AN INTEGRATED USED FUEL DISPOSITION AND GENERIC REPOSITORY MODEL

by

Kathryn D. Huff

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It is customary for authors of academic books to include in their prefaces statements such as this: "I am indebted to ... for their invaluable help; however, any errors which remain are my sole responsibility." Occasionally an author will go further. Rather than say that if there are any mistakes then he is responsible for them, he will say that there will inevitably be some mistakes and he is responsible for them....

Although the shouldering of all responsibility is usually a social ritual, the admission that errors exist is not — it is often a sincere avowal of belief. But this appears to present a living and everyday example of a situation which philosophers have commonly dismissed as absurd; that it is sometimes rational to hold logically incompatible beliefs.

— David C. Makinson (1965)

Above is the famous "preface paradox," a placeholder, **Do Not Believe**.

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ANDRA Agence Nationale pour la gestion des Déchets RAdioactifs, the French National Agency for Radioactive Waste Management. 52–54, 62

ANL Argonne National Laboratory. 27

CAFCA Code for Advanced Fuel Cycles Assessment. 22

COSI Commelini-Sicard. 21

CUBIT CUBIT Geometry and Mesh Generation Toolkit. 29

DANESS Dynamic Analysis of Nuclear Energy System Strategies. 21

DOE Department of Energy. vii, ix

EBS Engineered Barrier System. 27

EDZ Excavation Disturbed Zone. 27

FCT Fuel Cycle Technology. 12

FEHM Finite Element Heat and Mass Transfer. 29

FEPs Features, Events, and Processes. 26

GDSE Generic Disposal System Environment. 26, 27, 89

LANL Los Alamos National Laboratory. 28

LLNL Lawrence Livermore National Laboratory. 64

NAGRA National Cooperative for the Disposal of Radioactive Waste. 54

NFCSim Nuclear Fuel Cycle Simulator. 22

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OCRWM Office of Civillian Radioactive Waste Management. 23

PEI Peak Environmental Impact. 11

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UW University of Wisconsin. 69, 76

VISION the Verifiable Fuel Cycle Simulation Model. 20, 21

YMR YMR. 6, 10, 53

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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 Systems Analysis (SA) Campaign goals. Repository metrics such as necessary repository footprint and peak annual dose are affected by heat and nuclide 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 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 fuel cycle simulation tools such as the Cyclus tool developed at the University of Wisconsin - Madison.

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 Systems Analysis (SA) Campaign goals. Repository metrics such as necessary repository footprint and peak annual dose are affected by heat and nuclide 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 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 fuel cycle simulation tools such as the Cyclus tool developed at the University of Wisconsin - Madison.

1 INTRODUCTION

The scope of this work includes implementation of a software library of medium fidelity models to comprehensively represent the long-term disposal system performance of different disposal system concepts in various geologic media for deployment in a modular systems analysis platform. This work will model repository behavior as a function of arbitrary spent fuel composition by modularly incorporating dominant physics disposal system models into a computational fuel cycle analysis platform.

1.1 Motivation

The development of sustainable nuclear fuel cycles is a key challenge as the use of nuclear power expands 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 heavily dependent on upstream fuel cycle decisions, a relevant analysis of potential geological disposal and engineered barrier solutions therefore 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. Specifically, such models

will support efforts underway in focusing domestic research and development priorities as well as computational tools under development which quantify these metrics and understand the merits of different fuel cycle alternatives.

System level fuel cycle simulation tools must facilitate efficient simulation of a wide range of fuel cycle alternatives as well as sensitivity and uncertainty analyses. Efficiency is achieved with models at a level of detail which successfully captures significant aspects of the underlying physics while acheiving 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 are 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 geology, tunnel design, and appropriate loading strategies and schedule are all independent variables up for debate. That said, some 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 isotpic 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 [18].

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 [18].

A Once-Through Cycle represents the continuation of the business as usual case in the United States which neglects reprocessing and presents the 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 indicate that such a cycle will generate a volume of spent fuel that will necessitate the siting of two or more federal geological repositories to accomodate spent fuel [25].

A Full Recycle option, on the other hand, requires the research, development, and deployment of partititioning, 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 Gen-IV reactor technologies with 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 and waste treatment before ultimate disposal in a repository. Thus, a repository under the Full Recycle scenario must adaptively support highly variable waste stream composition, 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 volitilization 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 [18] .

Clearly, the myriad waste streams resulting from potential fuel cycles present an array of corresponding waste disposition, packaging, and engineered barrier system options. A

comprehensive analysis of the disposal system, dominant physics models must therefore be developed for 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 nuclide transport phenomena through, for example, vitrified glass as well as ceramic waste forms with with various loadings for arbitrary isotopic compositions is therefore required.

Future Waste Disposal System Options

In addition to reconsideration of the domestic fuel cycle policy, the uncertain future of the YMR (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 [31].

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 concrete in other lithologies.

The physical, hydrogeologic, and geochemical mechanisms which dictate nuclide and heat transport vary between the geological and engineered containment systems in the domestic option space. Therefore, in support of the system level simulation effort, models must be developed which capture the salient physics of these geological options and quantify associated disposal metrics and benefits. Furthermore, modular linkage between

subcomponent process modules and the repository envrionmental model must acheive a cohesively integrated disposal system model.

Thermal Modeling Needs

A thermal modeling capability must be included in this repository model in order to arrive at loading strategies which comply with regulatory limits in the engineered barrier system and the geological medium as well as in order to inform material and hydrogeologic phenomena which are thermally coupled.

Heat load limits within a used nuclear fuel disposal system are waste form, package, and geology dependent. Heat generation from the waste form and transport through the engineered barrier system and host environment constrains fuel loading in waste forms and packages as well as placing requirements on the size, design, and loading strategy in a potential geological repository.

Heat load limits of various waste forms have their technical basis in the temperature dependence of isolation integrity of the waste form. The waste form dissolution behavior as a function of waste form decay heat constrains loading density within the waste form. Plutonium, Americium, and their decay daughters dominate decay heat contribution within used nuclear fuels. Other contributing nuclides include Cesium, Strontium, and Curium [32].

Heat load limits of various engineered barrier systems similarly have a technical basis in the temperature dependent dissolution rate of the materials from whence they are constructed.

Heat load limits of the geologic environment on the other hand are usually not based

on the mechanical integrity of the rock. Rather, the isolating characteristics of a geological environment are most sensitive to minerologic, hydrologic and geochemical phenomena, so heat load contstraints are typically chosen to control hydrologic and geochemical response to thermal loading. In the United States, current regulations stipulate thermal limits in order to passively steward the repository's hydrologic and geochemical integrity against radionuclide release for the upcoming 10,000 years.

The two heat load constraints which primarily determined the heat-based 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 which this model will seek to capture for various geologies.

The first Yucca Mountain heat load constraint intended to prevent repository flooding and subsequent contaminated water flow through the repository. It requires that the minimum temperature in the granite tuff between drifts be no more than the boiling temperature of water which, at the altitude in question, is $96°C$. For a repository with homogenous waste composition in parallel drifts, this constraint is effectively a limit on the temperature halfway between adjacent drifts, where the temperature would be at a minimum.

The second constraint intended to prevent high rock temperatures that could induce fractures and would increase leach rates. 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.

Analgous constraints for a broader set of possible geological environments will depend on heat transport parameters of the matrix, hydrogeologic state, and 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 for reasons of complicance with 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 package dissolution rates, diffusive and advective 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 however, since time evolution of repository heat is such that thermal coupling can typically be neglected for long time scales [8].

Radiotoxicity and Source Term Modeling Needs

Domestically, the Nuclear Regulatory Commission 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 nuclide transport through the geological environment in order to calculate repository capacity and other benefit metrics.

The exposure limit set by the NRC is based on a 'reasonably exposed individual.' That is to say, 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 legistlative regulations limit total dose from the repository to 15 mrem/yr, and limit dose from drinking water to 4 mrem/yr. 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 leakages come in contact with water and travel through the rock 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. 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. 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 degredation, water flow, and other parameters during the long repository evolution time scale. However, source term remains a useful metric for the comparison of alternative separations and fuel cycle scenarios.

A generalized metric of probablistic risk is fairly difficult to arrive at. For example, the Peak Environmental Impact (PEI) metric from Berkeley (ref. [12]) 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 exposed individual radiotoxicity constraints 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 Fuel Cycle Technology (FCT) Used Fuel Disposition (UFD), the Separations and Waste Forms (SWF), and Systems Analysis (SA) 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 SA 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 upon 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. It will then incorporate dominant physics process models into the Cyclus computational fuel cycle analysis

1.2 Methodology

In this work, concise dominant physics models suitable for system level fuel cycle codes will be developed from 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.

Categorization and characterization of phyisical mechanisms by which nuclide and thermal transport take place within the materials and media under consideration will first be undertaken. In this way, the domain of applicability for which subprocesses may be generalized will be assessed. In so doing, a preliminary set of combinations of fuel cycles, waste forms, repository designs, and geologies can be chosen which covers a foundational subspace of the parametric domain.

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 hydrogeology and thermal physics which dominate nuclide transport and heat response in candidate geologies as a function of nuclide release and heat generation over long time scales from waste packages. D ominant

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 geology 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 hydrogeologic models and analytic regression of rich code results as well as existing empirical geologic data.

