AN INTEGRATED USED FUEL DISPOSITION AND GENERIC REPOSITORY MODEL

by

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Please insert a dedication here.

ACKNOWLEDGMENTS

> *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," which illustrates how to use the `wbepi` environment for epigraphs at the beginning of chapters. You probably also want to thank the Academy.

CONTENTS

LIST OF TABLES

LIST OF FIGURES

AN INTEGRATED USED FUEL DISPOSITION AND GENERIC REPOSITORY MODEL

Kathryn D. Huff

Under the supervision of Professor Paul P.H. Wilson
At the University of Wisconsin-Madison

FIXME: basically a placeholder; do not believe

I did some research, read a bunch of papers, published a couple myself, (pick one):

1. ran some experiments and made some graphs,
2. proved some theorems

and now I have a job. I've assembled this document in the last couple of months so you will let me leave. Thanks!

Paul P.H. Wilson

ABSTRACT

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1 INTRODUCTION

The scope of this work includes implementation of a comprehensive software library of medium fidelity models to represent the thermal behavior and long-term disposal system performance of different disposal system concepts in different geologic media for deployment in a modular systems analysis platform. This work will model repository behavior as a function of arbitrary spent fuel composition as well as modularly incorporate 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 waste package solutions therefore requires a system level approach. A simulation tool with top-level capability which will allow modular substitution of various fuel cycle facility, repository, and waste package models is needed. The development of such modular waste package and repository models 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 the development of computational tools to 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.

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. [**?**]

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 presenting 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 fuel cycle system by 2050. [**?**]

A Once-Through Cycle represents the continuation of the business as usual case in the United States, neglecting reprocessing, and presenting 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, but 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. [?]

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 Fully Recycle strategy will be reprocessed and cycled through a reactor numerous times and may undergo partitioning and waste treatment before ultimate disposal in a repository. Such 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 fully closed and fully open. 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. Spent fuel volumes and composition will vary dramatically among various possibilities within this scheme.

Clearly, the range of 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 the reconsideration of the domestic fuel cycle policy, the uncertain future of the Yucca Mountain repository 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. The physical, hydrogeologic, and geochemical mechanisms which dictate nuclide and heat transport vary between these geological systems. Therefore, in support of the 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

Heat 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 design basis in the temperature dependence of isolation integrity of the waste form. The waste form dissolution behavior under heat generation from the contained isotopics constrains loading density within the waste form in an isotope specific way.

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

Heat load limits of the geologies depend less on rock matrix degradation than on hydrogeology within the rock under heat evolution. The two heat load constraints which primarily determined the heat-based SNF capacity limit in the Yucca Mountain Repository design, for example, are fairly specific to 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.

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.

Radiotoxicity and Source Term Modeling Needs

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. The primary pathway of radionuclides from an accidental release will be from cracking aged canisters. 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 and 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. The probabilistic nature of these assessments mean a direct dependence of source term on repository capacity can be difficult to arrive at. In order to give informative values for the risk associated with transport of particular radionuclides, for example, studies make hundred thousand year predictions about waste form degredation, water flow, etc.

A generalized metric of probablistic risk is fairly difficult to arrive at. The Peak Environmental Impact metric from Berkeley [4], for example, is a complicated 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.

Importantly, due to the incredible time scale and intrinsic uncertainties required in probabilistic assessment it is in general not advisable to base any maximum repository capacity estimates on source term. However, source term is a useful metric for the comparison of alternative separations and fuel cycle scenarios.

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. Once complete, extended models and model variants will be developed to more comprehensively cover the option space.

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 shifting the emphasis between 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.

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 glass and ceramic 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 categorize and characterize detailed computational models of nuclide and heat transport available for regression analysis. Specifically, 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 4 will detail the analytical and regression analysis undertaken 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.

These models will focus on the hydrogeology and thermal physics dominating nuclide transport and heat response in candidate geologies as a function of isotope release and heat generation over long time scales from waste packages. Disposal site water chemistry (redox state) and dominant transport mechanism (advection or diffusion) 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 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 [**?**] or specific temperature change [**?**]) which approximate the thermal response from heat generation in the waste packages as linear along the repository drifts, and arrive at thermal evolution over time at any location in the rock as well as 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.). At this point, a regression analysis concerning those parameters will be undertaken with available detailed models (e.g. 3D finite element codes and full performance assessment models) 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, water presence etc.). 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. clay, salt, shale, granite). A similar process will be followed for nuclide transport models.

Verification and validation of abstracted models will be conducted through iterative benchmarking against more detailed repository models.

