AN INTEGRATED USED FUEL DISPOSITION AND GENERIC REPOSITORY MODEL

by

Kathryn D. Huff

A preliminary report submitted in partial fulfillment of
the requirements for the degree of

Doctor of Philosophy

(Nuclear Engineering and Engineering Physics)

at the

UNIVERSITY OF WISCONSIN–MADISON

2011

ACKNOWLEDGMENTS

I am grateful to a number of extraordinary professors and colleagues at the Universities of Wisconsin and Chicago who have inspired and encouraged me. Among them, I am especially indebted to my advisor, Paul P.H. Wilson, for his invaluable technical and practical guidance. I am also grateful to my laboratory advisor, Mark Nutt, and laboratory collaborator, Ted Bauer. They have been an outstanding resource for the work at hand and I look forward to learning a great deal from them in the upcoming phase of my research.

CONTENTS

LIST OF TABLES

LIST OF FIGURES

ACRONYMS

ANDRA Agence Nationale pour la gestion des Déchets RAdioactifs, the French National Agency for Radioactive Waste Management. 13, 21, 23, 25, 28, 73, 97, 103

ANL Argonne National Laboratory. 68, 69, 76, 98, 99

CAFCA Code for Advanced Fuel Cycles Assessment. 19

CEA Commissariat a l'Energie Atomique et aux Energies Alternatives. 18

COSI Commelini-Sicard. 18

CSNF Commercial Spent Nuclear Fuel. 36

CUBIT CUBIT Geometry and Mesh Generation Toolkit. 71

DANESS Dynamic Analysis of Nuclear Energy System Strategies. 18

DOE Department of Energy. v, vi, 4, 11, 12

DSNF DOE Spent Nuclear Fuel. 36

EBS Engineered Barrier System. 34, 35, 42, 43, 69, 77, 98

EDZ Excavation Disturbed Zone. 69

EPA Environmental Protection Agency. 8, 9

FCO Fuel Cycle Options. v, vi, 10, 93

FEHM Finite Element Heat and Mass Transfer. 70, 71

FEPs Features, Events, and Processes. 68

GDSM Generic Disposal System Model. 12, 13, 21, 67–69, 93, 97–99, 101, 103, 105

GPAM Generic Performance Asessment Model. 21, 67, 68, 103

HTGR High Temperature Gas Reactor. 36

INL Idaho National Laboratory. 17

LANL Los Alamos National Laboratory. 68, 69

LBNL Lawrence Berkeley National Laboratory. 68

LLNL Lawrence Livermore National Laboratory. 68, 77, 93, 98, 99, 101

MA Minor Actinide. 36

MIT the Massachusettes Institute of Technology. 19

NAGRA National Cooperative for the Disposal of Radioactive Waste. 25

NFCSim Nuclear Fuel Cycle Simulator. 19

NUWASTE Nuclear Waste Assessment System for Technical Evaluation. 17

NWTRB Nuclear Waste Technical Review Board. 17

OCRWM Office of Civillian Radioactive Waste Management. 20

PEI Peak Environmental Impact. 10

RD&D Research Development and Design. 10

SINDA\G Systems Improved Numerical Differencing Analyzer \ Gaski. 68, 74–76, 93, 98, 99, 101

SNL Sandia National Laboratory. 68, 69

SWF Separations and Waste Forms. 10

TSM Total System Model. 20

UFD Used Fuel Disposition. v, vi, 10–13, 30, 65, 67, 77, 92, 93, 97, 99, 103

US United States. 3, 11, 23, 25, 31

UW University of Wisconsin. 80, 85

VISION the Verifiable Fuel Cycle Simulation Model. 16, 17

WIPP Waste Isolation Pilot Plant. 28, 30

YMR Yucca Mountain Repository Site. 4, 5, 9, 18, 21, 22, 38, 63, 74

AN INTEGRATED USED FUEL DISPOSITION AND GENERIC REPOSITORY MODEL

Kathryn D. Huff

Under the supervision of Professor Paul P.H. Wilson

At the University of Wisconsin-Madison

As the United States Department of Energy (DOE) simultaneously considers alternative fuel cycles and waste disposal options, an integrated fuel cycle and generic disposal system analysis tool is increasingly necessary for informing domestic nuclear spent fuel policy. A generic repository model capabable of illuminating the distinct dominant physics of candidate repository lithologies, designs, and engineering components will provide an interface between the Used Fuel Disposition (UFD) and Fuel Cycle Options (FCO) Campaign goals. Repository metrics such as necessary repository footprint and peak annual dose are affected by heat and radionuclide release characteristics specific to variable spent fuel compositions associated with alternative fuel cycles. Computational tools capable of simulating the dynamic, heterogeneous spent fuel isotopics resulting from transition scenarios and alternative fuel cycles are, however, lacking in repository modeling options. This work proposes to construct such a generic repository model appropriate for systems analysis. By emphasizing modularity and speed, the work at hand seeks to provide a tool which captures the dominant physics of detailed repository analysis within the UFD Campaign and can be robustly and flexibly integrated within the Cyclus fuel cycle simulation tool.

Paul P.H. Wilson

ABSTRACT

As the United States Department of Energy (DOE) simultaneously considers alternative fuel cycles and waste disposal options, an integrated fuel cycle and generic disposal system analysis tool is increasingly necessary for informing domestic nuclear spent fuel policy. A generic repository model capabable of illuminating the distinct dominant physics of candidate repository lithologies, designs, and engineering components will provide an interface between the Used Fuel Disposition (UFD) and Fuel Cycle Options (FCO) Campaign goals. Repository metrics such as necessary repository footprint and peak annual dose are affected by heat and radionuclide release characteristics specific to variable spent fuel compositions associated with alternative fuel cycles. Computational tools capable of simulating the dynamic, heterogeneous spent fuel isotopics resulting from transition scenarios and alternative fuel cycles are, however, lacking in repository modeling options. This work proposes to construct such a generic repository model appropriate for systems analysis. By emphasizing modularity and speed, the work at hand seeks to provide a tool which captures the dominant physics of detailed repository analysis within the UFD Campaign and can be robustly and flexibly integrated within the Cyclus fuel cycle simulation tool.

1 INTRODUCTION

The scope of this work includes implementation of a software library of medium fidelity models to comprehensively represent various long-term disposal system concepts for nuclear material. This software library will be integrated with a computational fuel cycle systems analysis platform in order to inform repository performance metrics with respect to candidate fuel cycle options. By abstraction of more detailed models, this work will capture the dominant physics of radionuclide and heat transport phenomena affecting repository performance in various geologic media and as a function of arbitrary spent fuel composition.

1.1 Motivation

The development of sustainable nuclear fuel cycles is a key challenge as the use of nuclear power expands domestically and internationally. While fuel cycle performance may be measured with respect to a variety of metrics, waste management metrics are of particular importance to the goal of sustainability. Since disposal options are influenced by upstream fuel cycle decisions, a relevant analysis of potential geological disposal and engineered barrier solutions requires a system level approach that is both modular and efficient.

As the merits of numerous combinatoric fuel cycle possibilities are investigated, a top-level simulation tool capable of modular substitution of various fuel cycle facility, repository, and engineered barrier components is needed. The modular waste package and repository models resulting from this work will assist in informing current technology choices, identifying important parameters contributing to key waste disposal metrics, and highlighting the most promising waste disposal combinations with respect

to metrics chosen by the user. Specifically, such models will support efforts underway in focusing domestic research and development priorities as well as computational tools under development that quantify these metrics and demonstrate the merits of different fuel cycle alternatives.

System level fuel cycle simulation tools must facilitate efficient sensitivity and uncertainty analyses as well as simulation of a wide range of fuel cycle alternatives. Efficiency is achieved with models at a level of detail that successfully captures significant aspects of the underlying physics while achieving a calculation speed in accordance with use cases requiring repeated simulations. Often termed abstraction, the process of simplifying while maintaining the salient features of the underlying physics is the method by which used fuel disposal system models will be developed in this work.

Independent fuel cycle parameters of particular interest in fuel cycle systems analysis have been those related to the front end of the fuel cycle. Deployment decisions concerning reactor types, fast to thermal reactor ratios, and burnup rates can all be independently varied in fuel cycle simulation codes in such a way as to inform domestic policy decisions going forward. Some of these parameters are coupled, however, to aspects of the back end of the fuel cycle. For example, the appropriate fast reactor ratio is significantly altered by the chosen method and magnitude of domestic spent fuel reprocessing (or not).

However, independent variables representing decisions concerning the back end of the fuel cycle are of increasing interest as the United States further investigates repository alternatives to Yucca Mountain. Parameters such as the repository lithology, engineered barriers, appropriate loading strategies and schedules are all independent variables up for debate. All of these parameters are coupled with decisions about the fuel cycle.

Thus, while independent parameters can be chosen and varied within a fuel cycle

simulation, some parameters are coupled in such a way as to require full synthesis with a systems analysis code that appropriately determines the isotopic mass flows into the repository, their appropriate conditioning, densities, and other physical properties.

Future Fuel Cycle Options

Domestically, nuclear power expansion is motivated by the research, development, and demonstration roadmap being pursued by the United States Department of Energy Office of Nuclear Energy (DOE-NE), which seeks to ensure that nuclear energy remain a viable domestic energy option [22].

As the DOE-NE seeks to develop technologies and strategies to support a sustainable future for nuclear energy, various fuel cycle strategies and corresponding disposal system options are being considered. Specifically, the domestic fuel cycle option space under current consideration is described in terms of three distinct fuel cycle categories with the monikers Once Through, Full Recycle, and Modified Open. Each category presents unique disposal system siting and design challenges. Systems analyses for evaluating these options must be undertaken in order to inform a national decision to deploy a comprehensive fuel cycle system by 2050 [22].

The Once-Through Cycle category includes fuel cycles similar to the continuation of the business as usual case in the United States. Such fuel cycles neglect reprocessing and present challenges associated with high volumes of minimally treated spent fuel streams. In a business as usual scenario, conventional power reactors comprise the majority of nuclear energy production and fuel takes a single pass through a reactor before it is classified as waste and disposed of. In the open cycle, no reprocessing is pursued, but research and development of advanced fuels seek to reduce waste volumes. Calculations from the Electric Power Research Institute corroborated by the United

States (US) Department of Energy (DOE) in 2008 indicate that without an increase in the statutory capacity limit of the Yucca Mountain Repository Site (YMR), continuation of the current Once Through fuel cycle will generate a volume of spent fuel that will necessitate the siting of an additional federal geological repository to accommodate spent fuel [34, 21].

A Full Recycle option, on the other hand, requires the research, development, and deployment of partitioning, transmutation, and advanced reactor technology for the reprocessing of used nuclear fuel. In this scheme, conventional once-through reactors will be phased out in favor of fast reactor and so called Generation IV reactor technologies, which demonstrate transmutation capacity and greater fuel efficiency. All fuel in the Full Recycle strategy will be reprocessed. It may be reprocessed using an accelerator driven system or by cycling through an advanced fast reactor. Such fuel may undergo partitioning, the losses from which will require waste treatment and ultimate disposal in a repository. Thus, a repository under the Full Recycle scenario must support a waste stram composition that is highly variable during transition periods as well as myriad waste forms and packaging associated with isolation of differing waste streams.

Finally, the Modified Open Cycle category of options includes a variety of fuel cycle options that fall between once through and fully closed. Advanced fuel cycles such as deep burn and small modular reactors will be considered within the Modified Open set of fuel cycle options as will partial recycle options. Partitioning and reprocessing strategies, however, will be limited to simplified chemical separations and volatilization under this scheme. This scheme presents a dual challenge in which spent fuel volumes and composition will both vary dramatically among various possibilities within this scheme [22] .

Clearly, the myriad waste streams resulting from potential fuel cycles present an

array of corresponding waste disposition, packaging, and engineered barrier system options. For a comprehensive analysis of the disposal system, dominant physics models must therefore be developed for each of these subcomponents. Differing spent fuel composition, partitioning, transmutation, and chemical processing decisions upstream in the fuel cycle demand differing performance and loading requirements of waste forms and packaging. The capability to model thermal and radionuclide transport phenomena through, for example, vitrified glass as well as ceramic waste forms with with various loadings for arbitrary isotopic compositions is therefore required. This work will produce a repository model that meets this need.

Future Waste Disposal System Options

In addition to reconsideration of the domestic fuel cycle policy, the uncertain future of the YMR has driven the expansion of the option space of potential repository geologies to include, at the very least, granite, clay/shale, salt, and deep borehole concepts [44].

In accordance with various fuel cycle options, corresponding waste form, waste package, and other engineered barrier systems are being considered. Specifically, current considerations include ceramic (e.g. Uranium Oxide), glass (e.g. borosilicate glasses), and metallic (e.g. hydride fuels) waste forms. Waste packages may be copper, steel, or other alloys. Similarly, buffer and backfill materials vary from the crushed salt recommended for a salt repository to bentonite or concrete in other geologies. Therefore, a repository model capable of modular substitution of waste form models and data will be necessary to analyze the full option space.

The physical, hydrologic, and geochemical mechanisms that dictate radionuclide and heat transport vary between the geological and engineered containment systems in the domestic disposal system option space. Therefore, in support of the system level

simulation effort, models must be developed that capture the salient physics of these geological options and quantify associated disposal metrics and benefits. Furthermore, in the same way that system level modularity facilitates analysis, so too will modular linkage between subcomponent process modules. These subcomponent models and the repository environmental model must achieve a cohesively integrated disposal system model such as is proposed by this work.

Thermal Modeling Needs

The decay heat from nuclear material generates a significant heat source within a repository. In order to arrive at loading strategies that comply with thermal limits in the engineered barrier system and the geological medium, a thermal modeling capability must be included in the repository model. Such a model is also necessary to inform material and hydrologic phenomena that affect radionuclide transport and are thermally coupled.

Partitioning and transmutation of heat generating radionuclides within some fuel cycles will alter the heat evolution of the repository [57]. Thus, to distinguish between the repository heat evolution associated with various fuel cycles involving partitioning and transmutation, a repository analysis model, must at the very least, capture the decay heat behavior of dominant heat contributors. Plutonium, Americium, and their decay daughters dominate decay heat contribution within used nuclear fuels. Other contributing radionuclides include Cesium, Strontium, and Curium [48].

Thermal limits within a used nuclear fuel disposal system are waste form, package, and lithology dependent. The heat evolution of the repository constrains waste form loadings and package loadings as heat generated in the waste form is transported through the package. It also places requirements on the size, design, and loading

strategy in a potential geological repository as that heat is deposited in the engineered barrier system and host lithology.

Thermal limits of various waste forms have their technical basis in the temperature dependence of isolation integrity of the waste form. Waste form alteration, degradation, and dissolution behavior is a function of heat in addtition to redox conditions and constrains loading density within the waste form.

Thermal limits of various engineered barrier systems similarly have a technical basis in the temperature dependent alteration, corrosion, degradation, and dissolution rates of the materials from whence they are constructed.

Thermal limits of the geologic environment can be based on the mechanical integrity of the rock as well as mineralogical, hydrologic and geochemical phenomena. The isolating characteristics of a geological environment are most sensitive to hydrologic and geochemical effects of thermal loading. Thus, heat load constraints are typically chosen to control hydrologic and geochemical response to thermal loading. In the United States, current regulations necessitate thermal limits in order to passively steward the repository's hydrologic and geochemical integrity against radionuclide release for the first 10,000 years of the repository.

The two heat load constraints that primarily determined the heat-based spent nuclear fuel (SNF) capacity limit in the Yucca Mountain Repository design, for example, are specific to unsaturated tuff. These are given here as an example of the type of regulatory constraints that this model will seek to capture for various geologies.

The first Yucca Mountain heat load constraint is intended to promote constant drainage, thereby preventing episodic flow into waste package tunnels and subsequent contaminated water flow through the repository. It requires that the minimum temperature in the tuff between drifts be no more than the boiling temperature of water,

which is $96°C$ at the altitude in question. For a repository with homogeneous waste composition in parallel drifts, this constraint limits the temperature exactly halfway between adjacent drifts, where the temperature is at a minimum.

The second constraint is intended to prevent high rock temperatures that could induce fractures and alteration of the rock. It stated that no part of the rock reach a temperature above $200°C$, and was effectively a limit on the temperature at the drift wall, where the rock temperature is a maximum.

Analogous constraints for a broader set of possible geological environments will depend on heat transport properties and geochemical behaviors of the rock matrix as well as its hydrologic state. Such constraints will affect the repository drift spacing, waste package spacing, and repository footprint among other parameters.

In addition to development of a concept of heat transport within the repository in order to meet heat load limitations, it is also necessary to model temperature gradients in the repository in order to support modeling of thermally dependent hydrologic and material phenomena. As mentioned above, waste form corrosion processes, waste form dissolution rates, diffusion coefficients, and the mechanical integrity of engineered barriers and geologic environment are coupled with temperature behavior. Only a coarse time resolution will likely be necessary to capture that coupling however, since time evolution of repository heat is such that thermal coupling can typically be treated as quasi static for long time scales. [8].

Source Term Modeling Needs

Domestically, the Environmental Protection Agency (EPA) has defined a limit on human exposure due to the repository. This regulation places important limitations on capacity, design, and loading techniques for repository concepts under consideration. Repository

concepts developed in this work must therefore quantify radionuclide transport through the geological environment in order to calculate repository capacity and other benefit metrics.

The exposure limit set by the EPA is based on a 'reasonably maximally exposed individual.' For the YMR, the limiting case is a person who lives, grows food, drinks water and breathes air 18 km downstream from the repository. The Yucca Mountain Repository EPA regulations limit total dose from the repository to 15 mrem/yr, and limit dose from drinking water to 4 mrem/yr for the first 10,000 years. Predictions of that dose rate depend on an enormous variety of factors, most important of which is the primary pathway for release. In the YMR primary pathway of radionuclides from an accidental release will be from cracking aged canisters. Subsequently, transport of the radionuclides to the water table requires that the radionuclides come in contact with water and travel through the rock to the water table. This results in contamination of drinking water downstream.

Source term is a measure of the quantity of a radionuclide released into the environment whereas radiotoxicity is a measure of the hazardous effect of that particular radionuclide upon human ingestion or inhalation. In particular, radiotoxicity is measured in terms of the volume of water dilution required to make it safe to ingest. Studies of source term and radiotoxicity therefore make probabilistic assessments of radionuclide release, transport, and human exposure.

Importantly, due to the long time scale and intrinsic uncertainties required in such probabilistic assessments it is in general not advisable to base any maximum repository capacity estimates on source term. This is due to the fact that in order to give informative values for the risk associated with transport of particular radionuclides, for example, it is necessary to make highly uncertain predictions concerning waste form degradation, wa-

ter flow, and other parameters during the long repository evolution time scale. However, source term remains a pertinent metric for the comparison of alternative separations and fuel cycle scenarios as it is a fundamental factor in the calculation of risk.

Arriving at a generalized metric of probabilistic risk is fairly difficult. For example, the Peak Environmental Impact (PEI) metric from Berkeley (ref. [14]) is a multifaceted function of spent fuel composition, waste conditioning, vitrification method, and radionuclide transport through the repository walls and rock. Also, it makes the assumption that the waste canisters have been breached at $t = 0$. Furthermore, reported in m^3, PEI is a measure of radiotoxicity in the environment in the event of total breach. While informative, this model on its own does not completely determine a source-term limited maximum repository capacity. Additional waste package failure and a dose pathway model must be incorporated into it.

Domestic Research and Development Program

The DOE-NE Fuel Cycle Technology (FCT) program has three groups of relevance to this effort: these are the Used Fuel Disposition (UFD), the Separations and Waste Forms (SWF), and Fuel Cycle Options (FCO) (previously Systems Analysis) campaigns. The UFD campaign is conducting the Research Development and Design (RD&D) related to the storage, transportation, and disposal of radioactive wastes generated under both the current and potential advanced fuel cycles. The SWF campaign is conducting RD&D on potential waste forms that could be used to effectively isolate the wastes that would be generated in advanced fuel cycles. The SWF and UFD campaigns are developing the fundamental tools and information base regarding the performance of waste forms and geologic disposal systems. The FCO campaign is developing the overall fuel cycle simulation tools and interfaces with the other FCT campaigns, including UFD.

