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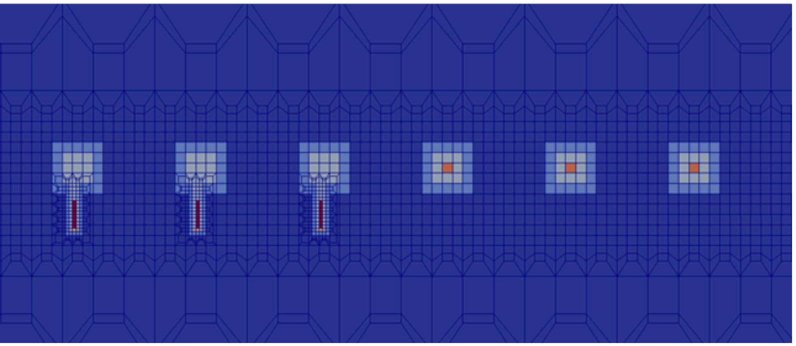

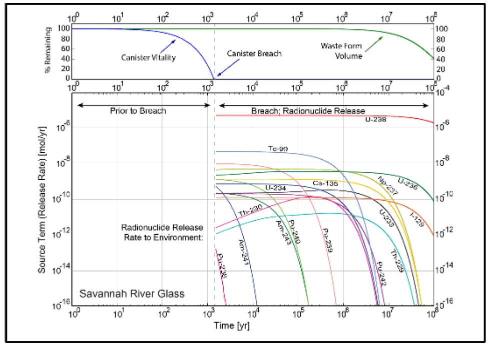

git

LGPLv3 Free as in Freedom

PFLOTRAN

Atlassian Bitbucket

MODELING WASTE PACKAGE DEGRADATION AND WASTE FORM DISSOLUTION FOR GEOLOGIC REPOSITORY PERFORMANCE ASSESSMENT IN PFLOTRAN

Jennifer M. Frederick, Glenn E. Hammond, Paul E. Mariner, Emily R. Stein, S. David Sevougian

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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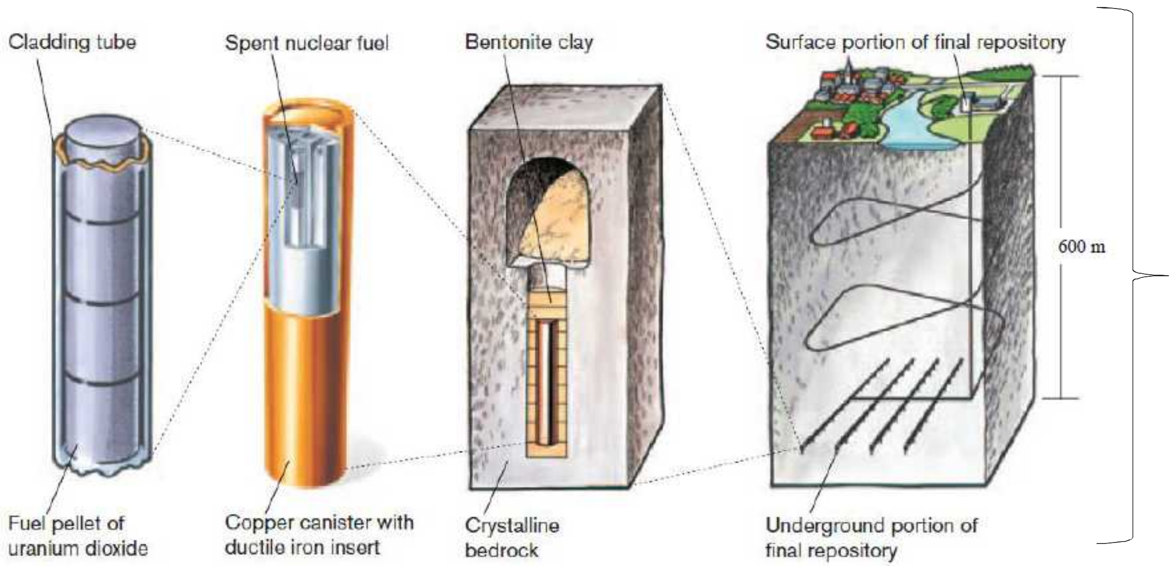
A Generic, Geologic Repository