For example, analytic models and semi-empirical models are available (i.e. specific temperature integrals (ref. [27]) or specific temperature change (ref. [35])) which approximate thermal response from heat generation in waste packages as linear along repository drifts. This analysis arrives at a thermal evolution over time at any location in the rock by superpositioning and integration. Subsequently, this result can be converted easily into conventional line loading and areal power density metrics. Such analytic models will first be assessed to determine likely parameters upon which thermal response will rely (e.g. tunnel spacing, nuclide inventories, etc.).

Thereafter, a regression analysis concerning those parameters will be undertaken with available detailed models (e.g. 2D and 3D finite differencing, finite element, and full 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

appropriate 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 nuclide transport models. The abstraction process in the development of waste form, package, and engineered barrier system models will be analgous 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.

For instance, in the case of nuclide release from waste packages, analytic models of nuclide release (e.g. congruent or solubility limited) will first be assessed to determine likely parameters upon which nuclide release will rely (e.g. nuclide concentration, water flow rates, etc.) [24]. Again, regression analysis concerning those parameters will be undertaken with available detailed models to further characterize the parametric dependence of nuclide release from specific waste packages. Finally, the nuclide release model so developed will depend on empirical data (e.g. the waste form dissolution rate). Determination of appropriate values to make available within the dominant physics model will rely on existing empirical data concerning the specific waste form materials being modeled (i.e. long time scale extrapolations of known glass failure rates).

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 nuclide release and transport as well as package degradation will necessarily be analyzed to determine the magnitude of coupling effects in the system.

1.3 Outline

The following chapter will present a literature review which organizes and reports upon previous relevant work. It will focus upon current analytical and computational modeling of nuclide 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 and the state of the art of repository modeling and integration within current systems analysis tools.

Chapter 3 will detail the computational paradigm of the Cyclus systems analysis platform as well as the components within the repository system. Models representing waste form, waste package, buffer, backfill, and engineered barier 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 equivalent models with varying levels of detail.

Chapter 4 will categorize and characterize detailed computational models of nuclide and heat transport available for regression analysis. Specificially, detailed codes in current use are categorized according to the physics which they model, the disposal system components with which they are concerned, and the level of detail and computational methodology with which they capture physical phenomena.

Chapter 5 will detail the analytical and regression analysis undertaken and forthcoming to acheive 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, hydrogeologic, 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.

Chapter 6 will summarize the conclusions reached concerning the appropriate analytical and detailed models to utilize in the process of abstraction for nuclide and heat transport through various components of the disposal system. Categorization of models and determination of the coverage within the option space domain will also be summarized. Finally, remaining future work and expected contributions to the field will be summarized.

2 LITERATURE REVIEW

The following literature review addresses five 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 review of analytical models of nuclide transport follows, after which follows a review of analytical models of heat transport. An overview of current detailed computational models, available data and algorithms characterizing nuclide transport follows, 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 hydrogeological 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, these analyses fail to address the impact of those waste streams on the performance of the geologic disposal system [40]. To fully inform the decision making process, metrics that depend on the performance of the geologic disposal system will be necessary.

A model for repository capacity was developed for the the Verifiable Fuel Cycle Simulation Model (VISION) fuel cycle simulator and recent efforts on the 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 [42] [34] [2].

NUWASTE

Nuclear Waste Assessment System for Technical Evaluation (NUWASTE) is a Nuclear Waste Technical Review Board code that determines many metrics about the fuel cycle according to various parameters [2]. This code 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 waste package, waste form, source term, and dose calculations.

VISION

VISION's repository model conducts decay calculations and tracks upwards of 80 isotopes of interest in the nuclear fuel cycle [42]. While it calculates some basic information about waste package heat production and heat based repository capacity, discrete waste packages are not modeled and emplaced spent fuel composition is assumed to be spatially homogeneous [34] [11].

DANESS

Dynamic Analysis of Nuclear Energy System Strategies (DANESS) is developed at Argonne National Laboratory and discretely models reactors within regional reactor parks. 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 and requires 15 minutes for a 100 year simulation on a modern PC. Input and output are in Microsoft Excel format and DANESS relies on the proprietary IThink simulation platform. The code therefore has a secure license sensitive to export control and requiring explicit developer approval [41, 38].

COSI

Commelini-Sicard (COSI) is a code from the CEA of France implemented in the Java programming language. It is capable of performing a large range of full fuel cycle scenarios. COSI6 is capable of making assessments of repository capacity as well as radiotoxicity and decay heat calculations of waste packages [11]. Nuclide transport through the repository post-emplacement is, however, not calculated and the distribution liscence 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 [36].

CAFCA

Code for Advanced Fuel Cycles Assessment (CAFCA) is a fuel cycle code from MIT. While CAFCA is capable of tracking processed fuel assemblies and isotopics, it does not calculate capacity metrics or conduct detailed nuclide or heat transport.

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 nuclide 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 $[W]$.

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 nuclide and heat transport are modeled in great detail . This level of detail results in a dramatically extended run time. The TSM model can only be run by its development team and runs a typical simulation, processing 70,000 MTHM in 12-15 hours [**?**].

The TSM framework is based on the proprietary 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 managment model which informs waste package emplacment.

Repository Focused Fuel Cycle Analyses

Focused fuel cycle sensitivity analyses emphasizing used fuel disposition and waste management in the Yucca Mountain Repository (YMR) have been conducted by Li, Piet, Wilson, and Ahn. With a focus on YMR capacity benefit, repository performance metrics of interest for these analyses were heat, source term, and more global envrionmental impact metrics. Sensitivity analyses for other geologies were conducted concerning repository concepts relevant to other nations as well. See Table 2.1.

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 2.1.

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 2.1: International repository concepts evaluated in the RED Impact Assessment.[26]

Fuel Cycle Technology, UFD Codes Under Development

The UFD campaign is currently conducting an effort to produce Generic Disposal System Environment (GDSE) models for various geological environments. Teams from Argonne Lawrence Berkeley, Los Alamos, and Sandia National Laboratories are developing models of generic clay, granite, and salt disposal environments. Sandia is simultaneously constructing a borehole disposal system model. Each generic disposal system model will perform detailed calculations of nuclide transport within its respective lithology. A longer term goal of the project includes an overarching generic model which incorporates the various geologically distinct submodels in order to provide a fully generic repository model.

The nuclide transport calculations for the geologically distinct models are performed within the GoldSim simulation platform. GoldSim is a commercial off the shelf simulation environment which ships with a contaminant transport system for modeling of release and transport of contaminants as well as an optional radionuclide transport module for decay calculations. Each models a single repeatable waste package cell to arrive a a full repository model. 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.

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

Thermal modeling for the GDSE models are conducted independently with associated codes capable of modeling thermal evolution for all geologies. For example, one thermal model is being created using the SINDA\G heat transport solver and another is under development which utilizes a combination of mathCAD and Excel.

Clay/Shale GDSE Model

The Clay GDSE model 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 GDSE models a single waste form, waste package, Engineered Barrier System (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 nuclide release pathways are considered. One is the nominal, undisturbed case, while the other is a fast pathway simulating a disturbed case [14].

Salt GDSE Model

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 nuclide 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. Nuclide transport into that interface is modeled as diffusive, advective, and solubility limited.

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

Two nuclide release pathways are considered. One is the nominal, undisturbed case, whicl the other is a fast pathway simulating a disturbed case [14].

Granite GDSE Model

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

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 which includes advection, diffusion and sorption. Specifically, the Finite Element Heat and Mass Transfer (FEHM) code was coupled into GoldSim to represent the far field.

Borehole GDSE Model

The 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 [14].

Models of Source Term for Various Geologies

Source (Who)	Nation (Where)	Geology (What)	Methodology (How)
Enresa [26]	Spain	Granite	GoldSim ^{129}I primary contributor
SCK·CEN [26]	Belgium	Clay	FEP ^{129}I primary contributor
GRS [26]	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) [27]	USA	Yucca Tuff	TSPA codes EBSREL and EBSFAIL
WIPP	USA	Salt	?
NAGRA [22, 23]	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 hydrologic transport code

Table 2.2: 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.

2.2 Analytical Models of Nuclide Transport

A comprehensive model of radiotoxic source term must address nuclide transport through the full release pathway including waste packages, engineered barrier systems, and geologic media. A model of transport through the waste package must incorporate waste package failure rate, nuclide release rate via waste form dissolution, and advective transfer rate into the engineered barrier system.

Waste package failure rate depends on near field environmental factors such as pH and humidity as well as decay heat and radiative damage anticipated from the contained waste.

In turn, the nuclide release rate from the waste package depends on the character of the waste form matrix, treatment of water flow, nuclide solubility and the elemental diffusion constant. Similarly, advective transfer through the engineered barrier system and into the geological medium also depends on water flow, nuclide solubility, and nuclide diffusion, but must be employed in the context of the hydrogeology of the rock.

Waste package failure rate varies 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 2.4, analytic models incorporate their own hydrogeologic approximations of canister degredation or make simpler assumptions of immediate waste canister failure in order to focus on dissolution and transfer.

Waste package release rate is the rate of mass transfer of a nuclide from its waste form into the saturation water. The mode of water flowthrough heavily effects nuclide 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 hydrogeologic activity.

