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Research paper

Rapid methods for radionuclide contaminant transport in nuclear fuel cycle simulation

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ABSTRACT

Nuclear fuel cycle and nuclear waste disposal decisions are technologically coupled. However, current nuclear fuel cycle simulators lack dynamic repository performance analysis due to the computational burden of high-fidelity hydrolgic contaminant transport models. The Cyder disposal environment and repository module was developed to fill this gap. It implements medium-fidelity hydrologic radionuclide transport models to support assessment appropriate for fuel cycle simulation in the Cyclus fuel cycle simulator.

Rapid modeling of hundreds of discrete waste packages in a geologic environment is enabled within this module by a suite of four closed form models for advective, dispersive, coupled, and idealized contaminant transport: a Degradation Rate model, a Mixed Cell model, a Lumped Parameter model, and a 1-D Permeable Porous Medium model. A summary of the Cyder module, its timestepping algorithm, and the mathematical models implemented within it are presented. Additionally, parametric demonstrations simulations performed with Cyder are presented and shown to demonstrate functional agreement with parametric simulations conducted in a standalone hydrologic transport model, the Clay Generic Disposal System Model developed by the Used Fuel Disposition Campaign Department of Energy Office of Nuclear Energy.

1. Introduction

Repository performance metrics provide an important basis for comparison among potential nuclear fuel cycles. Additionally, nuclear fuel cycle and nuclear waste disposal decisions are technologically coupled through the characteristics of spent fuel which vary among fuel cycles and impact repository design and performance (i.e. spent nuclear fuel (SNF) volume, isotopic composition, mass, disposition, and other variables). For this reason, dynamic integration of a generic disposal model with a fuel cycle systems analysis framework is necessary to illuminate performance distinctions of candidate repository host media, designs, and engineering components in the context of fuel cycle options. However, the computational burden of robust repository performance analysis has previously not been compatible with fuel cycle simulation. Therefore, current nuclear fuel cycle simulators lack coupled repository performance analysis capabilities.

Most current tools treat the waste disposal phase of fuel cycle analysis statically in post processing by reporting values such as mass, volumes, radiotoxicity, or heat production of accumulated SNF and high level waste(HLW). Such tools (e.g., Nuclear Waste Assessment System for Technical Evaluation) (NUWASTE) [1], Dynamic Analysis of Nuclear Energy System Strategies(DANESS) [2], Nuclear Fuel Cycle Simulator(NFCSim) [3], and ORION [4]) fail to address the dynamic impact of those waste streams on the performance of the geologic disposal system [5]. Two tools, Commelini-Sicard(COSI) [6] and the Verifiable Fuel Cycle Simulation Model(VISION) [5–8], dynamically perform heat based capacity calculations. However, those calculations are applicable only for specific repository concepts and cannot inform sensitivity to alternate geologic disposal system characteristics. Since repository capacity and loading strategies are impacted by SNF characteristics such as volume and composition, and since those may vary according to fuel cycle strategy and may over time in scenarios which include transitions between fuel cycles, a dynamic coupling between fuel cycle analysis and repository loading and performance more accurately captures reality.

This paper presents the Cyder software library [9] and its radionuclide contaminant transport models, which were developed to fill this capability gap. To enable dynamic analysis of waste metrics, Cyder provides medium fidelity models to conduct repository performance analysis on efficient timescales appropriate for fuel cycle analyses. It has been implemented as a Facility compatible

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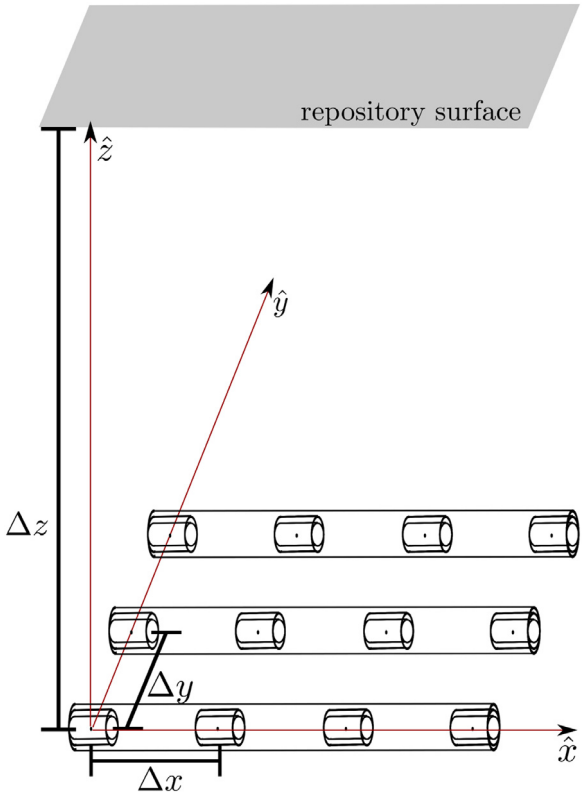

