

**AN INTEGRATED USED FUEL DISPOSITION AND GENERIC
REPOSITORY MODEL**

by

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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.

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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

1.1 CYCLUS : Fuel Cycle Simulator

CYCLUS is a fuel cycle simulation software created at the University of Wisconsin.

2 MOTIVATION

This is a motivational chapter.

3 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 applicable to likely advanced fuel cycle waste streams, 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.

3.1 Sensitivity Analyses of Repository Performance

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 environmental impact metrics. Sensitivity analyses for other geologies were conducted concerning repository concepts relevant to other nations as well. See Table 3.1.

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

Analyses Based On Heat Load

3.2 Repository Focused Sensitivity Analyses

Heat Load

Source Term

Two heat load constraints primarily determine the heat-based SNF capacity limit in the Yucca Mountain Repository design. Thermal limits in the current 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

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
SCK·CEN [7]	Belgium	Clay	Specific Temperature Integral
GRS [7]	Germany	Salt	HEATING (3D finite difference)
NCSU(Li) [9]	USA	Yucca Tuff	Specific Temperature Integral
NCSU(Nicholson) [11]	USA	Yucca Tuff	SRTA and COSMOL codes
Radel & Wilson [12]	USA	Yucca Tuff	Specific Temperature Change
NAGRA [? ?]	Switzerland	Opalinus Clay	3D Finite Element CGM code
ANDRA [?]	France	Argile Clay	3D Finite Element CGM code
ANDRA [?]	France	Granite	3D Finite Element CGM code
SKB [?]	Sweden	Forsmark	Site Descriptive Model (SDM)
		Laxemar	(thermal, hydrogeologic chemistry,
		metagranite	rock mechanics, and transport)

Table 3.2: Methods by which to calculate heat load vary slightly between geologies. Maximum heat load constraints also vary among host formations.

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.

Heat Load Metrics

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 situation has proven much more applicable to thermal performance studies of the repository, and the preferred method in the current literature relies on specific temperature integrals.

Specific Temperature Integrals model the thermal source as linear along the repository drifts, similar to the line loading and areal power density metrics. However, a temperature 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.[12]

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, 67 km.

Current Wisdom

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 Radcliff, Wilson, et al. find a maximum thermal capacity of 1.09 tonnes/m for commercial SNF (at an ELF of $49\text{GWd}_{th}/\text{m}$).[13]

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.[11] 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.[14]

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]

Author	Max. Capacity <i>tonnes</i>	Footprint <i>km²</i>	Details
OCRWM	70,000 97,000 119,000	4.65 6 7	“statutory case” “full inventory case” “additional case”
Yim, M.S.	75,187 76,493 95,970 82,110	4.6 4.6 4.6 4.6	SRTA code STI method 63m drift spacing 75 yrs. cooling
Nicholson, M.	103,600	4.6	drift spacing
EPRI	63,000 option 1 option 2 option 3 options 2+3 options 1+(2or3) options 1+2+3	6.5 13 6.5 6.5 6.5 13 13	Base Case CSNF expanded footprint multi-level design grouped drifts hybrid hybrid hybrid

Related Questions

- What is the thermal dependence on wasteform characteristics?
- What thermal effect does separation have?
- What kind of costs are related to drift-spacing redesign, footprint

expansion, age based mixing, extended cooling times, etc..?

3.3 Capacity Dependence on Source Term

Radiotoxicity and Source Term Constraints

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 legislative 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.

Radiotoxicity and Source Term Metrics

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 degradation, water flow, etc.

A generalized metric of probabilistic 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.

Current Wisdom

It has been shown with a great degree of uncertainty (50%) that the peak dose rate from a full, base case repository will occur in 300,000 years, and will reach no greater than 2.6 mrem/yr.[8]

The Total System Performance Assessment on the other hand conservatively predicts a peak mean dose rate in the first million years (where the peak occurs at approximately 300,000 years) to be on the order of 150 mrem/yr.[14]

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.

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 3.3: The above represent current methods by which waste package failure rates are modeled.

Factors Affecting Source Term

A source term model will incorporate waste package failure rate, nuclide dissolution rate, and advective transfer rate. 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 granite tuff also depends on water flow, nuclide solubility, and nuclide diffusion, but is employed in the context of the hydrogeology of the rock.

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 degradation, 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

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.

$$J = -D \frac{\delta \phi}{\delta x} \quad (3.1)$$

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. 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.

Ahn Models ([1, 2])

Basic Flowthrough Path 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 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 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 $5 \times 10^{-2} [\text{mol}/\text{m}^3]$ 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:

$$\dot{m}_i = 8\epsilon D_e S_i L \sqrt{\frac{U r_0}{\pi D_e}} \quad (3.2)$$

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

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 EPSREL 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:

$$w_{ci}(t) = C_i(t)q_{out}(t) \quad (3.3)$$

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:

$$T_a = \frac{X_u}{U_u} R_{du} \quad (3.4)$$

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.

Related Questions

- More detail on development of TSPA modules/solubility values?
- Effect of wasteforms on source term?
- More studies making probabilistic risk assessments of source term?

Independent Fuel Cycle Parameters

Independent fuel cycle parameters of particular interest to academics 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.

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 isotopic mass flows into the repository, their appropriate conditioning, densities, and other physical properties.

Repository Performance Metrics

On the back end, dependent variables are interesting as well.

Criticality Safety

Source Term

Peak Dose (Sv/y)

Integrated Dose (Sv)

Maximum Environmental Release (Sv/y)

Integrated Environmental Release (Sv)

Necessary Repository Volume

Thermal Load

Cost

Current Methodologies

3.4 Repository Models

Stand Alone Models

FSCNE

A³MCNP

SCANS 1A

ReFREP

Refrep is a near-field model. A. Hautajarvi and T. Vieno Model For A Spent Fuel Technical Research Centre of Finland (VTT) Repository.[10]

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 Assessment ^{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 3.4: 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.

Models Incorporated into Systems Analysis Codes

NUWASTE

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

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). MAFIC (hydraulic resolution of the networks, 3D modelling, 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 barrier). Porflow.
Transport in discrete fracture networks.	PROPER (FARF-31 component, 1D modelling in stream tube concept). PathPipe (conversion of networks of tubes for transport). and Goldsim (modelling in networks of 1D pipes).

Table 3.5: Similar to the Total System Performance Assessment, ANDRA's analyses are a coupled mass of many codes. Table reproduced from Argile Dossier 2005 [?]

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

3.5 Geochemical Migration Models

3.6 Waste Form Models

TAD Canisters

Borosilicate Glass

Glass Ceramic

Metal Alloy

Advanced Ceramic

Separated Streams

Classes A, B, and C waste

GTCC LTHLW

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