An Integrated Used Fuel Disposition and Generic Repository Model

A Nuclear Engineering and Engineering Physics PhD Preliminary Report

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Outline

Future Disposal System Options

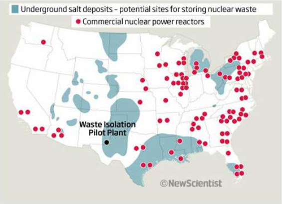


Figure: ref. [12]

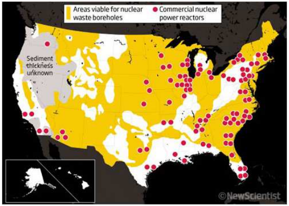


Figure: ref. [12]

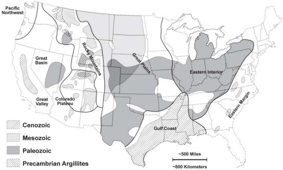


Figure: ref. [7]

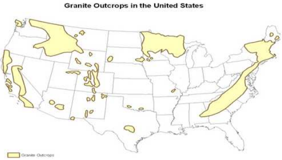


Figure: ref. [6]

Future Fuel Cycle Options

Domestic Fuel Cycle Options

Title	Description	Challenges
Open	Once Through	High Temperatures, Volumes
Modified Open	Partial Recycling	Both high volumes and myriad fuel streams
Closed	Full Recycling	Myriad fuel streams

Table: Domestic Fuel Cycle Options

Methodology : Modularity

Interchangeable Subcomponents, integration with fuel cycle model.

Methodology : Abstraction for Efficiency

Abstratction GPAM GDSM

Outline

Top Level Fuel Cycle Simulators

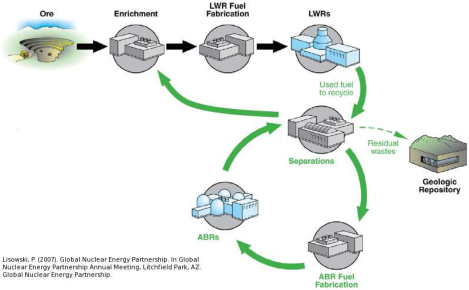


Figure: Top level simulators are intended to model the collective behavior of various fuel cycle decisions and strategies.[?]

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 geolgies.

Clay Disposal Environments

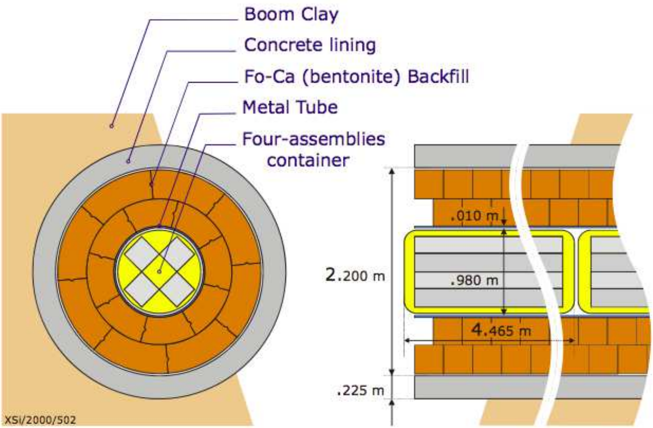


Figure: Belgian reference concept in Boom Clay.[?]

Granite Disposal Environments

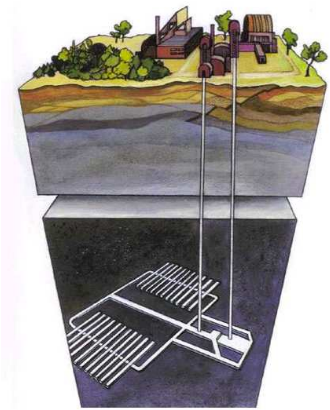


Figure: Czech reference concept in Granite.[?]

Salt Disposal Environments

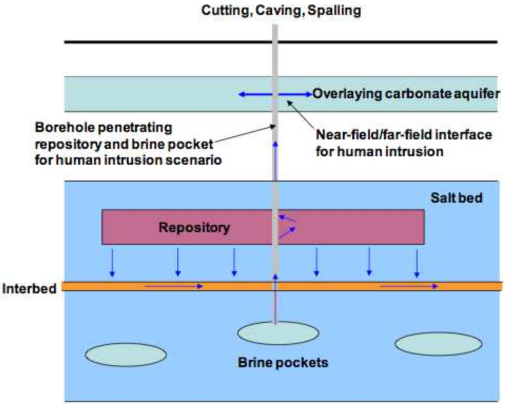


Figure: Used Fuel Division reference concept in Salt.[?]