This effort will interface with those campaigns to develop the higher level dominant physics representations for use in fuel cycle system analysis tools. Specifically, this work will leverage conceptual framework development and primary data collection underway within the Used Fuel Disposition Campaign as well as work by Radel, Wilson, Bauer et. al. to model repository behavior as a function of the contents of the waste [52]. It will then incorporate dominant physics process models into the Cyclus computational fuel cycle analysis tool [28].

1.2 Methodology

In this work, concise dominant physics models suitable for system level fuel cycle codes will be developed by comparison of analytical models with more detailed repository modeling efforts. The ultimate objective of this effort is to develop a software library capable of assessing a wide range of combinations of fuel cycle alternatives, potential waste forms, repository design concepts, and geological media.

Current candidate repository concepts have been investigated and reviewed here in order to arrive at a fundamental set of components to model. A preliminary set of combinations of fuel cycles, repository concepts, and geologies has been chosen that fundamentally captures the domestic option space. Specifically, three candidate geologies and four corresponding repository concepts under consideration by the DOE UFD campaign have been chosen for modeling in this work. These will be expected to interface with Cyclus simulations of a canonical set of potential fuel cycles within three broad candidate scenarios put forth by the US DOE.

A review and characterization of the physical mechanisms by which radionuclide and thermal transport take place within the materials and media under consideration was first undertaken. Potential analytical models to represent these phenomena were

investigated and categorized within the literature review.

A review and characterization of current detailed computational tools for repository focused analysis was next conducted. Both international and domestic repository modeling efforts were summarized within the literature review. Of these, candidate computational tools with which to perform abstraction and regression analyses were identified. Specifically, a suite of Generic Disposal System Model (GDSM) tools under development by the DOE UFD campaign will inform radionuclide transport models and a pair of corresponding thermal analysis codes will inform the thermal models.

Continuation of this work will consist of the development of a suite of subcomponent modules appropriate for use within the Cyclus fuel cycle simulator. This process will include the development of a robust architecture within the repository module that will allow for interchangeable loading of system components. Within the system components, dominant physics will be modeled based on domain appropriate approximation of analytical models and supported by abstraction with the chosen GDSM tools and thermal tools.

In general, such concise models are a combination of two components: semi-analytic mathematical models that represent a simplified description of the most important physical phenomena, and semi-empirical models that reproduce the results of detailed models. By combining the complexity of the analytic models and regression against numerical experiments, variations can be limited between two models for the same system. Different approaches will be compared in this work, with final modeling choices balancing the accuracy and efficiency of the possible implementations.

Specifically, geological models will focus on the hydrology and thermal physics that dominate radionuclide transport and heat response in candidate geologies as a function of radionuclide release and heat generation over long time scales. Dominant

transport mechanism (advection or diffusion) and disposal site water chemistry (redox state) will provide primary differentiation between the different geologic media under consideration. In addition, the concise models will be capable of roughly adjusting release pathways according to the characteristics of the natural system (both the host geologic setting and the site in general) and the engineered system (such as package loading arrangements, tunnel spacing, and engineered barriers).

The abstraction process in the development of a geological environment model will employ the comparison of semi-analytic thermal and hydrologic models and analytic regression of rich code results from more detailed models as well as existing empirical geologic data. Such results and data will be derived primarily from the UFD campaign GDSMs and data, as well as European efforts such as the RED-IMPACT assessment and Agence Nationale pour la gestion des Déchets RAdioactifs, the French National Agency for Radioactive Waste Management (ANDRA) Dossier efforts [36, 8, 18] .

Thereafter, a regression analysis concerning those parameters will be undertaken with available detailed models (e.g. 2D and 3D finite difference, finite element, and thermal performance assessment codes) to further characterize the parametric dependence of thermal loading in a specific geology.

Finally, the thermal behavior of a repository model so developed will depend on empirical data (e.g. heat transfer coefficients, hydraulic conductivity). Determination of representative values to make available within the dominant physics model will rely on existing empirical data concerning the specific geologic environment being modeled (i.e. salt, clay/shale, and granite).

A similar process will be followed for radionuclide transport models. The abstraction process in the development of waste form, package, and engineered barrier system models will be analogous to the abstraction process of repository

environment models. Concise models will result from employing the comparison of semi-analytic models of those systems with regression analysis of rich code in combination with existing empirical material data.

Coupling effects between components will have to be considered carefully. In particular, given the important role of temperature in the system, thermal coupling between the models for the engineered system and the geologic system may be important. Thermal dependence of radionuclide release and transport as well as package degradation will necessarily be analyzed to determine the magnitude of coupling effects in the system.

The full abstraction process will be iterated to achieve a balance between calculation speed and simulation detail. Model improvements during this stage will seek a level of detail appropriate for informative comparison of subcomponents, but with sufficient speed to enable systems analysis.

By varying input parameters and comparing with corresponding results from detailed tools, each model's behavior on its full parameter domain will be validated.

1.3 Outline

The following chapter will present a literature review that organizes and reports upon previous relevant work. First it summarizes the state of the art of repository modeling integration within current systems analysis tools. It then describes current domestic and international disposal system concepts and geologies. Next, the literature review focuses upon current analytical and computational modeling of radionuclide and heat transport through various waste forms, engineered barrier systems, and geologies of interest. It will also address previous efforts in generic geology repository modeling in order to categorize and characterize detailed computational models of radionuclide and heat transport available for regression analysis.

Chapter 3 will detail the computational paradigm of the Cyclus systems analysis platform and repository model which constitute this work. Models representing waste form, waste package, buffer, backfill, and engineered barrier systems will be defined by their interfaces and their relationships as interconnected modules, distinctly defined, but coupled. This modular paradigm allows exchange of technological options (i.e. borosilicate glass and concrete waste forms) for comparison but also exchange of models for the same technological option with varying levels of detail.

Chapter 4 will summarize the conclusions reached concerning the appropriate analytical and detailed models to utilize in the process of abstraction for radionuclide and heat transport through various components of the disposal system. It will then detail the analytical and regression analysis necessary to achieve a generic repository model for the chosen base repository type. A concise, dominant physics geological repository model of the base case disposal environment will be developed. Informed by semi-analytic mathematical models representing important physical phenomena, existing detailed computational efforts characterizing these repository environments will be appropriately simplified to create concise computational models. This abstraction will capture fundamental physics of thermal, hydrologic, and radionuclide transport phenomena while remaining sufficiently detailed to illuminate behavioral differences between each of the geologic systems under consideration. Verification and validation of abstracted models will be conducted through iterative benchmarking against more detailed repository models. Finally, remaining future work and expected contributions to the field will be summarized.

2 LITERATURE REVIEW

The following literature review addresses areas of current research integral to the work at hand. The contribution of computational nuclear fuel cycle simulation tools to sensitivity analyses of repository performance metrics is first summarized. A discussion of the disposal system concepts and geologies under consideration domestically and internationally are then also summarized. A review of analytical models of radionuclide transport and a review of analytical models of heat transport follow. An overview of current detailed computational models, available data and algorithms characterizing radionuclide transport are addressed next, including both standalone and those incorporated into nuclear fuel cycle simulation tools. Finally, a review of current computational models of heat transport in the waste disposal system context is given. Special focus is paid to the availability of supporting data and algorithms informing geochemical and hydrological transport on long time scales and in various geologies.

2.1 Repository Capabilities within Systems Analysis Tools

Current top-level simulators largely disregard the waste disposal phase of fuel cycle analysis. Choosing instead to report metrics such as mass or volumes of accumulated spent nuclear fuel, current tools fail to address the impact of those waste streams on the performance of the geologic disposal system [62]. To fully inform the decision making process, metrics that depend on the performance of the geologic disposal system will be necessary within the tool proposed here.

A model for repository capacity was developed for the the Verifiable Fuel Cycle

Simulation Model (VISION) fuel cycle simulator and recent efforts on the Nuclear Waste Assessment System for Technical Evaluation (NUWASTE) simulator have made some progress in addressing this deficiency, but despite a proliferation of sophisticated fuel cycle simulators, similar efforts are lacking in this regard [64, 51, 2].

NUWASTE

NUWASTE is a Nuclear Waste Technical Review Board code under development that determines many metrics about the fuel cycle according to various parameters and for various fuel cycles [2]. Its use is limited to the Nuclear Waste Technical Review Board (NWTRB) and access is further restricted by its utilization of commercial Microsoft Access and Visual Basic database and functional capabilities.

NUWASTE tracks 65 isotopes within material objects, discretely models individual shipping casks and incorporates cooling time in both dry and wet intermediate storage facilities. Though it tracks the number of assemblies through a simulation and their isotopic composition, NUWASTE lacks radionuclide transport and heat based capacity calculations.

VISION

VISION, a fuel cycle simulator created at Idaho National Laboratory (INL) is built on the commercial systems analysis platform, PowerSim. The code therefore has both commercial and governmental license restrictions and is sensitive to laboratory export control requiring explicit developer approval [63, 60]. VISION is capable of modeling an array of fuel cycle options. It tracks and conducts decay calculations for upwards of 80 isotopes of interest [64, 62].

While its repository model calculates YMR specific information about waste package heat production and heat based repository capacity, continuous masses are modeled rather than discrete waste packages, and no radionuclide transport calculations are conducted [51, 13].

DANESS

The Dynamic Analysis of Nuclear Energy System Strategies (DANESS) tool is developed at Argonne National Laboratory and discretely models reactors within regional reactor parks for a flexible array of fuel cycles. Material movement is based on a fuel ordering paradigm and is written in a combination of FortranIV and C, but is limited to a 10 reactor simulation. Repository capabilities are also limited to mass accounting and perform no radionuclide or heat transport calculations.

Input and output are in Microsoft Excel format and DANESS relies on the proprietary IThink simulation platform. The code therefore has both commercial and governmental license restrictions and is sensitive to export control requiring explicit developer approval [63, 60].

COSI

Commelini-Sicard (COSI) is a code from the Commissariat a l'Energie Atomique et aux Energies Alternatives (CEA) of France and is implemented in the Java programming language. It is capable of performing a large range of full fuel cycle scenarios in great detail. COSI6 utilizes fully detailed physics analysis packages and is capable of making assessments of repository capacity as well as radiotoxicity and decay heat calculations of waste packages [13]. Radionuclide transport through the repository post-emplacement is, however, not calculated and the distribution license is very restrictive.

NFCSim

The Nuclear Fuel Cycle Simulator (NFCSim) code was implemented in the Java programming language by Erich Schneider and Los Alamos National Lab. Primarily a mass tracking code, the repository model was limited to a heat analysis. Uniquely, in NFCSim the transportation of each waste package was modeled discretely [54].

CAFCA

Code for Advanced Fuel Cycles Assessment (CAFCA) is a fuel cycle code from the Massachusettes Institute of Technology (MIT) based on the VENISIM system dynamics platform. While CAFCA is capable of tracking processed fuel assemblies and isotopics, it does not calculate capacity metrics or conduct detailed radionuclide or heat transport. Its license, held by MIT, is of a less restrictive academic nature, but the source is not in wide distribution and the dependence on VENISIM necessitates that potential developers acquire a proprietary license for that software.

ORION

This code is a proprietary code developed at the United Kingdom's National Nuclear Laboratory. While there is no heat-limited capacity model or calculation of radionuclide transport, the material destined for the repository can be described with a number of mass indexed metrics such as activity $[Bq]$, radiotoxicity $[Sv]$, toxic potential $[m^3]$, spontaneous neutron emission $[s^{-1}]$, and heat production $[W]$. None of these metrics, however, incorporate a dose pathway or calculate radionuclide transport.

OCRWM Yucca Mountain Total System Model

The Total System Model (TSM) code, developed at Office of Civillian Radioactive Waste Management (OCRWM) is a very detailed model of the Yucca Mountain disposal system. It includes transportation issues and detailed emplacement timing and strategy models, but considers only the fuel cycle associated with the current U.S. reactor fleet. Casks are modeled discretely and radionuclide and heat transport are modeled in great detail. This level of detail results in a dramatically extended run time making this model inappropriate for top level fuel cycle systems analysis. The TSM model can only be run by its development team and runs a typical simulation, processing 70,000 MTHM, in 12-15 hours [58].

The TSM framework is based on the commercial SimCAD platform. The simulation steps through times in 8 hour time steps during the waste cask transportation, processing and emplacement. This event based simulator is primarily focused on the operation stage of the Yucca Mountain repository, but is equipped with a thermal management model that informs waste package emplacement.

Repository Focused Fuel Cycle Analyses

While top level fuel cycle system analyses fail to incorporate repository models, some repository focused fuel cycle sensitivity analyses have been conducted. Some repository focused analyses emphasizing used fuel disposition and waste management in the Yucca Mountain Repository (YMR) have been conducted by Ahn, Li, Piet, Wigeland, Wilson, and others . With a focus on YMR capacity benefit, repository performance metrics of interest for these analyses were heat, source term, and more global environmental impact metrics. Sensitivity analyses for other geologies were conducted concerning repository concepts relevant to other nations as well.

2.2 Conceptual Discussion of Disposal Environments

A suite of three geologic media and four disposal concepts of interest were chosen to capture the primary geologies and concepts found in the following review of international and domestic efforts. Granite, clay, and salt geologic environments will be modeled with flexible layouts and an array of available canonical engineered subcomponent models. The detailed Generic Performance Asessment Model (GPAM) effort and associated GDSM tools were chosen to support the for this work will support abstraction for these concepts and further comparison with ANDRA and RED-IMPACT results will provide further benchmarks for validation.

The concepts that have been investigated internationally and will be investigated in this work are dominated by saturated, closed concepts. Saturated concepts are those located below the water table such that, in contrast to YMR, the porosity within the rock matrix as well as fractures and other open spaces is suffused with water. A closed concept is one that neither relies on ventilation shafts nor an extended open period after waste emplacement.

Enclosed modes are appropriate for low permeability rock formations (clay/shale, granite, salt). Low permeability does not permit oxygen entry, so these are chemically reducing environments. Chemically reducing environments are reducing insofar as they induce redox reactions to proceed in the reduction direction. This attribute has the primary effect of slowing corrosion, dissolution, and alteration rates in materials that are subject to degradation. A reducing disposal environment also lowers solubility limits and increases sorption of many actinide species. The dominant dose contributors in reducing environments are therefore the soluble, long lived fission and activation products such as ^{129}I and ^{79}Se [45, 36]. Furthermore, rather than being primarily kinetically limited, as in an oxidizing environment, sorption behavior is primarily thermodynamically

limited [43, 55]. The models created here will be designed such that these distinctions between reducing and oxidizing environments may be parsed in the event that an extension model simulates an oxidizing environment.

Since heat is carried away less effectively once closure has occurred, heat limits are lower in closed repository concepts than in open ones, such as YMR, where drift tunnels are ventilated for a number of years after emplacement before closure.

A number of waste form options will be modeled as a part of this effort. To sufficiently model the fuel cycles of interest, it will be necessary to model a borosilicate glass high level waste form as well as an oxide ceramic waste form. These together will be provide a sufficient but not comprehensive option space for modeling candidate domestic disposal systems. They will also provide enough diversity to demonstrate the validity of the abstraction methodology here applied. Additional waste forms of interest are listed in Table 2.6. Waste forms will be distinguished by their alteration, corrosion, and other degradation behaviors.

Various engineered barrier system components will also be modeled as a part of this effort. Sufficient waste package, buffer, backfill, and other sealing components will be modeled in order to cover the option space demonstrated by both domestic and international repository concept research. Fundamentally, concrete, salt, and bentonite buffer and backfill options will be modeled and copper, carbon steel, and stainless steel waste package concepts will be modeled.

Distinctions between the four repository concepts that will be considered here include varying coefficients of hydraulic conductivity, thermal conductivity, sorption, solubility, etc.

Clay Disposal Environments

Clays, including a range of claystones, shales, and argillites, have been investigated in Belgium, France, Japan, and Switzerland as well as the US [36, 18]. Attractive qualities of clay for repository investigations include its ease of excavation as well as the tendency, particularly for some very plastic clays under consideration, to coalesce over time around waste packages within the zone disturbed by excavation. A less attractive quality of clay is a low thermal limit around $100°C$ temperature limit to prevent alteration [25]. Some characteristics of clay disposal concepts are given in Table 2.1.

Clay Repository Features

Hydrology	Geochemistry	Design Concepts	Thermal Behavior
Very low conductivity High porosity (up to 0.5) Low effective porosity Slow water velocity diffusion dominated	Reducing Saline Saturated	no/bentonite/concrete backfill $\sim 500m$ deep closed horizontal or vertical emplacement	alteration limited $100°C$ limit

Table 2.1: Clay geological repository concept demonstrates certain dominant physical phenomena.

Disposal System Components

The French ANDRA analysis modeled borosilicate glass as well as ceramic oxide waste forms within carbon steel waste packages in combination with a bentonite buffer material and a crushed clay or shale backfill [8]. The Belgian reference concept focused on a highly plastic Boom Clay, which eventually completely seals around stainless steel, nickel, or titanium waste packages [46]. The Swiss concept modeled glass waste forms in stainless steel waste packages with a bentonite buffer and a bentonite and sand backfill [32]. Each of these analyses considered horizontal emplacement in multiple-package emplacement drifts.

Hydrology

In the clay disposal environment, an exceptionally low interconnected porosity, diffusion dominated water movement and no fracturation result in a very low overall hydraulic conducitivity . Hydrology in the far field is typically assumed to be diffusion dominated.

Geochemistry

This environment is very reducing in both the near and far field. The salinity of this environment increases with depth and it is expected that the pH will be near neutral in this environment. However, for some concepts incorporating cementitious backfill materials for protection of steel, the pH can become significantly alkaline, resulting in expedited alteration of glass wasteforms, bentonite buffers, and the clay matrix [8].

Highly mobile radionuclides which dominate dose from clay repository concepts for most fuel cycles include ^{129}I, ^{79}Se, and ^{36}Cl [57].

Thermal Behavior

Heat limits in clay are based on the domain of known behavior in clay and the tendency for bentonite fill material to lose its isolating properties with high temperatures [8, 50]. Limits in clay are fairly low as the thermal conductivity of clay is typically lower than $2[W/m^{\circ}K]$[1].

The alteration of high smectite bentonite to non-expandable clays is a primary limitation for heat tolerance in the clay concept. The isolation characteristics of bentonite buffer materials are reduced after this alteration. The time integral of this phenomenon determines total bentonite alteration. While short bursts of heat might be allowable,

[1]Belgium (ref. [46]) used values between 1.25 and 1.7 $[W/m \cdot^{\circ} K]$.
France (ref. [8]) used values between 1.9 and 2.7 $[W/m \cdot^{\circ} K]$.
Switzerland (ref. [**?**]) used 1.8 $[W/m \cdot^{\circ} K]$.

because the bentonite will not alter immediately, the kinetic alteration into smectite clays is hastened by temperatures above approximately $100°C$[50]. The Belgian program has considered increasing the thermal limit of the clay in the buffer region by adding graphite. Conversely, well understood behavior for argillaceous clay and bentonite buffer backfill is conservatively assumed by the ANDRA assessment to occur only under $90°C$, which is effectively a limit at the waste package interface with the bentonite buffer material[8] . The National Cooperative for the Disposal of Radioactive Waste (NAGRA) Opalinus Clay assessment less conservatively uses a maximum heat limit in the bentonite buffer of $125°C$ [31] .

Granite Disposal Environments

Granite disposal concepts have been considered in Finland, Japan, Sweden, China, Spain, the Czech Republic, South Korea and Switzerland as well as the US [25, 9, 36].