Nuclide transfer rate through the lithology is dependent upon diffusion as well as advection. The diffusion coefficient varies per nuclide and is heavily dependent upon the concentration of that nuclide in the flowthrough water. The way in which diffusion affects nuclide concentration is described by Fick's Second Law,

$$\frac{\partial C_i}{\partial t} = D_i \nabla^2 C_i. \tag{2.1}$$

Source term dependence on concentration has a significant effect on potential repository capacity. Sensitivity to concentration complicates the viability of alternate loading schemes as well as waste separation scenarios. Specifically, Fick's Second Law becomes

$$\frac{\partial C_i}{\partial t} = \nabla \cdot (D_i \nabla C_i). \tag{2.2}$$

Radionuclide concentration has been shown to be proportional to the waste package loading configuration for the Yucca Mountain case [6, 24].

The most important geochemical processes to source term that occur within the waste, waste matrix, and near field as well as the host rock are dissolution, precipitation, and sorption [13].

Dissolution

Dissolution is the "most important prerequisite" for contribution of a radionuclide to source term[13]. That is, the initial dissolution of a radionuclide from its waste from is a breach of the ultimate barrier, or final line of defense. Dissolution rates depend strongly on pH, Eh, speciation of radionuclides (chemical oxidative state), and radiolysis of the dissolving fluid.

Precipitation

Precipitation is the reverse of dissolution and occurs when a soubility limit is reached. Interestingly the chemical equillibrium of dissolution and precipitation is rate dependent and is highly dependent on thermodynamics. Predictions are not reliable in may cases.

Sorption

Sorption is the interaction of a dissolved species with surfaces that removes that species from the dissolving medium models.

Sorption into the rock matrix is a method by which contaminants (and water?) are removed from a fracture during flow through that fracture. However, this is a reversible process , which means the contaminant might be returned to the fracture from the matrix with the same ”distribution coefficient“ with which they entered the rock matrix [3] .

Colloidal Mobility

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 exist.

Waste Form Release Models

Hedin Model ([19])

In a saturated fractured rock matrix representative of the KBS-3 granitic Swedish repository concept, copper canister waste packages contain a 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 which takes place within the waste package void. Nuclides are released congruently until the waste form is completely degraded. [19]

Ahn Models ([4, 5])

Waste canisters are modelled as compartments of waste form surrounded by a buffer layer which 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. Nuclides with higher solubilities are preferentially dissolved and treated with a 'congruent release' model discussed below. Nuclides 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.

Congruent Release Model

In the Ahn models, nuclides with a high solubility coefficient are modeled with the congruent release model. Nuclides 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.

Solubility Limited Release Model

In the Ahn models, nuclides with lower solubility coefficients are modeled with the solubility limited release model. Solubility values are assumed from TSPA for this model, and a

solubility of $5 \times 1^{-2}[mol/m^3]$ are taken to be 'low.' Elements in this 'low' category include the toxic actinides such as Zr, Nb, Sn, Th, and Ra. This model suggests that a dominant mode of dissolution of the nuclide into the flowthrough water is dominated instead by the diffusion coefficient, which is largely dependent upon the concentration gradient between the waste matrix and the water. The mass balance driving nuclide release takes the form:

$$\dot{m}_i = 8\epsilon D_e S_i L \sqrt{\frac{U r_0}{\pi D_e}} \tag{2.3}$$

where ϵ, U, r_0, and L are the geometric and hydrogeologic factors porosity, water velocity, waste package radius, and waste package length, repsectively. D_e is the diffusion coefficient (m^2/yr) of the element *e* and S_i is the isotope's solubility (kg/m^3).

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

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

where the mass m_{1i} $[g]$ of a nuclide, i relased into the waste package void volume v_1 in $[m^3]$, at a time t, is limited by constant the maximum concentration, C_{sol} in $[g/m^3]$ at which that nuclide is soluble [19].

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 2.3: The above represent current methods by which waste packeage failure rates are modeled.

Waste Package Failure Models

Instantaneous

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[19].

Other models also use an instantaneous waste package failure mode for all waste packages simultaneously, assuming that either at the beginning of the simulation or at the onset of the simulation. The mathematical representation of this probability density function is clearly just the delta function, with n_F being the number of failed waste packages, N being the total number of waste packages, and t_F being the time to failure,

$$n_F(t) = N\delta(t - t_F). \tag{2.4}$$

Rate Based

When enough data exists, waste package failure 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 hydrologic and thermal conditions. Specificially, corrosion rates for the same material are very different under dry oxidising conditions and wet reducing conditions.

An expression of the number of failed waste packages per year is a simple functional relationship

$$n_F = Nf(t, T, \cdots). \tag{2.5}$$

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 30,000 years, a gaussian distribution around that number would provide a probabilistic number of waste package failures per time step

$$n_F = Nf(t). \tag{2.6}$$

The instantaneous case is a special case of the probabilistic situation. Specfically, it is the Dirac delta function mentioned in equation (2.4).

A particularly attractive probability distribution for use in the case of failed engineered barriers is the Weibull distribution.

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Nuclide Transport Through Secondary Engineered Barriers

When the waste package is breached, nuclides are transported through secondary engineered barriers which includes the buffer zone and tunnel walls. After transportation through the secondary EBS nuclides reach the geological matrix.

Barrier Dissolution and Failure

The same models of waste package failure (instantaneous, rate based, and probabilistic) can be applied to buffers.

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 is primarily advective. Cracking can be modeled explicitly or as a continuum model.

Hydrogeologic Transport Models

Clay, shale, granite, and salt can largely be characterized as permeable porous media. Solute transport in permeable porous media involves advection, hydraulic dispersion, and diffusion.

Advection is transport congruent with the water velocity, diffusion is the result of brownian motion accross concentration gradients, and hydraulic dispersion is transport resulting from anisotropies in the water velocity field.

The equation representing solute transport in a permeable medium of homogenous porosity can be written (as in Schwartz and Zhang [**?**])

$$\frac{\partial \omega C}{\partial t} = -\nabla \cdot (F_c + F_{dc} + F_d) + m \tag{2.7}$$

where

$$\begin{aligned}
\omega &= \text{solute accessible porosity } [\%] \\
C &= \text{ concentration } [kg \cdot m^{-3}] \\
F_c &= \text{ convetive flow } [kg \cdot m^{-2} \cdot s^{-1}] \\
&= qC \\
F_{dc} &= \text{ dispersive flow } [kg \cdot m^{-2} \cdot s^{-1}] \\
&= \alpha q \nabla C \\
F_d &= \text{ diffusive flow } [kg \cdot m^{-2} \cdot s^{-1}]
\end{aligned}$$

$$= D_e \nabla C$$

$$m = \text{ solute source } [kg \cdot m^{-2} \cdot s^{-1}].$$

In the expressions above,

$$q = \text{ Darcy velocity } [m \cdot s^{-1}]$$

$$\alpha = \text{ dispersivity } [m]$$

and

$$D_e = \text{ effective diffusion coefficient } [m^2 \cdot s^{-1}].$$

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,

$$Pe = \frac{qL}{\alpha q + D_e},$$
$$= \frac{\text{advective rate}}{\text{diffusive rate}}$$

where

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

For a high Pe number, advection is the dominant transport mode, while diffusive transport dominates for a low Pe number.

The analytical expression in equation (2.7) will be the foundation of simplification by regression analyses for the nuclide transport interface between components of the repository system model representing permeable porous media.

From Schwartz and Zhang Ch. 23

Fundamentally, flow through a control volume is bounded by the mass conservation equation:

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

which can be stated more precisely as

$$\nabla \left(nD\nabla C \right) - \nabla \left(nv \right) = \frac{\partial (nC)}{\partial t} \tag{2.8}$$

Adding a chemical reaction rate, r,

$$\nabla\left(nD\nabla C\right)-\nabla\left(nv\right)+r=\frac{\partial(nC)}{\partial t} \tag{2.9}$$

Adding sorption, by accounting for a change in mass storage

$$\nabla\left(nD\nabla C\right)-\nabla\left(nv\right)+r=\frac{\partial(nC)}{\partial t}+\frac{\partial(s\rho_b)}{\partial t} \tag{2.10}$$

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

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

equation (2.10) becomes

$$\nabla\left(nD\nabla C\right)-\nabla\left(nv\right)+r=R_f\frac{\partial(nC)}{\partial t} \tag{2.11}$$

where

$$R_f=\text{retardation factor} \tag{2.12}$$

$$=1+\frac{\rho_b K_d}{n} \tag{2.13}$$

$$\rho_b=\text{bulk density of the rock matrix} \tag{2.14}$$

and

$$K_d = \text{species distribution coefficient.} \tag{2.15}$$

To incorporate radioactive decay it is necessary to represent the reaction rate, r, as a function of λ and R_f such that equation (2.11) becomes

$$\nabla\left(nD\nabla C\right) - \nabla\left(nv\right) + nR_f\lambda C = R_f\frac{\partial(nC)}{\partial t}. \tag{2.16}$$

For uniform flow, the dispersion tensor, D, becomes

$$\begin{aligned} D_x &= D_L \\ &= \alpha_L v_x + \tau D_m \qquad (2.17) \\ D_y &= D_{TH} \\ &= \alpha_{TH} v_x + \tau D_m \qquad (2.18) \\ D_z &= D_{TV} \\ &= \alpha_{TV} v_x + \tau D_m \qquad (2.19) \end{aligned}$$

where

$$\alpha_L = \text{longitudinal dispersivity [m]}$$

$$\alpha_{TH} = \text{horizontal dispersivity [m]}$$

$$\alpha_{TV} = \text{vertical dispersivity [m]}$$

and

$$\tau = \text{tortuosity}. \tag{2.20}$$

The unidirectional dispersion tensor gives

$$D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} + v_x \frac{\partial C}{\partial x} - \lambda R_f C = R_f \frac{\partial (nC)}{\partial t} \tag{2.21}$$

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

$$D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} + -\lambda R_f C = R_f \frac{\partial (nC)}{\partial t} \tag{2.22}$$

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 bouncary of the representative volume.