Deep Borehole Disposal Environment

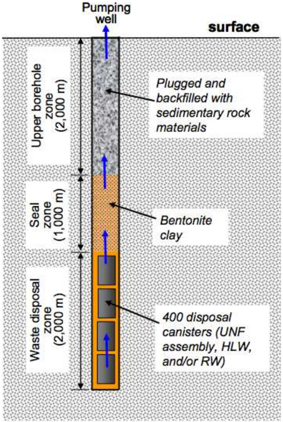
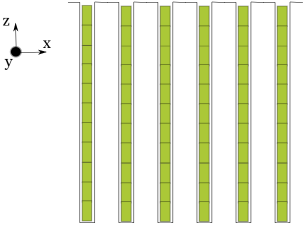


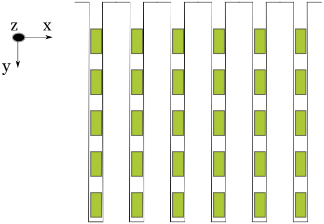
Figure: Used Fuel Division reference Deep Borehole concept.[?]

Repository Layouts

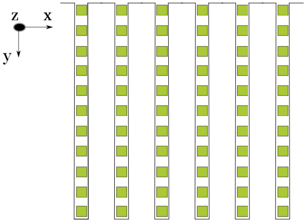
Deep Boreholes



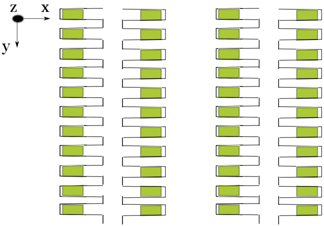
Horizontal In-Tunnel



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	Near & Far Field	NF only	NF only	NF only
Oxidizing	none	Slight in FF	Slight in FF	Slight in FF
Salinity	higher at depth	higher at depth	high	high
pH	~ 7	≥ 7	≥ 7	~ 7
Design				
Waste Package	Steel or Cu	Steel	Steel	Steel,Cement
Buffer	-,Fo-Ca,Cement	Fo-Ca,Cement	Crushed Salt	-,Fo-Ca,Cement
Depth	100-500 m	100-500 m	100-500m	3-5km
Emplacement	Vert.,Horiz,Alcove	Vert.,Horiz.	Alcove	Vert.
Packages/Gallery	one, many	one, many	one, two	400
Thermal Behavior				
Buffer Limit [$^\circ C$]	100 (Fo-Ca)	100 (Fo-Ca)	180	100 (Fo-Ca)
Host Limit [$^\circ C$]	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

Radionuclide Transport

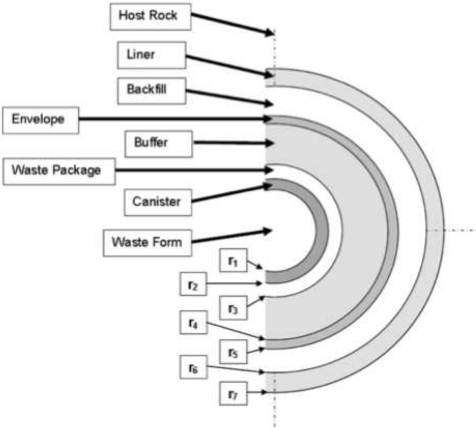


Figure: After waste package failure, radionuclides pass through successive layers of the engineered barrier system [?].

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 [5]

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Waste Package Failure Models

Current Waste Package Failure Models

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

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

Solute Transport in Permeable Porous Media

$$\frac{\partial nC}{\partial t} = -\nabla \cdot (F_c + F_{dc} + F_d) + m \tag{1}$$

where

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

$$\begin{aligned}
m &= \text{ solute source } [kg \cdot m^{-3} \cdot s^{-1}]. \\
v &= \text{ pore velocity } [m \cdot s^{-1}] \\
\alpha &= \text{ dispersivity } [m] \\
D_e &= \text{ effective diffusion coefficient } [m^2 \cdot s^{-1}]
\end{aligned}$$

and

$$n \cdot v = \text{ Darcy velocity } [m \cdot s^{-1}]. \tag{2}$$

Dispersion

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

$$D = \alpha v + D_e \tag{3}$$

such that the mass conservation equation becomes:

$$\nabla\left(nD\nabla C\right) - \nabla\left(nv\right) = \frac{\partial(nC)}{\partial t} \tag{4}$$