Attributes of granite that make it an attractive candidate geology for nuclear waste disposal include its very low porosity and permeability and high thermal conductivity. Fracturation in granite, however, has a negative effect on the isolation properties of the rock. Some characteristics of granite disposal concepts are given in Table 2.2.

Granite Repository Features

Hydrology	Geochemistry	Design Concepts	Thermal Behavior
Low porosity (~ 0.01) High Fracturation Low permeability High Water Velocity	Reducing in Near Field Slightly Oxidizing in Far Field Increasing saline with depth [36] Cement causes alkalinity [9] Saturated or Unsaturated	Single WP tunnels Carbon-Steel [9]or Copper overpack Bentonite buffer Crushed granite backfill [36] $\sim 500m$ deep	Closed Bentonite Limit $100°C$

Table 2.2: Granite repository concepts demonstrate certain dominant physical phenomena.

Disposal System Components

The Swedish KBS-3 concept includes ceramic oxide spent fuel waste forms within a steel shell and copper waste package buffered by bentonite clay and backfilled with clay and sand and emplaced vertically in horizontal drifts [1]. A similar Czech Republic repository concept consists of borosilicate glass waste forms within a stainless steel Universal Canister waste package, vertically emplaced in horizontal drifts and with a bentonite buffer and backfilled with a clay and sand mixture. The Spanish concept is almost exactly similar to these, except emplacement is horizontal within the horizontal repository drifts [36].

This work will model borosilicate glass and ceramic oxide waste forms, carbon steel and copper waste packages, and bentonite and concrete buffer options. A flexible repository layout model will support approximated modeling of each of these designs.

Hydrology

In the granite disposal environment, with a low porosity combined with higher expected water velocity (relative to other repository concepts in this work) and significant fracturation, the overall granite hydraulic conductivity is low, typically [55, 25]. Within this environment, the water behavior in the far field must be modeled as both diffusive and advective.

Geochemistry

This environment is very reducing in the near field and less reducing in the near surface far field. Far field fracturation in the granite near the surface of the site exposes the medium to the atmosphere, resulting in a slightly oxidizing condition in the near surface far field, most importantly resulting in higher actinide solubilities in that region. Salinity

in the granite environment increases monotonically with depth. At a typical concept depth of 500m, the repository is therefore expected to be in a location of high salinity, an indicator of historically low fluid flow but resulting in increased corrosion rates and for some radionuclides, changed solubilities [9]. It is expected that the pH will be near neutral in this environment except with the introduction of concretes, due to which the pH becomes significantly alkaline, resulting in more rapid alteration of bentonite buffers.

The relatively fast advective pathway provided by fracturation of granite has the effect of increasing the importance of ^{234}U in the initial waste stream. While ^{234}U and its decay daughter ^{230}Th are not very mobile in a reducing environment, their subsequent decay daughter ^{226}Ra is highly mobile. In clay, the 1601 year half life of ^{226}Ra is too short for a significant quantity to traverse the diffusive pathway. In granite, however, ^{226}Ra is a dominant dose contributor [57].

Thermal Behavior

Granite repository concepts are limited by the bentonite buffer in a manner similar to that of clay. However, in the absence of the bentonite limitation, a thermal limit within the granite itself is greater than $200°C$, limited by the increased risk of micro-cracking. This relatively high resistance to heat induced mechanical failure is due to the high thermal conductivity of granite, which is typically [2] found to be between 2.4 and 4 $[W/m \cdot^{\circ} K]$.

The effective thermal limit for granite disposal concepts, however, is usually related to the bentonite limit, which is conservatively assumed by the ANDRA assessment to

[2]Sweden (ref. [1]) used 3.4 - 4 $[W/m \cdot^{\circ} K]$ and 2.45 - 2.9 $[W/m \cdot^{\circ} K]$.
France (ref. [8]) used 2.4 - 3.8 $[W/m \cdot^{\circ} K]$.
Finland (ref. [49]) used 2.3 - 3.2 $[W/m \cdot^{\circ} K]$.

occur under 90°C at the waste package interface with the buffer material. Mechanical stresses and strains in the matrix due to heating at this level were analyzed by ANDRA and shown to have a negligible effect of flow behavior in granite. Similarly, thermo-hydraulic effects due to thermally induced fluid density changes are expected to be slight [9]. Similarly, for reasons of buffer isolation integrity, the Czech and Spanish granite disposal concepts both maintained a thermal limit at the waste package interface with the buffer of $100°C$. [36]

Salt Disposal Environments

The salt disposal concept has been investigated in Germany and demonstrated for non-heat-generating waste at the Waste Isolation Pilot Plant (WIPP) facility in the US. Salt demonstrates many attractive properties including ease of mining, creep behavior over time, which is expedited by heat, low permeability, and a high thermal conductivity, which affords a high temperature limit near $200°C$ [25] . Some characteristics of salt disposal concepts are given in Table 2.3.

Salt Repository Features

Hydrology	Geochemistry	Design Concepts	Thermal Behavior
Dry Waste Package	Reducing in Near Field	Alcove Emplacement	$180°C$ limit [36]
Dry Backfill	Far Field Slightly Oxidizing	Crushed Salt Backfill	Heat induced creep sealing
Saturated Far Field	Very saline brines	$\sim 500m$deep	Closed
Very low permeability		Multiple Packages	limited data
Brine pockets in far field		Breached only from intrusion	

Table 2.3: Salt geological repository concept demonstrates certain dominant physical phenomena.

Disposal System Components

The German reference concept in a salt dome has hundreds of drifts in which are placed thick steel waste packages and backfilled with crushed salt [36].

The consolidation properties of the backfill and salt are of great isolation importance. The infinitesimally small hydraulic conductivity of consolidated rock salt has the effect of nullifying the possibility of any releases without a disruption scenario. Thus, the accurate characterization of the site for both normal and high temperature will provide the fundamental confidence for repository behavior [16].

Hydrology

In a rock salt or salt dome disposal environment, a very low porosity combined with negligible water velocity and effectively no fracturation results in a salt hydraulic conductivity that is exceptionally low. Within this environment, extraordinarily slow diffusive speed out of the repository dominates the isolation behavior in a manner similar to the crystalline basement rock of the deep borehole concept. Candidate salt formations are remarkably uniform and their accessible porosity is near negligible, so almost no water movement is expected to occur except that which is potentially induced by the thermal output of the repository.

Geochemistry

This environment is very reducing in the near field and slightly less so in the far field [18]. The very high salinity in the salt environment expedites corrosive processes, but the engineered barrier system is of limited importance in this concept in which the diffusive rock barrier dominates isolation integrity. It is expected that the pH will be near neutral in this environment [36, 18].

Thermal Behavior

Response of a salt repository to heat has a significant mechanical component. Bulk heating of a salt repository matrix causes coalescing of the salt surrounding the heat source. In the case of a nuclear waste repository, this phenomenon increases isolation capability of the salt. A heat limit, then, is difficult to characterize, but evolution of the heat in a salt environment is of great importance to radionuclide transport modeling.

The German salt repository concept maintains a $180°C$ temperature limit. The technical basis for this limit has to do with the concern that at temperatures above $220°C$ the salt formation may release brines capable of facilitating radionuclide transport [36, 16].

A model of temperature dependent salt coalescent behavior is in order. While coalescent phenomena has been observed within the WIPP facility, the emplaced material in WIPP is not high heat generating. Thus, high heat salt coalescent behavior warrants further study [17].

The UFD salt repository concept was based on some experience with construction and maintenance of the horizontal borings at WIPP. The current geometry involves emplacement of waste packages arranged at the corner of an alcove. This alcove is then backfilled with crushed salt. Notably, crushed salt has low conductivity, which increases the sensitivity of rock salt temperature on emplaced package temperature. However, as the crushed salt coalesces with heat over time, its thermal conductivity approaches that of intact salt. Further investigation toward a comprehensive model of the thermal behavior of dry salt has been recommended both domestically and internationally [17].

The behavior of moisture in a salt repository under high heat is also not well characterized . Though it is clear that the salt will creep and coalesce with increased temperature, the potential generation of brines within the salt at high heat is a pertinent issue for salt disposal characterization.

Deep Borehole Disposal Environments

Deep Borehole disposal system concepts are being evaluated in the UK, Sweden and the United States. Attributes of this concept that are favorable for waste isolation include the stability of the crystalline basement rock in which the borehole emplacement would occur and the elongated diffusion path length for release. The potential technical difficulty of well controlled emplacement at great depth is an unfavorable attribute, however [25]. Some characteristics of deep borehole disposal concepts are given in Table 2.4.

Borehole Repository Features

Hydrology	Geochemistry	Design Concepts	Thermal Behavior
Crystalline rock Low porosity (~ 0.01) Limited fracturation at depth Rock Permeability ($\sim 10^{-19}$) EBS Permeability ($\sim 10^{-16}$) Very Limited Upward Flow	Reducing at depth Less Reducing at surface limited solubility enhanced sorption high salinity saturated	$\sim 5km$ deep disposal in lower 2km 1km betonite seal bentonite grout bentonite plugs 400 packages per borehole closed	cracking unimportant may affect flow high conductivity high density

Table 2.4: Borehole geological repository concept demonstrates certaindominant physical phenomena.

Disposal System Components

In deep borehole concepts many types of waste form and waste package material are equivalently emplaced at great depths, typically between 2 and 5 km [3] in a crystalline rock such as granite basement rock. In each borehole, hundreds of canisters are stacked vertically in the deepest section. In some concepts, dense bentonite plugs are stacked between the packages. Above the packages, swelling bentonite clay, asphalt and concrete provide a seal for the upper few kilometers [18].

[3] 4km in the Swedish concept and 5km in US concept [25, 18]

Hydrology

In the deep borehole crystalline rock disposal environment, a low porosity combined withonly minor fracturation results in an overall crystalline basement hydraulic conductivity which is very low. Thermally driven, upward water velocity is the primary driver for solute movement upward into the many kilometer diffusive path to the surface where fresh water aquifers may exist [18]. Without the introduction of a fast pathway such as an intersecting fracture or human intrusion, the length of the diffusive pathway has the effect of making the engineered barrier component choices irrelevant since no known engineered barrier choice can be expected to outlast the timescale of the diffusive pathway.

Geochemistry

This environment is very reducing in the near field and less in the very far field near the earth's surface. The very high salinity of this environment is due to its depth indicates historically low flow. While this increases corrosion rates of engineered barriers, the isolation worth of this concept does not depend significantly on the engineered barrier components, relying instead on the diffusion path length.

Thermal Behavior

Since the crystalline basement rock in which deep borehole concepts are envisioned is typically granite, the thermal behavior of the deep borehole environment is exactly similar to the granite case, except the bentonite buffer limitation is no longer applicable. Also, the $200°C$ limitation in order to avoid microfissures could be shown to be irrelevant in light of the great distance to the surface. That is, even if the damage zone in the vicinity of the emplaced waste packages is enlarged significantly by high heat load, the

kilometers of diffusion length to the surface will still dominate the isolation behavior of the repository.

2.3 Analytical Models of Radionuclide Transport

A comprehensive model of radiotoxic source term must address radionuclide transport through the full release pathway including waste packages, engineered barrier systems, and geologic media. A model of transport through the repository must incorporate a waste package failure model, a radionuclide release model via waste form dissolution, and advective and diffusive transport through the engineered barrier system and lithology. A number of efforts to model radionuclide transport through a geologic repository concept have been made internationally and domestically. These efforts, the geologies they address, and some features of their methodologies will be discussed here and appear in Table 2.5.

Waste package failure depends on near field environmental factors such as pH as well as decay heat and water chemistry due to radiolysis anticipated from the contained waste. In turn, the radionuclide release rate from the waste package depends on the character of the waste form matrix, water flow, radionuclide solubility and the elemental diffusion constant. Similarly, advective transfer through the engineered barrier system and into the geological medium also depends on water flow, radionuclide solubility, and radionuclide diffusion, but must be employed in the context of the hydrology of the rock which sets the boundary condition.

Waste package failure modes vary between models. While some employ detailed computational tools such as GoldSim or EBSFAIL (a part of the EBSPAC module used in the TSPA code), which will be discussed in section 2.5, some analytic models incorporate their own hydrologic approximations of canister degradation or make simpler

Models of Source Term for Various Geologies

Source (Who)	Nation (Where)	Geology (What)	Methodology (How)
Enresa [36]	Spain	Granite	GoldSim Proprietary Framework ^{129}I primary contributor
SCK·CEN [36]	Belgium	Clay	Features, events, processes ^{129}I primary contributor
GRS [36]	Germany	Salt	Systematic Performance Asessment ^{135}Cs, ^{129}I, ^{226}Ra, ^{229}Th
Ahn [4, 5]	USA	Yucca Tuff	Solubility Limited Release & Congruent Release
NCSU(Nicholson) [37]	USA	Yucca Tuff	TSPA codes EBSREL and EBSFAIL
NAGRA [31, 32]	Switzerland	Opalinus Clay	TAME code
ANDRA [8]	France	Argile Clay	Very detailed CEA code Mostly homogeneous medium ^{129}I primary contributor
ANDRA [9]	France	Granite	Very detailed CEA code Involves fracturation of medium ^{129}I primary contributor
SKB [1]	Sweden	Forsmark Laxemar	HYDRASTAR solute transport FracMan for fracturation

Table 2.5: Methods by which to evaluate source term dependence of waste package failure, transport through the EBS and hydrogeologic transport. The latter two parts vary significantly among host formations.

assumptions of immediate waste canister failure in order to focus on dissolution and transfer.

Waste form release rate is the rate of mass transfer of a radionuclide from its waste form into surrounding water. The mode of water flowthrough heavily affects radionuclide dissolution rate and is treated differently in various models. While some, inspired by the TSP assessment, assume water moves through the waste packages at a constant volumetric rate ('flowthrough model'), others adopt less conservative assumptions incorporating weather based predictions of hydrologic activity.

Radionuclide transport through the EBS and host rock is dependent upon diffusion as well as advection. Radionuclide transport is retarded by sorption, limited by solubility, and enhanced by colloidal mobility [15].

Dissolution is prerequisite to contribution of a radionuclide to source term [15]. That

is, the initial dissolution of a radionuclide from its waste form is a breach of the primary barrier. Dissolution rates depend strongly on pH, Eh, speciation of radionuclides (chemical oxidative state), and radiolysis of the dissolving fluid, but primarily on material properties of the waste form.

Precipitation is the reverse of dissolution and occurs when a solubility limit is reached. In a reducing environment, the approach to chemical equilibrium of dissolution and precipitation is rate dependent and is highly dependent on thermodynamics.

Sorption includes both absorption and adsorption. Absorption is the incorporation of a substance of one state into another of a different state. Adsorption is the interaction of a dissolved species with a surface that removes that species from the dissolving medium models. During sorption, contaminants are removed from the flowthrough water and taken up by the walls of pores or fractures in the rock matrix. Importantly, sorption is a reversible process, the counter process of which is desorption in which the contaminant is returned to the pore or fracture fluid from the matrix [3] . Reversible sorption is typically expressed in terms the mass of a radionuclide sorbed into the rock and the mass left in solution. K_d values are heavily radionuclide and geochemically dependent.

Finally, a phenomenon called colloidal mobility can enhance radionuclide transport. Mineral colloids, which are suspended molecular solids within a liquid emulsion, are expected in the solution saturating the geological environment. Colloids present in the near field dissolving solution have an effect on the mobility of radionuclides. Studies addressing the subtle differences between resultant behavior of various isotopes indicate that colloidal mobility can be modeled as a correction factor to the sorption coefficient [15].

Waste Form Release Models

Radionuclide release from various possible waste form types will be dominated by an array of degradation, alteration, and dissolution phenomena. These phenomena begin when surrounding waste packages are breached, exposing the waste form to water. Some phenomena dominating the release from canonical waste forms such as Commercial Spent Nuclear Fuel (CSNF), DOE Spent Nuclear Fuel (DSNF), and High Temperature Gas Reactor (HTGR) are listed in Table 2.6.

Waste Form Types

WF Type	SubTypes	Contents	Release Drivers
Once Through	CSNF Ceramic Oxide	Nominal Burnup UOx & MOX	redox reactions
	CSNF Ceramic Oxide	High Burnup	redox reactions, heat
	HTGR TRISO Graphite	High Burnup	graphite reactions
	DSNF Metal	High Burnup N Reactor Fuel	metal reactions, heat
	DSNF Carbides	Fast Reactor Fuels	carbide reactions, heat
	DSNF Ceramic Oxides	Research Reactor Fuels	redox reactions, heat
Borosilicate Glass	Current	Minor Actinides (MAs) Cs/Sr	heat, glass alteration
	Future	Mo, no MA no Cs/Sr	glass alteration
Glass Ceramic	Glass Bonded Sodalite	Echem processed oxide fuels	ceramic, redox, glass reactions
Metal Alloy	From Echem	Cladding, noble metals	metal reactions, heat
	From Aqueous	ransition metals	metal reactions, heat
Advance Ceramic		volatized iodine	ceramic reactions, redox
Salt	Cementitious Sodium	separated streams	alkaline reactions, dissolution

Table 2.6: An array of waste forms developed for nuclear wastes will have a corresponding array of dominant release mechanisms [12]

.

Hedin Model ([26])

In a saturated fractured rock matrix representative of the KBS-3 granitic Swedish repository concept, copper canister waste packages contain a spent fuel waste matrix, and a bentonite buffer surrounds the canisters within repository drift tunnels. Waste form dissolution within the Hedin model is a rate based model that takes place within the

waste package void. Radionuclides are released congruently with the flowthrough water at a fractional degradation rate until the waste form is completely degraded. [26]

Ahn Models ([4, 5])

In an oxidizing, unsaturated environment, waste canisters are modelled as compartments of waste form surrounded by a buffer layer that is in turn surrounded by layers of near field rock and far field rock. Water is introduced to the system at a constant rate, and encounters an array of failed waste packages (at $t = 0$ in the 2004 model, and at $T_f = 75,000$ years in the 2007 model). The water immediately begins dissolving the waste matrix. Radionuclides with higher solubilities are preferentially dissolved and treated with a "congruent release" advective transport model discussed below. Radionuclides with lower solubilities are transported through the buffer with the alternative "solubility limited" release model. The water flow begins at one waste package and travels through the matrix and buffer space to the next waste package, contacting each waste package consecutively and then flowing on into the near field. In this way, the water is increasingly contaminated as its path through the waste packages proceeds.

Ahn Congruent Release Model

In the Ahn models, radionuclides with a high solubility coefficient are modeled with the congruent release model. Radionuclides of this type include most of the fission products, but not the actinides. This model states that the release from the waste packages is congruent with the dissolution of the waste matrix and is transported through the rock by advective transfer with the water that flows through the waste packages.

Ahn Solubility Limited Release Model

In the Ahn models, radionuclides with lower solubility coefficients are modeled with the solubility limited release model. Solubility values are assumed from TSPA for this model, and elements with a solubility of less than $5 \times 10^{-2}[mol/m^3]$ are taken to be 'low.' Elements in this 'low' category include Zr, Nb, Sn and some toxic actinides such as Th and Ra for an oxidizing, unsaturated environment similar to YMR. It should be noted that in a reducing environment, the actinides are not as mobile, and the high and low solubility radionuclides will differ from this model. This model suggests that dissolution of radionuclides into the flowthrough water is dominated by diffusion, which is largely dependent upon the concentration gradient between the waste matrix and the water. The mass balance driving radionuclide release takes the form:

$$\dot{m}_i = 8\epsilon D_e S_i L \sqrt{\frac{U r_0}{\pi D_e}} \tag{2.1}$$

where ϵ, U, r_0, and L are the geometric and hydrologic factors porosity, water velocity, waste package radius, and waste package length, respectively. D_e is the effective diffusion coefficient (m^2/yr) and S_i is the solubility (kg/m^3) of isotope i.

