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September 1, 2011



Outline





Future Disposal System Options

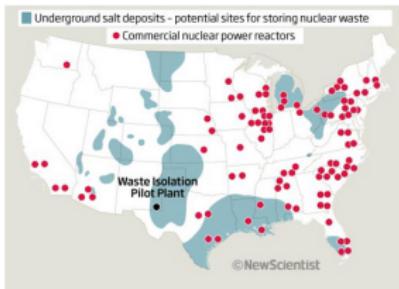


Figure: ref. [11]



Figure: ref. [11]

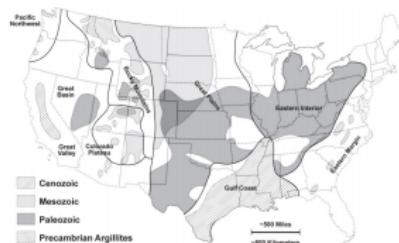


Figure: ref. [7]



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

Abstraction GPAM GDSM



Outline



Top Level Fuel Cycle Simulators

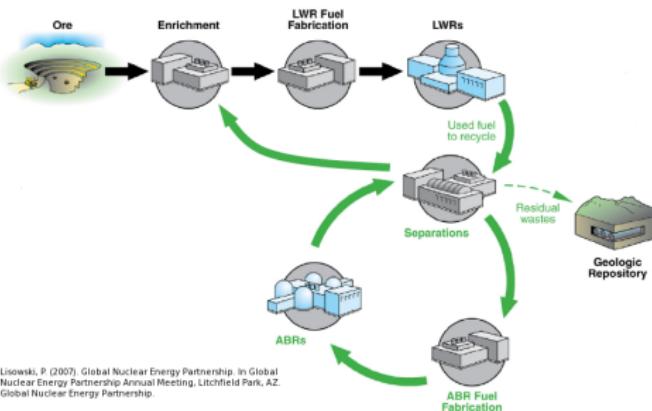


Figure: Top level simulators are intended to model the collective behavior of various fuel cycle decisions and strategies.[?]



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.



Clay Disposal Environments

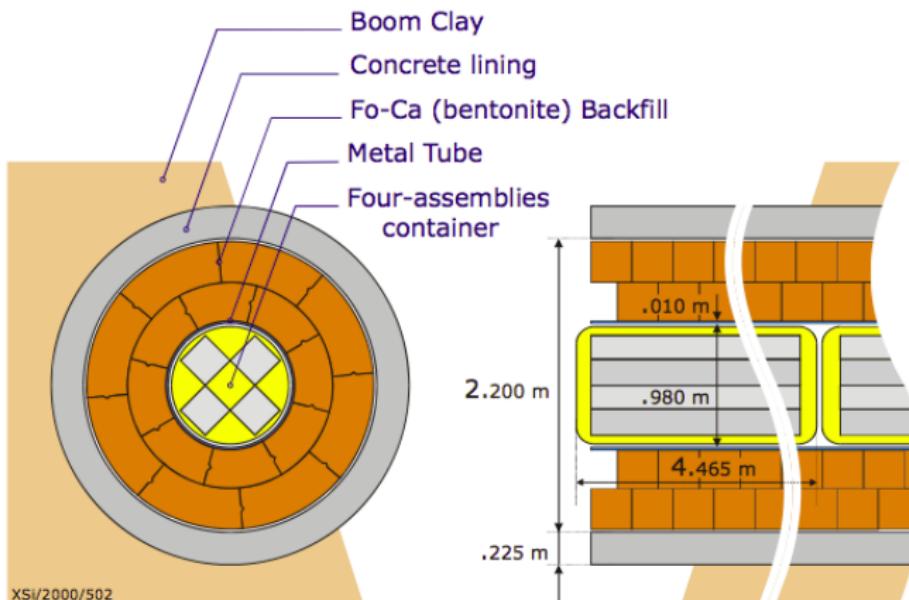


Figure: Belgian reference concept in Boom Clay.[?]



Granite Disposal Environments

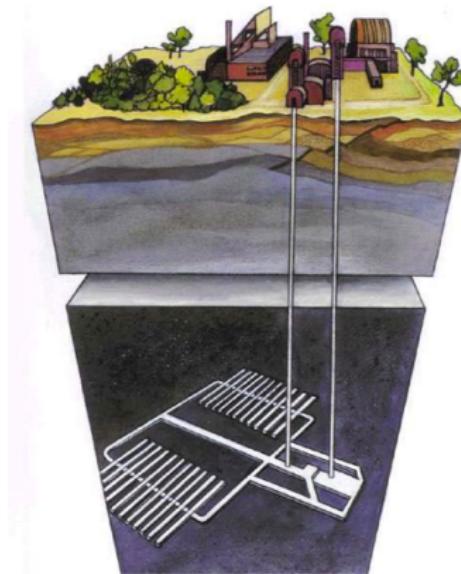


Figure: Czech reference concept in Granite.[?]