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

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

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

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.

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

Continuum Models

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 very unfractured situations. This approximation is not suitable for ituations in which the fracture width or frequency varies greatly.

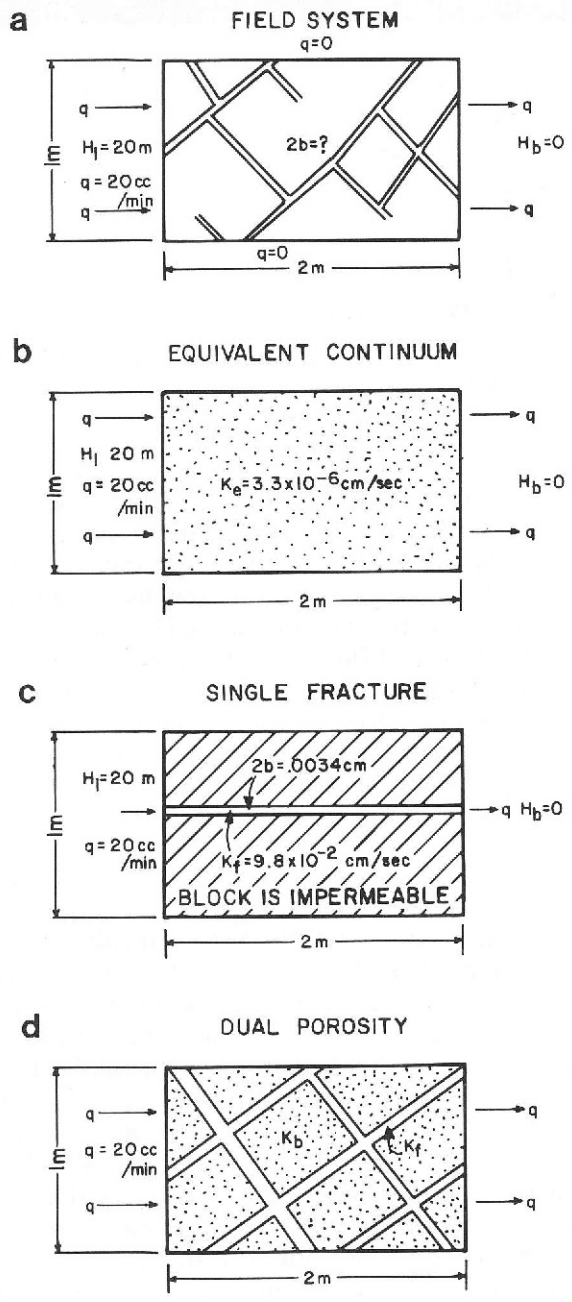

Fig. 12.6 Conceptual models of a fractured rock system (modified from Gale, 1982).
(a) A simplified fracture network of aperture $2b$ with groundwater flow from left to right.
(b) Equivalent porous medium model of (a).
(c) Discrete fracture model of (a).
(d) Dual porosity medium model of (a).

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

Equivalent Porous Medium (EPM) models assert that a uniformly fractured medium can be approximated as a fractureless matrix with an effective porosity high enough to account for real fracturation [10][7].

Dual Porosity Models make up one type. This model incorporates advective transport in simplistic, uniform fractures and diffisive sorption and desorption into the stagnant (no advective transfer) water contained in the pores of the rock matrix [37] [20].

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[37] [20].

Discrete Fracture Network Models Discrete fracture network models approximate that water and contaminants move only through the fracture network [7] [**?**].

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 [**?**]. For a fracture perpendicular to gravitational acceleration, g, the hydraulic conductivity, K, is described according to the cubic law as

$$K = \frac{\rho_w g b^2}{12\mu} \tag{2.23}$$

where

$$\rho_w = \text{water density},$$

$$\mu = \text{viscosity}.$$

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

$$Q = -Kbw\frac{\partial h}{\partial L}. \tag{2.24}$$

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, s, apart,

$$\begin{aligned} N &= \text{fracture frequency} \\ &= \frac{cos(\theta_f)}{s}. \end{aligned} \tag{2.25}$$

The fracture network permeability is then defined as,

$$k_f = \frac{b^3}{12N}. \tag{2.26}$$

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

$$k = \frac{k_m + \frac{A_f}{A_m} k_f}{1 + \frac{A_f}{A_m}}. \tag{2.27}$$

Geochemical Transport Models

Reducing Environments

¡++¿

Oxidizing Environments

¡++¿

2.3 Analytical Models of Heat Transport

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 equillibrium. The general form of the conduction equation can be expressed

$$\nabla^2 T + \frac{q'''}{k} = \frac{1}{\alpha}\frac{\partial T}{\partial t}, \tag{2.28}$$

which with no heat source becomes the transient Fourier equation,

$$\nabla^2 T = \frac{1}{\alpha}\frac{\partial T}{\partial t}, \tag{2.29}$$

or to the Laplace equation in steady state,

$$\nabla^2 T = 0. \tag{2.30}$$

Replacing the source gives the steady state Poisson equation,

$$\nabla^2 T + \frac{q'''}{k} = 0. \tag{2.31}$$

An areal heat flux, $q''[W \cdot m^{-2}]$ can be derived from an integration of Poisson's equation

(2.31) and expressed in terms of the thermal conductivity of the material, $k[W \cdot m^{-1} \cdot^{\circ} K^{-1}]$, and the temperature gradient $\nabla T[K \cdot m^{-1}]$ by the expression

$$q'' = -k\nabla T. \tag{2.32}$$

For the one dimensional case, equation 2.32 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,

$$\begin{aligned} q''_x &= -k_x \frac{dT}{dx} \\ &= -k_x \frac{(T_1 - T_2)}{x_1 - x_2}. \end{aligned}$$

A one dimensional heat flux rate can be found by integration over the surface area of the representative volume,

$$\dot{q} = -kA\frac{\Delta T}{\Delta x}.$$

Convection

Convective heat transfer occurs advectively in accordance with fluid movement. The form of Fourier's Law which describes convection is very similar to equation 2.32 for conduction,

though the convective heat transfer coefficient $h[Wm^{-2}K^{-1}]$ and the surface area of heat transfer $A[m^2]$ replace the conductivity coefficient. Convection is typically expressed as

$$q'' = -hA\nabla T \tag{2.33}$$

such that

$$q''_x = hA\frac{dT}{dx} \tag{2.34}$$

$$= -h_x A\frac{(T_1 - T_2)}{x_1 - x_2}. \tag{2.35}$$

Radiation

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

$$q'' = \sigma A_1 F_{1\to 2}(T_1^4 - T_2^4) \tag{2.36}$$

where

$$\sigma = 5.670373 \times 10^8 [W \cdot m^2 \cdot^\circ K^4]. \tag{2.37}$$

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 conductance is simply,

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

Lumped Parameter Model

The lumped heat capacitance model makes an analogy to electrical circuit by reducing a thermal system into discrete lumps. 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 quantitatively expressed by comparison of the internal thermal resistance to the external thermal resistance. The Biot number,

$$Bi = \frac{hA}{k} \tag{2.38}$$

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[21]. 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 $[W \cdot m^{-2} \cdot^{\circ} K \cdot s]$ through a circuit is simply given as the quotient of the temperature difference and the thermal resistance of the multiple lumps,

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

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,

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

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

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

For example, in the case of a simple conductive circuit between two bodies, i and j, the resistance of j can be described as

$$R_{cond} = 1/hA$$

such that

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

Under integration a time constant appears which describes the speed with which the body i changes temperature with respect to the maximum temperature change,

$$\begin{aligned} \int_{T_j=T_0}^{T_j(t)} \frac{dT_j(t)}{T_i - T_j} &= \frac{hA_j}{c_j \rho_j V_j} \int_0^t dt \\ -ln \frac{T_i - T_j(t)}{T_i - T_0} &= \frac{hA_j}{c_j \rho_j V_j} t \\ \frac{T_i - T_j(t)}{T_i - T_0} &= e^{-(hA_j / c_j \rho_j V_j) t} \end{aligned}$$

such that

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

where

$$\tau = \left(c_j \rho_j V_j / hA_j \right).$$

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, analgous to an electrical circuit. [17] This is the case for all resistances, R_i representing modes of heat transfer. Thus, one can say, in general

$$\tau_j = c_j \rho_j V_j R_j.$$

Impact of Repository Designs

Heat Limits in Various Waste Packages

Various waste package constraints exist which 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, confinement capabilities of bitumen waste packages are only known with confidence below $70°C$. Inside the "disposal cells" a maximum temperature of $30°C$ is adopted in the Agence Nationale pour la gestion des Déchets RAdioactifs, the French National Agency for Radioactive Waste Management (ANDRA) analysis. [8]

¡++¿

Heat Limits in Various Geologies

The repository concepts under consideration are so called 'closed' concepts. That is, closure of the repository happens very shortly after emplacement. Enclosed modes are appropriate for low permeability rock formations (clay/shale, granite, salt). Low permeability does not

permit oxygen entry, so these are reducing environments. Since heat is carried away less effectively once closure has occured, 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.