Hedin Solubility Limited Release Model

In the Hedin model of the waste matrix, the amount of solute available within the waste package is solved for, and for radionuclides with low solubility, the mass fraction released from the waste matrix is limited by a simplified description of their solubility. That is,

$$m_{1i}(t) \leq v_{1i}(t) C_{sol} \tag{2.2}$$

where the mass m_{1i} in $[kg]$ of a radionuclide i dissolved into the waste package void volume v_1 in $[m^3]$, at a time t, is limited by the solubility limit, the maximum concentration, C_{sol} in $[kg/m^3]$ at which that radionuclide is soluble [26].

Waste Package Failure Models

Waste package failure can, in general, be represented with an expression of the number of failed waste packages, n_F failing per unit time. This is a simple product between the initial number of waste packages, N, and the rate, f, of failure

$$n_F = N \cdot f(). \tag{2.3}$$

Some current common models addressed in this literature review appear in Table **??**.

Current Waste Package Failure Models

Model	WP Failure Mode	Waste Form	Details
TSPA	EBSFAIL		$300,000$ years
Ahn 2003	Instantaneous Failure	Borosilicate Glass	$t = 0$
Ahn 2007		CSNF UO_2 matrix	$T_f = 75,000$ years
		Borosilicate Glass	$T_f = 75,000$ years
		Naval UO_2 matrix	$T_f = 75,000$ years
Li	EBSFAIL		$300,000$ years
Hedin 2003	Instantaneous	Copper KBS-3 Concept	$t_{delay} = 300$ years

Table 2.7: The above represent some current methods by which waste package failure rates are modeled.

Physical Model

When enough data exists, the waste package failure rate f can be represented more realistically by fractional destruction according to experimentally observed corrosion and dissolution rate functions.

However, this can be complicated to model even if the data exists. In particular, the corrosion rate will depend dramatically on the chosen material as well as hydrologic and thermal conditions. Specifically, corrosion rates for the same material are very different under dry oxidizing conditions and wet reducing conditions.

The rate f of package failure in this case will be a function of time t, temperature T, and other physical parameters.

$$f() = N \cdot f(t, T, \cdots). \tag{2.4}$$

Probabilistic

When a probability distribution of waste package failure is available, the discrete waste packages can be modeled to fail according to that distribution. For example, if the expected lifetime of a waste package is some known t_F, a Gaussian distribution around t_F would provide a probability density function for waste package failures per time step, $f(t)$,

$$f() = f(t). \tag{2.5}$$

Expressed with a cumulative distribution function $F(t)$ rather than the probability

distribution function, equation (2.4) becomes

$$\sum_{t=0}^{t=t} n_F = N \cdot F(t). \tag{2.6}$$

A particularly appripriate probability distribution for use in the case of failed engineered barriers is the Weibull distribution,

$$f(t, \lambda, k) = \begin{cases} \frac{k}{\lambda} \left(\frac{t}{\lambda}\right)^{k-1} e^{-(t/\lambda)^k} & t \geq 0, \\ 0 & t < 0. \end{cases} \tag{2.7}$$

In this expression, k is a shape parameter and λ is a scale parameter. The time to failure, t in the Weibull distribution gives a distribution for which the failure rate is proportional to a power of time [47]. Its complementary cumulative distribution function is

$$f(t, \lambda, k) = 1 - e^{-(t/\lambda)^k}. \tag{2.8}$$

For $k < 1$, the rate of failure will decrease over time, while for a value of $k > 1$, the rate increases over time, appropriate for the aging process of materials [47].

Instantaneous

The instantaneous case is a special case of the probabilistic situation. Specifically, the probability density function is clearly just the Dirac delta function, with n_F being the

number of failed waste packages per unit time, N being the total number of waste packages, and t_F being the time to failure,

$$f() = \delta(t - t_F). \tag{2.9}$$

The Hedin model of waste package failure is effectively instantaneous, but limited by a release resistance coefficient. The release is assumed to occur through a hole in the waste canister that exists throughout the simulation, and the resistance coefficient limiting flow through the hole represents the magnitude of the canister flaw in combination with the buffer-geosphere interface[26]. Other models also use an instantaneous waste package failure mode for all waste packages simultaneously, in which failure occurs either at the onset of the simulation or at some distinct time during the simulation.

Radionuclide Transport Through Secondary Engineered Barriers

When the waste package is breached and radionuclides are released from the waste form, radionuclides are transported through the secondary engineered barrier, which includes the buffer, backfill, and tunnel wall. After transport through the secondary EBS, radionuclides reach the geosphere.

Barrier Dissolution and Failure

The same models of waste package failure (instantaneous, rate based, and probabilistic) can be applied to buffers. While concretes are expected to degrade over time, bentonite buffers are quite stable in a reducing environment and help to keep the environment reducing. Furthermore, if preserved by a low heat environment, plastically deforming

bentonite clays tend to swell over time and exhibit increased isolating behavior.

Transport Through Degraded Barrier Matrix

Diffusive and advective transport occur in the barrier matrix both before and after degradation. Before degradation, transport is primarily diffusive. Thereafter, transport can become advective due to cracking. Cracking can be modeled explicitly or as a continuum model.

Hydrologic Transport Models

Transport out of the EBS and through the geosphere in clay, shale, granite, and salt can largely be characterized as solute transport in permeable porous medi. While clay, shale and salt do not exhibit significant fracturation and can often be modeled as homogeneous, granite is characterized as a fractured permeable porous media. Solute transport in both fractured and homogeneous permeable porous media has both porous and fracture flow paths and involves advection, hydraulic dispersion, and diffusion phenomena.

Advection is transport driven by bulk water velocity, diffusion is the result of Brownian motion across concentration gradients, and hydraulic dispersion is transport resulting from heterogeneities in the water velocity field.

Fundamentally, the effect of these flows on mass transport is captured by the conceptual expression

$$\text{In} - \text{Out} = \text{Change in Storage} \tag{2.10}$$

Rearranging 2.10 and defining incoming and outflowing fluxes in a control volume, solute transport in a permeable medium of homogeneous porosity can be written (as in

Schwartz and Zhang [55])

$$\frac{\partial nC}{\partial t} = -\nabla \cdot (F_c + F_{dc} + F_d) + m \tag{2.11}$$

where

$$\begin{aligned}
n &= \text{solute accessible porosity } [\%] \\
C &= \text{ concentration } [kg \cdot m^{-3}] \\
t &= \text{ time } [s] \\
F_c &= \text{ advective flow } [kg \cdot m^{-2} \cdot s^{-1}] \\
&= nvC \\
F_{dc} &= \text{ dispersive flow } [kg \cdot m^{-2} \cdot s^{-1}] \\
&= \alpha nv \nabla C \\
F_d &= \text{ diffusive flow } [kg \cdot m^{-2} \cdot s^{-1}] \\
&= nD_e \nabla C \\
m &= \text{ solute source } [kg \cdot m^{-3} \cdot s^{-1}].
\end{aligned}$$

In the expressions above,

$$\begin{aligned}
v &= \text{ advective velocity } [m \cdot s^{-1}] \\
\alpha &= \text{ dispersivity } [m] \\
D_e &= \text{ effective diffusion coefficient } [m^2 \cdot s^{-1}]
\end{aligned}$$

and

$$n \cdot v = \text{ Darcy flux } [m \cdot s^{-1}]. \tag{2.12}$$

The method by which the dominant solute transport mode (diffusive or advective) is determined for a particular porous medium is by use of the dimensionless Peclet number,

$$\begin{aligned} Pe &= \frac{nvL}{\alpha nv + D_e}, \\ &= \frac{\text{advective rate}}{\text{diffusive rate}} \end{aligned} \tag{2.13}$$

where

$$L = \text{ transport distance } [m].$$

For a high Pe number, advection is the dominant transport mode, while diffusive or dispersive transport dominates for a low Pe number. If one of these terms can be neglected, the solution is simplified.

Otherwise, the analytical expression in equation (2.11) will be the foundation of simplification by regression analyses for the radionuclide transport interface between components of the repository system model representing permeable porous media.

It is customary to define the combination of molecular diffusion and mechanical mixing as the dispersion tensor, D,

$$D = \alpha v + D_e \tag{2.14}$$

such that the mass conservation equation becomes:

$$\nabla \left(nD\nabla C \right) - \nabla \left(nv \right) = \frac{\partial (nC)}{\partial t} \tag{2.15}$$

Adding sorption, by accounting for a change in mass storage,

$$\nabla \left(nD\nabla C \right) - \nabla \left(nv \right) = \frac{\partial (nC)}{\partial t} + \frac{\partial (s\rho_b)}{\partial t} \tag{2.16}$$

where

$s =$ sorption coefficient

$\rho_b =$ bulk (dry) density $[kg/m^3]$.

If it is assumed that sorption can be approximated as a linear equilibrium, reversible reaction,

$$\frac{\partial (s\rho_b)}{\partial t} = (R_f - 1) \frac{\partial (nC)}{\partial t} \tag{2.17}$$

equation (2.16) becomes

$$\nabla\left(nD\nabla C\right)-\nabla\left(nv\right)=R_f\frac{\partial(nC)}{\partial t} \tag{2.18}$$

where

$$R_f = \text{retardation factor} \tag{2.19}$$

$$= 1+\frac{\rho_b K_d}{n} \tag{2.20}$$

$$\rho_b = \text{bulk density of the rock matrix} \tag{2.21}$$

and

$$K_d = \text{species distribution coefficient.} \tag{2.22}$$

For uniform flow, the dispersion tensor, D, becomes

$$D_x = D_L$$

$$= \alpha_L v_x + \tau D_e \tag{2.23}$$

$$D_y = D_{TH}$$

$$= \alpha_{TH} v_x + \tau D_e \tag{2.24}$$

$$D_z = D_{TV}$$

$$= \alpha_{TV} v_x + \tau D_e \tag{2.25}$$

where

$$D_e = \text{effective diffusion coefficient}[m^2/s]$$
$$\alpha_L = \text{longitudinal dispersivity}[m]$$
$$\alpha_{TH} = \text{horizontal dispersivity}[m]$$
$$\alpha_{TV} = \text{vertical dispersivity}[m]$$

and

$$\tau = \text{tortuosity}. \tag{2.26}$$

For unidirectional flow, the unidirectional dispersion tensor gives

$$D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} + D_z\frac{\partial^2 C}{\partial z^2} + v_x\frac{\partial C}{\partial x} = R_f\frac{\partial (nC)}{\partial t}. \tag{2.27}$$

A special case of uniform flow, no flow, simplifies to the diffusion equation,

$$D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} + D_z\frac{\partial^2 C}{\partial z^2} = R_f\frac{\partial (nC)}{\partial t}. \tag{2.28}$$

Solutions to these equations can be categorized by their boundary conditions. The first, or Dirichlet type boundary conditions define a specified species concentration on some section of the boundary of the representative volume,

$$C(\vec{r}, t) = C_0(\vec{r}, t) \text{ for } \vec{r} \in \Gamma. \tag{2.29}$$

The second type or Neumann type boundary conditions describe a full set of fluxes at the boundary of the domain

$$\frac{\partial C(\vec{r},t)}{\partial r} = nD\vec{J} \text{ for } \vec{r} \in \Gamma. \tag{2.30}$$

where

$$\vec{r} = \text{ position vector}$$
$$\Gamma = \text{ domain boundary}$$
$$\vec{J} = \text{ solute mass flux } [kg/m^2 \cdot s].$$

The third, Cauchy, type describes a combination of the Dirichlet and Neumann type conditions, defining both a concentration at a boundary and a flux at that boundary,

$$C(\vec{r},t) = C_0(\vec{r},t) \text{ for } \vec{r} \in \Gamma \tag{2.31}$$
$$\frac{\partial C(\vec{r},t)}{\partial r} = nD\vec{J} \text{ for } \vec{r} \in \Gamma. \tag{2.32}$$

One Dimensional Solution with Constant Concentration

An analytical solution for the one dimensional case with a continuous source of constant concentration is known. For the boundary conditions

$$C(0,t) = C_0 \tag{2.33}$$

and

$$\left.\frac{\partial C}{\partial x}\right|_{x=\infty} = 0 \tag{2.34}$$

as well as the initial condition

$$C(x,0) = 0 \text{ for } x \in (0,\infty), \tag{2.35}$$

the so called Ogata and Banks solution gives

$$C(x,t) = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{x-\frac{v_x t}{R_f}}{2\sqrt{\frac{D_x t}{R_f}}}\right) + e^{\frac{v_x x}{D_x}}\operatorname{erfc}\left(\frac{x+\frac{v_x t}{R_f}}{2\sqrt{\frac{D_x t}{R_f}}}\right)\right]. \tag{2.36}$$

where

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}dt \tag{2.37}$$

$$\begin{aligned}\operatorname{erfc}(x) &= 1 - \operatorname{erf}(x)\\ &= \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-t^2}dt\end{aligned} \tag{2.38}$$

Equation (2.36) is an appropriate one dimensional solution to the situation in this work where a constant concentration at the internal boundary of each control volume is available at each time step. Abstraction-based approximations based on this solution will be used to advance the concentration values at each time step within each control volume.

Temperature Dependent Diffusion : Arrhenius

The Arrhenius relationship,

$$D = D_0 e^{-\frac{E_A}{RT}} \tag{2.39}$$

where

$$D = \text{the diffusion coefficient} \tag{2.40}$$

$$D_0 = \text{the maximum diffusion coefficient} \tag{2.41}$$

$$E_A = \text{molar activation energy of diffusion} [J/mol] \tag{2.42}$$

$$R = \text{the ideal gas constant} [J/\text{mol}K], \tag{2.43}$$

$$T = \text{is the temperature} [^\circ K] \tag{2.44}$$

$$\tag{2.45}$$

gives the diffusion coefficient of solids as a function of temperature and apparent activation energy of the medium.

Temperature Dependent Diffusion : Stokes Einstein

The Stokes-Einstein relationship,

$$D(T) = \frac{k_B T}{6\pi\eta r} \tag{2.46}$$

gives an equation for the diffusion coefficient in a fluid, as a function of T, the temper-

ature of the surrounding medium, k_B, the Boltzmann constant, and η, the viscosity of the medium. The Stokes-Einstein relationship relies on the linearization of the Navier-Stokes equation that preserves only the viscous components [24]. This is most valid for media where diffusion dominates and therefore inherently have a low Reynolds number,

$$Re = \frac{\rho v L}{\mu} \tag{2.47}$$

where

$$\rho = \text{fluid density}[kg/m^3] \tag{2.48}$$

$$v = \text{mean relative velocity of fluid}[m/s] \tag{2.49}$$

$$L = \text{characteristic length of system}[m] \tag{2.50}$$

$$\mu = \text{dynamic fluid viscosity}[kg/m \cdot s]. \tag{2.51}$$

Continuum Models of Fractured Media

There exist various conceptual models for incorporating fractures into a porous medium model. Some examples are given in Figure 2.1.

The models arrived at via a continuum approximation are appropriate for very fractured or purely porous media. This approximation is not suitable for situations in which the fracture width or frequency varies greatly.

Equivalent Porous Medium (EPM) models assume that a uniformly fractured medium can be approximated as a fractureless matrix with an effective porosity high enough to account for real fracturation [11, 7].

Dual continuum models are the most widely employed models of fracture flow

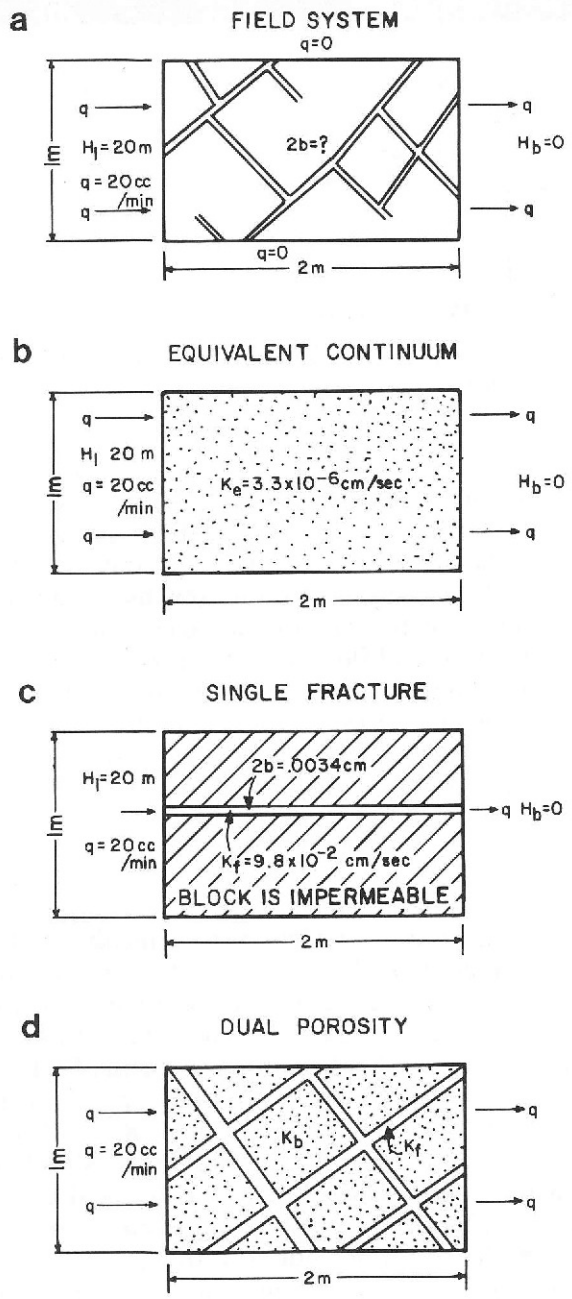

Fig. 12.6 Conceptual models of a fractured rock system (modified from Gale, 1982).
(a) A simplified fracture network of aperture $2b$ with groundwater flow from left to right.
(b) Equivalent porous medium model of (a).
(c) Discrete fracture model of (a).
(d) Dual porosity medium model of (a).

Figure 2.1: Various conceptual models may be used for the same natural system [7].

[19]. Dual Porosity Models make up one type of dual continuum model. This model incorporates advective transport in simplistic, uniform fractures and diffusive sorption and desorption into the stagnant (no advective transfer) water contained in the pores of the rock matrix [59, 27].

Dual Permeability Models are another type. These are similar to dual porosity models, but incorporate advective transfer within the rock matrix and between the rock matrix and the fracture volume [59, 27]. The incorporation of advective transfer in the dual permeability model is more appropriate for modeling granite since it incorporates advective solute transport through the rock matrix as well as diffusion.

Discrete Fracture Network Models

Discrete fracture network models approximate that water and contaminants move only through the fracture network [7, 55]. Such an approximation is appropriate when flow through fractures is fast relative to porous flow. This modeling formulation is complex and requires detailed knowledge of the candidate lithology.

The flow in each fracture can be approximated, as in Schwartz and Zhang, with the flow between two parallel plates having an aperture b, the mean fracture height [55]. For a fracture perpendicular to gravitational acceleration, g, the hydraulic conductivity, K, is described according to the cubic law as

$$K = \frac{\rho_w g b^2}{12\mu} \tag{2.52}$$

where

$$\begin{aligned}\rho_w &= \text{ water density } [kg/m^3] \\ g &= \text{ gravitational acceleration } [m/s^2] \\ b &= \text{ plate aperture } [m] \\ \mu &= \text{ dynamic fluid viscosity } [kg/m \cdot s].\end{aligned}$$

Accordingly, the volumetric flow rate in the single fracture of width, w, can be described in terms of the hydraulic head gradient, $\frac{\partial h}{\partial L}$, as

$$Q = -Kbw\frac{\partial h}{\partial L}. \tag{2.53}$$

Calculation of the volumetric flow rate and corresponding solute transport in a discrete fracture network model for many non-parallel fractures is an intensive numerical computation. However, for uniformly fractured media, a fracture network can be approximated by a set of parallel plates fractures.