Fig. 1. In Cyder, as in a canonical drift-tunnel repository, waste form components (the innermost components) are contained by waste package components which are, in turn, emplaced in a buffer component (the backfilled emplacement tunnel into which waste packages are loaded). That buffer component contains many other waste packages, spaced evenly in a horizontal grid. The geosphere (the outermost component) occupies all space below the repository surface and outside of the buffer components (emplacement tunnels). The Cyder repository layout has a depth (Δz) and package spacing defined by the user input (Δx within the drifts and Δy between drifts).

with version 0.3 of the Cyclus framework [10], but since it is compiled as a dynamically loadable shared object library with a well defined application programming interface(API), it can also be used as a standalone library. An overview of the Cyder framework and mathematical descriptions of its radionuclide transport models appear in Section 2.

The present work also verifies the hydrologic modeling capability in Cyder through parametric simulations performed with Cyder within Cyclus. Those results are presented in Section 3 alongside comparable parametric simulations conducted using a more detailed computational model, the Clay Generic Disposal System Model(GDSM). The Clay GDSM was developed by the Used Fuel Disposition(UFD) Campaign within the Department of Energy(DOE) Office of Nuclear Energy [11] and relies on the GoldSim simulation environment [12] and its contaminant transport module [12].

2. Radionuclide mass transport In Cyder

Cyder conducts radionuclide contaminant transport through a generic geologic repository concept to determine the contaminants expected to reach the environment. This calculation informs repository containment and environmental impact performance assessment metrics.

To achieve this, Cyder represents engineered and natural containment barriers as distinct control volumes. These *components* are arranged in a regular grid at a single vertical depth within a geologic component as in Fig. 1.

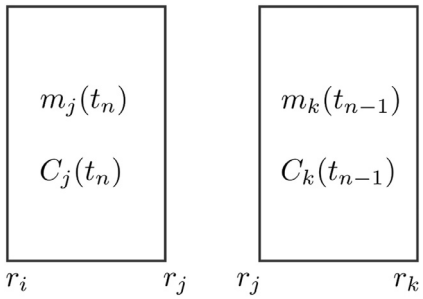

Fig. 2. Two components (j and k) share an interface at r_j. They each contain mass (m) and concentration (C) profiles at the beginning of timestep t_n.

Component mass inventory is a simple sum of in and out flows while mass distribution within the component is determined by the dominant physics of the mass balance model selected for that volume. Adjacent components share mass transfer interfaces across which mass transfer is calculated based on internal component mass inventory and distribution.

In Cyder, the mass transfer and mass balance solution follows an implicit *time stepping algorithm*. The solution behavior is determined by selecting among *mass balance models* within the components and selecting among *mass transfer modes* at boundaries between them. This section will describe the mathematics behind these three aspects of the Cyder paradigm, beginning with the phases of the time stepping algorithm.

2.1. Time stepping algorithm

In Cyder, radionuclide contaminants flow outward from the central component, usually the waste form. An implicit time stepping method arrives at the updated state of each component, radially outward, as a function of both the past state and the current state of the system. Mass balance is conducted in each component at each time step. These calculations proceed from the innermost component (e.g. the waste form) to the outermost component (e.g. the far field), with mass transfer calculations conducted at the boundaries. As mass flows from inner components to outer components, the mass balances in both components are updated. Thus, nuclide release information passes radially outward from the waste stream sequentially through each containment layer to the geosphere in a generic geometry of the form in Fig. 1. The default timestep in Cyclus, and therefore in Cyder, is one month.

At each component interface where mass transfer occurs and within each component where mass balances take place, the flow model is solved with the most up to date information available. To illustrate the algorithm by which mass flow calculations are conducted through the system of components at each time step, the phases of a single time step for a simple pair of components will be described.

The flow of the timestepping algorithm is seen in Figs. 2–4 and is detailed further in the following sections. For the remaining discussion, the source of material, *i*, is the inner component (i.e. the waste form) and the next destination of the material, *j*, is the adjacent outer component (i.e. the waste package). This example will be carried through the explanation of all five phases of the timestepping algorithm.

2.1.1. Phase 1: initial conditions

At the beginning of a timestep, the initial conditions in both the source and the sink are equal to the final updated state of the previous time step. On the first time step, initial mass inventories of each component in the repository system must be defined. In

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