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

$$\nabla\left(nD\nabla C\right) - \nabla\left(nv\right) = \frac{\partial(nC)}{\partial t} + \frac{\partial(s\rho_b)}{\partial t} \tag{5}$$

where

$$s = \text{sorption coefficient}$$
$$\rho_b = \text{ bulk (dry) density } [kg/m^3].$$

Dispersion

For unidirectional flow, the unidirectional dispersion tensor gives

$$D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} + v_x \frac{\partial C}{\partial x} = R_f \frac{\partial (nC)}{\partial t}. \tag{6}$$

Diffusion

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

$$D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} + D_z\frac{\partial^2 C}{\partial z^2} + = R_f\frac{\partial (nC)}{\partial t}. \tag{7}$$

Precipitation

Sorption

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

$$\frac{\partial(s\rho_b)}{\partial t} = (R_f - 1)\frac{\partial(nC)}{\partial t} \tag{8}$$

equation (5) becomes

$$\nabla\left(nD\nabla C\right) - \nabla\left(nv\right) = R_f\frac{\partial(nC)}{\partial t} \tag{9}$$

where

$$\begin{aligned} R_f &= \text{retardation factor} \\ &= 1 + \frac{\rho_b K_d}{n} \\ \rho_b &= \text{bulk density of the rock matrix} \end{aligned} \tag{10}$$

and

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

Dimensionality

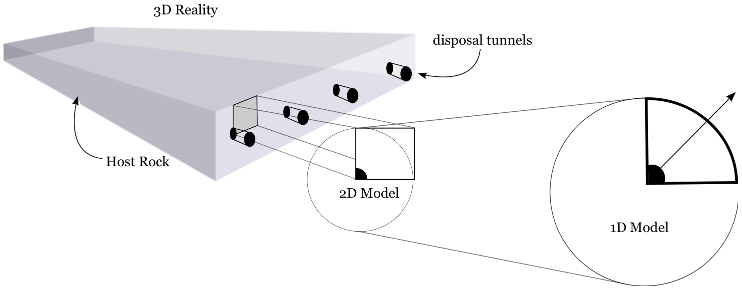


Figure: Employing the symmetries of the disposal layout can enable lower dimensional models.

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

$$C(0,t) = C_0 \tag{11}$$

and

$$\frac{\partial C}{\partial x}\Big|_{x=\infty} = 0 \tag{12}$$

as well as the initial condition

$$C(x,0) = 0 \text{ for } x \in (0,\infty), \tag{13}$$

the so called Ogata and Banks solution gives

$$C(x,t) = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{x - \frac{v_x t}{R_f}}{2\sqrt{\frac{D_x t}{R_f}}}\right) + e^{\frac{v_x x}{D_x}} \operatorname{erfc}\left(\frac{x + \frac{v_x t}{R_f}}{2\sqrt{\frac{D_x t}{R_f}}}\right)\right]. \tag{14}$$

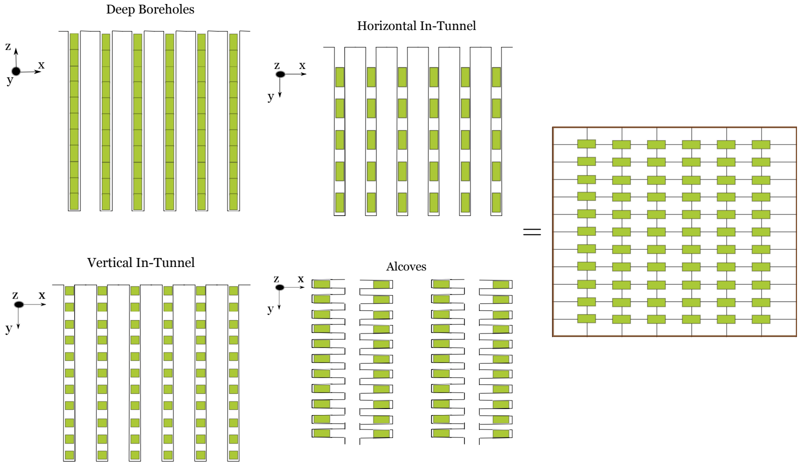
where

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-t^2}dt \tag{15}$$

Analytical Models

- Specific Temperature Integral
- Specific Temperature Change
- Lumped Parameter Model and ANL model
- Fully Analytic LLNL Model

Repository Layouts



Heat Limits In Geology

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

Heat Based Capacity

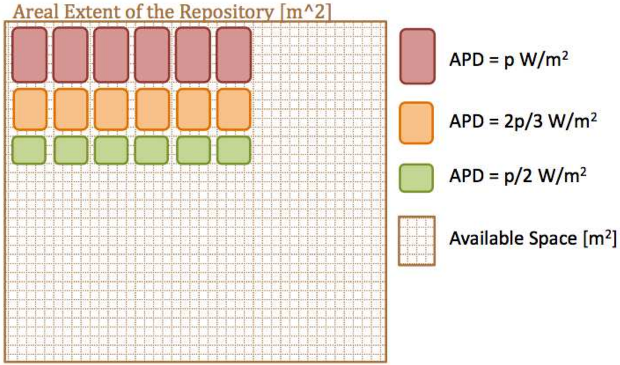


Figure: Areal Power Density (APD) can be used to determine appropriate repository loading for arbitrary waste strems.