If flow is expect in the θ_f direction, and the fractures of the set are spaced a distance, d, apart,

$$\begin{aligned}N &= \text{fracture frequency} \\ &= \frac{cos(\theta_f)}{d}.\end{aligned} \tag{2.54}$$

The fracture network permeability is then defined as,

$$k_f = \frac{b^3}{12N}. \tag{2.55}$$

The permeability, k, in an equivalent permeability model is thereby obtained by the permeabilities of the fracture network, k_f, and the permeability of the host matrix, k_m. Following the derivation in Schwartz and Zhang, in terms of the cross-sectional contact areas of the matrix and fractures A_m and A_f, the equivalent permeability, k, can be expressed

$$k = \frac{k_m + \frac{A_f}{A_m} k_f}{1 + \frac{A_f}{A_m}}. \tag{2.56}$$

This permeability is then used as the effective permeability of the rock in expressions that utilize it to determine the Darcy velocity, such as Equation (2.11).

2.4 Analytical Models of Heat Transport

A comprehensive model of a repository must arrive at an appropriate notion of heat-based waste loading and repository capacity. This requires a model which addresses heat transport through the repository as a function of spatial repository layout, waste stream decay heat, and heat transfer properties of the engineered barrier system and host rock lithology. This model must sufficiently solve for peak temperatures at heat limited locations, which are in most cases at the waste package interface with the buffer material and the buffer material interface with the lithology. These heat limits were discussed in section 2.2.

Heat transfer in these concepts will be dominated by conductive heat transfer. In a saturated closed system, very few air gaps will exist. For this reason, heat transfer by radiation is likely to be negligible. Similarly, since water velocities are comparatively low, heat transfer by mass transfer or by convection will be small relative to conduction.

A discussion of analytical models of heat transport follows that quantifies these modes of heat transfer and addresses their applicability to the model at hand.

Conduction

Conductive heat transfer occurs as a result of a temperature gradient. Heat flows diffusively from the hotter material to the cooler material over time and steadily approaches thermal equilibrium. The general form of the conduction equation can be expressed

$$\nabla^2 T + \frac{q'''}{k} = \frac{1}{\alpha}\frac{\partial T}{\partial t}, \tag{2.57}$$

which with no heat source becomes the transient Fourier equation,

$$\nabla^2 T = \frac{1}{\alpha}\frac{\partial T}{\partial t}, \tag{2.58}$$

or to the Laplace equation in steady state,

$$\nabla^2 T = 0. \tag{2.59}$$

Replacing the source gives the steady state Poisson equation,

$$\nabla^2 T + \frac{q'''}{k} = 0. \tag{2.60}$$

An areal heat flux, $q''[W/m^2]$ can be derived from an integration of Poisson's equation (2.60) and expressed in terms of the thermal conductivity of the material, $k[W/m \cdot^{\circ} K]$, and the temperature gradient $\nabla T[K/m]$ by the expression

$$q'' = -k\nabla T. \tag{2.61}$$

For the one dimensional case, equation 2.61 can be reduced using a finite difference approximation. For a body at x_1 with temperature T_1 and a body with temperature T_2 at position x_2,

$$q''_x = -k_x \frac{dT}{dx} \tag{2.62}$$

$$= -k_x \frac{(T_1 - T_2)}{x_1 - x_2}. \tag{2.63}$$

Convection

Convective heat transfer occurs advectively in accordance with fluid movement. Convection can be expressed as

$$\dot{q} = -hA\Delta T. \tag{2.64}$$

Radiation

Heat transfer by radiation is the result of the emission of electromagnetic waves. Planck black body radiation is analytically described, using σ, the Stefan-Boltzmann constant as

$$\dot{q} = \sigma A_1 F_{1\to 2}(T_1^4 - T_2^4) \tag{2.65}$$

where

$$\sigma = 5.670373 \times 10^8 [W/m^2 K^4]$$

and

$$F_{1\to 2} = \begin{cases} \epsilon_1 & \text{for a point source,} \\ \frac{1}{\frac{1}{\epsilon_1}+\frac{1}{\epsilon_2}-1} & \text{for parallel plates,} \\ \frac{2\pi r_1 L}{\frac{1}{\epsilon_1}+\frac{1}{\epsilon_2}-1}\frac{r_1}{r_2} & \text{for concentric cylinders} \end{cases} \tag{2.66}$$

where

$$\epsilon_i = \text{emissivity of surface i } [-]$$
$$r_i = \text{radius of cylinder i } [m]$$
$$L = \text{cylinder length } [m].$$

Mass Transfer

Heat transfer by mass transfer is straightforward, resulting in the change in temperature in adjacent volumes as a result of matter movement. If the specific heat capacity of the transferred mass can be expressed as c_p, then the heat transfer is simply,

$$\dot{q} = \dot{m} c_p \left(T_j - T_i\right) \tag{2.67}$$

where

$$c_p = \text{ specific heat capacity } [J/kg^\circ K].$$

Lumped Parameter Model

The lumped heat capacitance model makes an analogy to electrical circuit by reducing a thermal system into discrete lumps for an approximate solution of transient heat transfer. Such an approximation is appropriate when it can be assumed that the temperature gradient within each lump is approximately uniform. The appropriateness of this approximation can be quantitatively expressed by comparison of the internal thermal resistance to the external thermal resistance. The Biot number,

$$Bi = \frac{hA}{k} \tag{2.68}$$

indicates the relative speeds with which heat conducts within an object and across the boundary of that object. If the Biot number is low (< 0.1), and therefore conduction

is faster within the object than at the boundary, the assumption of a uniform internal temperature is appropriate and the lumped parameter model may be expected to give a result within 5% error[29]. This assists in choosing the size of distinct lumps within a conceptual model.

The lumped capacitance model can address multiple media and multiple heat transfer modes. The rate of heat transfer $\dot{q}$ $[Wm^{-2}K^{-1}s^{-1}]$ through a circuit is simply given as the quotient of the temperature difference and the sum of thermal resistances, $R_i[W \cdot K^{-1}]$, of the multiple lumps

$$\dot{q} = \frac{\Delta T}{\sum_{i=0}^{N} R_i}. \tag{2.69}$$

By representing the various modes of heat transport (i.e. conduction, convection, radiation, and mass transfer) with various expressions for resistance, the lumped capacitance model provides a solution to the transient problem described by the energy balance,

$$\text{(Energy added to body j in dt)} = \text{(Heat out of adjacent bodies into body j)}$$

$$c_j \rho_j V_j dT_j(t) = \sum_{i=0}^{i=N} [\dot{q_{i,j}}]\, dt, \tag{2.70}$$

where $c_j \rho_j V_j$ is the total lumped thermal capacitance of the body.

For example, in the case of a simple convective circuit between two bodies, i and j,

the resistance of j can be described as

$$R_{conv} = 1/hA \tag{2.71}$$

such that

$$c_j \rho_j V_j dT_j(t) = \sum_{i=0}^{i=N} \left[hA_j (T_i - T_j(t)) \right] dt. \tag{2.72}$$

$$\tag{2.73}$$

A time constant appears under integration that describes the speed with which the body i changes temperature with respect to the maximum temperature change,

$$\int_{T_j=T_0}^{T_j(t)} \frac{dT_j(t)}{T_i - T_j} = \frac{hA_j}{c_j \rho_j V_j} \int_0^t dt \tag{2.74}$$

$$-ln \frac{T_i - T_j(t)}{T_i - T_0} = \frac{hA_j}{c_j \rho_j V_j} t \tag{2.75}$$

$$\frac{T_i - T_j(t)}{T_i - T_0} = e^{-(hA_j / c_j \rho_j V_j) t} \tag{2.76}$$

such that

$$\frac{T_j(t) - T_i}{T_i - T_0} = 1 - e^{-t/\tau} \tag{2.77}$$

where

$$\tau = \left(c_j \rho_j V_j / hA_j \right). \tag{2.78}$$

The time constant, τ is the time it takes for the body to change $(1-(1/e))\%\Delta T$ and is equal to the product of the thermal capacitance and thermal resistance of the body, CR, analogous to an electrical circuit.

[23] This is the case for all resistances, R_i representing modes of heat transfer. Thus, one can say, in general

$$\tau_j = c_j \rho_j V_j R_j. \tag{2.79}$$

Impact of Repository Designs

The repository layout has a significant influence on its heat transfer properties. Waste package spacing in drifts, boreholes, or alcoves, tunnel spacing, and multiple gallery level designs all affect available heat loading. For example, in the YMR, a variety of parameters have been shown to affect the potential repository waste loading density.

The YMR statutory limit of once-through, thermal PWR waste is 70,000 tonnes SNF. That is to say, the statutory line load limit is approximately 1.04 tonnes/m for 67km of planned emplacement tunnels (with 81 meters between drifts). The Office of Civilian Radioactive Waste Management Science and Engineering Report gives this basic "statutory limit", but suggests an inherent design flexibility that could allow for expansion. Multiple efforts have adjusted various repository layout parameters in order to develop expanded capacity models of the YMR. Some of these efforts are detailed in Table 2.8.

This inherent flexibility can come from an increase in the areal extent of the repository footprint, the density of drifts, or vertical expansion. The "full inventory" Yucca Mountain design alternative gives a maximum repository capacity of 97,000 tonnes. In

Yucca Mounting Footprint Expansion Calculations

Author	Max. Capacity $tonnes$	Footprint km^2	Details
OCRWM	$70,000$	4.65	"statutory case"
	$97,000$	6	"full inventory case"
	$119,000$	7	"additional case"
Yim, M.S.	$75,187$	4.6	SRTA code
	$76,493$	4.6	STI method
	$95,970$	4.6	63m drift spacing
	$82,110$	4.6	75 yrs. cooling
Nicholson, M.	$103,600$	4.6	drift spacing
EPRI			
	$63,000$	6.5	Base Case CSNF
option 1	$126,000$	13	expanded footprint
option 2	$189,000$	6.5	multi-level design
option 3	$189,000$	6.5	grouped drifts
options 2+3	$252,000$	6.5	hybrid
options 1+(2or3)	$378,000$	13	hybrid
options 1+2+3	$567,000$	13	hybrid

Table 2.8: Various analyses based on heat load limited repository designs have resulted in footprint expansion calculations of the YMR.

addition, the current design for the repository has flexibility for "additional repository capacity" which would give a 119,000 tonne capacity at 1.04 tonnes/m.[20]

In addition to variable drift spacing, other modifications to repository layout have had promising results in terms of heat-limited repository capacity. The Electric Power Research Institute (EPRI) in their Room at the Mountain study found that with redesign of the repository an increased capacity of at least 400% (295 tonnes once-through SNF) and up to 900% (663 tonnes) could be expected to be achieved. Proposed design changes include decreased spacing between drifts, a larger areal footprint, vertical expansion into second and third levels of repository space, and hybrid solutions involving combinations of these ideas. In particular, EPRI suggests either an expansion of the footprint with redesign of the current line load design plan or a multi-level plan that repeats the

footprint and line load design of the current plan[34].

Layout options such as age based fuel mixing also allows for decreases in drift spacing. In aged based fuel mixing, aged (long cool time) SNF is loaded in a mixture with young SNF. This age based fuel mixing has been shown to achieve a 48% increase in the repository capacity as constrained by heat load[42]. This factor uses a fiducial default footprint of $4.6km^2$ used in the NRC TSPA. The reported 48% increase in capacity results in total repository capacity of 103,600 tonnes[61].

Heat Limits in Engineered Components

Various waste form constraints exist that limit fuel loading. These are in general less restrictive than heat limits resulting from geological medium constraints, however in some cases they are more restrictive.

For example, the current constraining heat limit in borosilicate glass reported by the UFD campaign is $500°C$, corresponding to the temperature at which the glass can be expected to begin devitrifying [**?** 25, 56]. For ceramic oxide fuel pellet waste forms, zirconium cladding has a heat limit of $350°C$ to prevent rupture [56].

Specific Temperature Integral

Linear mass loading ($tonnes/m$), linear thermal loading (W/m) and areal power density (W/m^2) are common metrics for describing the loading of the repository. While these metrics are informative for mass capacity and power capacity respectively, they fail to reflect differences in thermal behavior due to varying SNF compositions. A closer look at the isotopics of the situation has proven much more applicable to thermal performance studies of the repository, and the preferred method in the current literature relies on specific temperature integrals.

Specific temperature integrals model the thermal source as linear along the emplacement paths, similar to the line loading and areal power density metrics. However, a temperate integral takes account of heat transfer behavior in the rock, includes the effects of myriad SNF compositions, and gives the thermal integration over time for any specific location within the rock. Man-Sung Yim calls this the Specific Temperature Increase method[39] though other researchers have other names for this method. Tracy Radel calls her temperature metric at a point in the rock the Specific Temperature Change[51].

In a repository with linear drifts, the heat flux from the drifts can be expressed as the superposition of the linear heat flux contributions of all the radionuclides in the waste. The temperature change, more importantly can be expressed as a superposition of the temperature change contributions due to each radionuclide. Each radionuclide contributes in proportion to its decay heat generation and its weight fraction of the SNF. With information about isotopic composition of the SNF, the Specific Temperature Increase can determine the maximum thermal capacity of the repository in terms of tonnes/m. The length based accounting in $\frac{t}{m}$ is converted to $\frac{t}{Repository}$ by multiplication with the total emplacement tunnel length of the repository. In the case of Yucca Mountain, this was 67 km.

2.5 Detailed Computational Models of Radionuclide Transport

Detailed computational models of radionuclide transport seek to quantify the spatial movement of radionuclides within a repository environment due to heat generating waste forms. Such models are detailed with respect to their fine spatial and temporal resolution or with respect to the incorporation and coupling of numerous physical

phenomena. Current detailed computational models addressing various repository geologies and geometries will be reviewed here that utilize finite difference and finite element methods in many dimensions, sophisticated numerical solvers, and other high fidelity approaches.

European RED-IMPACT

The RED-IMPACT assessment compared results from European fuel cycle codes for various specific waste package forms, radioactive and radiotoxic inventories, reprocessing discharges, waste package thermal power, corrosion of matrices, transport of radioisotopes and resulting doses. Granite, clay and salt were analyzed by various countries and codes as listed in table 2.9.

International Repository Concepts

Geology	Nation	Waste Stream	Metric	Institution
Granite	Spain	HLW	Heat Load	Enresa
Granite	Czech Rep.	HLW	Heat Load	NRI
Clay	Belgium	HLW	Heat Load	SCK·CEN
Salt	Germany	HLW	Heat Load	GRS
Granite	Spain	HLW	Dose	Enresa
Clay	Belgium	HLW	Dose	SCK·CEN
Clay	France	HLW	Dose	CEA
Salt	Germany	HLW	Dose	GRS
Granite	Czech Rep.	ILW	LT Dose	NRI
Granite	Spain	ILW	LT Dose	Enresa
Clay	Belgium	ILW	LT Dose	SCK·CEN
Granite	Spain	HLW/ILW/Iodine	LT Dose	Enresa
Clay	Belgium	HLW/ILW/Iodine	LT Dose	SCK·CEN

Table 2.9: International repository concepts evaluated in the RED Impact Assessment.[36]

UFD Generic Performance Assessment Model

The UFD campaign is currently conducting an effort to produce a Generic Performance Asessment Model for analysis of GDSMs for various geological environments.

Teams from Argonne National Laboratory, Lawrence Berkeley National Laboratory, Los Alamos National Laboratory, and Sandia National Laboratory are developing models of generic clay, granite, and salt disposal environments respectively. Sandia is simultaneously constructing a deep borehole disposal system model in crystalline rock. Each generic disposal system model will perform detailed calculations of radionuclide transport within its respective lithology [18]. A 2012 goal of the project includes an overarching generic model that incorporates the various geologically distinct submodels in order to provide a fully generic repository model. This overarching GPAM work will be used in this effort.

The radionuclide transport calculations for the geologically distinct models are performed within the GoldSim simulation platform. GoldSim is a commercial simulation environment [35]. Probabilistic elements of the GoldSim modelling framework enable the models to incorporate Features, Events, and Processes (FEPs) expected to take place probabilistically during the evolution of the repository [18].

Cells within GoldSim represent components of the waste disposal system and are linked by diffusive, advective, precipitated, direct, or otherwise filtered mass transfer links.

Thermal modeling for the GDSMs are conducted independently with associated codes capable of modeling thermal evolution for all geologies. For example, one thermal model is being created using the Systems Improved Numerical Differencing Analyzer \ Gaski (SINDA\G) heat transport solver and another is under development at Lawrence Livermore National Laboratory (LLNL) that utilizes a combination of MathCAD and Excel.

Clay/Shale GDSM

The Clay GDSM is being pursued by the team at Argonne National Laboratory (ANL) and will be the primary model with which this work will conduct parametric regression analyses.

The Clay GDSM models a single waste form, waste package, EBS, Excavation Disturbed Zone (EDZ), and far field zone. This waste unit cell is modeled with boundary conditions such that it may be repeated throughout the extent of a repository configuration.

The waste form and engineered barrier system are modeled as well-mixed volumes and radial transport away from the cylindrical base case unit cell is modeled as one dimensional.

Two radionuclide release pathways are considered. One is the nominal, undisturbed case, while the other is a fast pathway simulating a disturbed case [18].

Granite GDSM

Los Alamos National Laboratory (LANL) and Sandia National Laboratory (SNL) have created a model of the granite repository concept in a saturated, reducing environment.

Waste form degradation is modeled as a constant, fractional rate to represent dissolution for both canonical borosilicate glass and commercial used fuel waste forms.

Though waste package failure is conservatively assumed to be instantaneous, waste package release into the near field is solubility limited as is the near field to far field interface.

Transport through the buffer is modeled as entirely diffusive coupled with sorption. Advection is neglected.

The far field was represented using a model that includes advection, diffusion and sorption. Specifically, the Finite Element Heat and Mass Transfer (FEHM) code was coupled into GoldSim to represent the far field.

Salt GDSM

The salt repository concept has an alcove gallery geometry and is located in a bedded salt formation. The formation is located in a reducing, saturated environment. Once waste packages are horizontally placed in a corner of the alcove, the space is backfilled with crushed salt.

Decay heat induced salt consolidation and brine flow are primary focuses of this analysis and inform radionuclide transport calculations.

A constant, temperature independent annual degradation rate model is used to represent waste form dissolution for both canonical borosilicate glass and commercial used fuel waste forms. Waste package failure is conservatively assumed to be instantaneous, and all near field components are modeled as a single mixed cell, the water volume of which is determined by the bulk volumes and degraded porosities of contained materials (e.g. bentonite buffer). A block of rock below the salt provides the pathway interface to an aquifer below. Radionuclide transport into that interface is modeled as diffusive, advective, and solubility limited.

The far field is modeled using an equilibrium sorption model in addition to solubility limited diffusion and advection. In such an equilibrium sorption model, the sorption to precipitation balance is assumed to be at a reaction equilibrium. In this way, the partitioning coefficient K_d is used to quantify the ratio between dissolved and undissolved reactant. Radionuclide transport in the far field takes place for 5km, and ends in a biosphere model.

Two radionuclide release pathways are considered. One is the nominal, undisturbed case, which the other is a fast pathway simulating a disturbed case [18].

Deep Borehole GDSM

The deep borehole model concept consists of some 400 waste canisters in a 5km deep hole within a low permeability, high salinity region characteristic of crystalline rock formations at depth. The lower 2km of the hole are filled by waste packages as well as spacing and sealing plugs. A 1km sealing zone extends above the waste disposal region.

As with the salt model, a constant, temperature independent annual degradation rate model is used to represent waste form dissolution for both canonical borosilicate glass and commercial used fuel waste forms. Waste package failure is conservatively assumed to be instantaneous.

Flow in the vicinity of the borehole was modeled using tabulated groundwater flow velocities obtained from simulations run using the FEHM code meshed in three full dimensions with the CUBIT Geometry and Mesh Generation Toolkit (CUBIT) meshing tool [18].