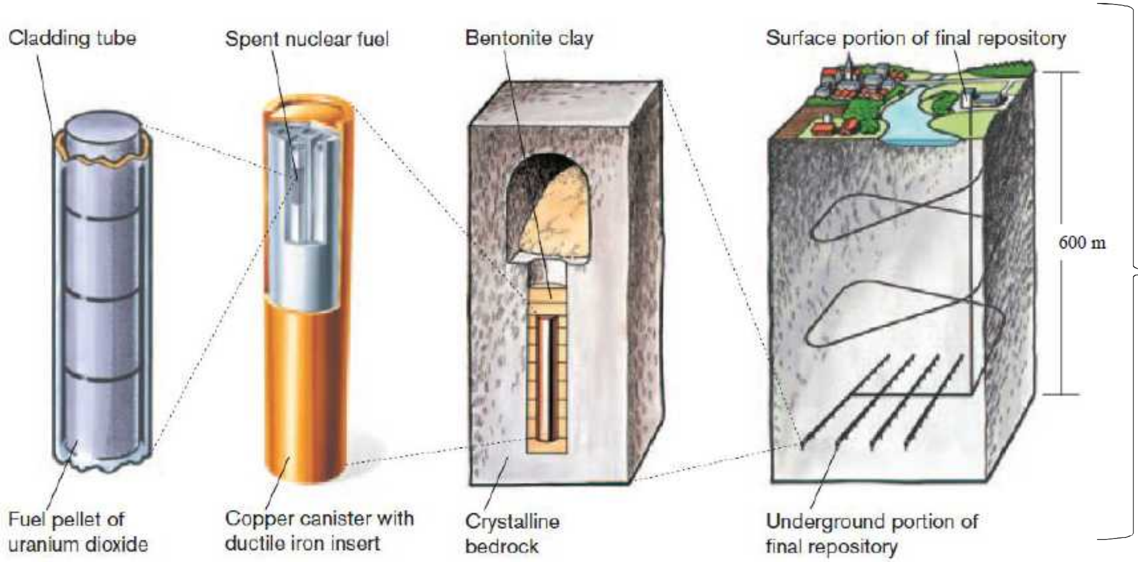
- A performance assessment (PA) for a nuclear waste repository requires a **comprehensive model** that can **simulate plausible scenarios and processes** that may affect **repository performance and safety**.



An example geologic repository in crystalline bedrock consists of a waste form within a copper canister that is surrounded by a bentonite clay 'buffer' and placed in the floor of mined drifts deep underground. The repository footprint at the surface is very small. Wang et al. (2014)

A Generic, Geologic Repository

- Disposal options for spent nuclear fuel and high-level nuclear waste include:
  - mined repository concepts in salt, argillite, and crystalline rock
  - deep borehole disposal in crystalline rock.



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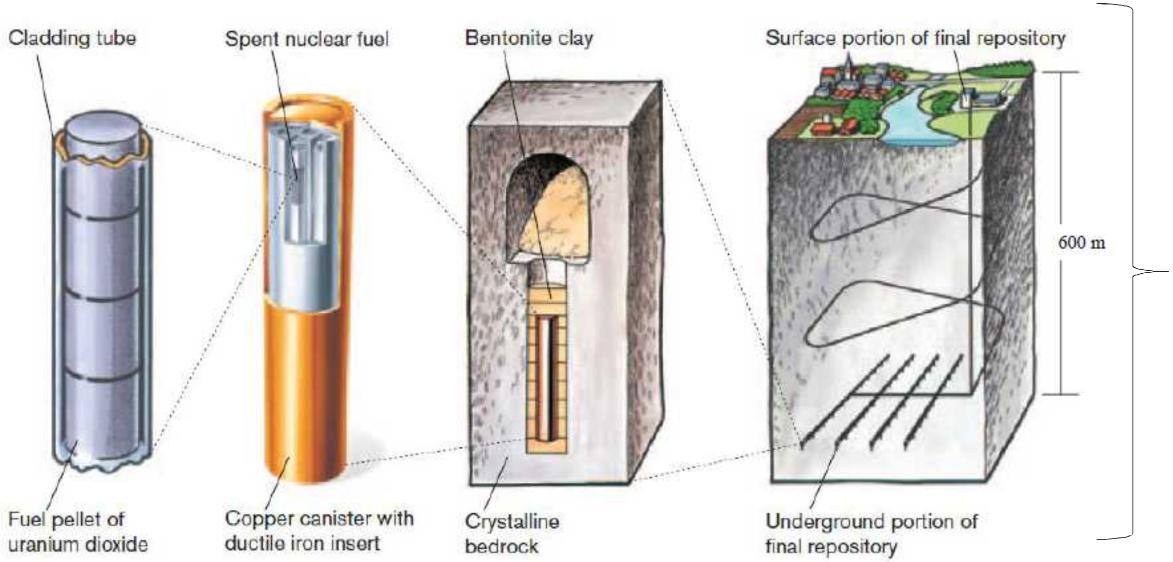
A Generic, Geologic Repository

- A major modelling challenge is accurately representing processes across **multiple spatial and temporal scales**:



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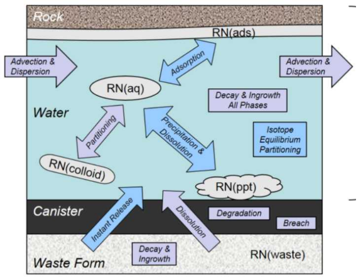
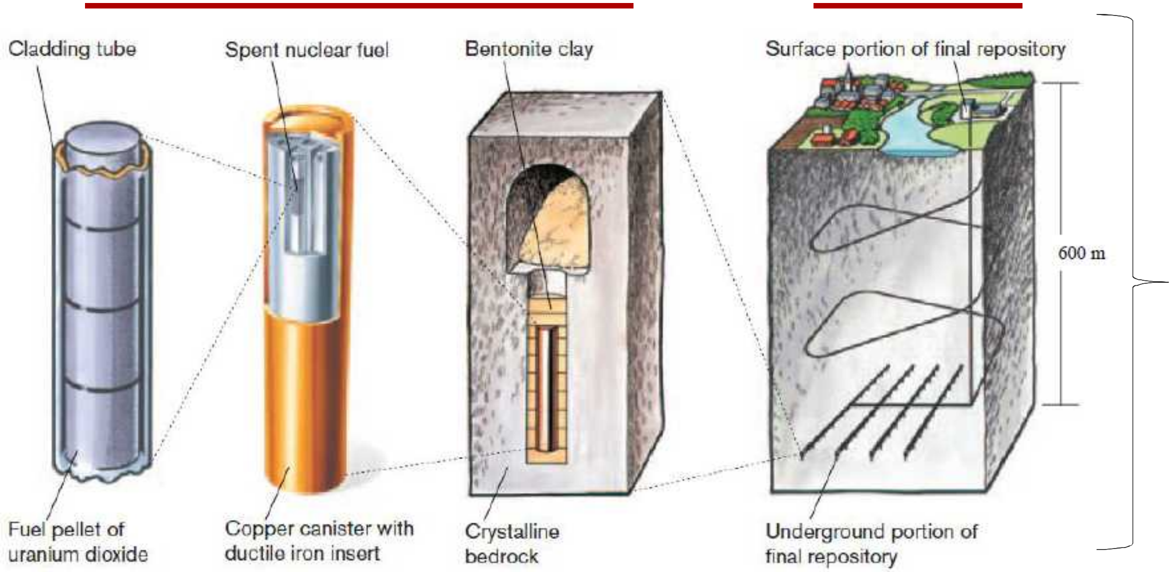


O(<<m^3), O(sec < t 1e8yr)

O(m^3)

O(km^3), O(t=1e8yr)



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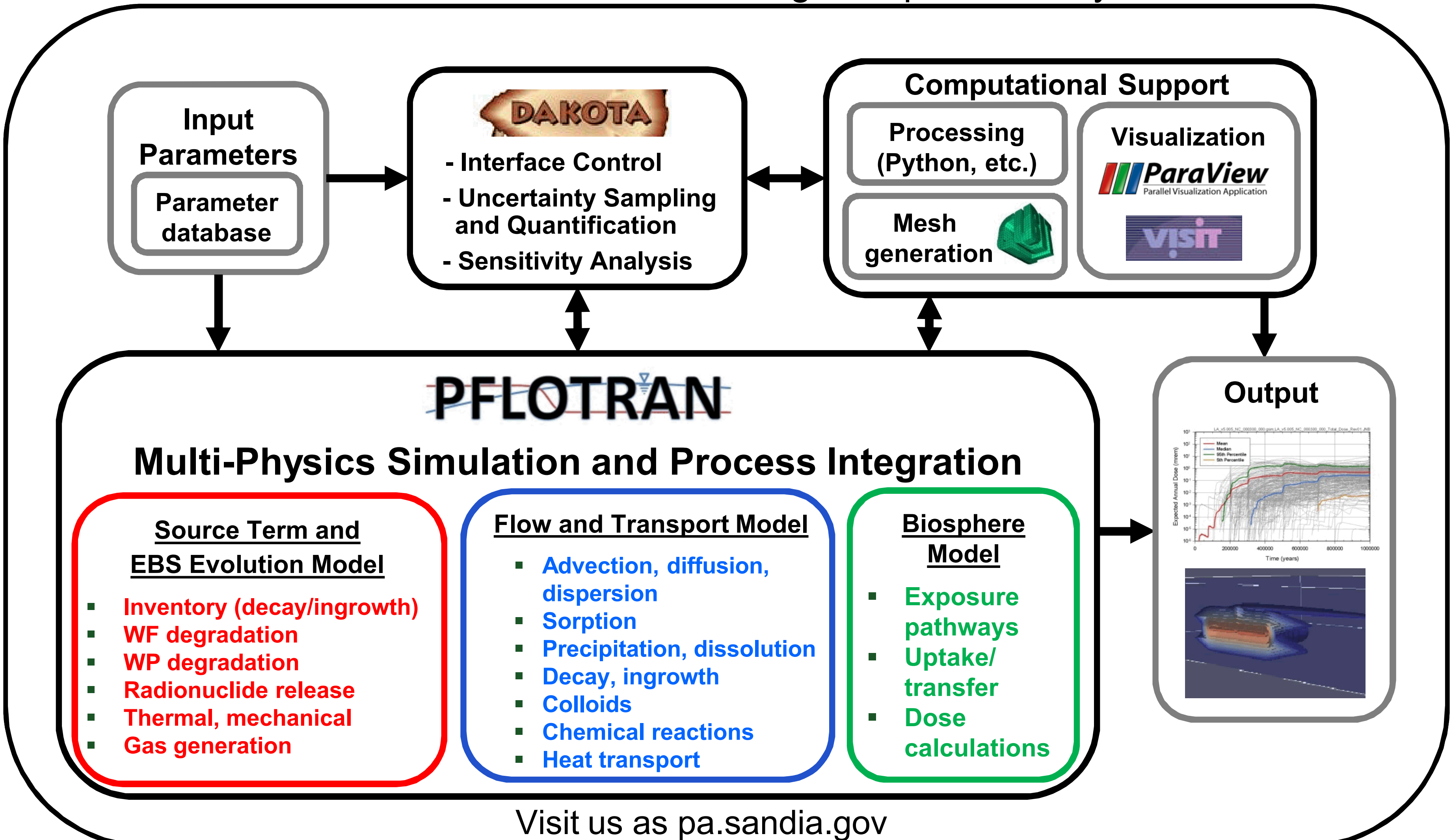
GDSA Framework