Clay/Shale

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. The alteration 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 is reduced after this alteration. The time integral of this phenomenon determines total bentonite alteration. While short bursts of heat might be allowable, because the bentonite will not alter immediately, the kinetic alteration into smectite clays is hastened by temperatures above approximately $100°C$[33]. Well understood behavior for agrillaceous clay and bentonite buffer backfill is conservatively assumed by the ANDRA assessment to occur 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 $125°C$. [22]

Granite

Granite repository concepts are limited by the bentonite buffer in a manner similar to that of clay. Well understood behavior for generic granite and bentonite buffer backfill is

conservatively assumed by the ANDRA assessment to occur under $90°C$, a limit that must be imposed at the waste package interface with the buffer material. Mechanical stresses and strains due to heating at this level were analyzed by ANDRA and shown to have a negligible effect of flow behavior. Similarly, thermo-hydraulic effects due to thermally induced fluid density changes are expected to be slight. [8] 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 $100°C$. [26]

Salt

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 nuclide transport modeling.

A model of temperature dependent salt coalescent behavior is in order. ¡++ ¡++»

The UFD salt repository concept was based on some experience trying to construct and maintain the horizontal borings at WIPP. The current geometry involves emplacement of crushed salt in an alcove over waste packages which are arranged at the corner of the alcove. Notably, crushed salt has low conductivity, which increases the sensitivity of rock salt temperature on emplaced package temperature.

The behavior of moisture in a salt repository under high heat is 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.

The German salt repository concept maintains a $180°C$ temperature limit salt. At temperatures above $220°C$ the salt formation may release brines capable of facilitating nuclide transport. [26][**?**]

Unsaturated Tuff

For comparision with the geologic media under consideration, it is important to note that two heat load constraints primarily determine the heat-based SNF capacity in the Yucca Mountain Repository design, which is located in unsaturated tuff. Thermal limits in that design are intended to passively steward the repository's integrity against radionuclide release for the upcoming 10,000 years.

The first constraint intends to prevent repository flooding and subsequent contaminated water flow through the repository. It requires that the minimum temperature in the granite tuff between drifts be no more than the boiling temperature of water which, at the altitude in question, is $96°C$. This is effectively a limit on the temperature halfway between adjacent drifts, where the temperature will be at a minimum.

The second constraint intends to prevent high rock temperatures that induce fractures and would increase leach rates. It states that no part of the rock reach a temperature above $200°C$, and is effectively a limit on the temperature at the drift wall, where the rock temperature is a maximum.

The 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. The "full inventory" Yucca Mountain design alternative gives a maximum repository capacity of 97,000 tonnes. In 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.[16]

Specific Temperature Change analysis by Radel, Wilson, et al. find a maximum thermal capcity of 1.09 tonnes/m for commercial SNF (at an ELF of $49GWd_{th}/m$)[35].

Elongation of cooling times has the potential to expand the capacity of the repository. 'Cooling time' refers to delaying complete loading of the repository. Longer cooling times allow high heat, short lived isotopes to decay to lower activity before they begin to heat the repository. Much of the benefit to repository capacity comes from the advantage that the cooling time allows a decrease in the space between emplacement drifts. Aged SNF has lower heat flux and so, the drift spacing can be decreased from 81 to 70 meters. A study by Man-Sung Yim and colleagues at North Carolina state found that for a representative commercial SNF composition a cooling time of 75 years allows for over 100 MTU SNF disposal without expanding the Yucca Mountain footprint[28].

Similarly, 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[30]. 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[39].

In addition to variable drift spacing, other modifications to repository layout have had

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

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 Upper Block line load design plan or a multi-level plan that repeats the footprint and line load design of the current plan[25].

Specific Temperature Integral

Line loading (t/m) and areal power density (W/km^2) are two common metrics for describing the fullness 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 situtation 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 repository drifts, 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[29] 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[34].

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. 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.

2.4 Detailed Computational Models of Nuclide Transport

Li Model[27]

As a function of time, water enters the Engineered Barrier System and corrodes the waste packages. These fail and from the failed waste packages nuclides are released according to advective transfer. Further transportation 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 nuclide 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 nuclide release from those failed waste packages. Mass balance governing the nuclide 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:

$$w_{ci}(t) = C_i(t)q_{out}(t). \tag{2.39}$$

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. characteristics and is independent of or weakly dependent on concentration. [27]

ANDRA Dossier 2005

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

Clay/Shale

More 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 nuclides of importance. These are chosen to be those with halflives over 1000 years and most toxicity or mobility. [8] The behavior of radionuclides in glassvitrification forms can be summarized by categorizing them into mobile, intermediate, and well retained elements.

Some specific codes used in the ANDRA clay assessment are listed in Table 2.5.

Detailed Nuclide Transport Models Used in the ANDRA analysis.

Models	Codes
Hydrogeology and particle tracking in continuous porous media	Connectflow (NAMMU component, 3D modelling, finite elements). Geoan (3D modelling, finite differences). Porflow (3D modelling, finite differences).
Hydrogeology and particle tracking in discrete fracture networks.	Connectflow (NAMMU component, 3D modelling, finite elements). FracMan (generation of discrete fracture networks) and MAFIC (hydraulic resolution of the networks, 3D, finite elements).
Transport in continuous porous media.	PROPER (COMP-23 component, modelling in segments of the engineered barrier, finite differences). Goldsim (volume modelling of engineered barriers). Porflow.
Transport in discrete fracture networks.	PROPER (FARF-31 component, 1D modelling 1D stream tube concept). PathPipe (conversion of networks of tubes for transport) and Goldsim (modelling in networks of 1D pipes).

Table 2.5: 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 was available. Vitrified waste package releases were either modeled with a simple model or a two phase phenomenological model.

Transportation through the backfill is modeled as diffusive, with high permeability.

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 nuclide transport and Prediver and Colonbo for waste package failure.

SKB Model

SKB used ConnectFlow to model Forsmark particle transport. It also used a model called MIKE SHE in conjunction with ConnectFlow in order to model "uses locally measured meteorological data to simulate transient water flow in the saturated (groundwater) and unsaturated zones, overland flow, and water losses due to evapotranspiration processes (interception, evaporation and transpiration)". CF contains an elaborate description of flow within the rock, whereas the MS model provides more detailed information on near-surface water flow paths and the associated discharge paths.

2.5 Detailed Computational Models of Heat Transport

LLNL MathCAD Model

This model, created at Lawrence Livermore National Laboratory (LLNL) for the UFD campaign, is written in a combination of MathCAD and Excel. The model consists of two parts. The first is a MathCAD solution of the transient homogeneous conduction equation

$$\nabla^2 T = frac1\alpha \frac{\partial T}{\partial t}. \tag{2.40}$$

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,

$$\nabla^2 T + \frac{q'''}{k} = 0. \tag{2.41}$$

which in turn calculates a resulting gradient through the geometry. 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.

Bauer SINDA\G Model

This model, created at Argonne National Lab by Ted Bauer uses a lumped capacitance solver, called SINDA.

The Bauer model is geometrically adjustable.

The SINDA lumped capacitance solver solves a thermal circuit, for which conducting nodes may be of four types corresponding to the four modes of heat transfer.

For heat flux rate through each conducting node, the SINDA lumped parameter model solves the Fourier equation,

$$\dot{q} = \frac{1}{R}(T_i - T_j) \tag{2.42}$$

(2.43)

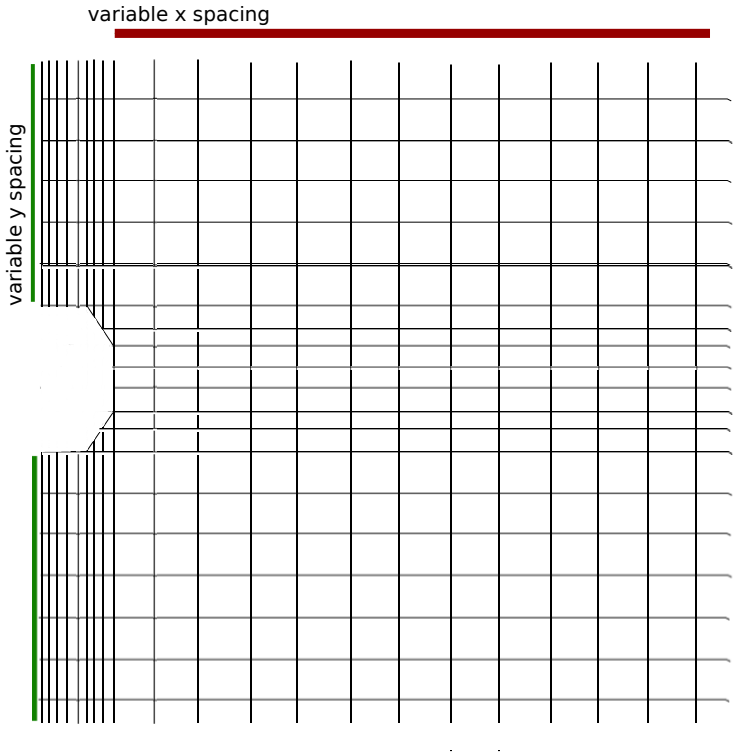

Figure 2.2: The geometry of the thermal model can be adjusted in two dimensions, altering the tunnel spacing and the vertical distance from the aquifer.

where

$R =$ resistance

$T =$ temperature

and

$$\dot{q} = \text{ heat rate.}$$

Lumps are connected by conduction, convection, radiation, and mass flow heat transfer links. Briefly, these are represented by

$$\begin{aligned} R_{cond} &= \frac{L}{kA} \\ R_{conv} &= \frac{1}{h \cdot A} \\ R_{mf} &= \frac{1}{\dot{m} c_p} \\ R_{rad} &= \frac{1}{\sigma F_{ij} A \left[T_i + T_A + T_j + T_A\right] \left[(T_i + T_A)^2 + (T_j + T_A)^2\right]} \end{aligned}$$

where

$$
\begin{aligned}
k &= \text{conductivity}[] \\
A &= \text{area}[m^2] \\
c_p &= \text{specific heat capacity}[] \\
h &= \text{heat transfer coefficient}[] \\
\dot{m} &= \text{mass transfer rate}[kg \cdot s^{-1}] \\
T_i &= \text{lump temperature}[^\circ C] \\
T_A &= \text{absolute temperature}[^\circ C] \\
F_{ij} &= \text{radiation interchange factor}[-].
\end{aligned}
$$

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

Finite Difference Codes

An array of finite difference codes exist which have been used to make repository heat evaluations. See Table **??**.