Loading is subject to the constraints,

Impact of Repository Designs

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

Lumped Parameter Technique

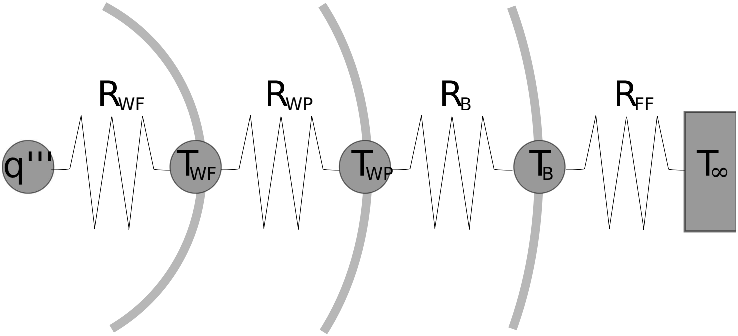


Figure: The lumped parameter analogy used for heat transfer can be applied to the one dimensional approximation to the disposal system concept.

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.

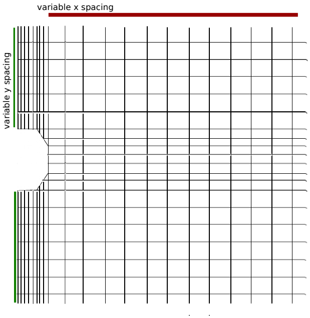


Figure: Two adjustable geometric dimensions of the ANL model [?].

LLNL Model : Geometry

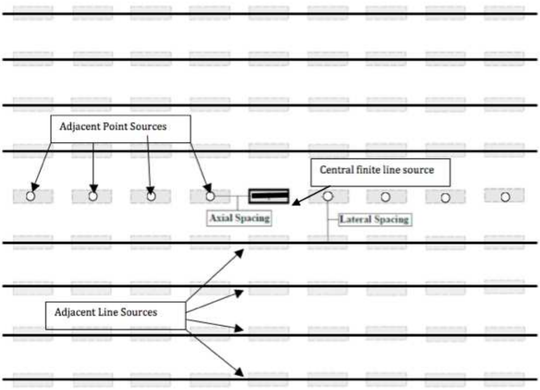


Figure: Vertical, horizontal, alcove, and borehole emplacement layouts can be represented by a line of point sources and adjacent line sources [?].

LLNL Model : Solution Strategy

A MathCAD solution of the transient homogeneous conduction equation,

$$\nabla^2 T = \frac{1}{\alpha}\frac{\partial T}{\partial t}. \tag{20}$$

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

$$\dot{q} = UA_{out}\left(T_{in} - T_{out}\right) \tag{21}$$

where

$$U = \frac{1}{\sum_i R_i} \tag{22}$$

which, for the detailed EBS becomes

$$U = \frac{1}{R_{WF} + R_{WP} + R_{buffer} + \cdots} \tag{23}$$

which calculates a resulting temperature gradient through the geometry at each

Heat Based Drift Loading

Detailed Techniques

Models of Heat Load for Various Geologies

Source (Who)	Nation (Where)	Geology (What)	Methodology (How)
Enresa [15]	Spain	Granite	CODE_BRIGHT 3D Finite Element
NRI [15]	Czech Rep.	Granite	Specific Temperature Integral
ANDRA [4]	France	Granite	3D Finite Element CGM code
SKB [1]	Sweden	metagranite	1D-3D Site Descriptive Models
SCK·CEN [15]	Belgium	Clay	Specific Temperature Integral
ANDRA [3]	France	Argile Clay	3D Finite Element CGM code
NAGRA [9, 10]	Switzerland	Opalinus Clay	3D Finite Element CGM code
GRS [15]	Germany	Salt	HEATING (3D finite difference)
NCSU(Li) [11]	USA	Yucca Tuff	Specific Temperature Integral
NCSU(Nicholson) [13]	USA	Yucca Tuff	COSMOL 3D Finite Element
Radel & Wilson [14]	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.