Chapter 5 will adapt existing models and data to the development of concise dominant physics waste form, waste package, and other engineered barriers (i.e., bentonite or cementitious materials) models appropriate for treatment of key radionuclides within the waste streams. Material/barrier degradation, radionuclide release, and radionuclide transport, and thermal processes and effects will be included, as necessary, in the concise representations that will be developed for subsequent use in the system-level architecture. A range of waste forms, waste package materials, and other engineered barrier materials (buffer, backfill) under consideration by the DOE-NE FCT program (SWF and UFD campaigns) will be evaluated. The concise dominant physics models will include appropriate load limiting factors such as waste characterization, classification, stabilizing medium limitations, and waste form heat loading behavior.

The abstraction process will employ the comparison of semi-analytic models and analytic regression of rich code results as well as existing empirical material data. For instance, in the case of nuclide release for 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.) [**?**].

At this point, a 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 package dissolution rate). Determination of appropriate values to make available within the dominant physics model will rely on existing empirical data concerning the specific package materials being modeled (i.e. extrapolations of known material failure rates).

Feedbacks from the geologic media response model on the response of the engineered system, including waste forms, 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 will 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.

Chapter 6 will discuss the future work necessary to extend developed models to comprehensively cover the potential disposal system option space.

The path forward for extension of the geological base case model to cover all five geologic concepts of interest (clay, granite, salt, shale, and deep boreholes) will be discussed. Similarly, gaps in waste form and engineered barrier system models and data will be addressed and a plan for data and model coverage for that options space will be described.

Chapter 7 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 option space parametric domain coverage 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 current computational repository models follows, including both standalone and those incorporated into nuclear fuel cycle simulation tools. 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. Next, an overview is presented of available waste form performance models, and finally, work is reviewed that concerns the need for simplified first order, physics based models of fuel cycle processes within the context of top level simulation.

2.1 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 matrix 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 Matrix Release Models

Hedin Model ([?])

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. Matrix dissolution within the Hedin model a rate based model which takes place within the waste package

Ahn Models ([1, 2])

Waste canisters are modelled as compartments of waste matrix 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.

In the Hedin model of the Swedish KBS repository, waste matrix dissolution is taken to occur at a steady rate within the waste package. That is, degradation and congruent nuclide release occur at a constant rate until the the fuel matrix is wholly degraded, but remain within the waste package until its failure. Gradual dissolution of the initial mass M_{oi} of a nulcide i can be described by a production rate $P(t)$,

$$P(t) = M_{oi} D_F e^{-\lambda t}$$

where D_F is the dissolution rate of fuel matrix (mass fraction per time) and t is the time since emplacement.

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:

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

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

Current Waste Package Failure Models

Model	WP Failure Mode	Waste Form	Time at first failure
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
Jun	EBSFAIL		$300,000$ years

Table 2.1: The above represent current methods by which waste packeage failure rates are modeled.

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. [**?**]

Waste Package Failure Models

Continuous

Instantaneous

The Hedin model of waste package failure is effectively instantaneous, but limited by 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. [?]

Probabilistic

Nuclide Transport Through Engineered Barriers

Barrier Dissolution and Failure

Transport Through EBS Matrix

Hydrogeologic Transport Models

Solute Transport in Permeable Porous Media

Clay, granite, salt, and shale can larely be characterized as permeable porous media.

The equation representing solute transport in a permeable medium of homogenous porosity can be written

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

where

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

In the expressions above,

$$
\begin{aligned}
q &= \text{ Darcy velocity } [m \cdot s^{-1}] \\
\alpha &= \text{ dispersivity } [m]
\end{aligned}
$$

and

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

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

$$Pe = \frac{qL}{\alpha q + D_e},$$

where

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

Reducing Environments

Saturated Environments

Unsaturated Environments

Oxidizing Environments

Saturated Environments

Unsaturated Environments

Fracturation

Sorption Into Matrix

Diffusion Into Fracture

Advection Through Fracture

Effective Porosity

Major and Minor Fracturation

2.2 Analytical Models of Heat Transport

Impact of Repository Designs

Heat Limits in Various Waste Packages

Heat Limits in Various Geologies

Clay

Granite

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 is order.

Shale

Unsaturated Tuff Two heat load constraints primarily determine the heat-based SNF capacity limit 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.

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[**?**] 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.[11]

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.

2.3 Detailed, Stand-Alone Repository Codes

European RED-IMPACT

Yucca Mountain Total System Performance Assesment

WIPP Performance Assessment Code

Fuel Cycle Technology, UFD Codes Under Development

2.4 Repository Analysis Capbabilities Within Systems Analysis Codes

VISION

COSI

NUWASTE

DANESS

ETC. . .

