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Outline

Outline





Future Disposal System Options

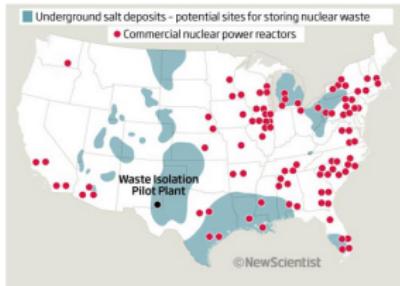


Figure: U.S. Salt Deposits, ref. [?].

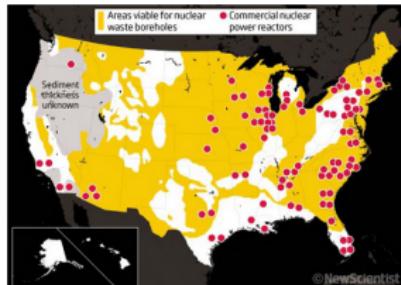


Figure: U.S. Crystalline Basement, ref. [?].

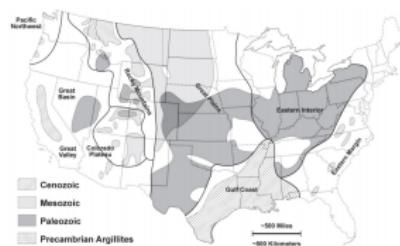


Figure: U.S. Clay Deposits, ref. [?].



Figure: U.S. Granite Beds, ref. [?].



Future Fuel Cycle Options

Domestic Fuel Cycle Options

Title	Description	Challenges
Open	Once Through Current US PWR Fleet No Separations No Recycling Higher Burnups	High Temperatures, Volumes
Modified Open	Partial Recycling Next Gen. PWR Fleet Limited Separations Limited Transmutation Advanced Fuel Forms HLW treatment	Both high volumes and myriad fuel streams
Closed	Full Recycling Full Separations Full Recycling VHTGR, SFRs, other transmutation HLW treatment	Myriad fuel streams

Table: Domestic Fuel Cycle Options



Methodology : Modularity

A modular repository framework facilitates

- interchangeable subcomponents (i.e. buffer material) so that the impact on the disposal system performance may be observed
- and simulations with varying levels of detail.

Integration with a fuel cycle simulator facilitates

- analysis of feedback effects upon the fuel cycle
- and investigation of fuel cycle choices on disposal system performance.



Methodology : Modularity

A modular repository framework facilitates

- interchangeable subcomponents (i.e. buffer material) so that the impact on the disposal system performance may be observed
- and simulations with varying levels of detail.



Methodology : Abstraction for Efficiency

Abstraction simplifies models while capturing salient physics. Parametric analysis with detailed models will inform simpler models at the level of detail important for fuel cycle analysis.

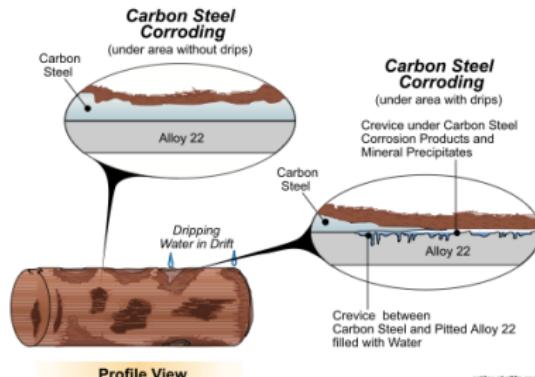


Figure 3-42. Waste Package Degradation Schematic

snl/nw/abc03a.sps
PV3034-3

Figure: A complex computational model is an abstraction of reality.

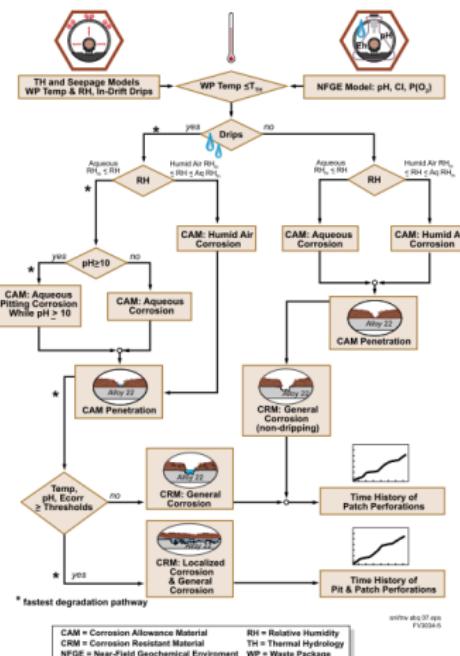


Figure 3-44. Waste Package Degradation Model Logic Diagram



Outline



Top Level Fuel Cycle Simulators

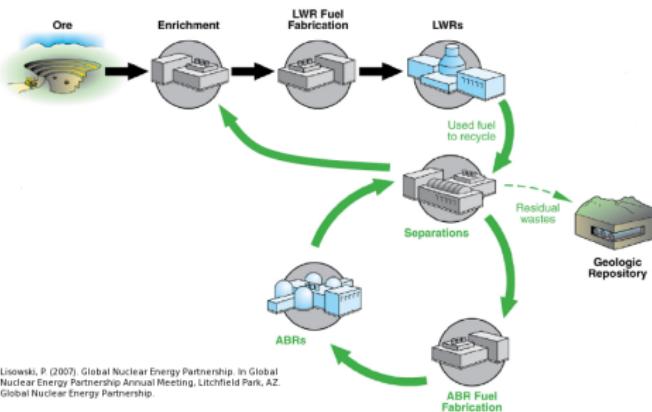


Figure: Top level simulators are intended to model the collective behavior of various fuel cycle decisions and strategies [?].



Need For an Integrated Repository Model

Current fuel cycle simulators neglect disposal system decisions and repository behavior. Most report masses and mass indexed metrics such as radiotoxicity, both meaningless without release pathway analysis and not informative for disposal system options.

Repository Capabilities within Systems Analysis Tools

Tool	Institution	Fuel Disposition	Radionuclide Transport	Heat Transport
NUWASTE [?]	NWTRB	yes	no	no
VISION [?]	INL	yes	no	YMR only
DANESS [?]	ANL	no	no	no
COSI [?]	CEA	yes	no	yes
NFCSim [?]	LANL	no	no	no
CAFCA [?]	MIT	no	no	no
ORION [?]	BNL	no	no	no
TSM [?]	OCRWM	yes	no	YMR only

Table: System tools are lacking in radionuclide transport and heat transport calculations in generic geologies.



Clay Disposal Environments

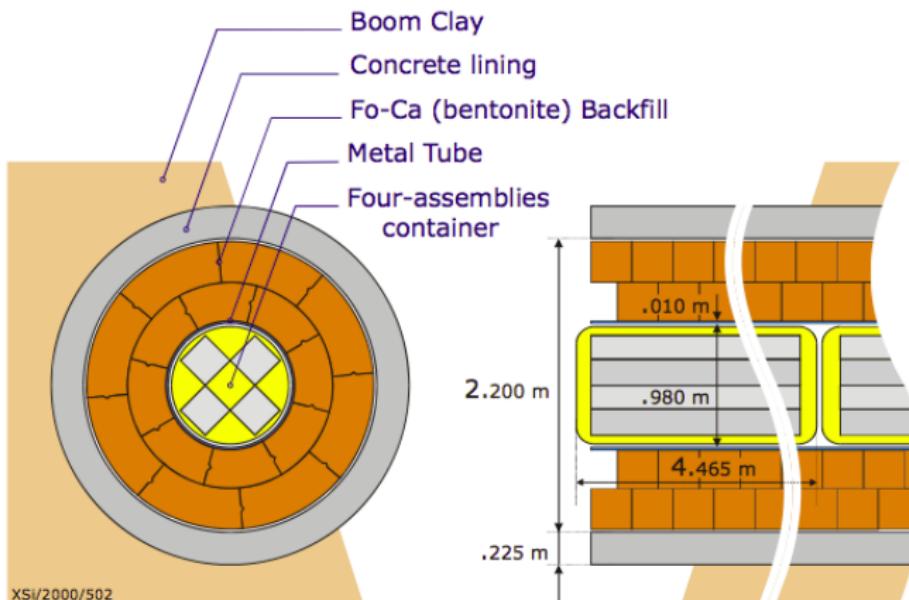


Figure: Belgian reference concept in Boom Clay [?].