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

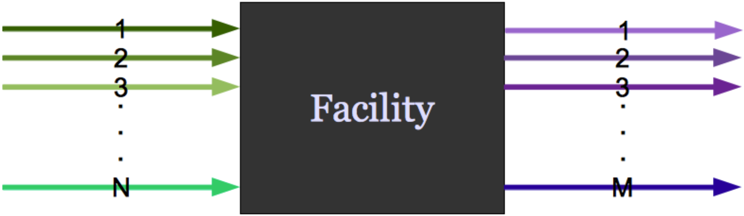


Figure: Regions, Institutions, Facilities, and Markets are all black boxes.

Module Interfaces

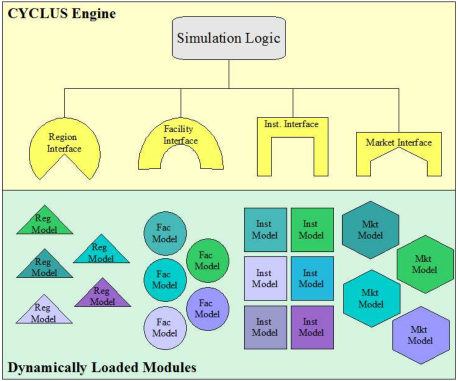


Figure: Well defined model interfaces facilitate model interchange. The user may choose the model at their desired level of detail.

Facilities Are Black Boxes

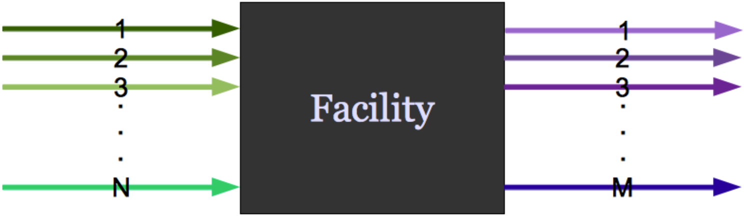


Figure: Each facility in the simulation makes requests and offers to fill its stocks and empty its inventory respectively.

Facilities Are Black Boxes

Figure: A facility might only make offers.

Facilities Are Black Boxes

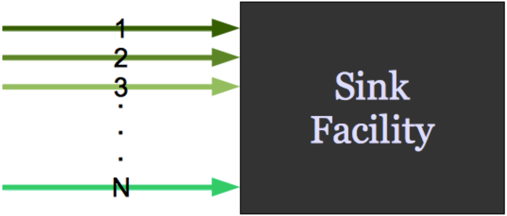


Figure: A facility might only make requests.

Each Commodity is Associated with a Market

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

The Market Solves the Matching Problem

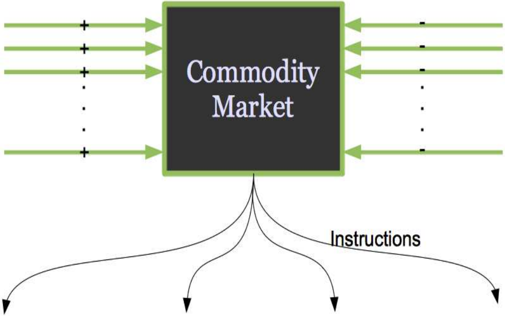


Figure: When the Market's arbitrary algorithm solves the matching problem, the Market sends instructions to the offering facilities.

A Simple Example

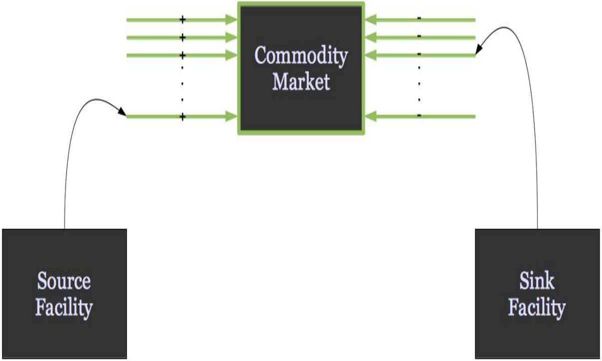


Figure: The source sends an offer and the sink sends a request.

A Simple Example

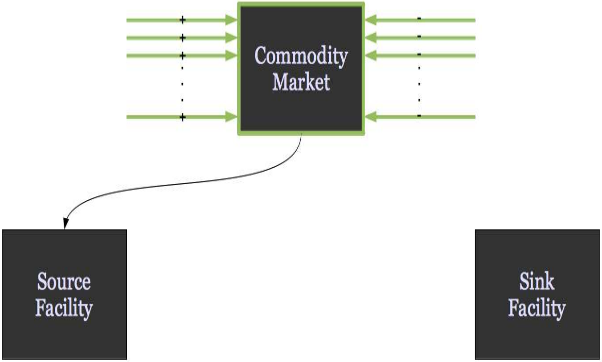


Figure: The Market solves the problem and instructs the source facility to send a certain amount to the sink facility.