Salt Disposal Environments

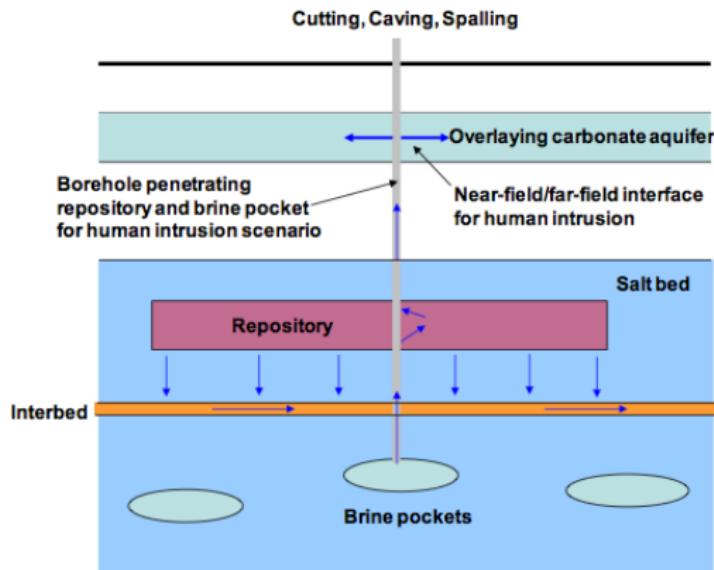


Figure: Used Fuel Division reference concept in Salt.[?]



Deep Borehole Disposal Environment

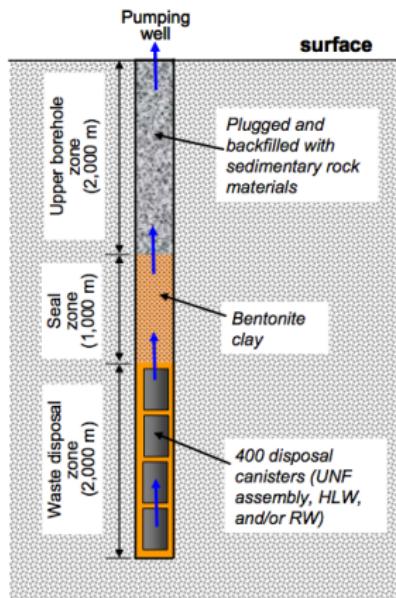


Figure: Used Fuel Division reference Deep Borehole concept.[?]



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 or Cu -,Fo-Ca,Cement 100-500 m Vert.,Horiz,Alcove one, many	Steel 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 [$^{\circ}C$] Host Limit [$^{\circ}C$] 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

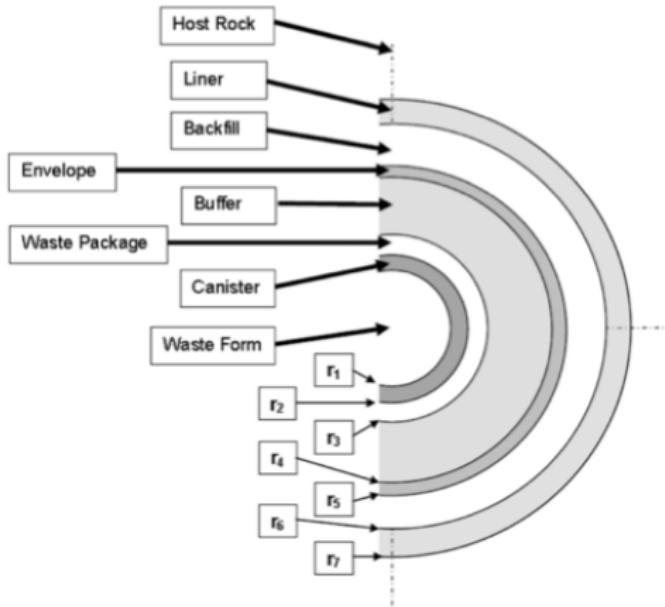


Figure: After waste package failure, radionuclides pass through successive layers of the engineered barrier system [?].



Waste Form Release Models

Waste Form Types				
WF Type	SubTypes	Contents	Release D	Notes
Once Through	CSNF Ceramic Oxide CSNF Ceramic Oxide HTGR TRISO Graphite DSNF Metal DSNF Carbides DSNF Ceramic Oxides	Nominal Burnup UO ₂ & MOX High Burnup High Burnup High Burnup N Reactor Fuel Fast Reactor Fuels Research Reactor Fuels	redox reactions redox reactions graphite reactions metal reactions carbide reactions redox reactions	
Borosilicate Glass	Current Future	MA, Cs/Sr Mo, no MA no Cs/Sr	heat, glass alteration	glass alteration
Glass Ceramic	Glass Bonded Sodalite	Echem processed oxide fuels	ceramic, redox, glass	
Metal Alloy	From Echem From Aqueous	Cladding, noble metals undissolved solids, transition metals	metal reactions metal reactions	
Advance Ceramic		volatized iodine	ceramic reactions	
Salt	Cementitious Sodium	separated streams	alkaline reactions	

Table: An array of waste forms developed for nuclear wastes will have a corresponding array of dominant release mechanisms [5]



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

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

where

n = solute accessible porosity [%]

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

t = time [s]

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

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

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

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 [$m \cdot s^{-1}$]. (2)



Dispersion

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

$$D = \alpha v + D_e \quad (3)$$

such that the mass conservation equation becomes:

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

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

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

where

s = sorption coefficient

ρ_b = bulk (dry) density [kg/m^3].