Granite Disposal Environments

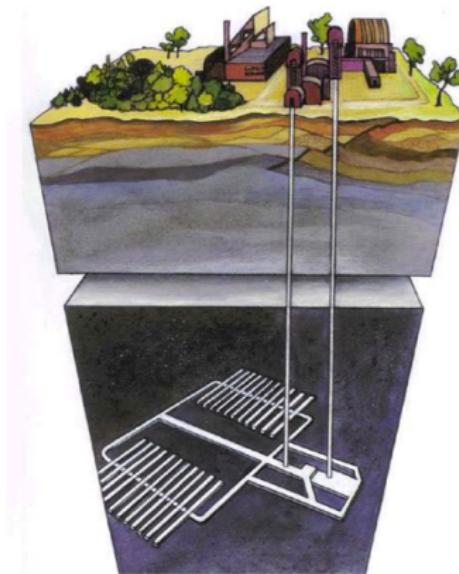


Figure: Czech reference concept in Granite [?].



Salt Disposal Environments

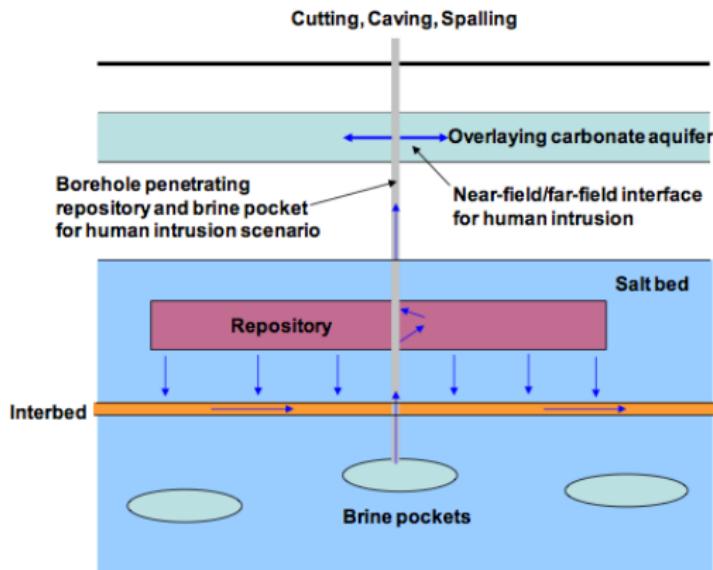


Figure: DOE-NE Used Fuel Disposition Campaign concept in Salt [?].



Deep Borehole Disposal Environment

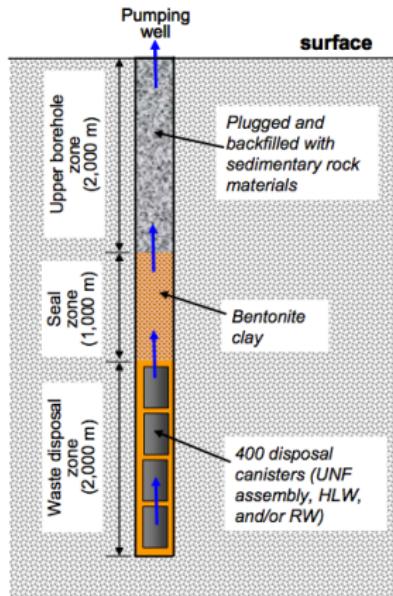
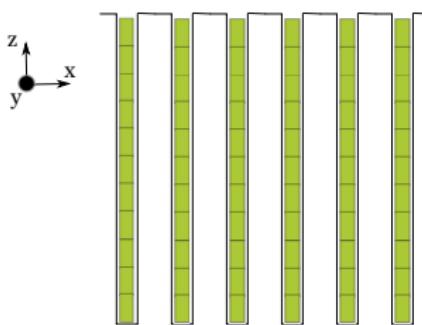


Figure: DOE-NE Used Fuel Disposition Campaign Deep Borehole concept [?].

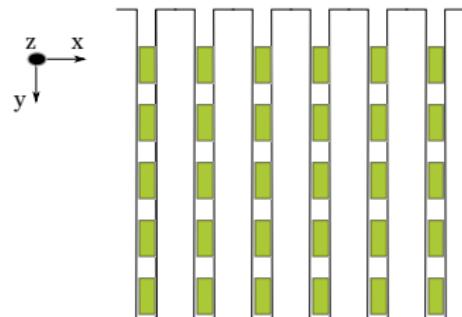


Repository Layouts

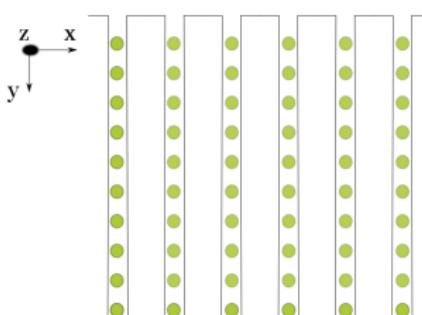
Deep Boreholes



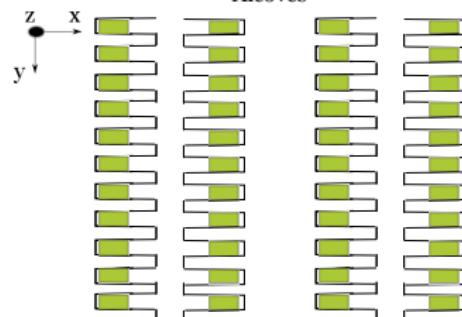
Horizontal In-Tunnel



Vertical In-Tunnel



Alcoves





All Disposal Environments

Features of Various Concepts

Feature	Clay	Granite	Salt	Deep Borehole
Hydrology				
Total Porosity [%]	34-60	0.1	0.5	0-0.5
Eff. Porosity [%]	0.5-5	0.0005	0.1	0.00005-0.01
Conductivity [m/s]	$10^{-11} - 10^{-9}$	$10^{-6} - 10^{-5}$	$10^{-12} - 10^{-10}$	$10^{-13} - 10^{-4}$
Fracturation	none	high	none	low at depth

Geochemistry

Reducing Oxidizing Salinity pH	Near & Far Field none higher at depth ~ 7	NF only Slight in FF higher at depth ≥ 7	NF only Slight in FF high ≥ 7	NF only Slight in FF high ~ 7
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Design

Waste Package Buffer Depth Emplacement Packages/Gallery	Steel, Cu -, Fo-Ca, Cement 100-500 m Vert., Horiz, Alcove one, many	Steel, Cu Fo-Ca, Cement 100-500 m Vert., Horiz. one, many	Steel Crushed Salt 100-500m Alcove one, two	Steel, Cement -, Fo-Ca, Cement 3-5km Vert. 400
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Thermal Behavior

Buffer Limit [$^{\circ}\text{C}$] Host Limit [$^{\circ}\text{C}$] Conductivity [$\frac{W}{m \cdot K}$] Coalescence	100 (Fo-Ca) 100 (alteration) 1 – 2 yes	100 (Fo-Ca) 200 (cracking) 2 – 4 no	180 180 (brines) ~ 4 yes	100 (Fo-Ca) none 2 – 4 no
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Radionuclide Transport

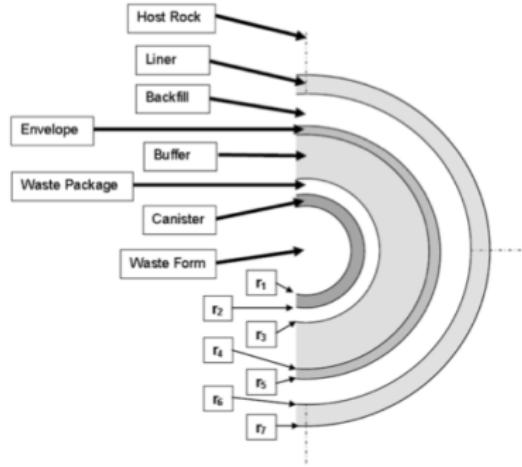


Figure: After waste package failure, radionuclides pass through successive layers of the engineered barrier system [?].