A Simple Example

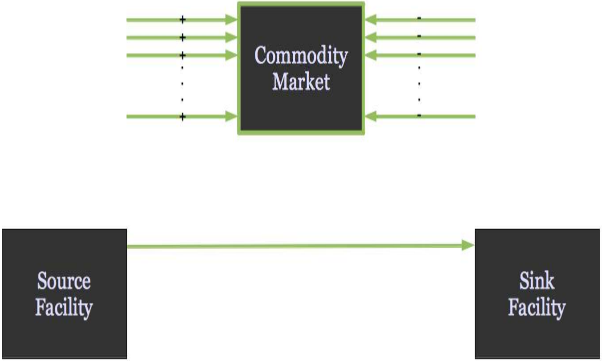


Figure: The source facility sends the material directly to the sink facility.

This Market Model Scales for Complex Systems

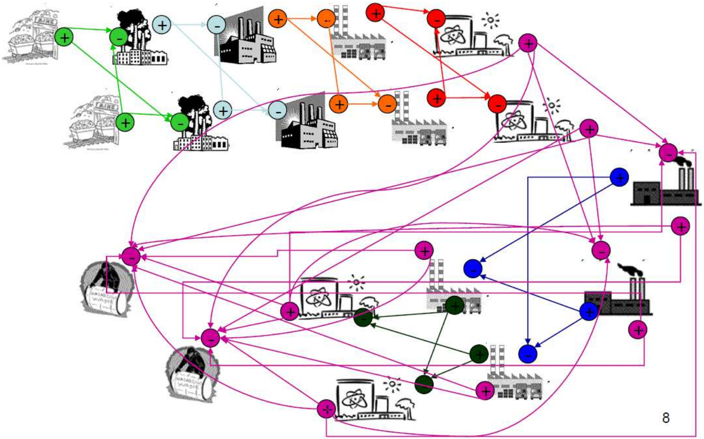


Figure: Well designed interfaces and strict encapsulation support scalability of the Market-based simulation paradigm [?]

Dynamic Module Loading : Developer

With a dynamic, plug-in implementation, the simulation logic is independent of the available models and models are loaded as shared libraries at runtime.

Model.cpp

```
#include Model.hpp
#include dlfcn.h
    .
    .
    .
 mdl_ctr* loadModel(name){
      void* model = dlopen(name.c_str(), RTD_LAZY)
      mdl_ctr* new_model = (mdl_ctor*) dlsym(model,"construct");
    .
    .
    .
 return new_model;
}
```

RecipeReactor.cpp

```
 #include RecipeReactor.hpp
      .
      .
      .
  extern "C" Model* construct() {
      return new RecipeReactor();
  }
      .
      .
      .
```

Figure: Dynamic c library loading separates simulation logic from knowledge of available models, supporting extensions by developers with minimal lines of code.

Dynamic Module Loading : User

With a dynamic, plug-in implementation, the simulation logic is independent of the available models and models are loaded as shared libraries at runtime.

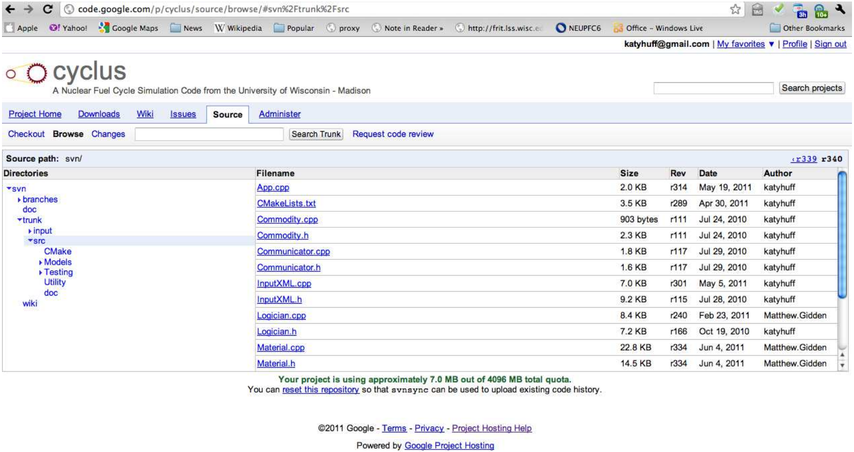
input.xml

```xml
<simulation>
  <startYear>1962</startYear>
  <duration>1200</duration>
  <region>
    <name>UChicago</name>
    <DeployRegionModel>
      <deployment>
        <facility>
          <name>ChiPile1</name>
          <model>RecipeReactor</model>
        </facility>
        <year>1942</year>
      </deployment>
      </DeployRegionModel>
      .
      .
      .
  </region>
  .
  .
  .
</simulation>
```

Figure: XML input parsing and a relaxNG schema provide a simplified XML interface is available for the end user to define available module implementations.