Dispersion

For unidirectional flow, the unidirectional dispersion tensor gives

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



Diffusion

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

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



Precipitation



Sorption

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

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

equation (5) becomes

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

where

R_f = retardation factor

$$= 1 + \frac{\rho_b K_d}{n} \quad (10)$$

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

$$C(0, t) = C_0 \quad (11)$$

and

$$\left. \frac{\partial C}{\partial x} \right|_{x=\infty} = 0 \quad (12)$$

as well as the initial condition

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

the so called Ogata and Banks solution gives

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

where

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



Heat Limits In Geology

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

Models of Heat Load for Various Geologies

Source (Who)	Nation (Where)	Geology (What)	Methodology (How)
Enresa [14]	Spain	Granite	CODE_BRIGHT 3D Finite Element
NRI [14]	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 [14]	Belgium	Clay	Specific Temperature Integral
ANDRA [3]	France	Argile Clay	3D Finite Element CGM code
NAGRA [8, 9]	Switzerland	Opalinus Clay	3D Finite Element CGM code
GRS [14]	Germany	Salt	HEATING (3D finite difference)
NCSU(Li) [10]	USA	Yucca Tuff	Specific Temperature Integral
NCSU(Nicholson) [12]	USA	Yucca Tuff	COSMOL 3D Finite Element
Radel & Wilson [13]	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.



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.



Dimensionality

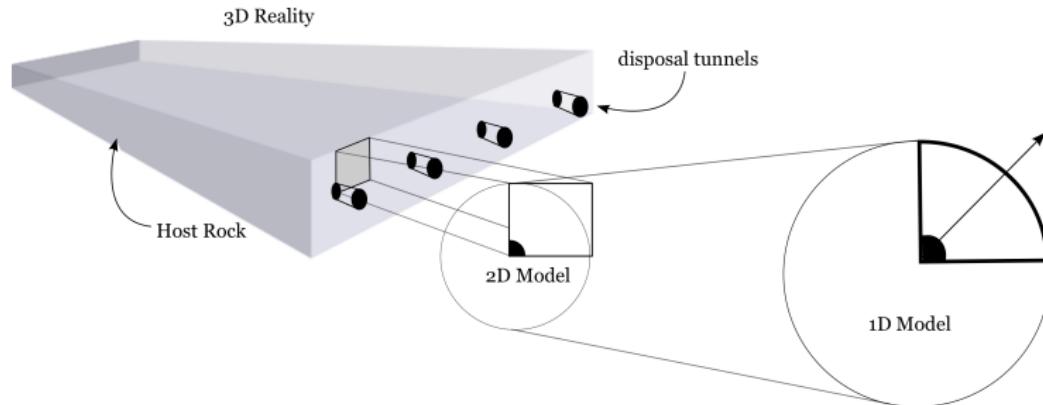


Figure: Employing the symmetries of the disposal layout can enable lower dimensional models.



Lumped Parameter Technique

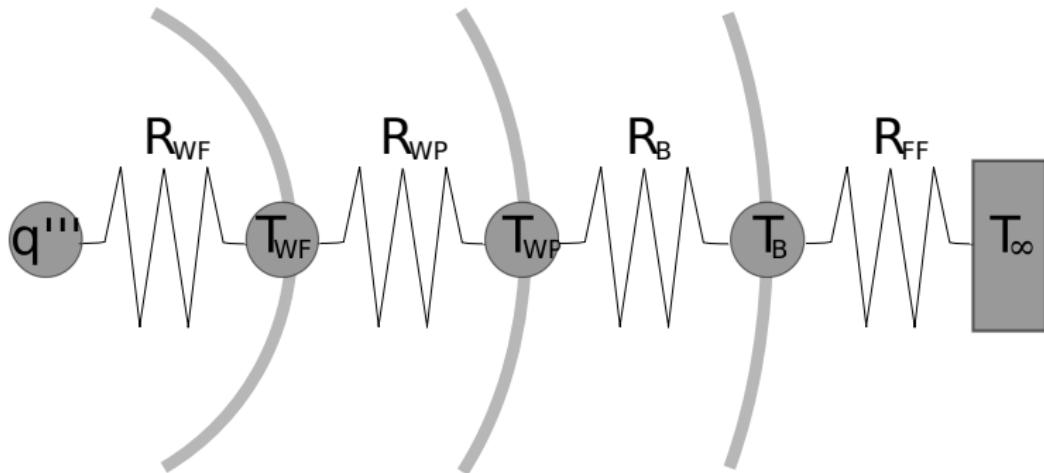


Figure: The lumped parameter analogy used for heat transfer can be applied to the one dimensional approximation to the disposal system concept.