GDSA = Geologic Disposal Safety Assessment



GDSA Framework

GDSA = Geologic Disposal Safety Assessment

Input Parameters

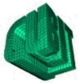
- Parameter database

DAKOTA

- Interface Control
- Uncertainty Sampling and Quantification
- Sensitivity Analysis

Computational Support

- Processing (Python, etc.)
- Mesh generation



- Visualization: ParaView (Parallel Visualization Application), VisIt

PFLOTRAN

Multi-Physics Simulation and Process Integration

Source Term and EBS Evolution Model

- Thermal, mechanical
- Gas generation

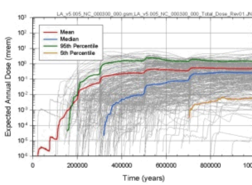
Flow and Transport Model

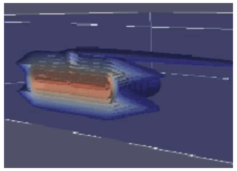
- Advection, diffusion, dispersion
- Sorption
- Precipitation, dissolution
- Decay, ingrowth
- Colloids
- Chemical reactions
- Heat transport

Biosphere Model

- Exposure pathways
- Uptake/ transfer
- Dose calculations

Output





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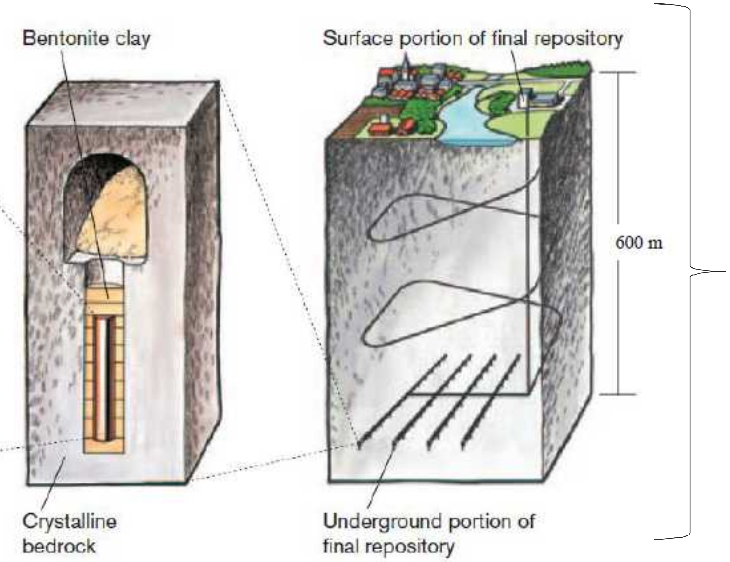
Modeling Waste Package/Form Degradation

- Waste package and waste form evolution involves:
  - Radionuclide decay and ingrowth
  - Waste package degradation processes and breach
  - Waste form dissolution



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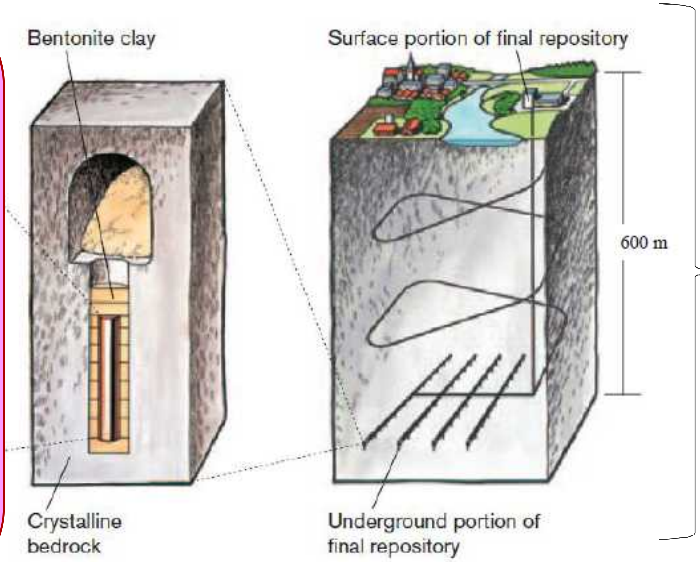
Modeling Waste Package/Form Degradation

- We represent this in PFLOTRAN using a nested process model:

`waste form process model`



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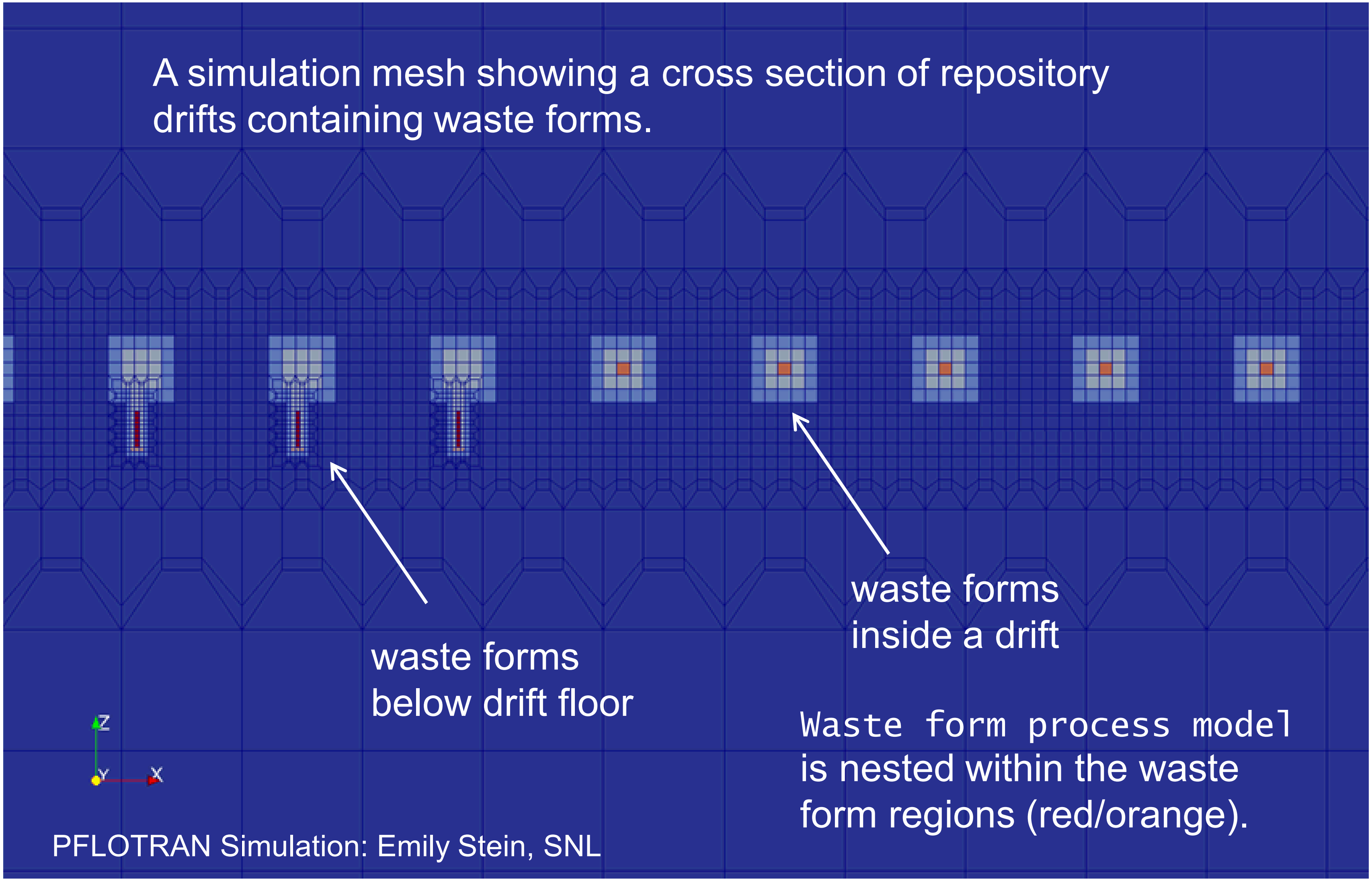
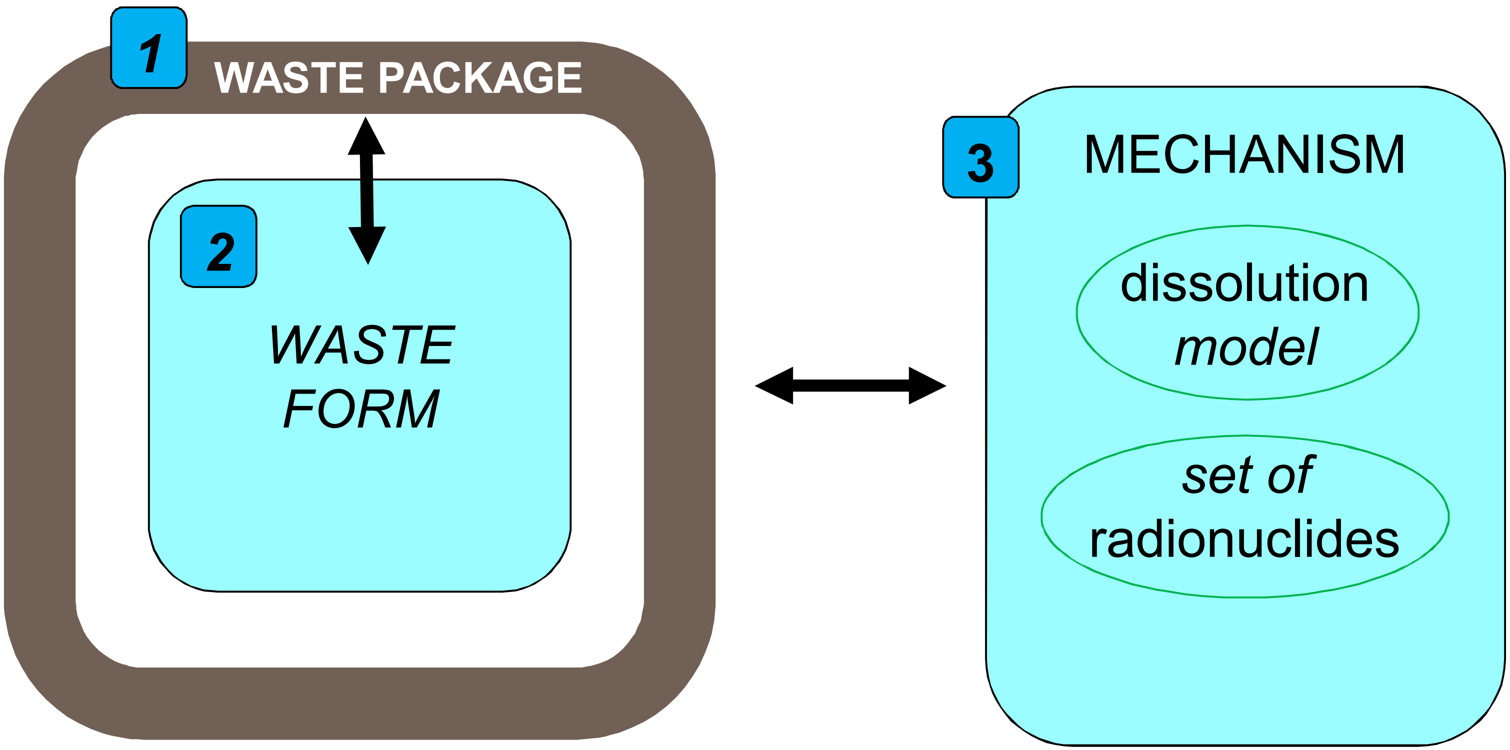
PFLOTRAN's Waste Form Process Model