- Source Term - Radionuclide mass flux to the environment
 - Safety and Risk Metric
 - EPA Regulation
- Radionuclide transport is a function of
 - Geochemistry - chemically induced material degradation, radionuclide solubility limits, sorption, colloid mobility, etc.
 - Hydrology - water induced material degradation, water movement through pores and fractures, dissolved contaminant dispersion.
 - Thermal Effects - thermally induced material degradation, thermal hydrological effects.



Waste Form Release Models

Waste Form Types

WF Type	SubTypes	Contents	Release Drivers
Once Through	CSNF Ceramic Oxide CSNF Ceramic Oxide HTGR TRISO Graphite DSNF Metal DSNF Carbides DSNF Ceramic Oxides	Nominal BU UOx & MOX High BU UOx & MOX High BU High BU N Reactor Fuel Fast Reactor Fuels Research Reactor Fuels	redox rxns redox rxns, heat graphite rxns metal rxns, heat carbide rxns, heat redox rxns, heat
Borosilicate Glass	Current Future	MA, Cs/Sr Mo, no MA no Cs/Sr	heat, alteration alteration
Glass Ceramic	Glass Bonded Sodalite	Echem treated UOx, MOX	redox, alteration
Metal Alloy	From Echem From Aqueous	Cladding, noble metals transition metals	metal rxns, heat metal rxns, heat
Advanced Ceramic		volatized iodine	ceramic rxns, redox
Salt	Cementitious Sodium	separated streams	alkaline rxns, dissolution

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



Waste Package Failure Models

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

$$n_F = N \cdot f(). \quad (1)$$

This rate may be a physical function,

$$f() = N \cdot f(t, T, \dots). \quad (2)$$

or any time dependent function,

$$f() = f(t). \quad (3)$$

of which instantaneous failure is a special case,

$$f() = \delta(t - t_F). \quad (4)$$

as is the Weibull distribution,

$$f(t, \lambda, k) = \begin{cases} \frac{k}{\lambda} \left(\frac{t}{\lambda} \right)^{k-1} e^{-(t/\lambda)^k} & t \geq 0, \\ 0 & t < 0. \end{cases} \quad (5)$$



Waste Package Failure Models

Current Waste Package Failure Models

Model	WP Failure Mode	Details
TSP	Physical WAPDEG Model	$t_{delay} = 300,000$ years
Ahn 2003	Instantaneous Failure	$t = 0$
Ahn 2007	Instantaneous Failure	$T_f = 75,000$ years
Li	Physical WAPDEG model	$t_{delay} = 300,000$ years
Hedin 2003	Instantaneous Failure	$t_{delay} = 300$ years
UFD 2011	Instantaneous Failure	$t = 0$

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



Solute Transport in Permeable Porous Media

$$\frac{\partial nC}{\partial t} = -\nabla \cdot (F_c + F_{dc} + F_d) + m \quad (6)$$

where

n = solute accessible porosity [%]

C = concentration [$kg \cdot m^{-3}$]

t = time [s]

F_c = advective transport [$kg \cdot m^{-2} \cdot s^{-1}$]
 $= nvC$

F_{dc} = dispersive transport [$kg \cdot m^{-2} \cdot s^{-1}$]
 $= \alpha nv \nabla C$

F_d = diffusive transport [$kg \cdot m^{-2} \cdot s^{-1}$]
 $= D_e \nabla C$

m = solute source [$kg \cdot m^{-3} \cdot s^{-1}$].

v = pore velocity [$m \cdot s^{-1}$]

α = dispersivity [m]

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

and

$n \cdot v$ = Darcy velocity [$m \cdot s^{-1}$]. (7)



Dispersion

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

$$D = \alpha v + D_e \quad (8)$$

such that the mass conservation equation becomes:

$$\frac{\partial(nC)}{\partial t} = \nabla(nD\nabla C) - \nabla(nvC) \quad (9)$$

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

$$\frac{\partial(nC)}{\partial t} + \frac{\partial(s\rho_b)}{\partial t} = \nabla(nD\nabla C) - \nabla(nvC) \quad (10)$$

where

s = sorption coefficient

ρ_b = bulk (dry) density [kg/m^3].



Dimensionality

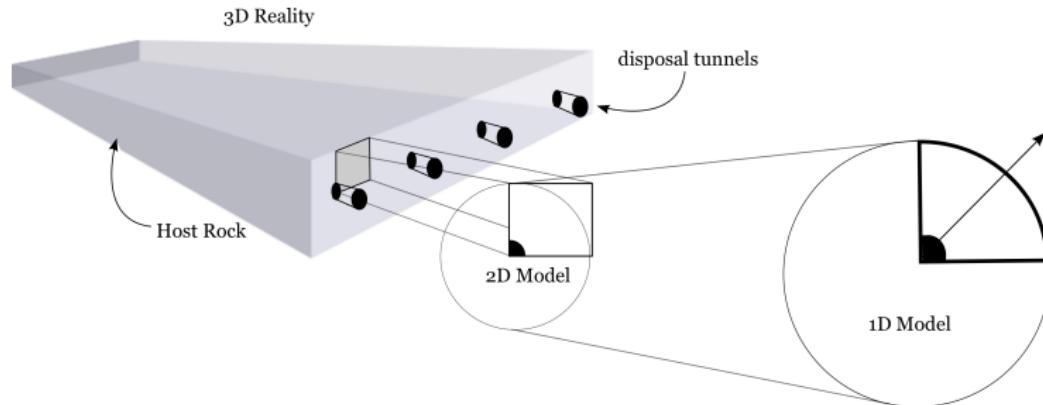


Figure: Employing the symmetries of the disposal layout can enable lower dimensional models.



Dispersion

For unidirectional flow, the unidirectional dispersion tensor gives

$$D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} + v_x \frac{\partial C}{\partial x} = R_f \frac{\partial(nC)}{\partial t}. \quad (11)$$



Diffusion

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

$$D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} + = R_f \frac{\partial(nC)}{\partial t}. \quad (12)$$



Precipitation

Elemental solubility limits are based on the maximum concentration of an element which can exist in solution.

$$m_{1i}(t) \leq v_{1i}(t) C_{sol} \quad (13)$$

where

m_{1i} = dissolved kg of radionuclide i

v_{1i} = void volume

C_{sol} = solubility limit



Sorption

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

$$\frac{\partial(s\rho_b)}{\partial t} = (R_f - 1) \frac{\partial(nC)}{\partial t} \quad (14)$$

equation (10) becomes

$$\nabla(nD\nabla C) - \nabla(nv) = R_f \frac{\partial(nC)}{\partial t} \quad (15)$$

where

R_f = retardation factor

$$= 1 + \frac{\rho_b K_d}{n} \quad (16)$$

ρ_b = bulk density of the rock matrix

and

K_d = species distribution coefficient.



One Dimensional Solution with a Constant Concentration Source

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

$$C(0, t) = C_0 \quad (17)$$

and

$$\left. \frac{\partial C}{\partial x} \right|_{x=\infty} = 0 \quad (18)$$

as well as the initial condition

$$C(x, 0) = 0 \text{ for } x \in (0, \infty), \quad (19)$$

the Ogata and Banks solution gives

$$C(x, t) = \frac{C_0}{2} \left[\operatorname{erfc} \left(\frac{x - \frac{v_x t}{R_f}}{2\sqrt{\frac{D_x t}{R_f}}} \right) + e^{\frac{v_x x}{D_x}} \operatorname{erfc} \left(\frac{x + \frac{v_x t}{R_f}}{2\sqrt{\frac{D_x t}{R_f}}} \right) \right]. \quad (20)$$

where

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2} dt. \quad (21)$$



Heat Limits In Geology

Important heat limits in materials of the repository restrict loading designs and capacity.