Finite Element Codes

An array of finite element codes exist which have been used to make repository heat evaluations. See Table **??**

Models of Heat Load for Various Geologies

Source (Who)	Nation (Where)	Geology (What)	Methodology (How)
Enresa [26]	Spain	Granite	CODE_BRIGHT
NRI [26]	Czech Rep.	Granite	Specific Temperature Integral
ANDRA [9]	France	Granite	3D Finite Element CGM code
SKB [1]	Sweden	metagranite	Forsmark / Laxemar Site Descriptive Model (SDM)
SCK·CEN [26]	Belgium	Clay	Specific Temperature Integral
ANDRA [8]	France	Argile Clay	3D Finite Element CGM code
NAGRA [22, 23]	Switzerland	Opalinus Clay	3D Finite Element CGM code
GRS [26]	Germany	Salt	HEATING (3D finite difference)
NCSU(Li) [28]	USA	Yucca Tuff	Specific Temperature Integral
NCSU(Nicholson) [30]	USA	Yucca Tuff	SRTA and COSMOL codes
Radel & Wilson [34]	USA	Yucca Tuff	Specific Temperature Change

Table 2.6: Methods by which to calculate heat load are independent of geology. Maximum heat load constraints, however, vary among host formations.

ANDRA/RED-IMPACT Codes

Codes used by ANDRA and other programs within the RED-IMPACT assessment may not fit in any of the categories above. They are listed in Table 2.6. ¡++¿

3 MODELING PARADIGM

The modeling paradigm with which this repository model and simulation platform are implemented are here described. 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 transacation 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

which comprise the bedrock 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.

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 modules 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.

Abstraction

Cyclus implements a 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 a region institution 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 RegionModel, InstitutionModel, FacilityModel, and MarketModel while their subclasses are the concrete types (e.g. RecipeReactorFacility). 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.

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.

Region-Institution-Facility Hierarchy

Many times in a fuel-cycle simulation, parameters describing relationships between facilities are required. For instance, one may wish to account for the presence of a contract between two facilities, or one may wish to model two facilities operated by the same entity. Accordingly, Cyclus implements this ability via a Region-Instituion-Facility hierarchy. Every discrete facility in Cyclus is considered to be owned by an institution that operates in a geographic region. An institution can be used to represent any entity that may own and operate a facility such as a private corporation, a government agency, or

a non-governmental organization, among others. A region can be used to represent any geographic area, typically a politically relevant area such a sub-national region (e.g. a U.S. State), a nation-state, or a supranational region (e.g. the E.U.). While some performance parameters of the facility may depend on its institutional ownership or geographical location, this capability is more useful in modeling the way in which a facility engages in a market for trade of nuclear material based on its ownership entity and/or region.

For each of the global regions, the user defines available facility configurations that can operate in those markets. Multiple facility configurations will typically be created in each region, including one or more reactor configurations (AP1000 vs ESBWR vs EPR or PWR vs. HTGR vs CANDU) and one or more configurations for other facility types. The user is free to choose the level of detail used in distinguishing one facility configuration from another. Each facility configuration will either be a supplier in one or more global markets, a consumer in one or more global markets, or both a supplier and consumer in non-intersecting sets of global markets. The set of facility configurations defines which facilities are available for deployment in a given scenario, but multiple instances of each facility configuration may exist.

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 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.

The repository model which is the subject of this work is a facility model within the Cyclus simulation paradigm.

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.

Each instance of a facility is associated with a defined Institution and each institution operates in a geographically defined Region.

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.

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 interchangably 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.

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.

Waste Stream Input

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

As the set of disposable material in the simulation is of heterogeneous composition and therefore heterogeneous heat production capability, the repository model will sometime need to recalculate its own capacity in terms of new materials.

Repository Performance Metrics Calculated

Repository performance metrics that may be calculated from the source term and heat data calculated by the model will cover a broad space of metrics of interest to sustainability

goals.

Some metrics support analyses which 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 which may be calculated from the calculations of the repository model include environmental metrics such as peak radiotoxic 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..

Nested Component Concept

The fundamental unit of information in the repository model is the nuclide release at each stage of containment, and the repository model in this work mimics reality treating them as nested elements in a release chain.

Structure and Linkages

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.

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

Each component model similarly requires information about the nuclides 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.

Concept Generality

The capability to allow each model to define the models within it gives this repository model concept the ability to model many types of repository concept while maintaining a simple interface with the simulation.

Components of the Nested System

Waste Stream

The waste stream data object contains spent fuel isotopics over the course of the simulation. As nuclides 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 nuclides are immediately accessible, and some tend to remain in the fuel matrix.

Waste Package

The waste package model calculates nuclide release due to waste pacakge 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 and borehole repositories may not have a buffer material.

Backfill

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

Borehole repository concepts may not have a backfill material.

Tunnel Lining

Much like the waste package model, nuclide release is typically modeled as either instantaneous and total or constant and partial.

Geological Environment

Various hydrogeological models exist to represent travel through porous media, fractured porous media, crystalline media, and clays.

Sudicky and Frind give a model for fractured porous media which analytically captures nuclide mobility due to advection through fractures as well as competing retardation factors including sorption on the fracture walls, diffusion into stagnant fluid in the rock matrix, and sorption into rock matrix walls.

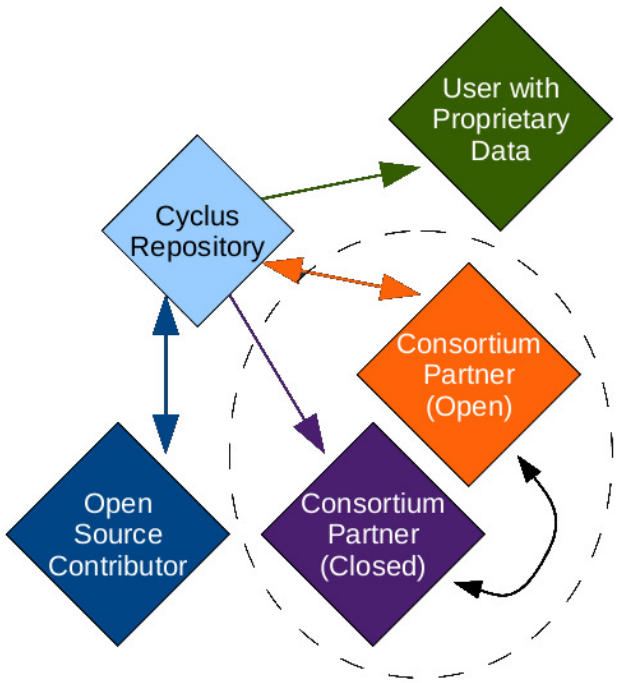

Figure 3.1: The Cyclus code repository allows for varied accessibility.

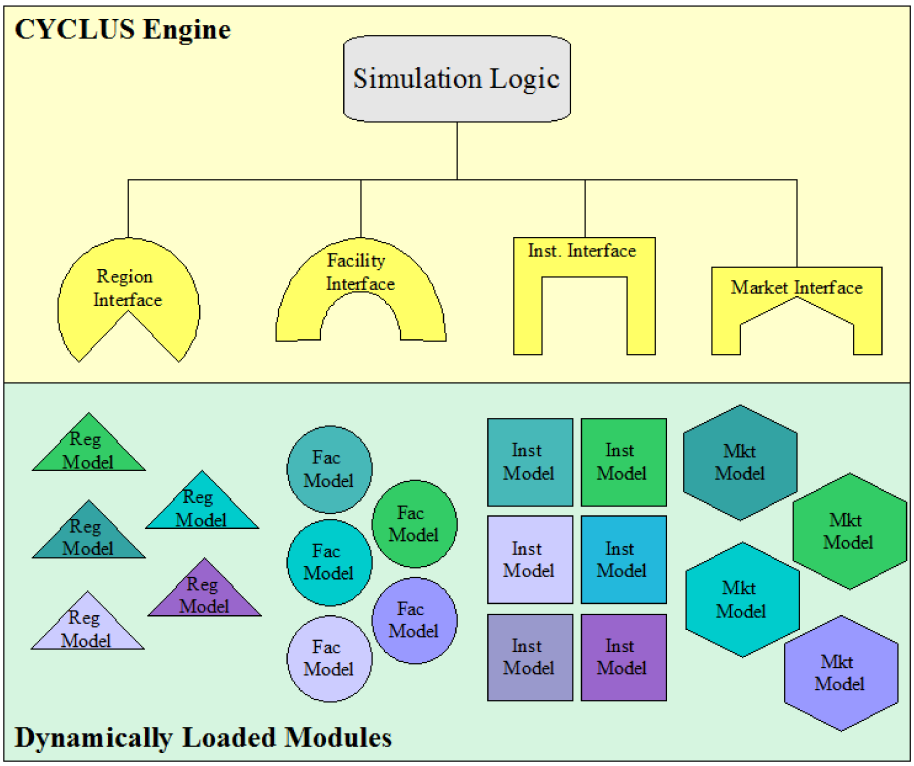

Figure 3.2: Modules are defined solely by their interfaces in a modular paradigm and can be arbitrarily interchanged with modules posessing equivalent interfaces.