Li Model[37]

As a function of time, water enters the Engineered Barrier System and corrodes the waste packages. These fail and from the failed waste packages radionuclides are released according to advective transfer. Further transport through the near and far field rock medium is modeled in two modes, one representing the unsaturated zone, and one representing the saturated zone.

Waste package failure and radionuclide release are modeled with two TSPA code modules called EBSFAIL and EBSREL. The waste package failure rate is determined from

EBSFAIL, which incorporates waste form chemistry, humidity, oxidation, etc and upon contact from water begins the degradation process. The results of EBSFAIL become the input to EBSREL, which models corresponding radionuclide release from those failed waste packages. Mass balance governing the radionuclide release rate in this model allows advective transfer to dominate and takes the form:

$$\dot{m}_i = w_{li}(t) - w_{ci}t - m_i\lambda_i + m_{i-1}\lambda_{i-1}.$$

In this expression, $w_{li}(t)$ is the rate $[mol/yr]$ of isotope *i* leached into the water. It is a function of water flow rate, chemistry, and isotope solubility. m_i describes the mass of isotope *i*, and λ_i $[s^{-1}]$ describes its decay constant. Finally, $w_{ci}(t)$ describes the advective transfer rate $[mol/yr]$ of the isotope *i*. This model defines w_{ci} as:

$$w_{ci}(t) = C_i(t)q_{out}(t). \tag{2.80}$$

where q_{out} is the volumetric flow rate of the water $[m^3/yr]$, and C_i is the concentration on isotope i in the waste package volume m_i/V_{wp} in $[mol/m^3]$. These assumptions fail to take into account any differences in the varying solubilities of the isotopes, but are quite sensitive to the concentration of an isotope *i* in the waste package volume.

ANDRA Dossier 2005

The ANDRA Dossier 2005 studies provided detailed radionuclide transport calculations for both argillaceous clay and granite formations.

ANDRA Clay Model

In the ANDRA clay model, complicated saturation and resaturation phenomena are neglected and it is assumed that the initial repository condition is fully resaturated. This is a conservative simplification. Another conservative assumption is one in which the evacuation disturbed zone does not heal. Rather, it is modeled in its damaged state immediately after excavation.

This model only tracks 15 radionuclides of importance. These are chosen to be those with half lives over 1000 years and most toxicity or mobility [8]. The behavior of radionuclides in glass vitrification forms can be summarized by categorizing them into mobile, intermediate, and well retained elements.

Some specific codes and the method with which they were used in the ANDRA clay assessment are listed in Table 2.10.

Detailed Nuclide Transport Models Used in the ANDRA analysis.

Models	Codes
Hydrogeology and particle tracking in continuous porous media	Connectflow (3D finite element) Geoan (3D finite differences). Porflow (3D finite differences).
Hydrogeology and particle tracking in discrete fracture networks.	Connectflow (3D finite elements). FracMan (discrete fracture networks) and MAFIC (3D finite elements).
Transport in continuous porous media.	PROPER (finite differences), Goldsim (control volumes), and Porflow (control volumes?).
Transport in discrete fracture networks.	PROPER (1D stream tube concept). PathPipe (networks of tubes) and Goldsim (networks of 1D pipes).

Table 2.10: Similar to the Total System Performance Assessment, ANDRA's analyses are a coupled mass of many codes. Table reprouced from Argile Dossier 2005 [8]

Waste form dissolution and package release was assumed to be immediate for some waste forms and corrosion rate based for those where appropriate data were available. Vitrified waste package releases were either modeled with a simple model or a two

phase phenomenological model.

Transport through the backfill is modeled as diffusive, with high permeability after degradation. The evacuation disturbed zone has both a fracture zone and a microfissure zone. In the host formation, movement is dominated by diffusion, and advection is modeled, but is negligible.

Tools used in the ALLIANCES software platform include Castem, PorFlow and Trace for hydraulic calculations and radionuclide transport and Prediver and Colonbo for waste package failure.

2.6 Detailed Computational Models of Heat Transport

Detailed heat transport models seek to quantify the heat evolution within a repository environment due to heat generating waste forms. Such models are detailed with respect to their detailed spatial and temporal resolution or with respect to the incorporation and coupling of numerous physical phenomena. Such codes typically utilize finite differencing or finite element methods in many dimensions or sophisticated numerical solvers, respectively.

ANL SINDA\G Model

This model, created at Argonne National Lab uses the SINDA\G lumped capacitance solver. Originally created for optimal waste loading analysis of the YMR, the model is geometrically adjustable in two dimensions, as is demonstrated in Figure 2.2. The tunnel size is a fixed parameter in the model, but the optimal drift spacing for a particular waste stream and package loading is solved for with an optimization loop within this model.

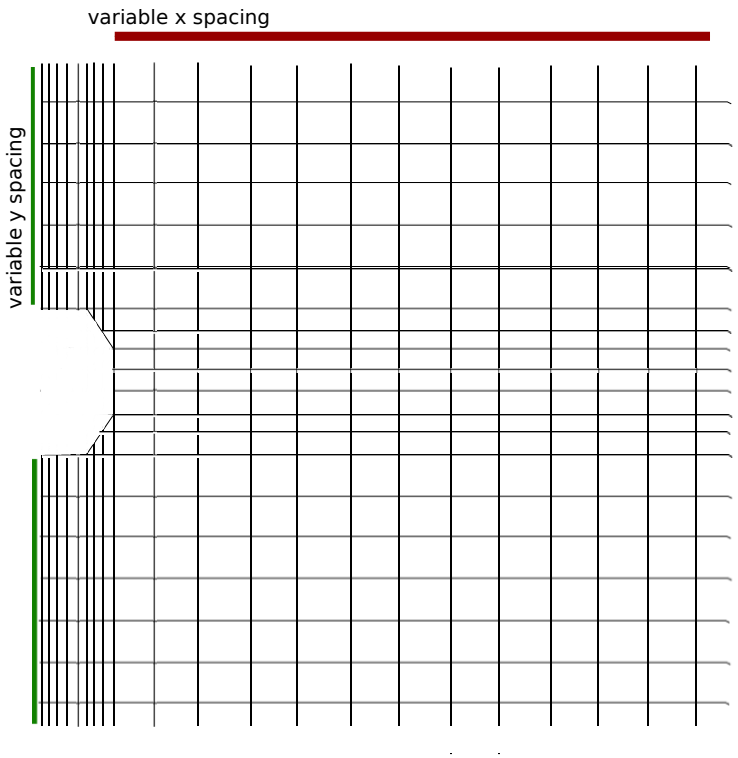

Figure 2.2: The geometry of the thermal model can be adjusted in two dimensions, altering the tunnel spacing and the vertical distance from the aquifer.

The SINDA\G lumped capacitance solver solves a thermal circuit, for which conducting nodes may be of four types corresponding to the four modes of heat transfer. Nodes are connected by conduction, convection, radiation, and mass flow heat transfer links. As discussed in section 2.4, these are represented by

$$R_{cond} = \frac{L}{kA} \tag{2.81}$$

$$R_{conv} = \frac{1}{hA} \tag{2.82}$$

$$R_{mf} = \frac{1}{\dot{m}c_p} \tag{2.83}$$

$$R_{rad} = \frac{1}{\sigma F_{ij} A \left[T_i + T_A + T_j + T_A\right] \left[(T_i + T_A)^2 + (T_j + T_A)^2\right]} \tag{2.84}$$

where

$k =$ thermal conductivity$[W \cdot m^{-1} \cdot K^{-1}]$

$A =$ area$[m^2]$

$c_p =$ specific heat capacity$[J \cdot K^{-1}]$

$h =$ heat transfer coefficient$[W \cdot m^{-1} \cdot K^{-1}$

$\dot{m} =$ mass transfer rate$[kg \cdot s^{-1}]$

$T_i =$ lump temperature$[^{\circ}C]$

$T_A =$ absolute temperature$[^{\circ}C]$

$F_{ij} =$ radiation interchange factor$[-]$.

With these representations of thermal resistance, a lumped parameter model will require an analysis that determines the appropriate length scale for the lumped parameter approximation.

Given one or more heat constraints, the ANL model optimizes spatial waste loading in order to meet those constraints with maximal waste loading. For example, given a constraint at the edge of the waste package, the model utilizes the SINDA\G lumped

capacitance solver to determine the two dimensional heat evolution of the repository as a result of a given waste package composition for various drift spacings and arrives at an ideal drift spacing by iteration.

LLNL MathCAD Model

This model, created at LLNL for the UFD campaign, is written in a combination of MathCAD and Excel. The model consists of two physical parts, the first is the host rock, and the second models the waste form, package, and buffer as a single EBS unit. Since the thermal mass of the EBS is small in comparison to the thermal mass of the host rock, it may be treated as quasi-steady state. Thus, the transient state of the transient temperature between the host rock and the EBS can be found with a MathCAD solution of the transient homogeneous conduction equation,

$$\nabla^2 T = \frac{1}{\alpha}\frac{\partial T}{\partial t}. \tag{2.85}$$

Superimposed point and line source solutions allow for a notion of the repository layout to be modeled in the host rock. The solution of this equation at the boundary of the EBS and the waste package is then treated as a boundary condition for the heterogeneous steady state equation,

$$\dot{q} = U A_{out} \left(T_{in} - T_{out}\right) \tag{2.86}$$

where

$$U = \frac{1}{\sum_i R_i} \tag{2.87}$$

which, for the detailed EBS becomes

$$U = \frac{1}{R_{WF} + R_{WP} + R_{buffer} + \cdots} \tag{2.88}$$

which calculates a resulting temperature gradient through the geometry at each point in time for each layer surface, assuming an infinite line source [25].

The process is then iterated with a one year resolution in order to arrive at a heat evolution over the lifetime of the repository. This model seeks to inform heat limited waste capacity calculations for each geology, for many waste package loading densities, and for many fuel cycle options.

Other Numerical Methods

Codes used by repository modeling efforts investigated in this review include finite difference codes, finite element codes, and specific temperature integrals. Some efforts and their methods are listed in Table 2.11.

Models of Heat Load for Various Geologies

Source (Who)	Nation (Where)	Geology (What)	Methodology (How)
Enresa [36]	Spain	Granite	CODE_BRIGHT 3D Finite Element
NRI [36]	Czech Rep.	Granite	Specific Temperature Integral
ANDRA [9]	France	Granite	3D Finite Element CGM code
SKB [1]	Sweden	metagranite	1D-3D Site Descriptive Models
SCK·CEN [36]	Belgium	Clay	Specific Temperature Integral
ANDRA [8]	France	Argile Clay	3D Finite Element CGM code
NAGRA [31, 32]	Switzerland	Opalinus Clay	3D Finite Element CGM code
GRS [36]	Germany	Salt	HEATING (3D finite difference)
NCSU(Li) [38]	USA	Yucca Tuff	Specific Temperature Integral
NCSU(Nicholson) [42]	USA	Yucca Tuff	COSMOL 3D Finite Element
Radel & Wilson [51]	USA	Yucca Tuff	Specific Temperature Change

Table 2.11: Methods by which to calculate heat load are independent of geology. Maximum heat load constraints, however, vary among host formations.

3 MODELING PARADIGM

The modeling paradigm with which this repository model and simulation platform are implemented are described here. Implications of the simulation platform architecture on the design of the repository model are discussed and the interfaces defining components of the repository model follow.

3.1 Cyclus Simulator Paradigm

The Cyclus project at the University of Wisconsin (UW) at Madison is the simulation framework in which this repository model is designed to operate. Modular features within this software architecture provide a great deal of flexibility, both in terms of modifying the underlying modeling algorithms and exchanging components of a fuel cycle system.

The Cyclus fuel cycle simulator is the result of lessons learned from experience with previous nuclear fuel cycle simulation platforms. The modeling paradigm follows the transaction of discrete quanta of material among discrete facilities, arranged in a geographic and institutional framework, and trading in flexible markets. Key concepts in the design of Cyclus include open access to the simulation engine, modularity with regard to functionality, and relevance to both scientific and policy analyses. The combination of modular encapsulation within the software architecture and dynamic module loading allows for robust but flexible reconfiguration of the basic building blocks of a simulation without alteration of the simulation framework.

The modeling paradigm adopted by Cyclus includes a number of fundamental concepts that comprise the foundation on which other, more flexible, design choices have been made.

Dynamic Module Loading

The ability to dynamically load independently constructed modules is a heavy focus of Cyclus development. Dynamically-loadable modules are the primary mechanism for extending Cyclus ' capability. The primary benefit of this approach is encapsulation: the trunk of the code is completely independent of the individual models. Thus, any customization or extension is implemented only in the loadable module. A secondary benefit of this encapsulation is the ability for contributors to choose different distribution and licensing strategies for their contributions. By allowing models to have varied availability, the security concerns of developers can be assuaged (See Figure 3.1).

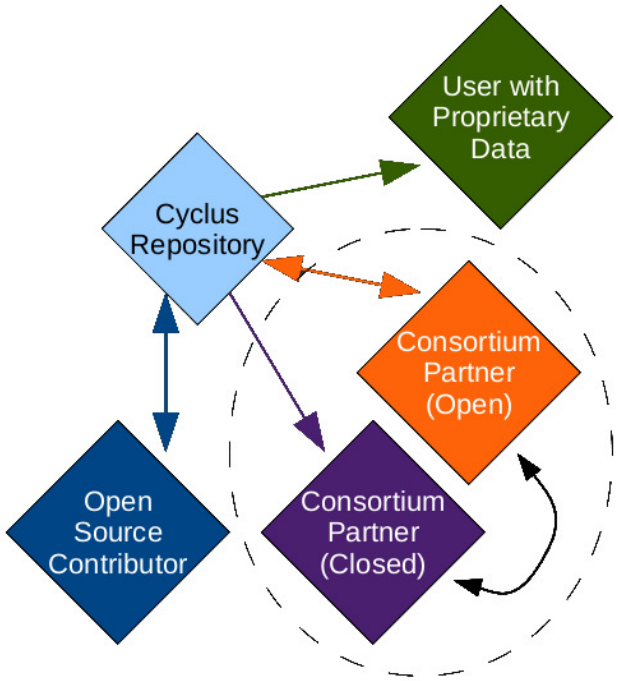

Figure 3.1: The Cyclus code repository allows for varied accessibility.

Finally, this strategy allows individual developers to explore different levels of complexity within their modules, including wrapping other simulation tools as loadable modules within the Cyclus framework. This last benefit of dynamically-loadable mod-

ules addresses another goal of Cyclus : ubiquity amongst its potential user base. By engineering Cyclus to easily handle varying levels of complexity, a single simulation engine can be used by both users keen on big-picture policy questions as well as users interested in more detailed, technical analyses.

Encapsulation

Cyclus implements an encapsulated structure that takes advantage of object-oriented software design techniques in order to create an extensible and modular user and developer interface. A primary workhorse for this implementation is the notion of dynamic module loading in combination with well defined module interfaces within a region, institution, and facility hierarchy. In this paradigm, the shared interface of polymorphic objects is abstracted from the logic of their instantiation by the model definition they inherit.

In this way, Cyclus allows a level of abstraction to exist between the simulation and model instantiation as well as between model instantiation and behavior. An interface defines the set of shared functions of a set of subclasses in an abstract superclass. In Cyclus main superclasses are Regions, Institutions, Facilities, and Markets while their subclasses are the concrete available model types (e.g. a RecipeReactorFacility). See Figure 3.2.

The interface for the FacilityModel class is the set of virtual functions declared in the Facility class such as getName, getID, executeOrder(), sendMaterial(), receiveMaterial() etc. Through such an interface, the members of a subclass can be treated as interchangeable (polymorphic) instantiations of their shared superclass.

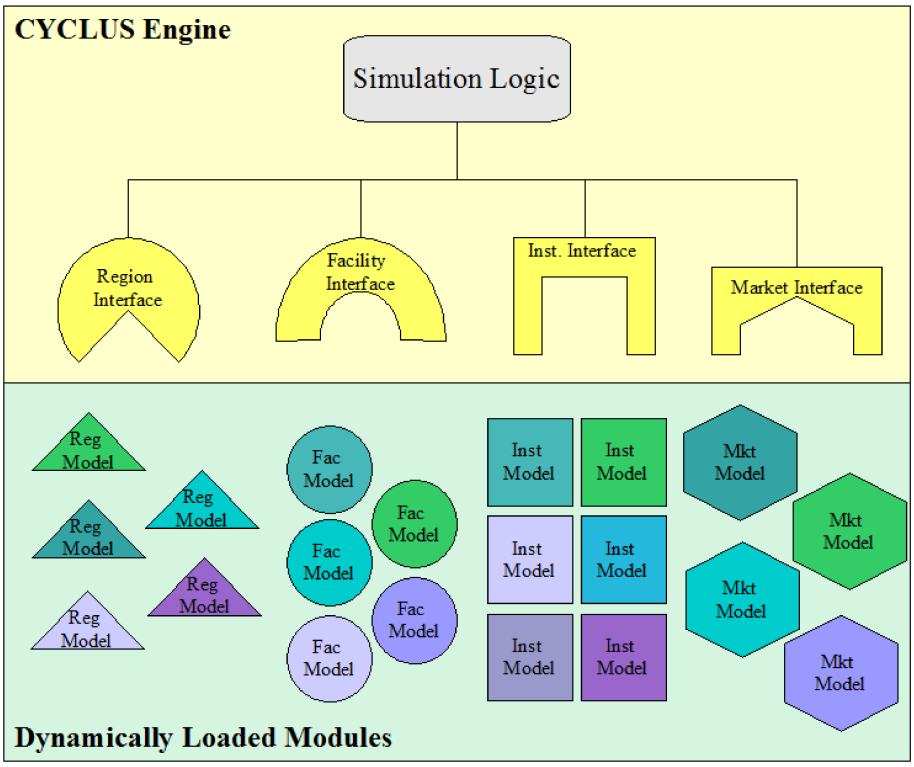

Figure 3.2: Modules are defined solely by their interfaces in a modular paradigm and can be arbitrarily interchanged with modules posessing equivalent interfaces.

Modularity and Extensibility

A modular code must have the traits of encapsulation and abstraction appropriate for a user or developer to flexibly make alterations to the simulation performance with minimal modification to the code. An extensible code should be both robustly suited to the addition of classes and subclasses as well as suited to communication with other codes. In Cyclus , addition of new models by dynamic loading is possible without any alteration of the software trunk. The modular design of Cyclus stresses avoidance of rigidity, in which changes to the code are potentially difficult, and fragility, in which changes to the code are potentially damaging.

Market-based Material Transactions

The foundation of a simulation is a commodity market that collects offers and requests and matches them according to some algorithm. The user is able to select which type of algorithm is used for each market by selecting a MarketModel and configure it with a particular set of parameters defined by that MarketModel. Changing the parameters of a market changes its performance and selecting a different MarketModel completely changes its behavior.

The transaction of nuclear materials takes place in markets that act as brokers matching a set of requests for material with a set of offers for that material. A variety of market models will be available to perform this brokerage role. It is important to note that each market is defined for a single commodity and acts independently of other markets. Once the requests and offers have been matched by each market in a simulation, the facilities exchange material objects.

Facilities are deployed to issue offers and requests in these markets. Like markets, the user may select which type of algorithm is used for each facility by selecting a FacilityModel and configure it with a particular set of parameters defined by that FacilityModel. Changing the parameters of a facility changes its performance and selecting a different FacilityModel completely changes its behavior. Unlike markets, multiple independent instances of each facility configuration can be deployed to represent individual facilities.

Discrete Materials and Facilities

The Cyclus modeling infrastructure is designed such that every facility in a global nuclear fuel cycle is treated and acts individually. While modeling options exist to allow collective action, this will be as a special case of the individual facility basis. Each facility has two fundamental tasks: the transaction of goods or products with other facilities

and the transformation of those goods or products from an input form to an output form. For example, a reactor will receive fresh fuel assemblies from a fuel fabrication facility, transform them to used used fuel assemblies using some approximation of the reactor physics, and supply those used fuel assemblies to a storage facility.