PFLOTRAN's Waste Form Process Model

Consists of 3 Main Components:

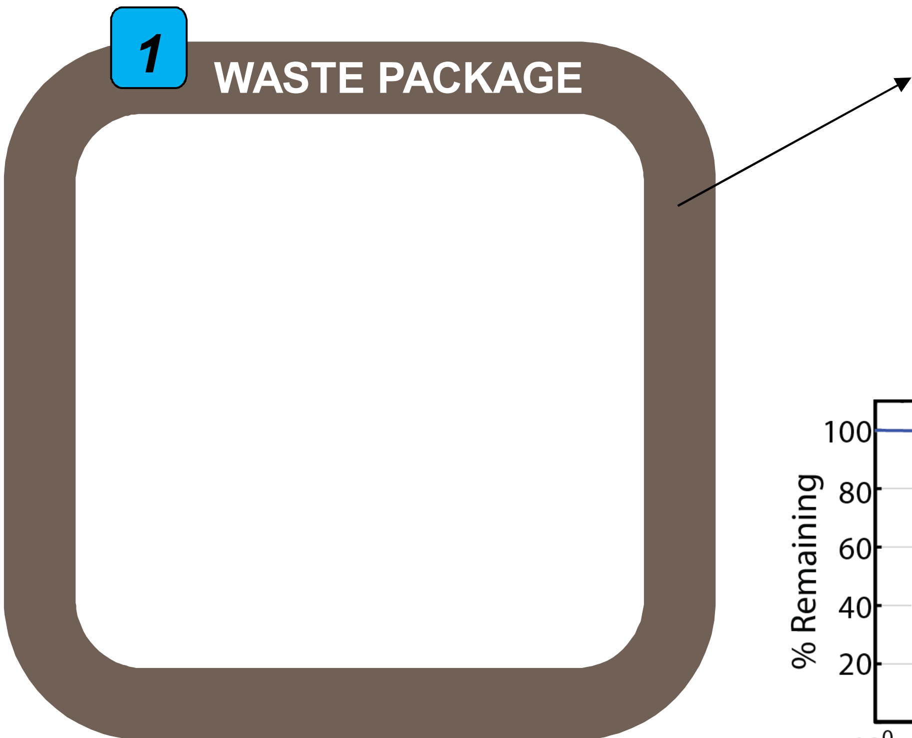


"waste form object"
"fruit"

"waste form type"
"banana, apple, orange, etc."

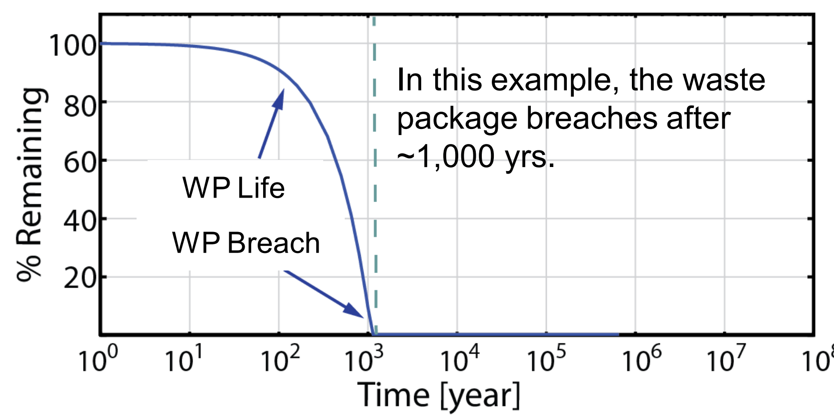
PFLOTRAN's Waste Form Process Model

1. Waste Package Degradation Model



Waste Package Life (Vitality)