2.5 System Level Analyses of Repository Performance

Fuel cycle sensitivity analyses emphasizing used fuel disposition and wastie management in the Yucca Mountain Repository (YMR) have been conducted

International Repository Concepts

Geology	Nation	Waste Stream	Metric	Institution	Code
Granite	Spain	HLW	Heat Load	Enresa	¡+CodeName+¿
Granite	Czech Rep.	HLW	Heat Load	NRI	¡+CodeName+¿
Clay	Belgium	HLW	Heat Load	SCK·CEN	SAFIR2
Salt	Germany	HLW	Heat Load	GRS	¡+CodeName+¿
Granite	Spain	HLW	Dose	Enresa	¡+CodeName+¿
Clay	Belgium	HLW	Dose	SCK·CEN	SAFIR2
Clay	France	HLW	Dose	CEA	ANDRA
Salt	Germany	HLW	Dose	GRS	¡+CodeName+¿
Granite	Czech Rep.	ILW	LT Dose	NRI	¡+CodeName+¿
Granite	Spain	ILW	LT Dose	Enresa	¡+CodeName+¿
Clay	Belgium	ILW	LT Dose	SCK·CEN	SAFIR2
Granite	Spain	HLW/ILW/Iodine	LT Dose	Enresa	¡+CodeName+¿
Clay	Belgium	HLW/ILW/Iodine	LT Dose	SCK·CEN	SAFIR2

Table 2.2: International repository concepts evaluated in the RED Impact Assessment.[7]

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 2.2.

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.[**?**]

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

Models of Heat Load for Various Geologies

Source (Who)	Nation (Where)	Geology (What)	Methodology (How)
Enresa [7]	Spain	Granite	CODE_BRIGHT
NRI [7]	Czech Rep.	Granite	Specific Temperature Integral
ANDRA [?]	France	Granite	3D Finite Element CGM code
SKB [?]	Sweden	metagranite	Forsmark / Laxemar Site Descriptive Model (SDM)
SCK·CEN [7]	Belgium	Clay	Specific Temperature Integral
ANDRA [?]	France	Argile Clay	3D Finite Element CGM code
NAGRA [? ?]	Switzerland	Opalinus Clay	3D Finite Element CGM code
GRS [7]	Germany	Salt	HEATING (3D finite difference)
NCSU(Li) [9]	USA	Yucca Tuff	Specific Temperature Integral
NCSU(Nicholson) [10]	USA	Yucca Tuff	SRTA and COSMOL codes
Radel & Wilson [11]	USA	Yucca Tuff	Specific Temperature Change

Table 2.3: Methods by which to calculate heat load are independent of geology. Maximum heat load constraints, however, vary among host formations.

of $49GWd_{th}/m$).[12]

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.[9]

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.[10] 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.[13]

In addition to variable drift spacing, other modifications to repository layout have had promising results in terms of heat-limited repository capacity. The Electric Power Research Institute (EPRI) in their Room at the Mountain study found that with redesign of the repository an increased capacity of at least 400% (295 tonnes once-through SNF) and up to 900% (663 tonnes) could be expected to be achieved. Proposed design changes include decreased spacing between drifts, a larger areal footprint, vertical expansion into second and third levels of repository space, and hybrid solutions involving combinations of these ideas. In particular, EPRI suggests either an expansion of the footprint with redesign of the current Upper Block line load design plan or a multi-level plan that repeats the footprint and line load design of the current plan.[6]

Due to the incredible time scale and intrinsic uncertainties required in the probabilistic assessment it is in general not advisable to base any maximum repository capacity estimates on source term. However, source term is a useful metric for the comparison of alternative separations and fuel cycle scenarios.

Factors Affecting Source Term

Waste package failure rate varies between models. While some employ a simulation code called EBSFAIL, a part of the EBSPAC module used in the TSPA code, other models incorporate their own hydrogeologic approximations of canister degredation, and still others assume immediate waste canister failure in order to focus on dissolution and transfer.

Nuclide dissolution rate can also be understood as nuclide release rate from the waste packages, and is the rate of mass transfer of a nuclide from

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.

its waste matrix into the saturation water. Models calculating nuclide dissolution rate have assumed waste package failure insofar as the water is assumed to saturate the waste matrix. 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. as directly proportional to the nuclide concentration in some cases,

Advective transfer rate through the granite tuff is dependent upon diffusion through the rock as well as water speed, etc. The diffusion coefficient varies per nuclide and is heavily dependent upon the concentration of that nuclide in the flowthrough water. This is just Fick's First Law.

$$J = -D\frac{\delta\phi}{\delta x} \tag{2.2}$$

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. Radionuclide concentration has been shown to be proportional to the waste package loading configuration.[3, 5]

The dissolution rate and the advective transfer rate of a nuclide through granite tuff are typically be taken to depend directly upon the diffusion coefficient of that nuclide, which for some nuclides is heavily dependent upon the concentration of that nuclide relative to the flowthrough water.