A facility configuration is created by selecting a FacilityModel and defining the parameters for that facility configuration. Each FacilityModel will define its own set of parameters that

The repository model that is the subject of this work is a facility model within the Cyclus simulation paradigm. govern its performance. The same FacilityModel may be used for multiple facility configurations in the same region, each with parameters values appropriate for that facility configuration.

Materials

Material movement is the primary unit of information in Cyclus . Materials passed, traded, and modified between and within facilities in the simulation are recorded at every timestep. This material history is stored in the output dataset of Cyclus . In addition to holding the map of isotopes and their masses, a material object holds a comprehensive history of its own path as it moves through models within the simulation.

Implications for Repository Model

The above sections outline the fuel cycle simulation platform currently under development at UW in which the repository model at hand is to be implemented. Implemented as a facility within this framework, the repository model interface is defined by the Facility Model interface defined within the Cyclus paradigm.

That interface requires that a capacity be defined by the repository at every CYCLUS timestep so that the repository may make appropriate requests of disposable material.

Furthermore, the capability for dynamic module loading possible within the CYCLUS paradigm allows the repository system subcomponents to be interchangeably loaded at runtime, enabling comparison of various repository subcomponents, physical models of varying levels of detail.

The repository is both a subclass and a superclass. It is a subclass of the FacilityModel class, and a superclass of its own subcomponents. That is, dynamically loaded subcomponents of the repository inherit data, parameters and behaviors from the repository itself.

3.2 Repository Modeling Paradigm

The repository model architecture is intended to modularly permit exchange of disposal system subcomponents, accept arbitrary spent fuel streams, and enable extending modules representing new or different component models.

Nested Component Concept

The fundamental unit of information in the repository model is the final nuclide release at the boundary of the far field resulting from nuclide release at each stage of containment. The repository model, in this way, is fundamentally a tool to determine the source term at the envrionmental surface as a result of an arbitrary waste stream. The repository model in this work conducts this calculation by treating each containment component as nested volumes in a release chain.

The capability to allow each component to define the components within it gives

this repository the ability to model many types of repository concept while maintaining a simple interface with the simulation.

Control Volumes

Each component of the repository system (i.e. waste form, waste package, buffer, and geologic medium) is modeled as a discrete control volume. Each control volume performs its own mass balance at each time step and assesses its own internal heat transfer and degradation phenomena separately from the other nested components.

Each control volume will initially be modeled as a mixed cell. That is, for permeable porous media, all contaminants released into the pore and fracture water are assumed to be uniformly distributed.

Thermal energy as well as mass will be conserved within each control volume by demanding continuity of thermal and mass fluxes accross the boundaries. Since radionuclide and thermal transport calculations internal to the control volumes may be represented by many models at varying levels of detail, abstraction on the component level against detailed models will be conducted to acheive appropriate detail in each component.

Information Passing Between Volumes

Each component passes some information radially outward to the nested component immediately containing it and some information radially inward to the nested component it contains. A diagram of the fundamental information being passed between components is described in Figure 3.3.

Most component models require external information concerning the water volume that has breached containment, so information concerning incoming water volumes is

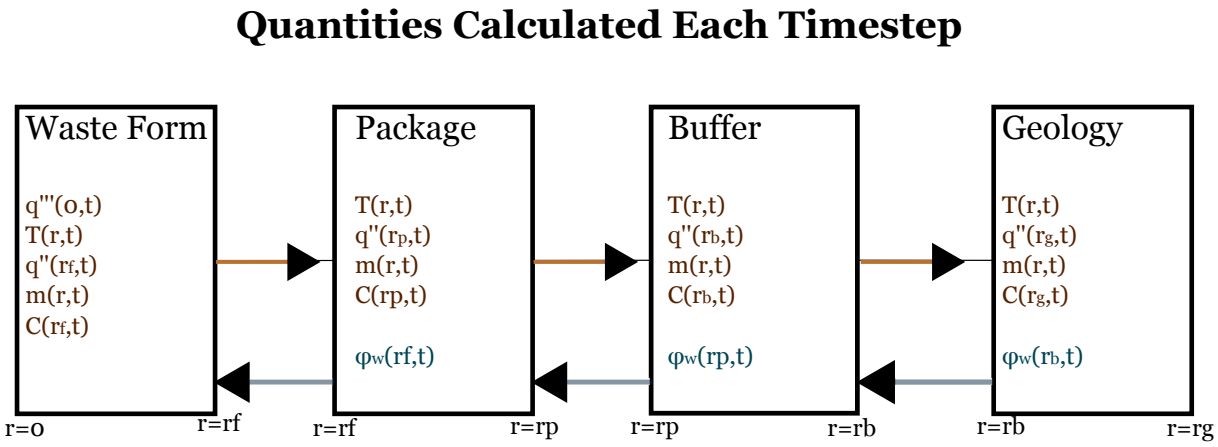

Figure 3.3: The nested components supply thermal flux and concentration information to each other at the boundaries.

passed radially inward.

Each component model similarly requires information about the radionuclides released from the component it immediately contains. Thus, nuclide release information is passed radially outward from the waste stream sequentially through each containment layer to the geosphere.

Components of the Nested System

The repository model is a collection of subcomponents which behave collectively to calculate repository metrics of interest. These subcomponents will be models of their own, and within the object oriented paradigm of the software will be a collection of module classes. Each component (i.e. waste form, waste package, buffer, lithology, etc.) will name a component superclass. Each superclass will be inherited by subclass models capable of representing that component in some level of detail specified by the model.

Waste Stream

The waste stream data object contains spent fuel isotopics over the course of the simulation. As radionuclides are gained, lost, and transmuted within the spent fuel object, a history of its isotopic composition is recorded.

For waste streams that vary from each other in composition, the thermal capacity of the repository must be recalculated. One way to model this will be to recalculate the appropriate lengthwise spacing of waste packages when the heat generation rate of a new package is significantly different than other waste packages in the repository.

Waste Form

The waste form model will calculate nuclide release due to dissolution of the waste form. Various heuristics by which nuclide release is modeled in accordance with waste form dissolution as well as the method by which the dissolution is modeled.

Dissolution can be instantaneous, rate based, water dependent, heat dependent, or coupled. Dissolution related release can be modeled as congruent, solubility limited, or both. Some radionuclides are immediately accessible, and some tend to remain in the fuel matrix.

Waste Package

The waste package model calculates nuclide release due to waste package failure. Waste package failure is typically modeled as instantaneous and complete or partial and constant. That is, a delay before full release, or a constantly present hole in the package.

Waste package time to failure is dependent on water contact and heat, but can be modeled as an average, probabilistic, or a rate.

In the case of highly deforming geologic media, such as salt, mechanical failure can be the primary mechanism for release from the waste package.

Buffer

Diffusion is the primary mechanism for nuclide transport through the buffer component of the repository system.

Salt, clay, and borehole repository concepts may not have a buffer material.

Backfill

Similarly, diffusion is the primary mechanism for nuclide transport through the buffer component of the repository system.

Clay concepts and borehole concepts may not have a backfill material.

Geological Environment

The literature review introduced various hydrological models that represent fluid and contaminant travel through permeable porous media and fractured porous media. These assume saturated flow and incorporate diffusive flow, advective flow, hydrodynamic dispersion, and equilibrium sorption. The geological environment control volume component will implement these models appropriately for each geology to provide a mass balance and to communicate concentrations to adjacent components. Dirichlet boundary conditions at the surfaces of the control volume will allow the simulation to step through transport in the rock. Additional boundary condition types maybe implemented as extensions to the base case model.

Simulation Interface

The interface of the repository model with the Cyclus fuel cycle simulation interface is intended to be minimally restrictive, requiring only that the simulation supply waste stream information and provide a bookkeeping framework with which to record repository performance metrics. The repository model, in order to participate in the simulation as a facility model, must make requests for spent material up to its capacity. Determination of the repository capacity for various types of spent fuel commodities will comprise the interfacing functionality of the repository model. With the intention of developing the repository model in such a way as to be capable of interfacing with other simulation tools, however, calculation of metrics including expected dose rates and component failures will be the model's primary functionality.

Waste Stream Input

The repository model must accept arbitrary spent fuel and high level waste streams. Material objects resulting from the simulated fuel cycle arrive at the repository and are emplaced if all repository capacity limits allow it.

Since disposable material in most simulations of interest will be of variable composition and therefore heterogeneous heat production capability, the repository model will repeatedly need to recalculate its own capacity as new materials are offered.

Repository Performance Metrics Calculated

Repository performance metrics that may be calculated from the source term and heat data calculated by the model will cover many metrics of interest to sustainability goals. Some metrics support analyses that seek to maximize safe repository capacity under

heat and source term limitations. Those include spatial dimensions, spatial dimensions per kWh or equivalent, repository footprint, and number of waste packages generated.

Still other metrics that may be calculated include those being considered by the UFD campaign in a Fuel Cycle Data Package task underway [43]. Additional metrics that will be considered in this context will likely include environmental metrics such as peak dose to the public, radiotoxic fluxes released to the biosphere integrated over time, and the minimum managed lifetime. These metrics are recorded in a database flexibly defined by the repository model.

Facility Functionality

The repository will behave as a facility within the Cyclus simulation paradigm. The fundamental facility behavior within Cyclus involves participating in commodity markets. The repository will participate as a requester of waste commodities. During reactor operation, the repository will make requests to markets dealing in spent fuel streams according to its available capacity. Possible optional intermediate storage facility model is available for cooling periods.

4 SUMMARY AND PROPOSED WORK

4.1 Summary

The need for this work has been shown by a summary of the current state of the art of fuel cycle simulator repository capabilities. The literature review concluded that most fuel cycle simulators lack repository analysis beyond basic mass tracking. The integrated radionuclide transport and thermal analysis to be pursued in this work will provide a currently unavailable tool for disposal system analysis. An immediate need for such a tool has been expressed in the UFD campaign roadmap for this year in which an interface with the FCO campaign was noted as a primary goal.

4.2 Proposed Work

A repository model, integrated in the Cyclus fuel cycle simulation platform, will be developed in three phases in parallel will supportive Cyclus development. A demonstration phase will implement an 'empty' repository structure which captures the fundamental software behavior of the subcomponents and integrated repository model. A base case phase will build upon the demonstration model by implementing the fundamental physics to represent key heat and radionuclide transport phenomena for simple unfractured media and canonical subcomponent concepts. The final extension phase will build upon the base case by implementing extending physics to capture the salient features of various competing repository concepts such as fracturation, sorption, and coalescent behavior. These phases will be completed within a test-driven software development paradigm and will rely on abstractions of the UFD GDSM and SINDA\G and LLNL thermal models.

Cyclus Framework

Development of the Cyclus fuel cycle simulator has generated a tool with which the systems analysis aspects of this work will be conducted. Development of the fundamental repository module concept appropriate for modular integration with Cyclus has laid the foundation for a software effort which will deliver a library of disposal system component models capable of analyzing current disposal concepts of interest both domestically and internationally.

Demonstration Case Development

A first milestone in the development of this software will be a proof of principle demonstration of the data structure and information passing schemes. That is, no physics will be implemented in the demonstration milestone. Rather, the component models will be developed in such a way that they are capable of passing physically arbitrary thermal and solute fluxes to neighboring components and placeholder functions will be implemented in place of physics.

Demonstration Case Concept

The demonstration will produce a complete but 'empty' repository model. That is, the appropriate facility interface will be implemented on the repository scale, which allows the repository modeled to be loaded into a Cyclus simulation. A structure of subcomponent control volumes will also be implemented which can be dynamically loaded at runtime.

At the subcomponent level, the demonstration will include information passing, bookkeeping, and mass and energy balances within and between the subcomponent control volumes. Information passing between subcomponents concerning heat and

radionuclide concentration boundary conditions will be implemented. A complementary output database structure will be defined and bookeeping for writing relevant radionuclide and heat transport information.

Volumes are defined by their dimensions, surfaces, temperature, contained matter, and contained contaminants. Interfaces are defined by a shared surface area, a flux type, and a flux direction. Any single volume may only interface with one inner and one outer volume. Contained matter must sum to the full volume of the control cell, in keeping with mass conservation.

This model treats matter in solid and liquid phases. Gaseous matter is not supported. Solids are assumed to be porous media and are defined by their porosity (n, $\%$), tortuosity (τ, $[-]$), and dry (bulk) density (ρ). Early phases of this work will assume just one liquid, water. Later extensions will incorporate varying water salinities and chemistries. In order to do so, liquids will be defined by their dynamic viscosities (μ, [Pascal seconds]), characteristic diffusivities (d_i, $[m^2/s]$) and solubility (K,$[kg/m^3]$) coefficients for each nuclide.

Demonstration Code Development

Initial code development on the base case model has begun with creation of the FacilityModel subclass, GenericRepository. This subclass meets the requirements defined by the Cyclus FacilityModel interface and can be dynamically loaded by the simulator.

A first phase in the demonstration milestone will be for the repository model to successfully load its subcomponent models from user input (i.e. the waste form, waste package, buffer, and lithology) with their corresponding defining parameters. A set of parameters that may be sufficient to model the base case is listed in Table 4.1.

A second phase will involve implementing an information exchange paradigm be-

Initialization Parameters for Subcomponents

Waste Form	Waste Package	Buffer	Geology
Inner Radius Outer Radius Length Density Specific Heat Capacity Initial Temperature Heat Transfer Coefficients			
Porosity Tortuosity Dissolution Model	Failure Model	Porosity Toruosity	Porosity Tortuosity

Table 4.1: A preliminary list of user-input initialization parameters for the four primary types of subcomponent models. Some parameters are necessary for all subcomponents.

tween the subcomponents. The purpose of this information passing scheme will be to communicate sufficient temperature fluxes and contaminant concentrations at the boundaries of the control volumes for neighboring subcomponents to solve their internal transport calculations. In addition to these Neumann type boundary conditions, additional types of boundary conditions may need to be anticipated.

When these aspects are implemented, a structure for the output database will be defined and appropriate bookkeeping will be implemented sufficient to communicate the heat and solute transport evolution within the repository.

Demonstration Testing

This work will be developed with a test driven development strategy. That is, before any new functionality is implemented, a suite of tests is written which as closely define its necessary behavior as possible. The software is then written with the goal of passing the test suite. In this way, the software developed in this work is expected to be comprehensively tested in parallel with its development.

Test problems which will help comprehensively define and confirm each unit of the

demonstration functionality will include very basic information passing tests as well as more complex multiple subcomponent integration tests. Every unit of functionality within the model should be tested as an integral part of development.

A null test of the demonstration case, for example, will release a single contaminant radionuclide through each subcomponent sequentially. This test will pass if the bookkeeper properly writes to the database its (aphysically unhindered) path through each control volume. Other tests might include a set of database writing tests, subcomponent loading tests, and tests of the facility interface.

When these unit tests pass, validation efforts will take place which show that the complete model behaves in agreement with the more detailed model on which it was based. If it does not behave as expected, sensitivity analyses, model abstraction, and computational development will be iterated through until the model is validated.

Base Case Development

The next phase in this work will be the development of the base case. This will build upon the demonstration repository module by implementing fundamental physics for each of the subcomponents. This will include mass and thermal conservation balances in each control volume, mixing models that include dissolution and solubility limitations as well as fundamental heat transport models within each subcomponent. These component models will be created using a dominant physics based approach that emphasizes the most important physics affecting radionuclide transport in each component. This milestone will result in a repository module capable of modeling the clay and salt GDSM concept modeled by the UFD campaign and the ANDRA and RED-IMPACT assessments. This step will implement the calculations in each subcomponent which will provide sufficient information to determine the heat based capacity of the repository for each

Categorization of Phenomena

Phenomenon	Simplest						Hardest
WF dissolution	instant	fractional	f(t)	f(H20)	f(T)	f(T,H20)	f(T,H20,etc.)
WP dissolution	instant	fractional	f(t)	f(H20)	f(T)	f(T,H20)	
WF release	instant	fractional	diffusive	advective	diff+adv	congruent	solubility limited
WP release	instant	fractional	diffusive	advective	diff+adv	congruent	solubility limited
Buffer failure	instant	fractional	f(t)	f(H20)	f(T)	f(T,H20)	f(T,H20,etc.)
Buffer release	instant	fractional	diffusive	advective	diff+adv	congruent	solubility limited
FF transport	diffusive	+fractures	+advective	congruent	+sorption	+colloids	solubility limited
WF Heat	indexed	decay					
WP Heat	conductive	+conv	+rad	+mass	2d	finite diff	finite element
Buffer Heat	conductive	+conv	+rad	+mass	2d	finite diff	finite element
FF Heat	conductive	+conv	+rad	+mass	2d	finite diff	finite element

Table 4.2: This table is a preliminary sketch of the various categories of phenomena which will occur in the components of the repository model.

request of material.

Base Case Component Abstraction

To fill in thermal and solute transport physics models for each component, it will be necessary to begin with a few fundamental models for each component. That is, it is possible to model each component (i.e. waste form, waste package, buffer, and lithology) in a simplistic way as well as a complex way. Table 4.2 categorizes some potential models for each component. The detail with which these models calculate thermal and radionuclide transport will be determined by component level abstraction against the GDSM models, the ANL SINDA\G model, and the LLNL heat model.

On the component level, the importance of input parameters on outgoing fluxes will be analyzed using abstraction. For example, the relationship of the dimensions of the waste package with the outgoing thermal flux will be analyzed by varying the waste package dimensions in the LLNL model and observing its calculation of the thermal evolution of the boundary between the waste package and buffer EBS components.

Base Case System Level Abstraction

In addition to abstraction on the component level, the collective behavior of the system will be analyzed via abstraction as well. That is, the appropriateness of model choices for each component and the behavior of combinations of collections of choices will be compared to results obtained from the detailed models.

For example, when enough buffer component models have been developed to give a suite of buffer options, the choice between a model that incorporates fracturation in the degraded buffer material and one that does not incorporate fracturation may be available. The choice between models will be informed by an analysis comparing results of each simulation and a similar full simulation with the detailed model.

This type of system level abstraction analysis will be performed with each component for which a range of models exist. This analysis will seek out models which capture differences in ultimate repository releases and other repository performance metrics, but neglect detailed calculations which have negligible effects on repository performance.

In conjunction with abstraction, system level benchmarking against the GDSM, LLNL, and ANL SINDA\G models will be undertaken at this point for assurance that the representation of a canonical repository concept within this model has expected results. Benchmarking will confirm behavior at many levels, ensuring detailed release and heat evolution for known incoming waste streams and repository configurations as well as ensuring trends in behavior for varied model parameters.

Much of this phase of the work will emulate the parametric and regression analysis that has begun with the base case Clay GDSM at ANL. The UFD campaign has reported sensitivity results for various parameters as they affect Peak Annual Dose. These preliminary analyses have focused on general trends and coefficients defining the relationships between these parameters and source term over time for each isotope.

For example, the vertical distance to the aquifer above the disposal configuration defines the distance separating source term nuclide contaminants from the biosphere. The clay model indicates that the mean annual dose is very sensitive to this distance [18].

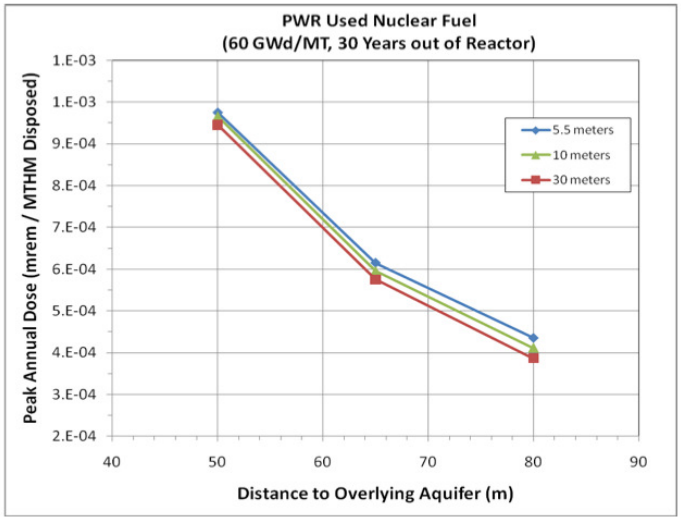

Figure 4.1: An analysis by the UFD campaign with the clay GDSM shows that the peak annual dose is very sensitive to the distance to the overlying aquifer[18].