Open Source Repository

This open source repository provides a centralized location for documentation, developer history, and unhindered developer access.


code.google.com/p/cyclus/source/browse/#svn%2Ftrunk%2Fsrc

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cyclus

A Nuclear Fuel Cycle Simulation Code from the University of Wisconsin - Madison

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Source path: svn/ ‹r339 r340

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Filename	Size	Rev	Date	Author
App.cpp	2.0 KB	r314	May 19, 2011	katyhuff
CMakeLists.txt	3.5 KB	r289	Apr 30, 2011	katyhuff
Commodity.cpp	903 bytes	r111	Jul 24, 2010	katyhuff
Commodity.h	2.3 KB	r111	Jul 24, 2010	katyhuff
Communicator.cpp	1.8 KB	r117	Jul 29, 2010	katyhuff
Communicator.h	1.6 KB	r117	Jul 29, 2010	katyhuff
InputXML.cpp	7.0 KB	r301	May 5, 2011	katyhuff
InputXML.h	9.2 KB	r115	Jul 28, 2010	katyhuff
Logician.cpp	8.4 KB	r240	Feb 23, 2011	Matthew.Gidden
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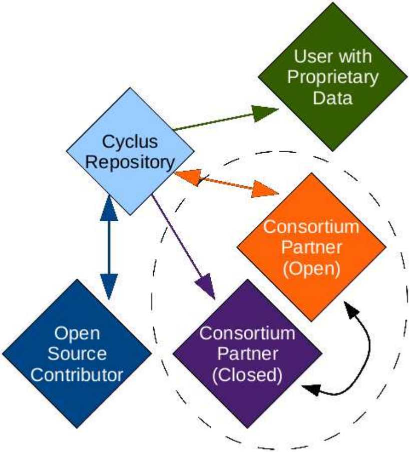

Figure: License, architecture, and development paradigm allow varying levels of code sharing and data security.

Version Control

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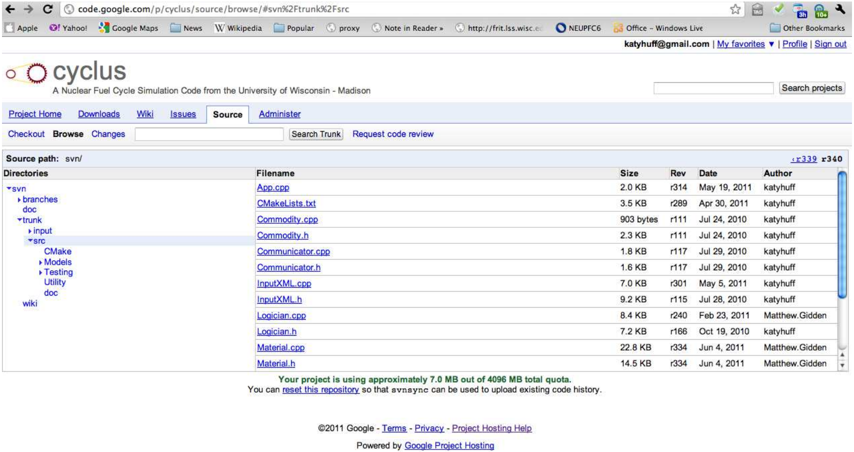
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A Nuclear Fuel Cycle Simulation Code from the University of Wisconsin - Madison