Li Model[8]

Basic Flowthrough Path 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 EPSREL. 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 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:

$$w_{ci}(t) = C_i(t)q_{out}(t) \tag{2.3}$$

where q_out is the volumetric flow rate of the water $[m^3/yr]$, and $C_i = m_i/V_{wp}$ 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.

The Unsaturated Zone lies between the repository and the water table. This model describes transport time in the porous rock as:

$$T_a = \frac{X_u}{U_u}R_{du} \tag{2.4}$$

where X is length of the unsaturated zone, U is the pore velocity of the water $[m/yr]$ and R_{iu} is the retardation factor for the isotope i. The retardation factor is poorly described here, but in general denotes migration distance of the solute over that of the solvent. Presumably, this factor incorporates isotope specific characteristics and is independent of or weakly dependent on concentration.

The Saturated Zone lies below the water table. At this point, the nuclide transport is taken to be completely advective, nuclide independent, and congruent with the volumetric flow of the water within the water table.

Independent Fuel Cycle Parameters

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 decisiong going forward. A 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.

The point then, is that 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.

Stand Alone Models

Models Incorporated into Systems Analysis Codes

To date, most of these top-level simulators ignore the waste disposal phase entirely and simply report a metric that measures the accumulated spent nuclear fuel and other wastes without considering the impact of those waste

Models of Source Term for Various Geologies

Source (Who)	Nation (Where)	Geology (What)	Methodology (How)
Enresa [7]	Spain	Granite	GoldSim ^{129}I primary contributor
SCK·CEN [7]	Belgium	Clay	FEP ^{129}I primary contributor
GRS [7]	Germany	Salt	Systematic Performance Asessment ^{135}Cs, ^{129}I, ^{226}Ra, ^{229}Th
Ahn [1, 2]	USA	Yucca Tuff	Solubility Limited Release & Congruent Release
NCSU(Nicholson) [8]	USA	Yucca Tuff	TSPA codes EBSREL and EBSFAIL
WIPP	USA	Salt	?
NAGRA [**?** **?**]	Switzerland	Opalinus Clay	TAME code
ANDRA [**?**]	France	Argile Clay	Very detailed CEA code Mostly homogeneous medium ^{129}I primary contributor
ANDRA [**?**]	France	Granite	Very detailed CEA code Involves fracturation of medium ^{129}I primary contributor
SKB [**?**]	Sweden	Forsmark Laxemar	HYDRASTAR hydrologic transport code

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

streams on the performance of the geologic disposal system. A wider variety of waste management metrics will be necessary to fully inform the decision making process, especially metrics that depend on the performance of the geologic disposal system. A model for repository capacity was developed for the VISION fuel cycle simulator [**?**] and recent efforts on the NUWASTE simulator [**?**] have made some progress in addressing this deficiency, but many similar efforts are lacking in this regard. The DOE-NE Fuel Cycle Technology (FCT) program has three groups of relevance to this effort. These are the FCT Used Fuel Disposition (UFD), the Separations/Waste Form (SWF), and System Analysis (SA) campaigns. The SA campaign is developing the overall fuel cycle simulation tools and interfaces with the

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

other FCT campaigns, including UFD. The UFD campaign is conducting the 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. This effort will interface with those campaigns to utilize the tools and information to develop the higher-level dominant physics representations for use in fuel cycle system analysis tools. The scope of work encompasses the implementation of a comprehensive software library of medium fidelity models to represent the thermal behavior and long-term disposal system performance of different disposal system concepts in different geologic media for deployment in a modular systems analysis platform. This work will leverage upon previous work by the lead institution (Lead) to model repository behavior as a function of the contents of the waste as well as recent developments by the Lead to modularly incorporate dominant physics process models into a computational fuel cycle analysis platform. It will also rely on conceptual framework development and primary data collection underway at the primary partner institution (Partner) and through interfaces with the FCT program participants (Partner). This integrated simulation tool will be demonstrated with performance analysis of potential advanced fuel cycle options. Key metrics will be demonstrated and initial uncertainty/sensitivity analyses will be conducted

NUWASTE

Nuclear Waste Technical Review Board code that determines many metrics about the fuel cycle according to various parameters. [**?**]

VISION

VISION's repository model conducts decay calculations and tracks upwards of 83 isotopes of interest in the nuclear fuel cycle. [**?**] Are there wasteform models in VISION?

DANESS

COSI

DYMOND

NFCSim

CAFCA

SMAFS

NFCSS

2.6 Geochemical Migration Models

2.7 Waste Form Models

TAD Canisters

Borosilicate Glass

Glass Ceramic

Metal Alloy

Advanced Ceramic

Separated Streams

Classes A, B, and C waste

GTCC LTHLW

3 CATEGORIZATION OF MODELS

4 REPOSITORY MODELS

5 ENGINEERED BARRIER SYSTEMS

6 MODEL EXTENSION

7 SUMMARY AND FUTURE WORK

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