- A measure of how much 'life' the waste package has remaining
- Normalized waste package thickness
- Range: 100% - 0%
- Once vitality drops to 0%, the waste package breaches



PFLOTRAN’s Waste Form Process Model

1. Waste Package Degradation Model

Waste Package Life (Vitality)

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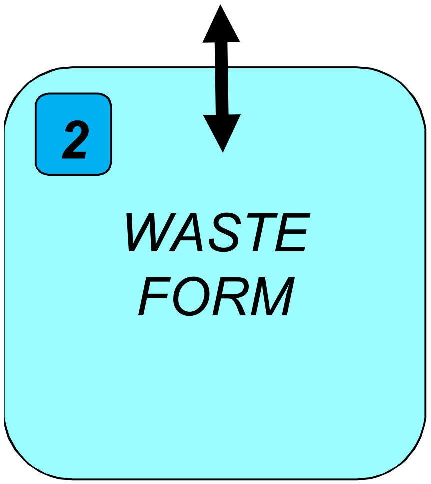
Waste Package Degradation Rate

- Rate at which waste package thickness decreases
- Unique to each waste form
- A base value is assigned via:
  - Directly as a user-provided value
  - ‘Random’ value from known distribution
- ‘Effective’ value is function of local conditions
- Provides a framework for future mechanistic processes that can control vitality degradation

$$R_{eff} = R \cdot e^{\left[\frac{1}{60℃} - \frac{1}{T(x,t)}\right]}$$

PFLOTRAN's Waste Form Process Model

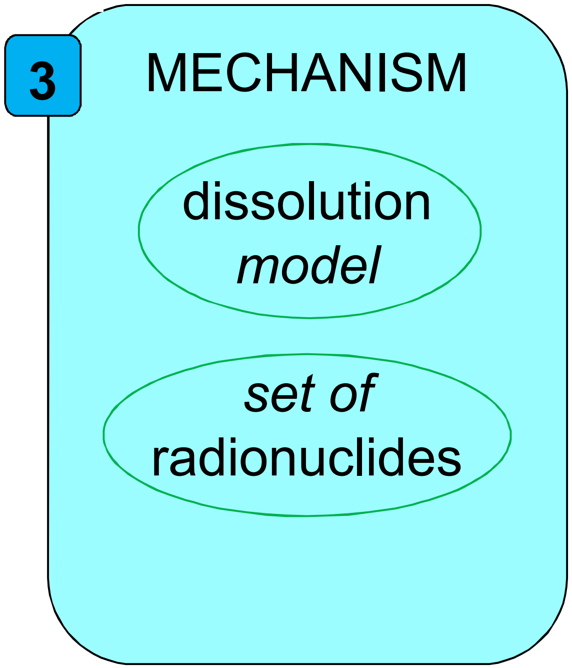
2. Waste Form Object



"waste form object"
"fruit"

PFLOTRAN's Waste Form Process Model

3. Waste Form Mechanism



"waste form type"
"banana, apple, orange, etc."

PFLOTRAN's Waste Form Process Model

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← varying local physical and chemical conditions →

waste package life (0-100%)

waste package degradation rate, R_{eff}

waste form 1
- region/coordinate
- RN concentrations
- eff. dissolution rate
- volume
- mech. pointer

waste form 2
- region/coordinate
- RN concentrations
- eff. dissolution rate
- volume
- mech. pointer

waste form 3
- region/coordinate
- RN concentrations
- eff. dissolution rate
- volume
- mech. pointer

waste form 4
- region/coordinate
- RN concentrations
- eff. dissolution rate
- volume
- mech. pointer

$$R_{eff} = R \cdot e^{\left[\frac{1}{60°\text{C}} - \frac{1}{T(x,t)}\right]}$$

PFLOTRAN's Waste Form Process Model

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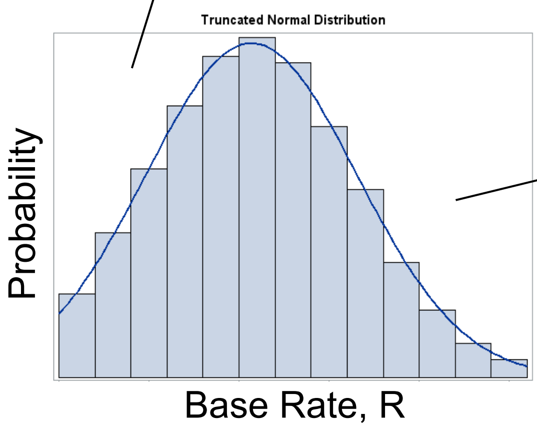