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.

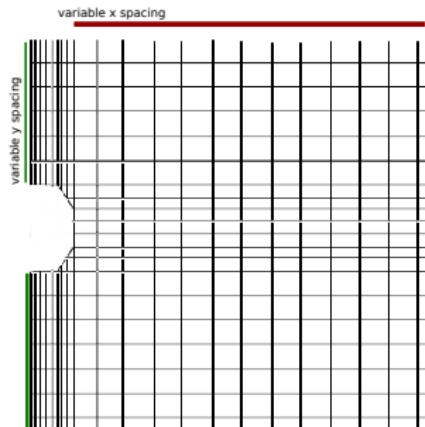


Figure: Two adjustable geometric dimensions of the ANL model [?].



LLNL Model

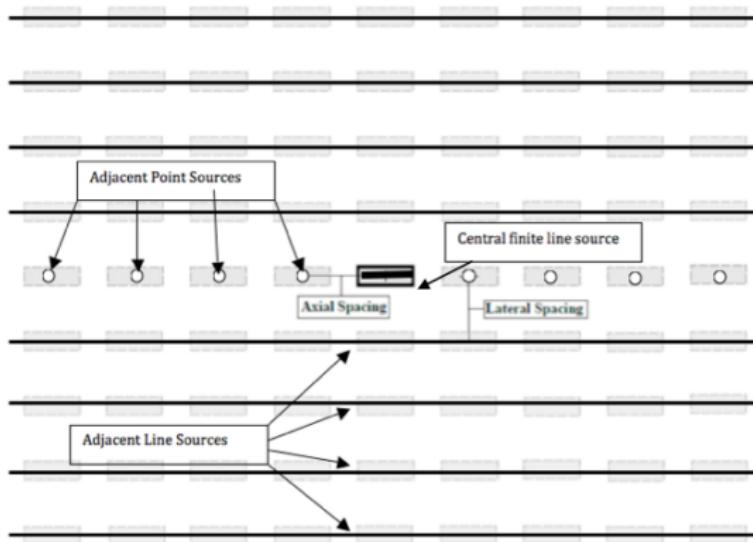


Figure: Vertical, horizontal, alcove, and borehole emplacement layouts can be represented by a line of point sources and adjacent line sources.

Heat Based Drift Loading



Analytical Models





Detailed Techniques

Outline





Cyclus Modular Architecture and Open Development

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



Encapsulation

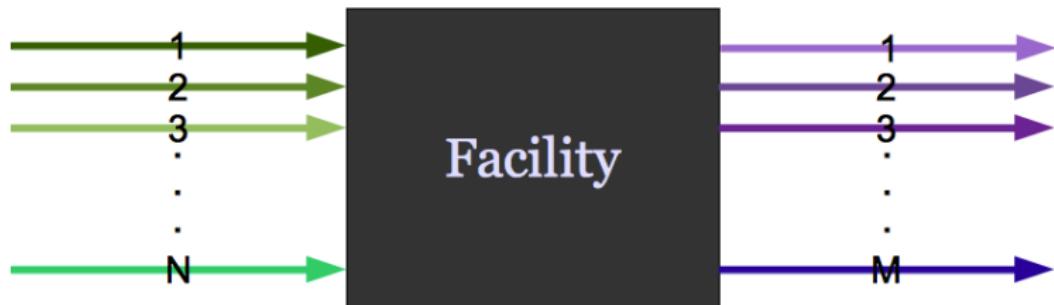


Figure: Regions, Institutions, Facilities, and Markets are all black boxes.



Module Interfaces

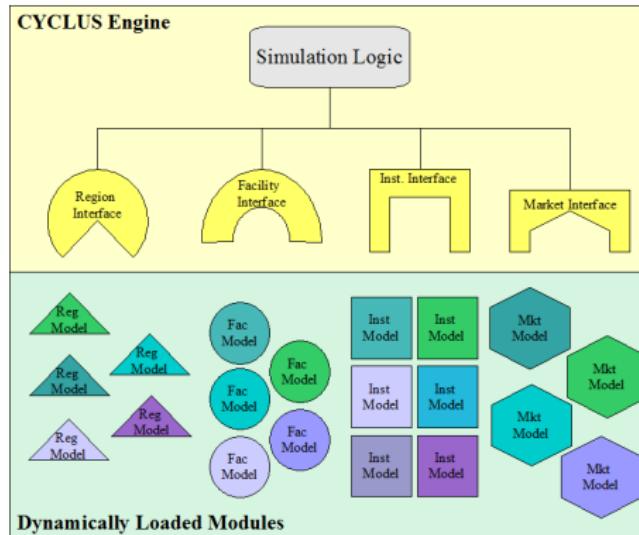


Figure: Well defined model interfaces facilitate model interchange. The user may choose the model at their desired level of detail.