4 CATEGORIZATION OF MODELS

The goal of this chapter is to categorize the available analytical and computational models into their salient characteristics according to the phenomena we are interested in modeling. For example, a table will be listed here detailing the phyical phenomena at work vs. the conceptual and mathematical models available, listed in order of complexity.

4.1 Fractures

Explicit Discrete Fracture Formulation

This modeling formulation is complex and requires detailed knowledge of the candidate lithology. While an extensibility to include such a model will be retained in the repository system, it is well out of scope of the level of detail being sought by this nature of simulation.

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

Dual-Continuum Formulation

The dual continuum formulation for either porosity or permeability allows a network of cracks to be

It is one of the most widely employed models of fracture flow [15].

Discrete Fracture Network

Single Equivalent Continuum

Unsaturated or Multiphase Flow

While some candidate repository geologies such as salt and granite are presumed to be unsaturated, the base case geology being modeled in this work is assumed to be saturated.

4.2 Mixing

Precipitates

Dissolved Concentrations

4.3 Matter Dissolution

Atomistic

Molecular Dynamics

Staged

Various stages of matter dissolution may include the initial attack, alteration, maturation, evolution, etc.

SWF/UFD/NEAMS data

These will presumably give simplified constant rates.

4.4 Diffusion Coefficients

Constant

Tabulated.

Temperature Dependent : Arrhenius Relationship

The Arrhenius relationship,

$$D = D_0 e^{-\frac{E_A}{RT}} \tag{4.1}$$

where

$$D = \text{the diffusion coefficient} \tag{4.2}$$

$$D_0 = \text{the maximum diffusion coefficient} \tag{4.3}$$

$$E_A = \text{the ctivation energy of diffusion}[J \cdot kg^{-1}] \tag{4.4}$$

$$T = \text{is the temperature}[^\circ K] \tag{4.5}$$

$$R = \text{the ideal gas constant}[J \cdot \text{mol}^{-1} \cdot^\circ K^{-1}], \tag{4.6}$$

$$\tag{4.7}$$

gives the diffusion coefficient of solids as a function of temperature.

Gives D as a function of temperature and apparent activation energy of the medium.

Temperature Dependent : Stokes Einstein Relationship

The Stokes-Einstein relationship,

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

gives an equation for the diffusion coefficient in a fluid, as a function of T, the temperature of the surrounding medium, k_B, the Boltzmann constant, and η, the viscosity of the medium. This relationship is appropriate for media which have a low Reynolds number,

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

where

$\rho =$ fluid density$[kg \cdot m{-}3]$

$v =$ mean relative velocity of fluid$[m \cdot s^{-1}] < ++ >$

$L =$ characteristic length of system$[m]$

$\mu =$ dynamic fluid viscosity$[kg \cdot m^{-1} \cdot s{-}1]$

where viscous forces dominate.

Concentration Dependent : ?

Maybe there is a generally known functional form.

4.5 Heat

I'll be using the lumped parameter model for everything. Maybe linking to SINDA or the LLNL program.

. . .

5 CURRENT WORK

5.1 Cyclus

The Cyclus framework discussed in chapter 3 provides a fuel cycle simulation platform on which to initially develop and deploy the repository model that is the subject of this effort. As a part of this effort also under development, Cyclus has been developed with an architecture that supports the goals of this effort and will continue to mature in parallel with the development of this model.

Framework

The Cyclus framework is available, and the product of some quantity of work.

This will be essential for implementing and testing the repository model.

Available Models

Cyclus has a base set of models which are currently available and will support open and some closed fuel cycle simulations. These include a source and a sink facility model as well as recipe based reactor models, an enrichment facility, an intermediate storage facility, and a fleet of markets which direct material movement in the simulation.

Further fuel cycle facility models are being developed within Cyclus which will be essential for providing interesting scenarios for comparison via repository metrics. For a modified open cycle, a separations facility is necessary which will be capable of conducting arbitrarily complex chemical separations of used fuel. Similarly, an associated reprocessing

facility will be neccessary which is equipped to handle the so called 'winery' problem of constructing critical fresh fuel assemblies appropriate for specific reactors from separated streams.

5.2 GDSE Analysis

Much of my future work is based on the parametric and regression analysis that has begun with the base case Clay GDSE model at ANL.

Sensitivity Analyses

The Used Fuel Cycle Division has reported sensitivity results for various parameters as they affect Mean Annual Dose. I've looked at a few parameters too. I'll repeat those calculations for source term rather than dose in order to provide some graphs for the parameters below and more. I will be interested in coefficients defining the relationships between these parameters and source term over time for each isotope.

Cooling Time

Extending the cooling time between discharge and emplacement results in an altered waste stream. The resulting source term releases of this waste stream were expected to differ from base case results. Nonetheless it was found that for the clay GDSE model there was approximately no Mean Annual Dose sensitivity to the cooling period length [14].

Burnup

The burnup of a used fuel assembly results in an altered waste stream at the time of emplacement. It was found that for the clay GDSE model, the mean annual dose sensitivity to waste form dissolution rate became more important linearly with increased burnup [14].

It is expected that the burnup will alter heat based capacity.

¡+sindaAnalysis+¿

¡+burnupVScapacityGRAPH+¿

Drift Spacing

The mean annual dose is not very sensitive to the horizontal spacing between drifts.

Vertical Distance to Aquifer

The vertical distance to the aquifer above the disposal configuration defines the distance separating source term nuclide contaminants from the biospere. The clay model indicates that the mean annual dose is very sensitive to this distance [14].

Vertical Darcy Velocity

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 [14].

It is assumed that the thermal model will not demonstrate any sensitivity to the vertical Darcy velocity. Since heat dissipation in the far field is taken to be completely diffusive in clay, the Darcy velocity and the thermal model are entirely independent.

Hypothetical Intersecting Fast Advective Pathway

A fast pathway model intended to demonstrate a disrupted scenario is modeled as a single intersecting fracture in the clay matrix. The importance of the various ways in which this fast pathway intersects the model is very nuclide specific [14]. In the clay model the fast pathway intersects the engineered barrier system either directly in the emplaced waste or just outside the secondary engineered barrier system.

It is assumed that the thermal model will not demonstrate any sensitivity to the presence of a fast pathway. Since advective heat dissipation in such a crack would be minimal at the water speeds being considered. The thermal mocel takes the far field to be completely advective, also, and does not currently have the capability to model a fast pathway.

Dimensions of Hypothetical Fast Pathway

That is, how important is the crack width?

J Ahn's PhD thesis had some analytical answers to this question.

Clay Porosity

This should have a very slight linear effect. A coefficient needs to be derived from the relationship.

Buffer Porosity

This should have a very slight linear effect. A coefficient needs to be derived from the relationship.

Waste Form Porosity

That is, the porosity within the waste form initially.

Waste Form Degradation Rate

This will be irrelevant for cases with low burnup or no fast pathway.

Waste Form Release Mode

Solubility limited? Continuous?

Waste Package Degradation Rate

This will be irrelevant for cases with low burnup or no fast pathway.

Waste Package Release Mode

Solubility limited? Continuous?

Nuclide Solubilities

For each nuclide.

Etc.

There are many parameters I haven't thought of.

Comparison with other geologies

A short comparison with each of the other models representing specific geologies will be begun in order to determine the differences in results for similar parameters.

5.3 SINDA Model Analysis

Sensitivity Analysis

Cooling Time

Extending the cooling time between discharge and emplacement results in an altered waste stream. The emplacement capacity of this waste stream may be expected to differ from base case results.

Since the cooling period will be modeled outside of the repository model within the CYCLUS analysis, this sensitivity will not be incorporated into the repository modeling effort at the heart of this work, but gives an intuition for appropriate sensitivity to altered waste streams.

It is expected that the cooling time alters heat based capacity.

¡+sindaAnalysis+¿

¡+coolingVScapacityGRAPH+¿

Burnup

The burnup of a used fuel assembly results in an altered waste stream at the time of emplacement. It was found that for the clay GDSE model, the mean annual dose sensitivity

to waste form dissolution rate became more important linearly with increased burnup [14].

It is expected that the burnup will significantly alter heat based capacity.

¡+sindaAnalysis+¿

¡+burnupVScapacityGRAPH+¿

Heat Generating Isotopes

Plutonium and minor actinides are dominant contributors to heat. Focusing on the sensitivity of the heat based capacity to the waste stream content of these nuclides could significantly simplify the heat analysis.

For each of these, a sensitivity analysis of capacity to the nuclide will be developed by analyzing the thermal repository capacity for a waste stream of that nuclide alone.