Thermal Behavior of Various Concepts

Feature	Clay	Granite	Salt	Deep Borehole
Buffer Limit [°C]	100 (Fo-Ca)	100 (Fo-Ca)	180	100 (Fo-Ca)
Host Limit [°C]	100 (alteration)	200 (cracking)	180 (brines)	none
Conductivity [$\frac{W}{m \cdot K}$]	1 – 2	2 – 4	~ 4	2 – 4
Coalescence	yes	no	yes	no



Impact of Repository Designs

Yucca Mounting Footprint Expansion Calculations

Author	Max. Capacity <i>tonnes</i>	Footprint <i>km</i> ²	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	6.5 126,000 189,000 189,000 252,000 378,000 567,000	Base Case CSNF expanded footprint multi-level design grouped drifts hybrid hybrid hybrid

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



Heat Based Capacity

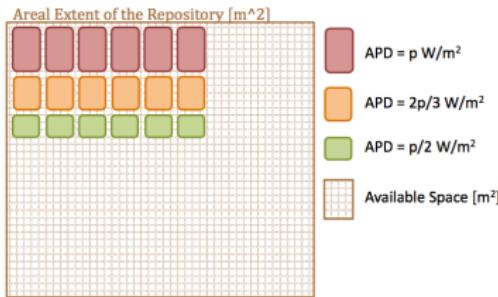


Figure: Areal Power Density (APD) can be used to determine appropriate repository loading for arbitrary waste streams.

Loading is subject to the constraints,

$$P_{\text{tot}} \leq P_{\max} \quad (22)$$

$$APD_i \leq APD_{\max} \quad (23)$$

where

$$P_{\max} = A \cdot APD_{\max} \quad (24)$$

$$P_{\text{tot}} = \sum_{i=0}^N n_i P_i \quad (25)$$

P_i = power of package i

n_i = ith package

N = number of packages

APD_{\max} = max areal power density



Detailed Techniques

Models of Heat Load for Various Geologies

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

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

Similar heat transport models can be used for all geologies, but are differentiated by material parameters (c_p, K, ρ) and different thermal constraints.



ANL model

A model created by the UFD team at Argonne national lab using the SINDA\G heat transport framework employs a lumped parameter model and an optimization loop to arrive at a minimal drift spacing for a given waste stream in agreement with user input thermal limits.

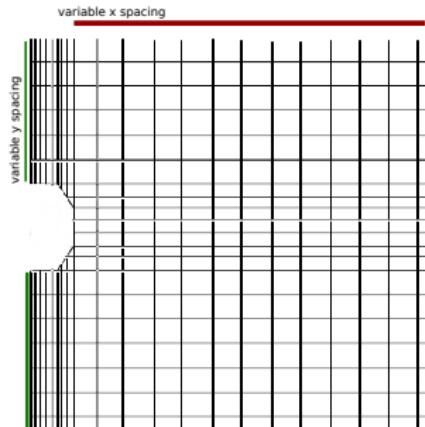


Figure: Two adjustable geometric dimensions of the ANL model [?].



Lumped Parameter Technique

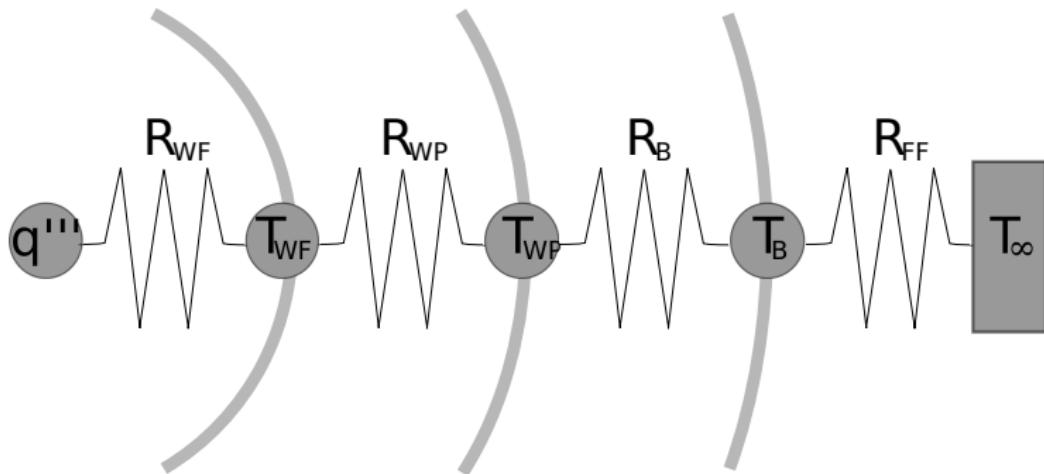


Figure: The lumped parameter analogy used for heat transfer can be applied to the one dimensional approximation to the disposal system concept.



LLNL Model : Geometry

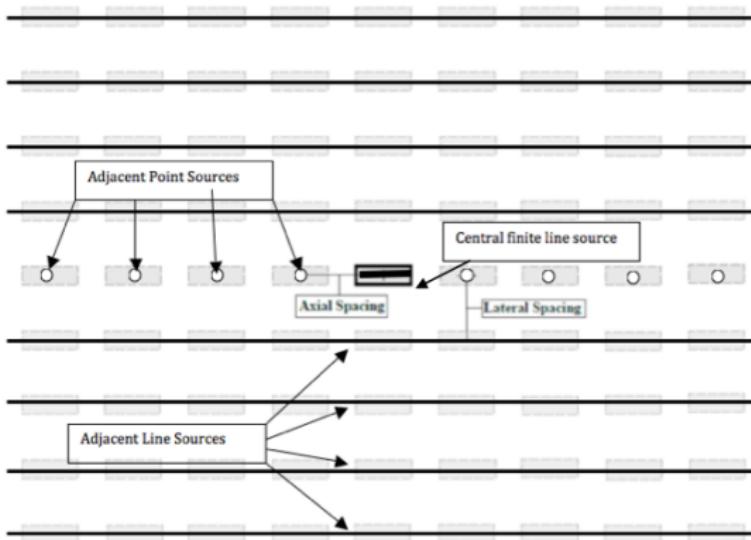
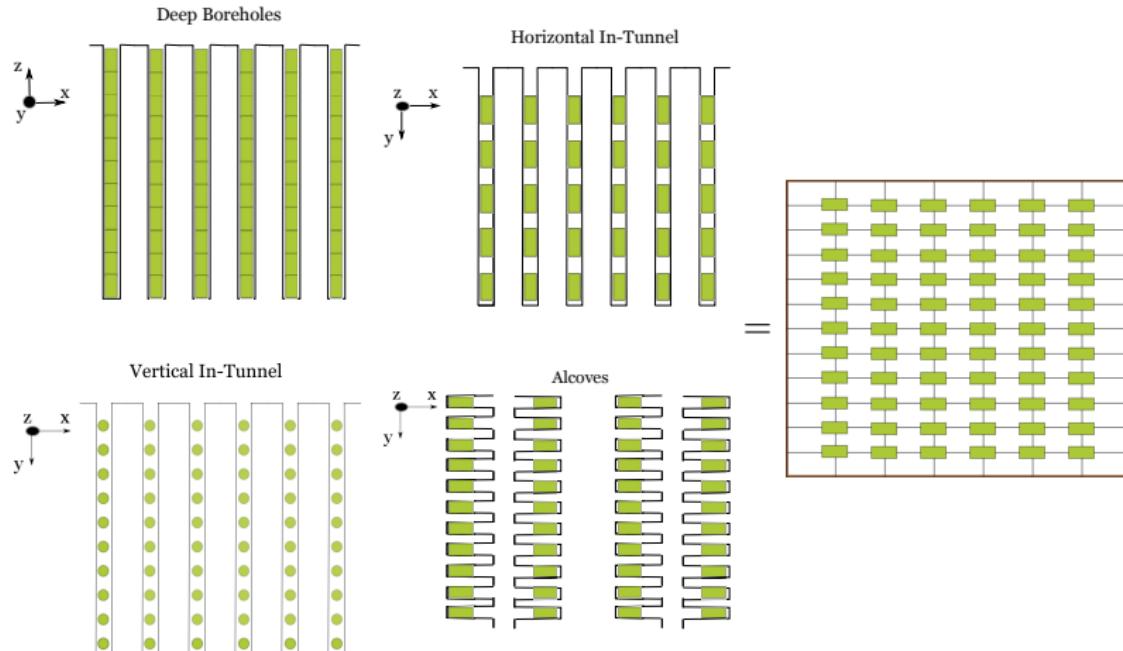


Figure: Vertical, horizontal, alcove, and borehole emplacement layouts can be represented by a line of point sources and adjacent line sources [?].