Facilities Are Black Boxes

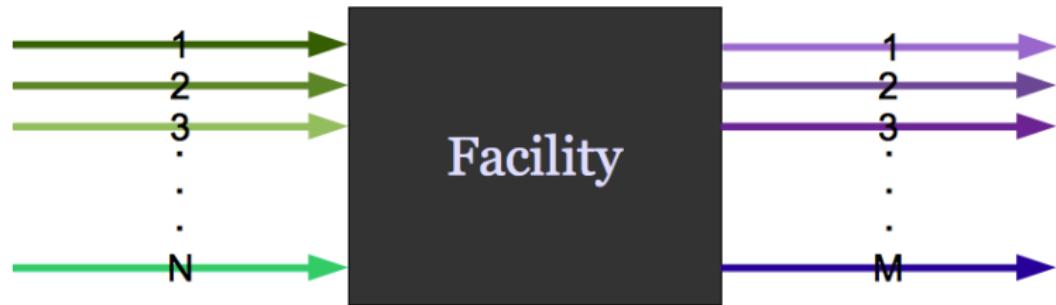


Figure: Each facility in the simulation makes requests and offers to fill its stocks and empty its inventory respectively.



Facilities Are Black Boxes



Figure: A facility might only make offers.



Facilities Are Black Boxes

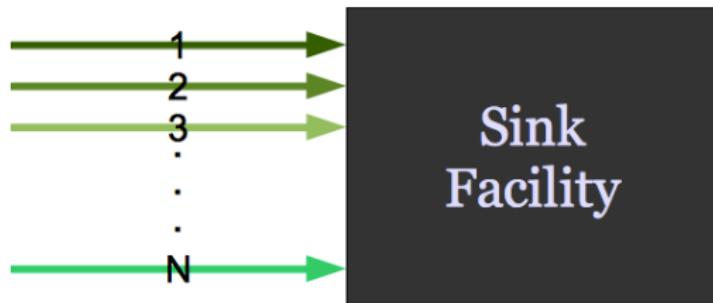


Figure: A facility might only make requests.



Each Commodity is Associated with a Market



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



The Market Solves the Matching Problem

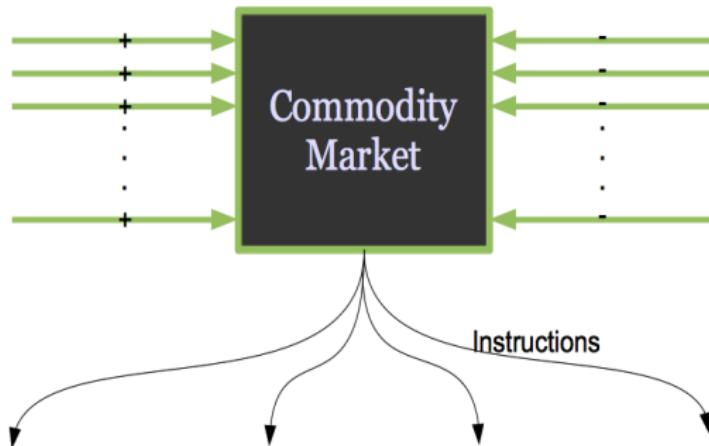


Figure: When the Market's arbitrary algorithm solves the matching problem, the Market sends instructions to the offering facilities.



A Simple Example

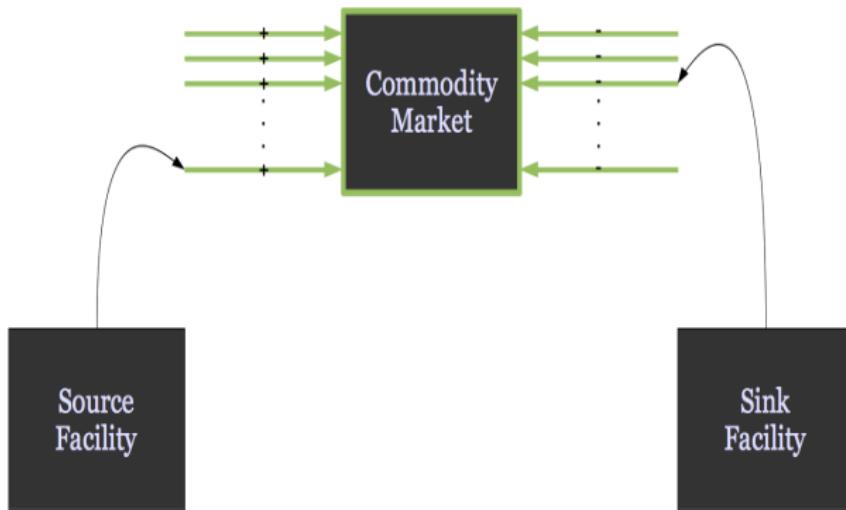


Figure: The source sends an offer and the sink sends a request.