¡+sindaAnalysis+¿

¡+contributorMassVSCapacityGRAPH+¿

Drift Spacing

It is expected that the heat based capacity will be highly sensitive to the spacing between drifts. A higher drift density produces larger amounts of heat generation per repository footprint area. Constrained by heat limits typically at the drift tunnel boundaries, the repository capacity is reduced by increased areal loading density.

¡+sindaAnalysis+¿

¡+spacingVScapacityGRAPH+¿

Waste Package Separation

It is expected that the heat based capacity will be highly sensitive to the spacing between packages linearly within the drifts. A higher line loading density produces larger amounts of heat generation per repository footprint area. Again, the repository capacity is reduced by increased areal loading density.

¡+sindaAnalysis+¿

¡+lineloadingVScapacityGRAPH+¿

Waste Package Loading Density

It is expected that the heat based capacity will be highly sensitive to the mass loading per waste package. A higher package loading density produces larger amounts of heat generation per repository footprint area. Constrained by heat limits typically at the drift tunnel boundaries, the repository capacity is reduced by increased areal loading density.

¡+sindaAnalysis+¿

¡+pkgloadingVScapacityGRAPH+¿

Clay Porosity

It is expected that the heat based capacity will be fairly sensitive to the clay matrix porosity. A higher porosity allows greater diffusive flowthrough and heat removal. Constrained by heat limits typically at the drift tunnel boundaries, the repository capacity is increased by increased clay porosity.

¡+sindaAnalysis+¿

¡+porosityVScapacityGRAPH+¿

Buffer Porosity

It is expected that the heat based capacity will be fairly sensitive to the buffer matrix porosity. A higher porosity allows greater diffusive flowthrough and heat removal. Constrained by heat limits typically at the drift tunnel boundaries, the repository capacity is increased by increased clay porosity.

¡+sindaAnalysis+¿

¡+porosityVScapacityGRAPH+¿

Vertical Distance to Aquifer

It is expected that the thermal model will not demonstrate significant sensitivity to the distance to the overlying aquifer. Heat disspiation over the length scales at hand, in the hundreds of meters, renders the distance of the boundary at the far field irrelevant.

Review of Radel Analysis

Maybe earlier in lit review instead.

Changing Geometry

The tunnel geometry can be altered in two dimensions.

Thermal Conductivities, etc.

Sensitivity to various physical parameters of the model will be found.

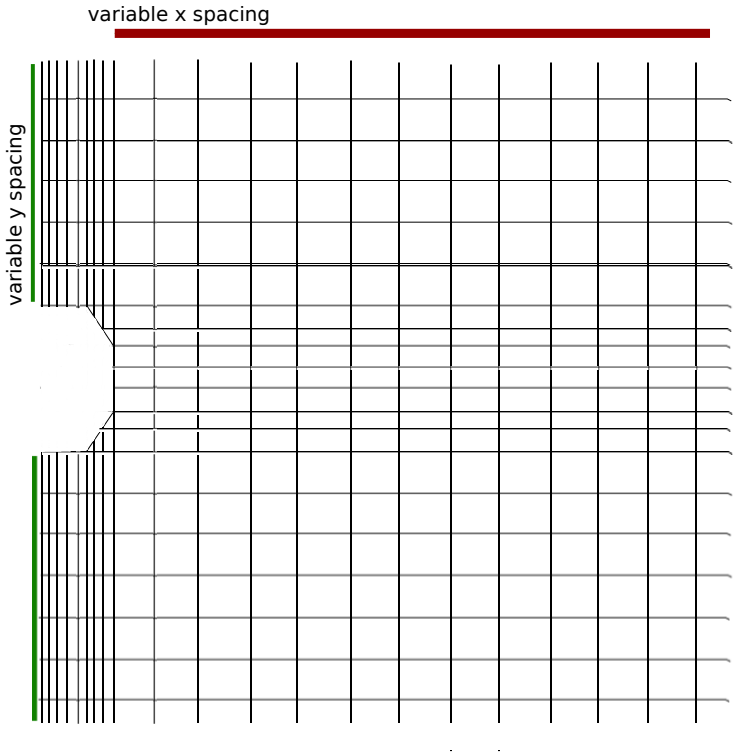

Figure 5.1: The geometry of the thermal model can be adjusted in two dimensions, altering the tunnel spacing and the vertical distance from the aquifer.

5.4 LLNL Model Analysis

An analysis similar to that conducted with the SINDA model will be conducted for the LLNL thermal model.

5.5 Demonstration

Conceptual Model

Volumes

Volumes are defined by their dimensions, surfaces, temperature, contained matter, and contained contaminants.

Dimensions fully define the shape and magnitude of the volume. **Volume shape? Can be more than just cylindrical?**

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 volume.

Matter

This model treats matter in solid and liquid phases. Gaseous matter is not supported.

Liquids are defined by their dynamic viscosities (μ, [Pascal seconds]) and by characteristic diffusivity (d_i, $[m^2/s]$) and solubility (K,$[kg/m^3]$) coefficients for each nuclide.

Solids are assumed to be porous media and are defined by their porosity (n, $\%$), tortuosity (τ, $[-]$), and dry (bulk) density (ρ). Fracturation is dealt with separateea, a flux type, and a flux direction.

Connections

Heat transfer connections include at least conductive and convective connections. Radiative and mass transfer heat connections will be a secondary extension to the modeling paradigm.

Nuclide transport connections will include at least diffusive and advective connections. These will incorporate available porosity of the surface interface. Solubility limitations will be a characteristic of the mixing volume cell rather than the release pathway.

Mathematical Model

Mass Balances Within Cells

This will describe the preliminary mixing model.

Mass Transfer Boundaries

Heat Diffusion

Equation, assumptions, B.C.s, I.C.s, solutions.

Fluid/Contaminant Diffusion

Equation, assumptions, B.C.s, I.C.s, solutions.

Heat Advection

Equation, assumptions, B.C.s, I.C.s, solutions.

Fluid/Contaminant Advection

Equation, assumptions, B.C.s, I.C.s, solutions.

Computational Model

Simplified Models

For a proof of principle, each repository subcomponent has been implemented with a first order model. The information passing system is thereby tested for completeness.

Information Exchange

The information exchange paradigm must provide a comprehensive set of module boundary information as described in the mathematical model.

6 SUMMARY AND FUTURE WORK

6.1 Summary

Motivation

Most fuel cycle simulators are lacking in repository analysis.

The UFD campaign needs an interface with the SA campaign.

Current Work

Abstraction of current detailed repository models in combination with the current CYCLUS framework has generated a fundamental modeling concept and demonstrated capability for modeling the nuclide transport and heat evolution of a generic geological repository.

6.2 Future Work

Sensitivity Analysis

The sensitivity analysis underway to arrive at simplified dominant physics relationships between the various input parameters of the simulation.

Nuclide Transport

These are the independent parameters I'm interested in.

A TABLE, perhaps. Including parametric domain.

This is how I'll vary them.

Show that these provide a largely complete set of input variables to define nuclide transport. Discuss variables that are being neglected for simplicity, perhaps to be added later.

Heat Evolution

These are the independent parameters I'm interested in.

A TABLE, perhaps. Including parametric domaie.

This is how I'll vary them.

Show that these provide a largely complete set of input variables to define heat evolution. Discuss variables that are being neglected for simplicity, perhaps to be added later.

Mathematical Model Abstraction

Using the results of these sensitivity analyses, regression analysis will be performed to develop simplified parametric dependencies for all independent variables for each model.

Computational Model Development

Base Case

Clay, bentonite backfill, no evacuation disturbed zone, some handfull of waste packages and waste forms.

TAD Canisters The canisters proposed for transportation, aging and disposal are called TAD canisters. They are two concentric cylinders of steel and alloy22 inside and out respectively.

Borosilicate Glass Current borosilicate glass: Includes processing chemicals from original separations, with U/Pu removed, but minor actinides and Cs/Sr remaining Potential borosilicate glass: No minor actinides and/or no Cs/Sr; Mo may be removed to increase glass loading of radionuclides; it has alower volumetric heat rate

Glass Ceramic Glass Ceramic: This is glass-bonded sodalite from Echem processing of EBR-II, and from potential future Echem processing of oxide fuels o Metal Alloy: This includes subcategories

Metal Alloy Metal alloy from Echem: Includes cladding as well as noble metals that did not dissolve in the Echem dissolution Metal alloy from aqueous reprocessing: Includes undissolved solids and transition metal fission products

Advanced Ceramic Advanced Ceramic: An advanced waste form that includes iodine volatilized during chopping, which is then gettered during head-end processing of used fuels

Separated Streams Other: Examples include radionuclides removed from other waste forms (e.g., Cs/Sr, I, C), as well as new waste forms such as a salt waste form

Classes A, B, and C waste Lower Than High Level Waste (LTHLW): Includes Classes A, B, and C

GTCC LTHLW Greater Than Class C (GTCC)

Demonstration

Show that the complete model behaves in agreement with the more detailed model on which it was based. Else, iterate through sensitivity analyses, model abstraction, and computational development until the model is validated.

Extension

This disposal system will at this point be extended to include a fleet of predefined model implementations to represent some canonical waste forms, packages, buffers, and clay types.

Fuel Cycle Analysis

Show some various fuel cycles have different repository needs and metrics. Specifically, compare a closed fuel cycle, an open one, and at least one modified fuel cycle.

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