Repository Layouts





LLNL Model : Solution Strategy

A MathCAD solution of the transient homogeneous conduction equation,

$$\nabla^2 T = \frac{1}{\alpha} \frac{\partial T}{\partial t}. \quad (26)$$

Superimposed point and line source solutions approximate the repository layout. The solution of this equation at the boundary of the EBS and the waste package is then treated as a boundary condition for the heterogeneous steady state equation,

$$\dot{q} = UA_{out} (T_{in} - T_{out}) \quad (27)$$

where

$$U = \frac{1}{\sum_i R_i} \quad (28)$$

which, for the detailed EBS becomes

$$U = \frac{1}{R_{WF} + R_{WP} + R_{buffer} + \dots} \quad (29)$$

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

Outline





Cyclus Modular Architecture and Open Development

The combination of modular encapsulation within the software architecture and an open development paradigm allows for simulation at multiple levels of simulation detail.



Encapsulation

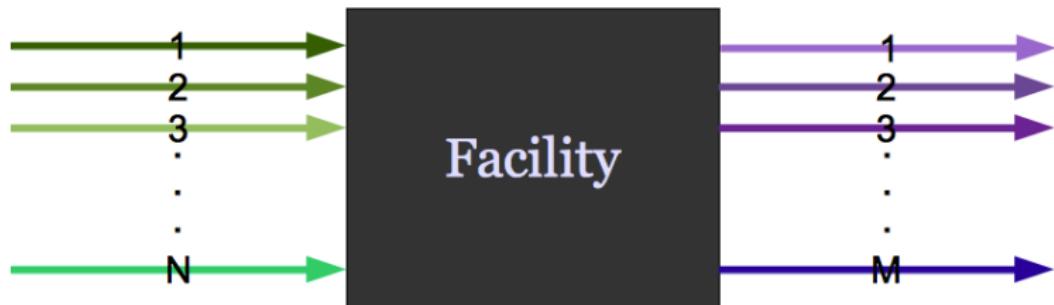


Figure: Regions, Institutions, Facilities, and Markets are all black boxes.



Module Interfaces

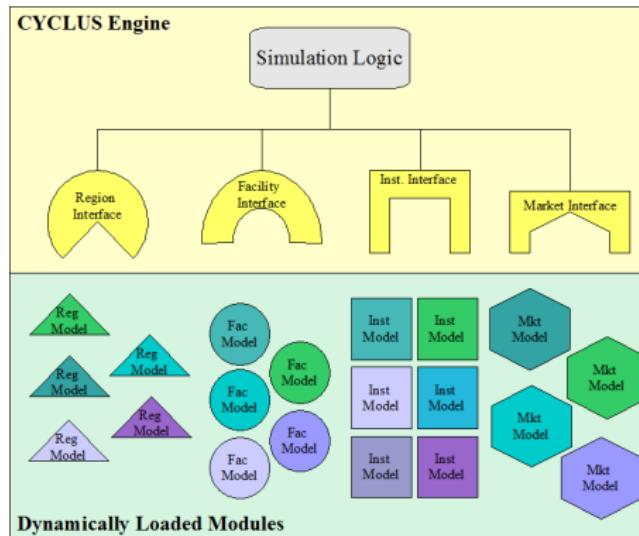


Figure: Well defined model interfaces facilitate model interchange. The user may choose the model at their desired level of detail.



Facilities Are Black Boxes

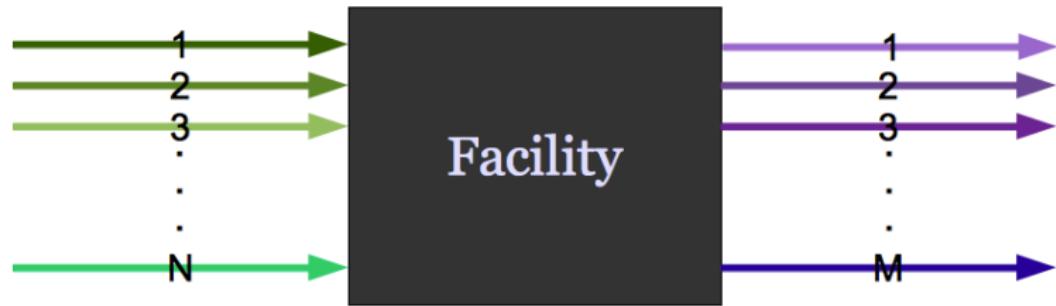


Figure: Each facility in the simulation makes requests and offers to fill its stocks and empty its inventory respectively.



Facilities Are Black Boxes



Figure: A facility might only make offers.



Facilities Are Black Boxes

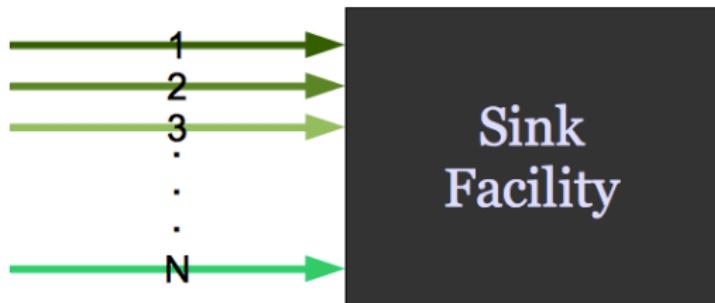


Figure: A facility might only make requests.



Each Commodity is Associated with a Market



Figure: A market receives offers and requests concerning its commodity.



The Market Solves the Matching Problem

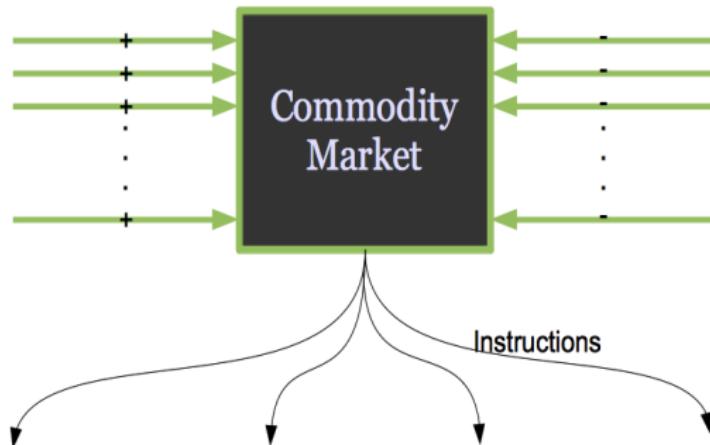


Figure: When the Market's arbitrary algorithm solves the matching problem, the Market sends instructions to the offering facilities.