Sensitivity to vertical Darcy velocity is similar to the sensitivity to vertical distance to aquifer in the sense that it directly determines the nuclide travel time to the biosphere. The clay model indicates that the mean annual dose is very sensitive to this parameter as well [18]. Other parameters such as the dimensions of the intersecting fast pathway, the permeable porous medium porosity, the waste form and waste package degradation rates, will be investigated with the GDSM models, the SINDA\G model, and the LLNL model.

Base Case Concept

The base case concept will model a generic, isotropic, permeable porous geological medium with reducing geochemistry, as well as waste form, waste package, and buffer models in the near field. This model will be appropriate for clay and salt geologies. The fracturation in the geologies of the granite and deep borehole concepts will not be appropriately modeled in the base case unless an equivalent porous medium calculation is conducted external to the code. The incorporation of fracture models will follow in subsequent extensions to the base case.

A waste form component module capable of modeling two canonical waste form concepts will be developed. It will be modeled with a rate based dissolution model and will be equipped with a heat limit which may constrict the waste form loading. Such a waste form component module will be appropriate for borosilicate glass, the dissolution of which is dominated by a surface alteration rate. It will be appropriate also for a ceramic oxide waste form, the dissolution of which is dominated by a corrosive degradation rate. A graphical representation of the base case waste form dissolution model is given in Figures 4.2 and 4.3.

An explicit time dependent probability distribution waste package failure model will

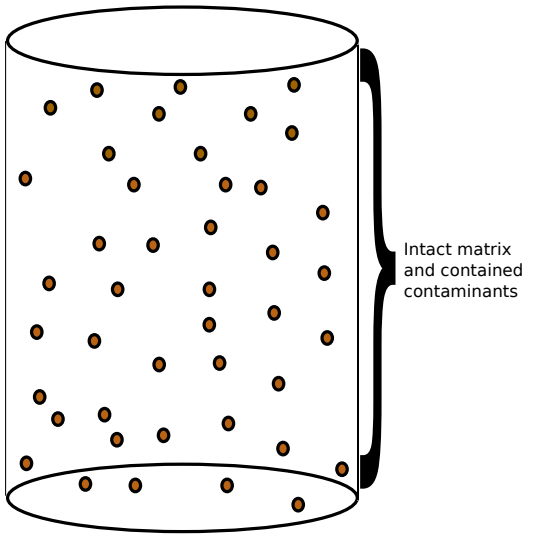

Figure 4.2: The control volume contains an intact waste form matrix and contaminants that are unavailable to neighboring subcomponents until dissolution has begun.

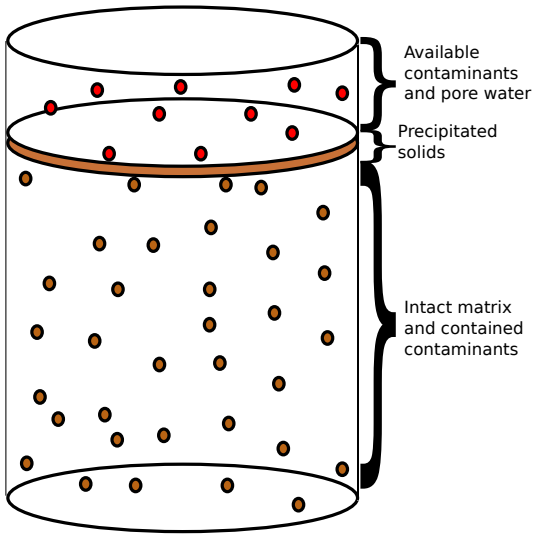

Figure 4.3: Once dissolution begins, the control volume contains a partially dissolved waste form matrix, contaminated pore water, and precipitated solids.

be employed that can accommodate instantaneous, constant, and more complex time dependent failure probability density functions. From a user-defined time dependent probability distribution (of which the Weibull distribution might be one), a waste package failure vector will be populated, which assigns a failure time to each waste package object. As the simulation progresses, these waste packages will fail discretely, triggering the initial degradation attack for the waste forms within them. The primary purpose of the waste package model, from a modeling perspective, is to initiate the beginning of waste form dissolution.

The buffer component will be modeled as an isotropic permeable porous medium that is chemically reducing and in which transport is diffusion dominated and solubility limited. For the base case, this model will involve only diffusive transport. Extensions to this model will include a model for sorption as well as fracturation and advective

transport.

Heat limits in the base case will be calculated at the boundary between the waste package and buffer as well as the boundary between the buffer or backfill and the rock matrix.

Base Case Testing, Verification, and Validation

For verification and validation during development, some comparisons to current detailed models such as the UFD GPAM and GDSMs will be incorporated into the testing framework. Additional verification and validation can be expected to be conducted with respect to known benchmarks such as ANDRA and RED-IMPACT results once the model is fully functional.

Extensions

When the base case is established, a series of extensions to these models will be pursued. This will build upon the base case repository module by incorporating sorption, fracturation, coalescence, and disruption models within each subcomponent. This milestone will result in a repository module capable of modeling the granite and borehole GDSM concepts modeled by the UFD campaign and the ANDRA assessments. Additional extension will also incorporate potentially important physical models of salt and clay coalescent behaviors.

Similar abstraction analysis will be undertaken for the phenomena involved in the extension models. Detailed physics in the extension concepts will be analyzed for their importance by regression analysis with the GDSM tools and iteratively compared to analytical models.

The code development in the extension phase will follow the same pattern as previous phases, but will focus on extending just one physics model in each component at a time in order to gauge the component level and system level impacts.

Extension Concepts

First, additional phenomena in radionuclide transport will be added to the modeling capability. Sorption, for example, will be added by incorporating sorption effects to the basic diffusive solute transport model, approaching a full solute transport solution such as equation (2.36). Additionally, solubility limited transport will be added with a simple restriction on the mixing calculations during mass balancing in the control volumes. Next, the capability to model fracturation features of granite and borehole geologies will be added to the modeling capability by adding a dual continuum fracture model.

Another anticipated extension will adapt the radionuclide transport model to incorporate the effects of heat and time driven coalescent behavior in clay and salt behavior. This extension will focus on the porosity decrease in those media as time and heat drive collapse around the waste packages. Time dependent coalescence will be addressed first, followed by temperature dependent coalescence.

A final potential extension may be implemented that will address the issue of modeling a disruption scenario with a fast advective pathway that intersects the repository. A fast pathway model intended to demonstrate a disrupted scenario is modeled as a single intersecting fracture in the clay matrix.

Extension Testing, Verification, and Validation

Unit testing, verification and validation will occur in a manner very similar to the previous milestones. Unit tests will assess the performance of each extension functionality as

well as their integrated behavior. Validation against GDSM results will also be performed for confidence building.

Fuel Cycle Analysis

As the model becomes capable of representing various repository concepts, these will be analyzed with relation to canonical closed, open, and modified fuel cycles as Cyclus is capable of them. As discussed before, these fuel cycles will present different repository challenges, and analysis with an integrated repository model is expected to demonstrate the dynamics of these challenges. While it is out of the scope of this work to perform comprehensive analysis of fuel cycle options, this work seeks to provide a tool with which to perform such analyses. Thus, some limited analysis of fuel cycle options will be performed to demonstrate that the tools developed in this work can illustrate the sensitivity of repository performance to upstream fuel cycle options.

REFERENCES

[1] AB, Svensk karnbranslehantering. 2006. *Long-term safety for KBS-3 repositories at forsmark and laxemar-a first evaluation: Main report of the SR-Can project*. SKB.

[2] Abkowitz, Mark. 2010. Nuclear waste assessment system for technical evaluation - NUWASTE.

[3] Ahn, J. 1988. Mass transfer and transport of radionuclides in fractured porous rock. Tech. Rep., California Univ., Berkeley, CA.

[4] Ahn, J. 2004. An environmental impact measure for nuclear fuel cycle evaluation. *Journal of Nuclear Science and Technology* 41(3):296 – 306.

[5] Ahn, J. 2007. Environmental impact of yucca mountain repository in the case of canister failure. *Nuclear technology* 157(1):87 – 105.

[6] Ahn, J., D. Kawasaki, and P. L Chambre. 2002. Relationship among performance of geologic repositories, canister-array configuration, and radionuclide mass in waste. *Nuclear Technology* 140(1).

[7] Anderson, M. P, and W. W Woessner. 1992. *Applied groundwater modeling: simulation of flow and advective transport*.

[8] ANDRA. 2005. Argile: Evaluation de la faisabilite du stockage geologique en formation argileuse. Tech. Rep., Paris.

[9] ANDRA. 2005. Granite: Evaluation de la faisabilite du stockage geologique en formation granite. Tech. Rep., Paris.

[10] Bateman, H. 1908. 1910. the solution of a system of differential equations occurring in the theory of radio-active transformations. In *Proc. cambridge philosophical soc*, vol. 15, 423.

[11] Berkowitz, Brian, Jacob Bear, and Carol Braester. 1988. Continuum models for contaminant transport in fractured porous formations. *Water Resources Research* 24(8):PP. 1225 – 1236.

[12] Blink, J. A., T. A. Buscheck, W. G. Halsey, and T. Wolery. 2010. Disposal systems evaluations and tool Development-Engineered barrier system evaluation. Tech. Rep., Lawrence Livermore National Laboratory (LLNL), Livermore, CA.

[13] Boucher, Lionel. 2010. International comparison for transition scenario codes involving COSI, DESAE, EVOLCODE, FAMILY and VISION. CEA France.

[14] Bouvier, E., J. Ahn, and T. Ikegami. 2007. *Comparison of environmental impacts for PWR-UOsub 2, PWR-MOX and FBR*. LaGrange Park, IL: American Nuclear Society.

[15] Bracke, G., T. Beuth, K. Fischer-Appelt, J. Larue, and M. Navarro. 2008. Safety functions derived from geochemistry for safety analysis of final disposal of high-level radioactive waste. *Uranium, Mining and Hydrogeology* 771—778.

[16] Brewitz, Wernt, and Ulrich Noseck. 2002. Long-term performance of spent fuel in geological repositories. *Comptes Rendus Physique* 3(7-8):879–889.

[17] Carter, Joe. 2011. Disposal of recycling facility waste in a generic salt repository. Predecisional SRNL-RP-2011-00149.

[18] Clayton, D, G Freeze, E Hardin, W.M. Nutt, J Birkholzer, H.H. Liu, and S Chu. 2011. Generic disposal system modeling - fiscal year 2011 progress report. Tech. Rep. FCRD-USED-2011-000184, U.S. Department of Energy, Sandia, NM.

[19] Diodato, D. M., and T. Center. 1994. A compendium of fracture flow modelsâĂŞ1994. *Work sponsored by US Department of Defense, United States Army, Europe, Combat Maneuver Training Center, Hohenfels, Germany*.

[20] DOE. 2002. Yucca mountain science and engineering report. *US Department of Energy, Las Vegas, NV DOE/RW-0539-1, Rev* 1.

[21] DOE. 2008. The report to the president and the congress by the secretary of energy on the need for a second repository | department of energy. Tech. Rep. DOE/RW-0595.

[22] DOE. 2010. Nuclear energy research & development roadmap: Report to congress.

[23] El-Wakil, Mohamed Mohamed. 1981. *Nuclear heat transport*. American Nuclear Society.

[24] Happel, J., and H. Brenner. 1991. *Low reynolds number hydrodynamics: with special applications to particulate media*, vol. 1. Kluwer Academic Print on Demand.

[25] Hardin, E, J Blink, Harris Greenberg, Mark Sutton, Massimo Fratoni, Joe Carter, Mark Dupont, and Rob Howard. 2011. Generic repository design concepts and thermal analysis - 8.8.2011 draft. Tech. Rep. FCRD-USED-2011-000143, Department of Energy Office of Used Fuel Disposition, Sandia.

[26] Hedin, A. 2002. Integrated analytic radionuclide transport model for a spent nuclear fuel repository in saturated fractured rock. *Nuclear Technology* 138(2).

[27] Ho, C. K. 2000. Dual porosity vs. dual permeability models of matrix diffusion in fractured rock. Tech. Rep., Sandia National Laboratories, Albuquerque, NM (US); Sandia National Laboratories, Livermore, CA (US).

[28] Huff, Kathryn, Paul P. H. Wilson, and Matthew Gidden. 2010. Cyclus: A nuclear fuel cycle code from the university of wisconsin madison. http://code.google.com/p/cyclus/.

[29] Incropera, Frank. 2006. *Fundamentals of heat and mass transfer*. 6th ed. Hoboken N.J.: Wiley.

[30] Johnson, L., C. Ferry, C. Poinssot, and P. Lovera. 2005. Spent fuel radionuclide source-term model for assessing spent fuel performance in geological disposal. part i: Assessment of the instant release fraction. *Journal of Nuclear Materials* 346(1): 56âĂŞ65.

[31] Johnson, L., B. Kunz, C. Frei, Nagra, and Projekt Opalinuston. 2002. *Project opalinus clay: Safety report: Demonstration of disposal feasibility for spent fuel, vitrified high-level waste and long-lived intermediate-level waste (Entsorgungsnachweis)*. Nagra, National cooperative for the Disposal of Radioactive Waste.

[32] Johnson, L. H., and Nagra. 2002. *Calculations of the temperature evolution of a repository for spent fuel, vitrified high-level waste and intermediate level waste in opalinus clay*. Nagra.

[33] Kawasaki, D., J. Ahn, P. L Chambre, and W. G Halsey. 2004. Congruent release of long-lived radionuclides from multiple canister arrays. *Nuclear technology* 148(2): 181 – 193.

[34] Kessler, J. H, J. Kemeny, F. King, A. M Ross, and B. Ross. 2006. Room at the mountain: Estimated maximum amounts of commercial spent nuclear fuel capable of disposal in a yucca mountain repository. Tech. Rep., The ASME Foundation, Inc., New York.

[35] Kossik, R. F., I. Miller, and S. Knopf. 2006. *GoldSim graphical simulation environment user's guide*. Version.

[36] von Lensa, W., R. Nabbi, and M. Rossbach. 2008. *RED-IMPACT impact of partitioning, transmutation and waste reduction technologies on the final nuclear waste disposal*. Forschungszentrum Julich.

[37] Li, J. 2006. A methodology to evaluate nuclear waste transmutation/fuel cycle systems.

[38] Li, J., M. Nicholson, W. C Proctor, M. S Yim, and D. McNelis. 2007. Examining repository loading options to expand yucca mountain repository capacity. In *Proceedings of GLOBAL*, 519 — 525.

[39] Li, J., M. S Yim, and D. McNelis. 2008. The specific temperature increase method for repository thermal analysis. *Transactions of the American Nuclear Society* 99:216 — 218.

[40] Li, J. 2007. A methodology to evaluate nuclear waste transmutation / fuel cycle systems. Ph.D. thesis, North Carolina State University.

[41] Miron, A., J. Valentine, J. Christenson, M. Hawwari, S. Bhatt, M. L Dunzik-Gougar, and M. Lineberry. 2009. Identification and analysis of critical gaps in nuclear fuel cycle codes required by the SINEMA program. Tech. Rep., University of Cincinnati.

[42] Nicholson, M. A. 2007. *Thermal loading and uncertainty analysis of high level waste in yucca mountain*. North Carolina State University.

[43] Nutt, Mark. 2011. Personal communication.

[44] Nutt, W. M. 2010. Used fuel disposition research and development roadmap-FY10 status. Tech. Rep., Argonne National Laboratory (ANL).

[45] OECD-NEA. 2006. *Advanced nuclear fuel cycles and radioactive waste management*. OECD Publishing.

[46] ONDRAF-NIRAS. 2001. Technical overview of the SAFIR 2 report. Tech. Rep. Nirond 2001-05 E, Belgium.

[47] Papoulis, A., and S. U. Pillai. 2002. *Probability, random variables, and stochastic processes*. 4th ed. Series in Electrical and Computer Engineering, McGraw-Hill.

[48] Piet, S., T. Bjornard, B. Dixon, D. Gombert, C. Laws, and G. Matthern. 2007. Which elements should be recycled for a comprehensive fuel cycle? *Proc. Global 2007* 1595.

[49] Posiva. 2010. *Interim summary report of the safety case 2009*. POSIVA.

[50] Pusch, R., L. Borgesson, and M. Erlstrom. 1987. *Alteration of isolating properties of dense smectite clay in repository environment as examplified by seven pre-quarternary clays*. Swedish Nuclear Fuel and Waste Management Co.

[51] Radel, T. E. 2007. *Repository modeling for fuel cycle scenario analysis*. University of Wisconsin – Madison.

[52] Radel, T. E, P. P.H Wilson, R. M. Grady, and T. H. Bauer. 2007. *Effect of separation efficiency on repository loading values in fuel cycle scenario analysis codes*. LaGrange Park, IL: American Nuclear Society.

[53] Savoye, S., F. Goutelard, C. Beaucaire, Y. Charles, A. Fayette, M. Herbette, Y. Larabi, and D. Coelho. 2011. Effect of temperature on the containment properties of argillaceous rocks: The case study of Callovo-Oxfordian claystones. *Journal of Contaminant Hydrology*.

[54] Schneider, E., M. Knebel, and W. Schwenk-Ferrero. 2004. NFCSim scenario studies of german and european reactor fleets. Tech. Rep., LA-UR-04-4911, Los Alamos National Laboratory.

[55] Schwartz, F. W., and H. Zhang. 2004. Fundamentals of ground water. *Environmental Geology* 45:1037âĂŞ1038.

[56] Soelberg, N., S. Priebe, D. Gombert, and T. Bauer. 2009. Heat management strategy trade study. *Advanced Fuel Cycle Initiative, AFCI-SYSA-PMO-MI-DV-2009-000169, INL/EXT-09-16708*.

[57] Swift, Peter, and Mark Nutt. 2010. Applying insights from repository safety assessments. San Francisco, CA.

[58] Turner, Stephen L. 2010. Discrete modeling: OCRWM total system model DRAFT. DOE FCRD-XXXX-2009-XXXXXX.

[59] Uleberg, K., and J. Kleppe. 1996. Dual porosity, dual permeability formulation for fractured reservoir simulation. In *Norwegian university of science and technology, trondheim RUTH seminar, stavanger*.

[60] Van Den Durpel, L., D. C Wade, and A. Yacout. 2006. DANESS: a system dynamics code for the holistic assessment of nuclear energy system strategies. *Proceedings of the 2006 System Dynamics Conference*.

[61] Williams, N. H. 2001. Total system performance AssessmentâĂŞAnalyses for disposal of commercial and DOE waste inventories at yucca MountainâĂŞInput to final environmental impact statement and site suitability evaluation REV 00 ICN 02. Tech. Rep.

[62] Wilson, P. P.H. 2011. Comparing nuclear fuel cycle options. *A report for the Reactor & Fuel Cycle Technology Subcommittee of the Blue Ribbon Commission on America's Nuclear Future*.

[63] Yacout, A. 2011. DANESS. www.anl.gov/techtransfer/Software_Shop/Daness/DANESS.html.

[64] Yacout, A. M., J. J. Jacobson, G. E. Matthern, S. J. Piet, D. E. Shropshire, and C. Laws. 2006. VISION – verifiable fuel cycle simulation of nuclear fuel cycle dynamics. In *Waste management symposium*.