A Simple Example

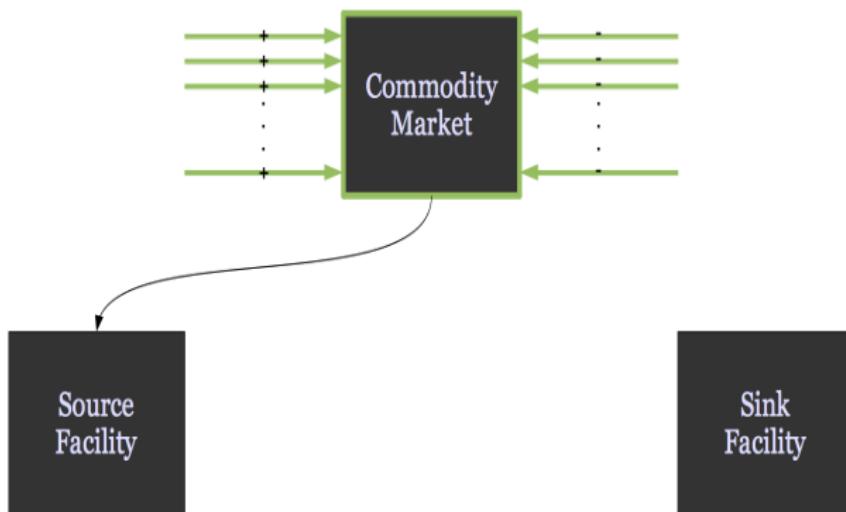


Figure: The Market solves the problem and instructs the source facility to send a certain amount to the sink facility.



A Simple Example

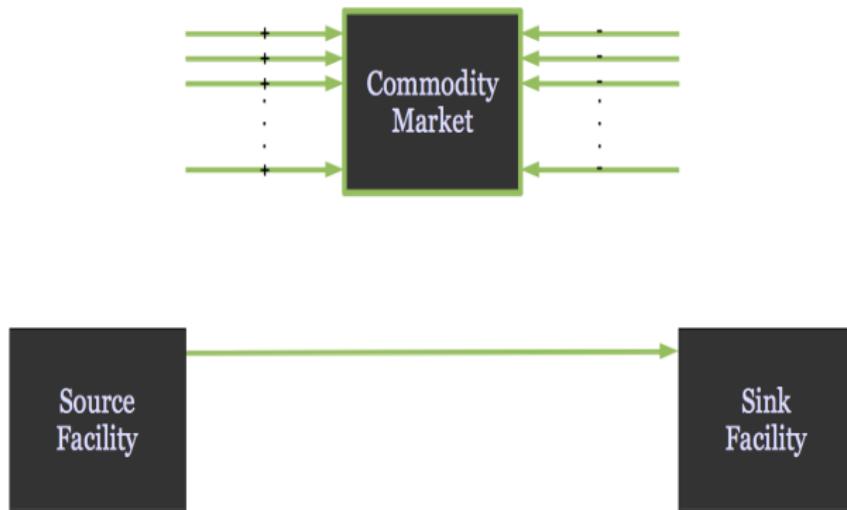


Figure: The source facility sends the material directly to the sink facility.



This Market Model Scales for Complex Systems

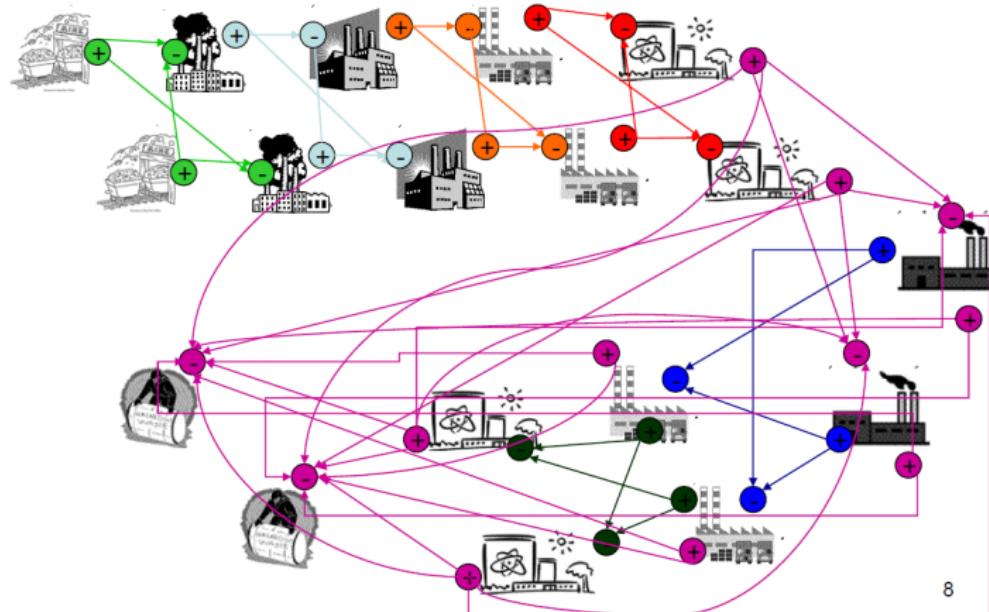


Figure: Well designed interfaces and strict encapsulation support scalability of the Market-based simulation paradigm [?]