A Simple Example

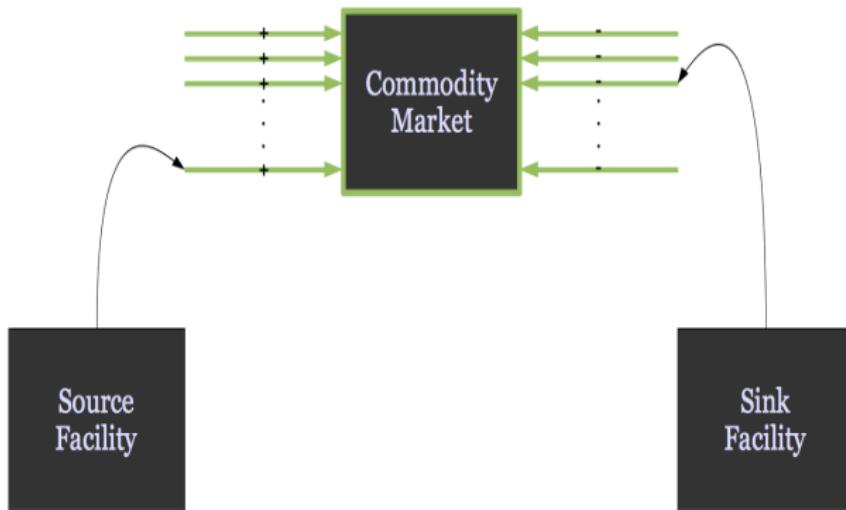


Figure: The source sends an offer and the sink sends a request.



A Simple Example

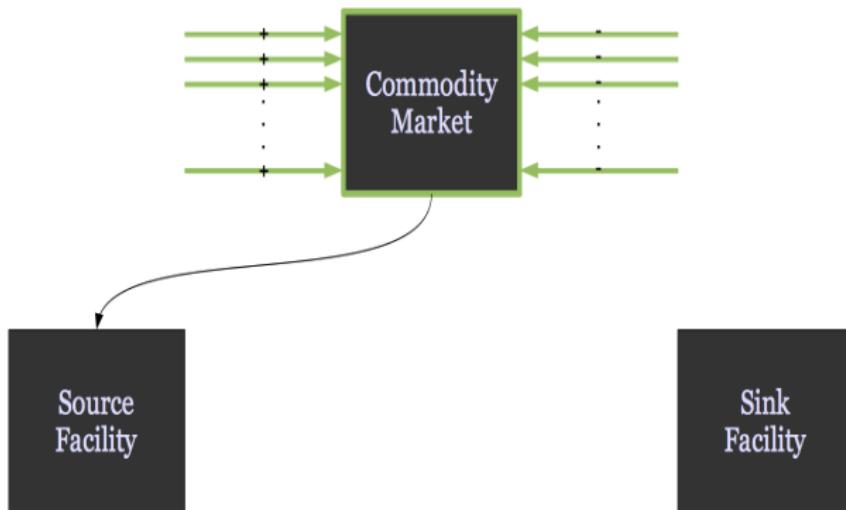


Figure: The Market solves the problem and instructs the source facility to send a certain amount to the sink facility.



A Simple Example

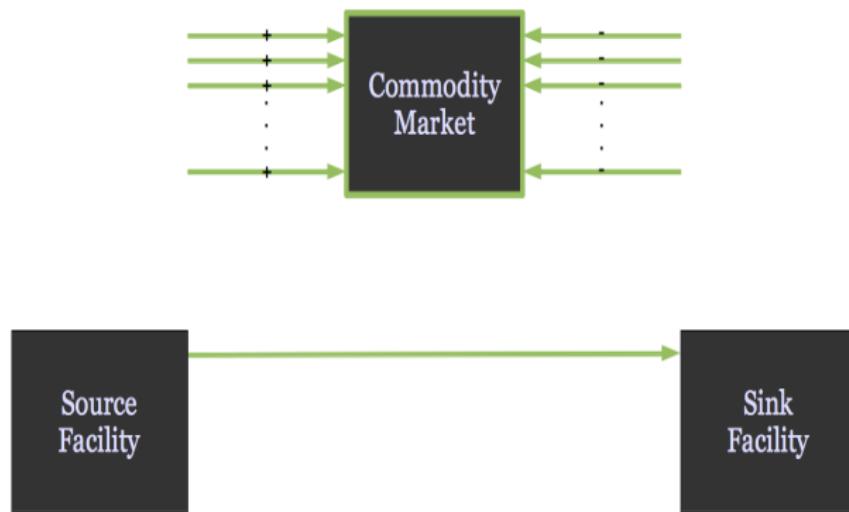


Figure: The source facility sends the material directly to the sink facility.



This Market Model Scales for Complex Systems

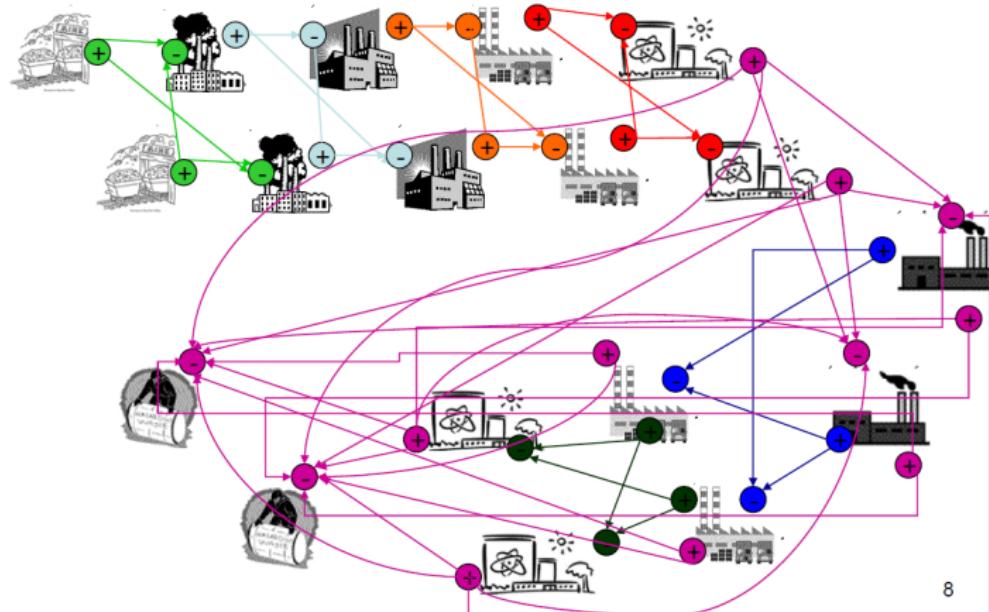


Figure: Well designed interfaces and strict encapsulation support scalability of the Market-based simulation paradigm [?]



Nested Components

Quantities Calculated Each Timestep

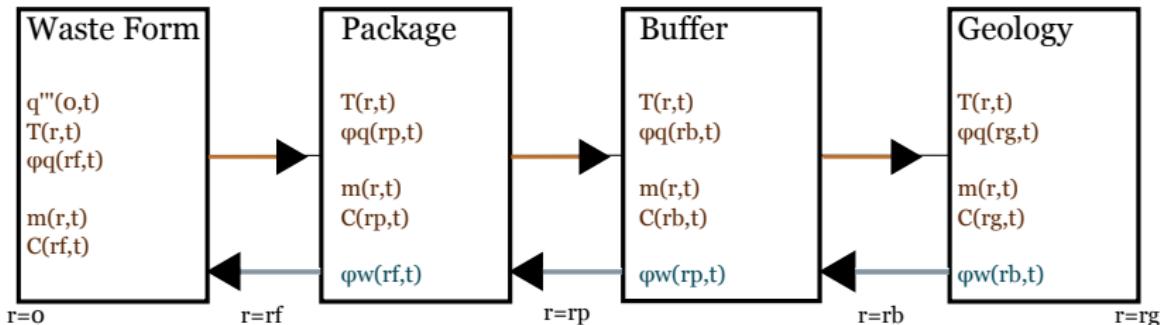
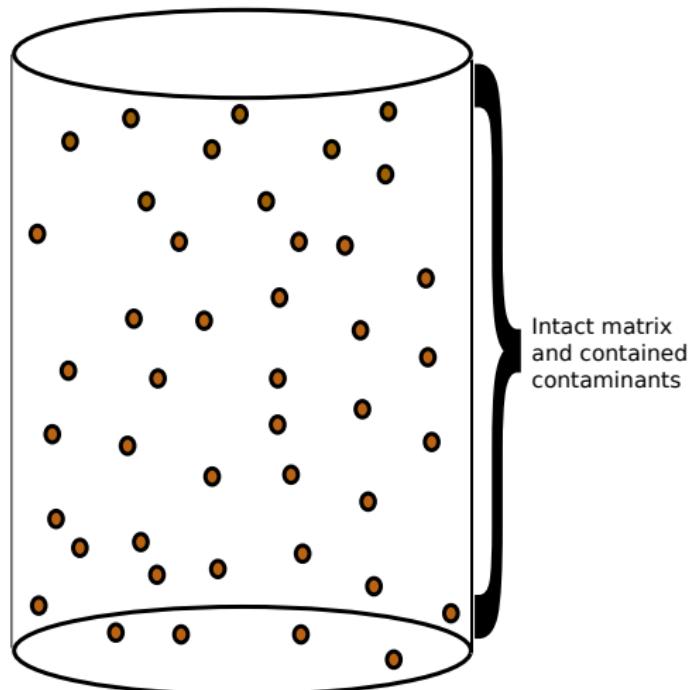