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Nested Components

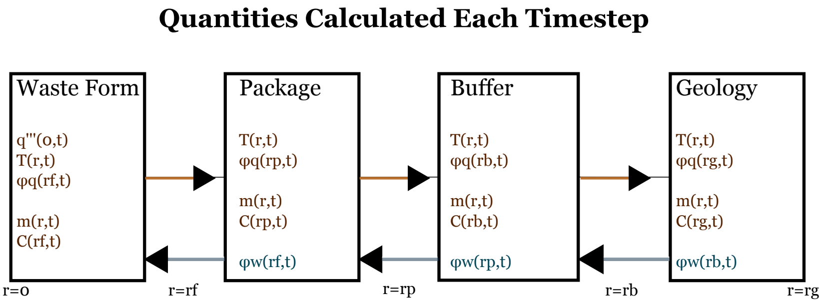
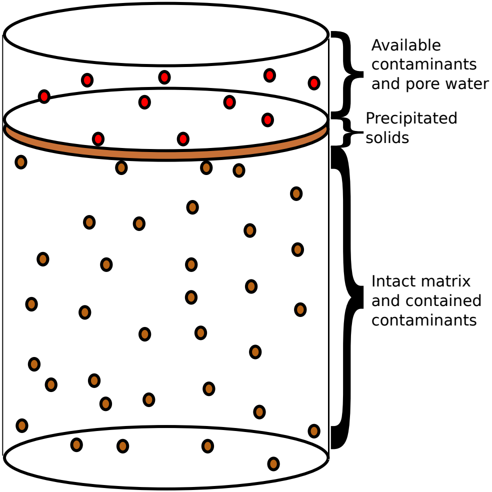


Figure: The nested components supply thermal flux and concentration information to each other at the boundaries.

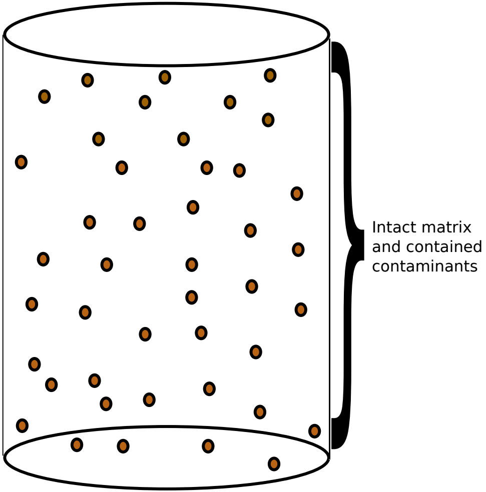
Waste Stream

A material may be any arbitrary isotopic vector

Waste Form


Available contaminants and pore water
Precipitated solids
Intact matrix and contained contaminants

Waste Form



Waste Package

$$n_F = N \cdot f(). \tag{24}$$

physical model

$$f() = N \cdot f(t, T, \cdots). \tag{25}$$

time dependent

$$f() = f(t). \tag{26}$$

Weibull

$$f(t, \lambda, k) = \begin{cases} \frac{k}{\lambda}\left(\frac{t}{\lambda}\right)^{k-1} e^{-(t/\lambda)^k} & t \geq 0, \\ 0 & t < 0. \end{cases} \tag{27}$$

instantaneous

$$f() = \delta(t - t_F). \tag{28}$$

Buffer

Geological Environment

Outline

Demonstration Case : Code Development

Empty Concept
Interfaces, information passing, module loading. Not in that order.
Information passing tests, Database writing tests, module loading tests.

Base Case : Component Abstraction

each component?

Base Case : System Level Abstraction

tell the difference between component models.

Extensions : Fracturation

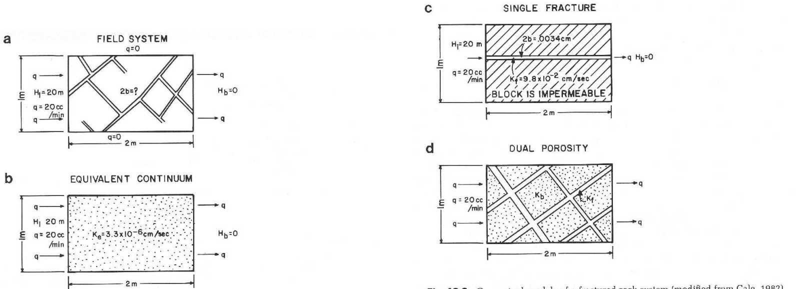


Fig. 12.6 Conceptual models of a fractured rock system (modified from Gale, 1982).
(a) A simplified fracture network of aperture 2b with groundwater flow from left to right.
(b) Equivalent porous medium model of (a).
(c) Discrete fracture model of (a).
(d) Dual porosity medium model of (a).

A dual continuum model will be implemented to more accurately represent fractured host media such as granite [2].

Extensions : Sorption

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

$$R_f = 1 + K_d \times \frac{\text{density of rock}}{\text{porosity of rock}} = \frac{\text{rate of groundwater movement}}{\text{rate of radionuclide movement}}$$

Element	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.

Figure: Sorption will be modeled using retardation factors in the mixed cell models [?]

Extensions : Coalescence

Salt and clay exhibit coalescent behavior under heat.

Integrated Used Fuel Disposition and Repository Model

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