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_ctr*)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
	<pre><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></pre>

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

Apple | Yahoo! | Google Maps | News | Wikipedia | Popular | proxy | Note in Reader > | http://frt.iss.wisc.edu | NEUPFC6 | Office – Windows Live | Other Bookmarks

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» branches	CMakeLists.txt	3.5 KB	r289	Apr 30, 2011	katyhuff
» doc	Commodity.cpp	903 bytes	r111	Jul 24, 2010	katyhuff
» trunk	Commodity.h	2.3 KB	r111	Jul 24, 2010	katyhuff
» Input	Communicator.cpp	1.8 KB	r117	Jul 29, 2010	katyhuff
» src	Communicator.h	1.6 KB	r117	Jul 29, 2010	katyhuff
CMake	InputXML.cpp	7.0 KB	r301	May 5, 2011	katyhuff
Models	InputXML.h	9.2 KB	r115	Jul 28, 2010	katyhuff
Testing	Logician.cpp	8.4 KB	r240	Feb 23, 2011	Matthew.Gidden
Utility	Logician.h	7.2 KB	r166	Oct 19, 2010	katyhuff
doc	Material.cpp	22.8 KB	r334	Jun 4, 2011	Matthew.Gidden
wiki	Material.h	14.5 KB	r334	Jun 4, 2011	Matthew.Gidden

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'Modified Open' Source

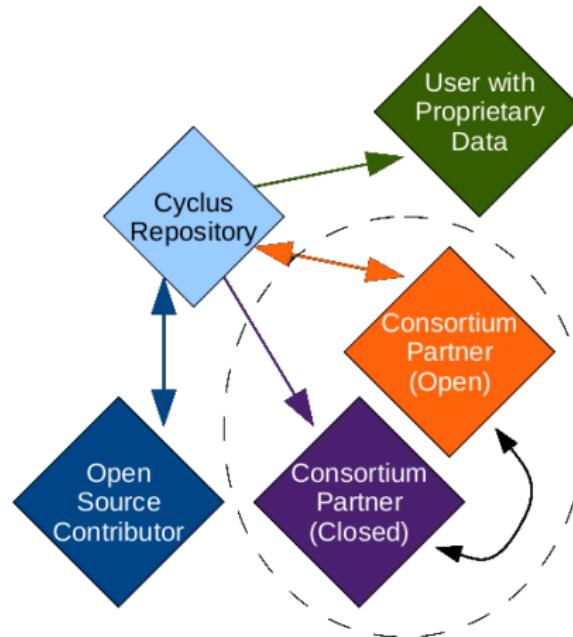


Figure: License, architecture, and development paradigm allow varying levels of code sharing and data security.



Version Control

This open source repository employs a version control system for provenance, developer access, and reproducibility of results.

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

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Nested Components

Quantities Calculated Each Timestep

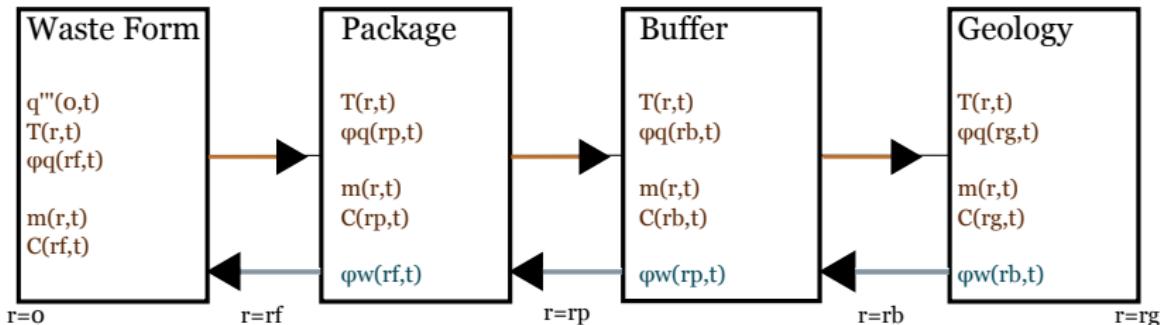


Figure: The nested components supply thermal flux and concentration information to each other at the boundaries.