Figure: The nested components supply thermal flux and concentration information to each other at the boundaries.

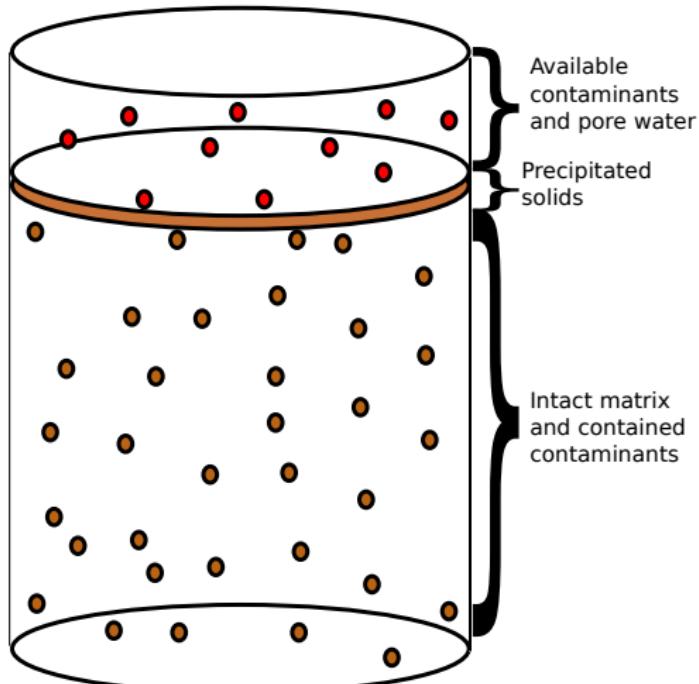


Mixed Cell : Permeable Porous Medium





Mixed Cell : Permeable Porous Medium with Degradation





Nested Components

- Waste Form
 - Mixed Cell
 - with Rate Based Degradation Model
 - and solubility limits
 - Data for various waste forms
- Waste Package
 - Rate Based Failure Model
 - Data for various waste packages
- Buffer
 - Mixed Cell
 - with Rate Based Degradation Model
 - Data for various buffers
- Geology
 - Solute transport model
 - Data for various geologies



Outline



Demonstration Case : Code Development

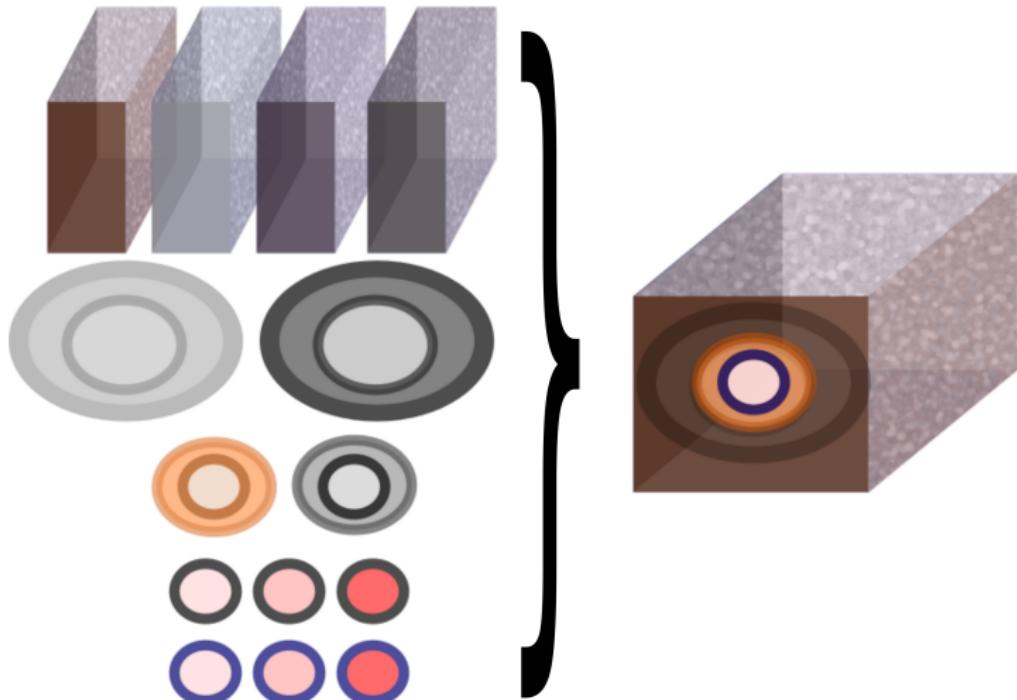
The demonstration case is an empty software architecture in which to implement the physical models. This demonstration will build and test

- component module loading of models and data
- information passing between modules
- and database writing.



Demonstration Case : Module Loading

With a dynamic, plug-in implementation, repository model can be loaded as a shared library at runtime.



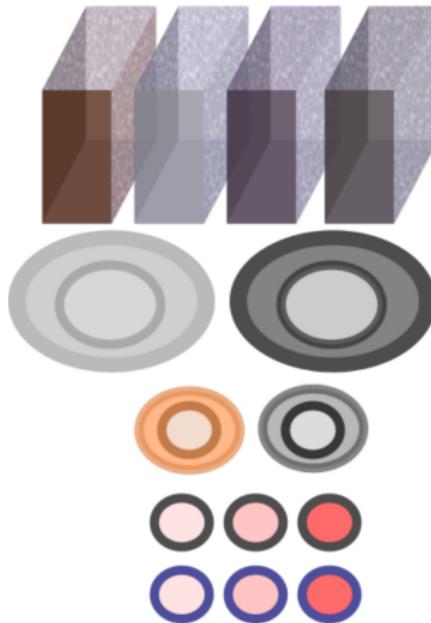


Base Case : Nested Components

- Waste Form
 - Mixed Cell with Rate Based Degradation Model
 - Glass and UOx Data
- Waste Package
 - Rate Based Failure Model
 - Steel and Copper Data
- Buffer
 - Mixed Cell with Rate Based Degradation Model
 - Bentonite (Fo-Ca), Salt, and Cement Data
- Geology
 - Ogata and Banks 1D Permeable Porous Medium Solute Transport
 - Data for Clay, Granite, Salt, and Crystalline Basement



Base Case : Components



Selection of geology

- Clay, Granite, Salt, Crystalline Basement
- Dimensions
- Porosity, n
- Tortuosity, τ
- Bulk Density, ρ
- Fracturation, k_{eff}

Selection of buffer

- Bentonite, cement, salt
- Dimensions
- Porosity, n
- Tortuosity, τ
- Bulk Density, ρ

Selection of Waste Package

- Copper, Steel
- Failure model function
- Dimensions

Selection of Waste Form

- Glass, UO₂
- Degradation function
- Dimensions
- Porosity, n
- Tortuosity, τ
- Bulk Density, ρ



Base Case : Waste Form Abstraction

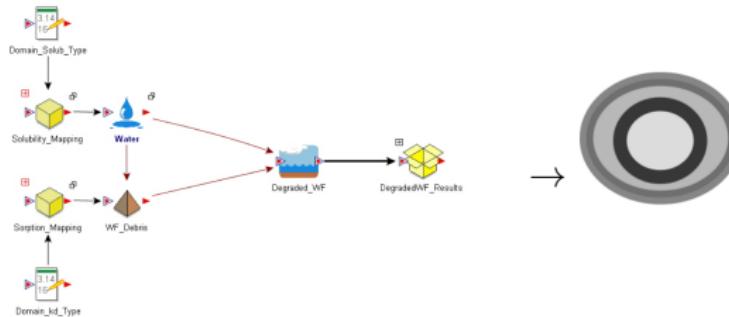


Figure 4-9. GoldSim GPAM Degraded Waste Form Domain Elements.

