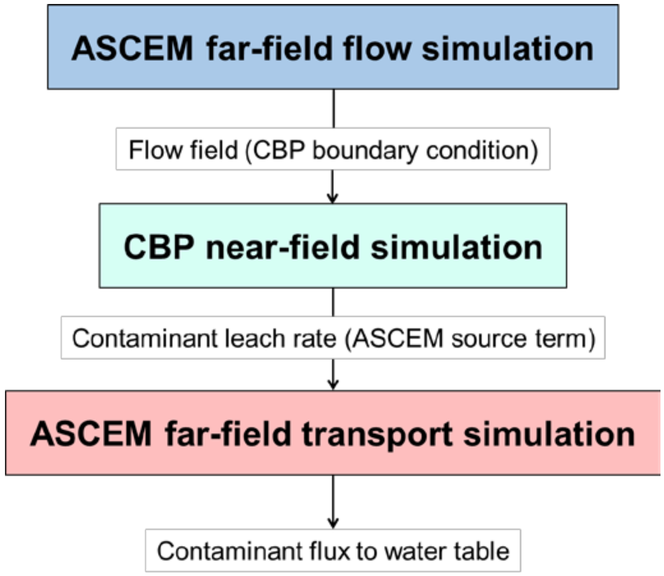

Fig. 2. Workflow for CBP and ASCEM Software Coupling.

MODEL DEVELOPMENT PROGRESS

Because the primary purpose of the model simulations is to demonstrate complementary linkage of CBP and ASCEM software, the waste release scenario chosen for modeling is hypothetical, although similar to those encountered in a DOE tank closure Performance Assessment. Figure 3 illustrates the primary phenomena considered in the CBP near-field model. Two radionuclide species of common interest in DOE-EM Performance Assessments are considered, I-129 and Tc-99. Of particular importance to redox sensitive Tc-99 is gas-phase ingress of oxygen in addition to dissolved oxygen. The multiphase CBP model incorporates both means of oxidation of reducing cementitious materials and Tc-99. Key boundary conditions needed for the CBP model are the volumetric water flux and saturation in the soil layer. These are defined in the joint demonstration by a variably saturated (Richard equation) flow simulation using the ASCEM Amanzi simulator following the workflow in Figure 2. The ASCEM flow model is being initially developed with at a surface infiltration rate of 10 cm/yr and water table positioned just beneath the waste tank, conditions representative of a humid environment such as the Savannah River Site. Additional simulations at much lower infiltration and material saturations are planned. The CBP near-field model is being developed based on the carbonation model described in Reference [1]. Model development is focused on adding gas-phase oxygen transport and oxidation reactions.

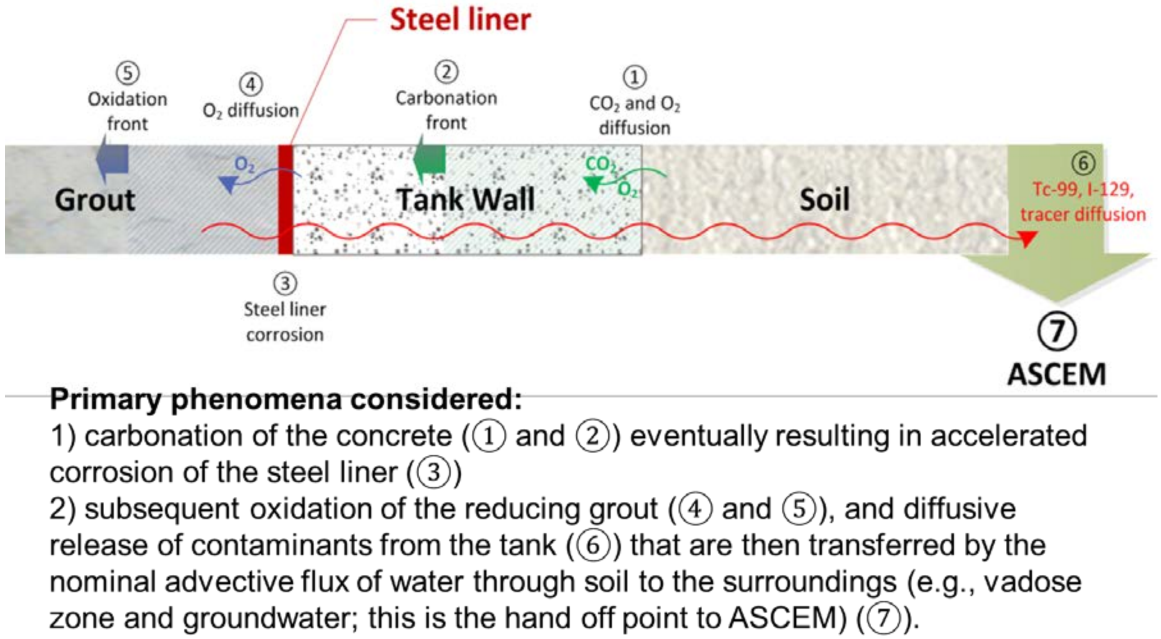

Fig. 3. CBP Near-Field Simulation Using LeachXS/ORCHESTRA.

CONCLUSIONS

CBP and the ASCEM software capabilities are being leveraged in a joint simulation of radionuclide release from a hypothetical closed waste tank. Specialized CBP capabilities for simulating reactive transport in cementitious materials were utilized in a near-field simulation of radionuclide leaching from the engineered system. The high-performance computing (HPC) capabilities of the ASCEM Amanzi simulator were utilized to simulate far-field flow and transport. The ASCEM flow simulation provided boundary conditions to the CBP near-field model, which in turn provided radionuclide source terms to the ASCEM far-field transport simulation. The joint demonstration illustrates how two crosscutting projects can be used in a complementary manner to enhance DOE-EM PA and risk assessment.

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