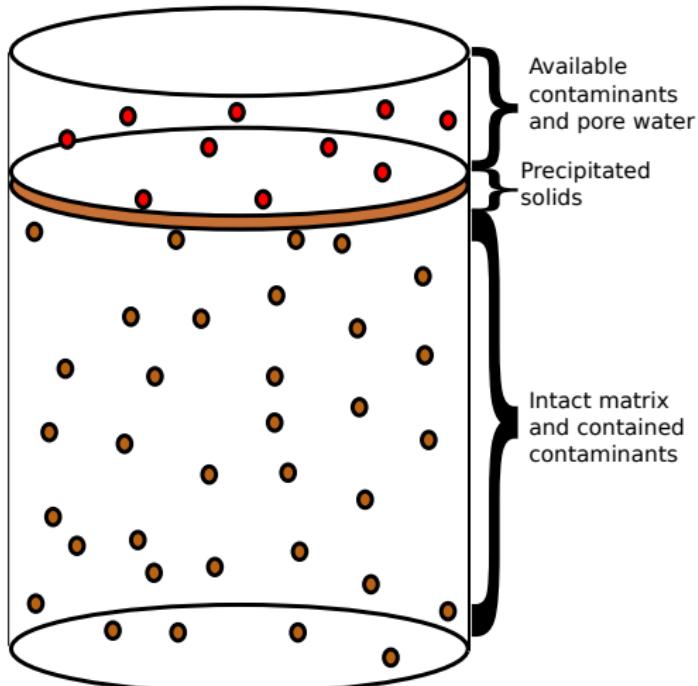


Waste Stream

A material may be any arbitrary isotopic vector

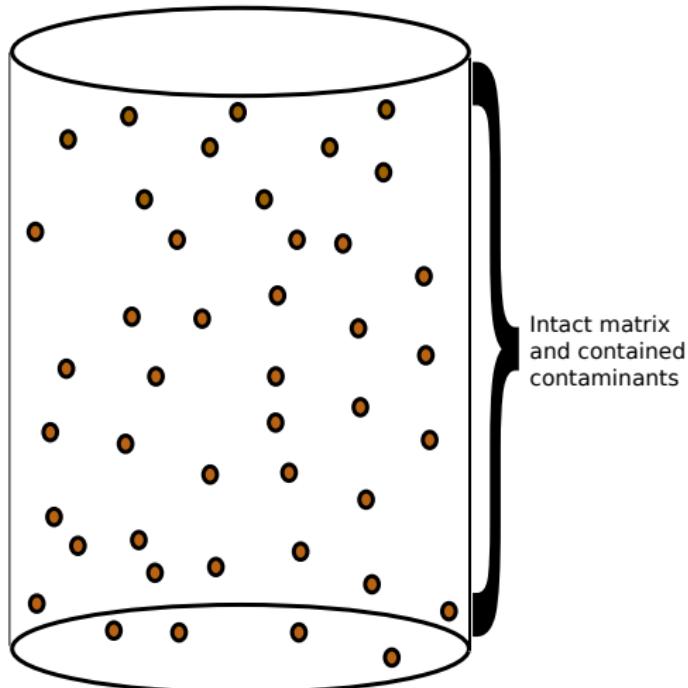


Waste Form





Waste Form





Waste Package

$$n_F = N \cdot f(). \quad (16)$$

physical model

$$f() = N \cdot f(t, T, \dots). \quad (17)$$

time dependent

$$f() = f(t). \quad (18)$$

Weibull

$$f(t, \lambda, k) = \begin{cases} \frac{k}{\lambda} \left(\frac{t}{\lambda} \right)^{k-1} e^{-(t/\lambda)^k} & t \geq 0, \\ 0 & t < 0. \end{cases} \quad (19)$$

instantaneous

$$f() = \delta(t - t_F). \quad (20)$$

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

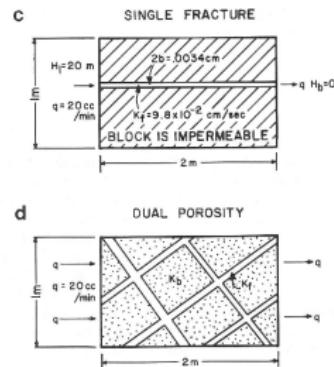
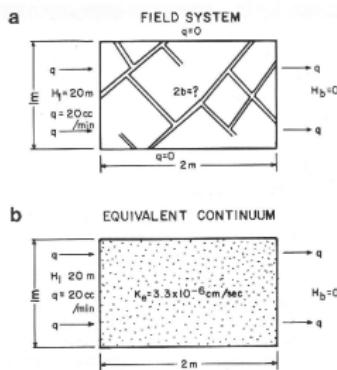


Fig. 12.6 Conceptual models of a fractured rock system (modified from Gale, 1982).
 (a) A simplified fracture network of aperture $2b$ with groundwater flow from left to right.
 (b) Equivalent porous medium model of (a).
 (c) Discrete fracture model of (a).
 (d) Dual porosity medium model of (a).

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

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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