Parameters of Interest

- Failure model function
- Dimensions
- Density, ρ



Base Case : Waste Package Abstraction

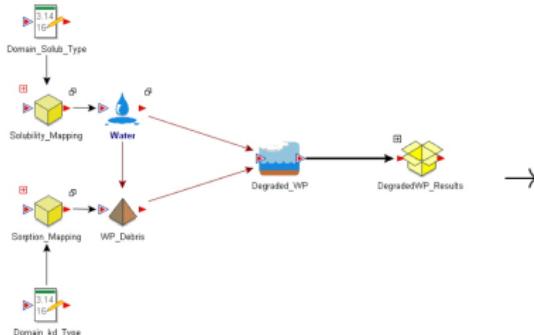


Figure 4-10. GoldSim GPAM Degraded Waste Package Domain Element.

Parameters of Interest

- Degradation function
- Dimensions
- Porosity, n
- Tortuosity, τ
- Bulk Density, ρ



Base Case : Buffer Abstraction

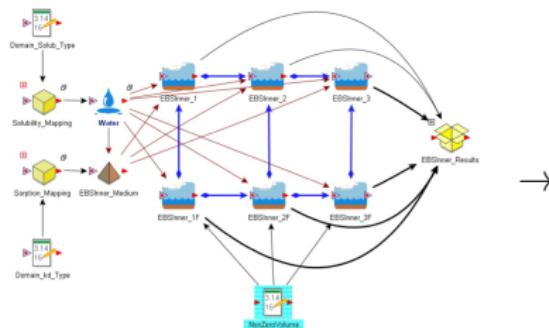
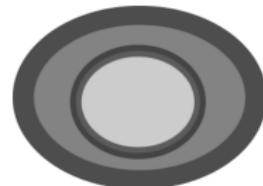


Figure 4-11. GoldSim GPAM EBS Inner Domain elements.



Parameters of Interest

- Dimensions
- Porosity, n
- Tortuosity, τ
- Bulk Density, ρ
- Sorption
- Precipitation



Base Case : Geology Abstraction

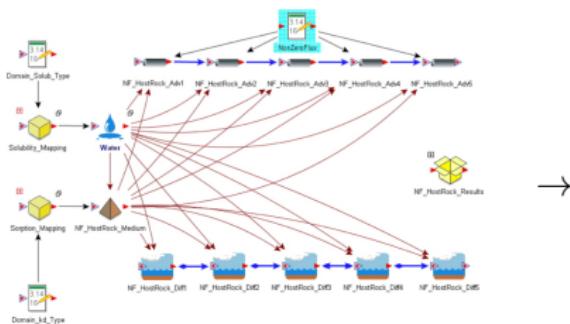
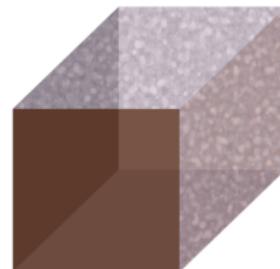


Figure 4-13. GoldSim GPAM Near Field Host Rock Domain elements.

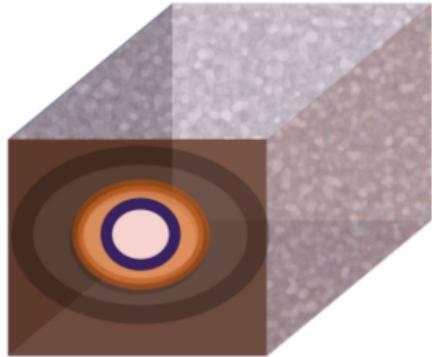


Parameters of Interest

- Tunnel Layout
- Porosity, n
- Tortuosity, τ
- Bulk Density, ρ
- Fracturation, k_x



Base Case : System Level Abstraction



Vs.

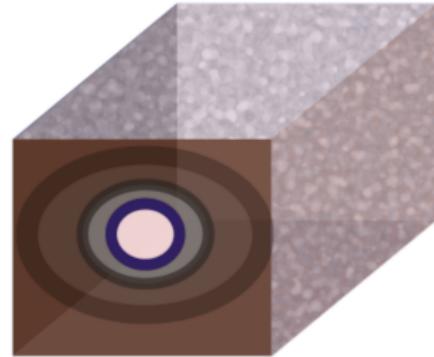


Figure: System level abstraction seeks to determine the systems level response to the change in models of subcomponents.



Extensions : Fracturation

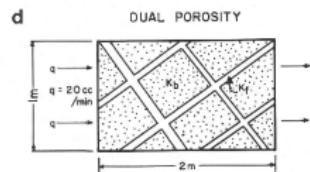
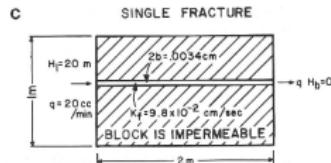
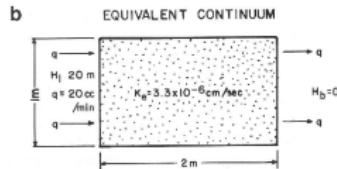
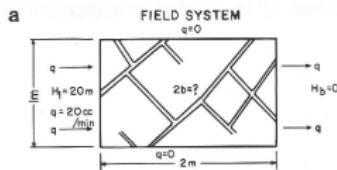


Fig. 12.6 Conceptual models of a fractured rock system (modified from Gale, 1982).
 (a) A simplified fracture network of aperture $2b$ with groundwater flow from left to right.
 (b) Equivalent porous medium model of (a).
 (c) Discrete fracture model of (a).
 (d) Dual porosity medium model of (a).

A dual continuum model will be implemented to more accurately represent fractured host media such as granite [?].



Extensions : Sorption

Table 3 Retardation factors for important radionuclides in rock materials being considered for repository siting^a

Element	$R_f = 1 + K_d \times \frac{\text{density of rock}}{\text{porosity of rock}} = \frac{\text{rate of groundwater movement}}{\text{rate of radionuclide movement}}$				
	Granite	Basalt	Tuff (volcanic ash)	Shale or clay	Salt
Sr	20–4,000	50–3,000	100–100,000	100–100,000	10–50
Cs	200–100,000	200–100,000	500–100,000	200–100,000	40–100
I	1	1	1	1	1
Tc	1–40	1–100	1–100	1–40	1–10
U	20–500	50–500	10–400	50–2,000	20–100
Np	10–500	10–200	10–200	40–1,000	10–200
Pu	20–2,000	20–10,000	50–5,000	50–100,000	40–4,000
Am	500–10,000	100–1,000	100–1,000	500–100,000	200–2,000

^a The table is compiled from reported experimental values in many sources. The high figure in each range is an estimate for assumed most common repository conditions ($Eh = -0.2$ to -0.3 V, $pH = 7$ to 9); the low figure is an estimate of the minimum value under less favorable conditions of Eh , pH , or complexing. The numbers for salt do not refer to sorption on salt itself, but rather on ordinary rock material in the vicinity of a salt repository, where the groundwater may be fairly concentrated brine.



Extensions : Coalescence

Salt and clay exhibit coalescent behavior under heat.



Integrated Used Fuel Disposition and Repository Model



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