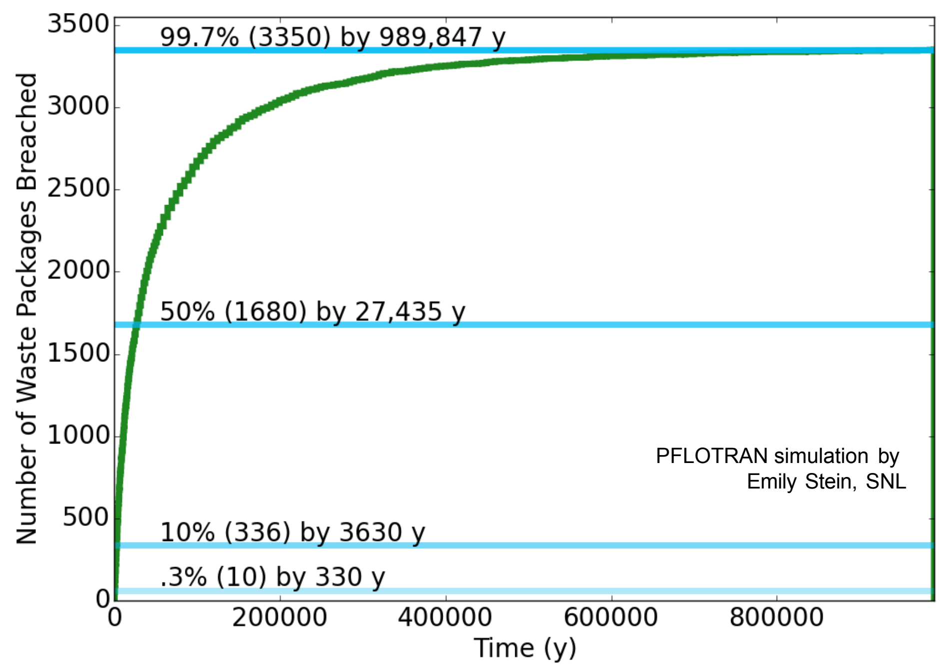

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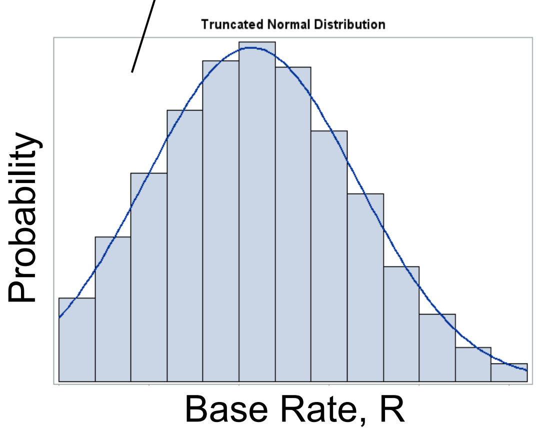

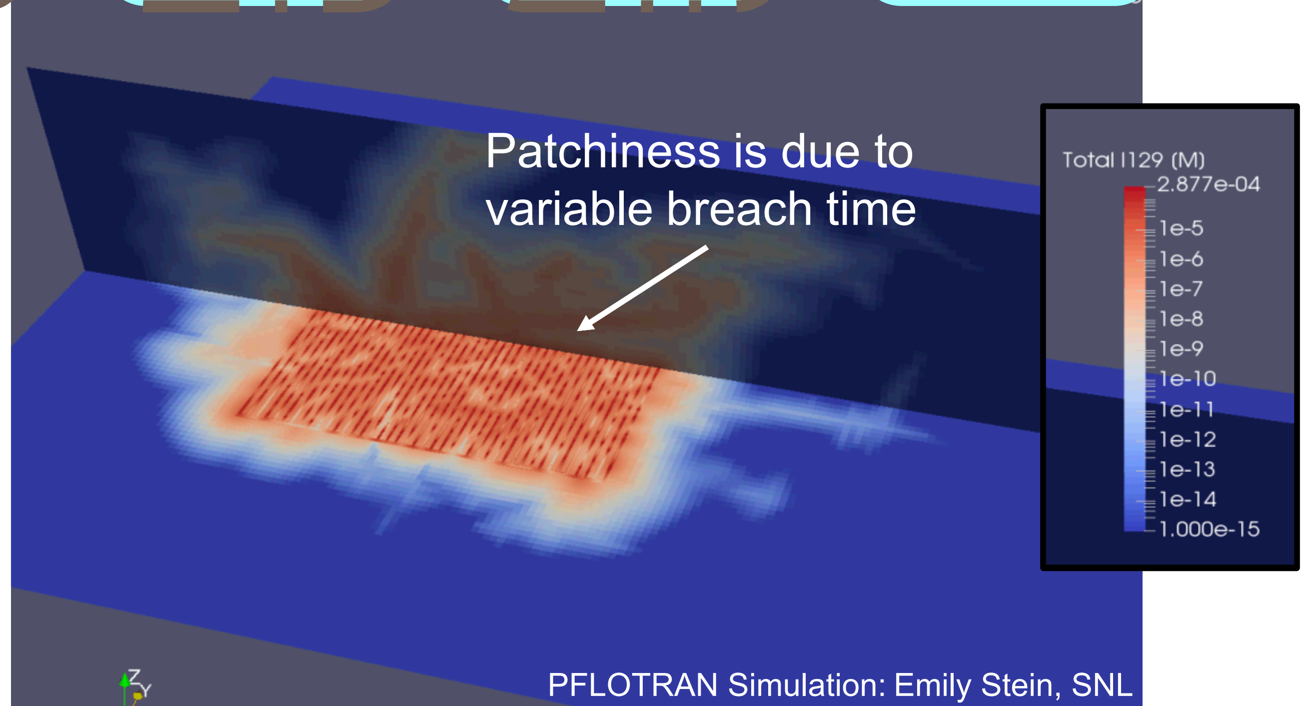

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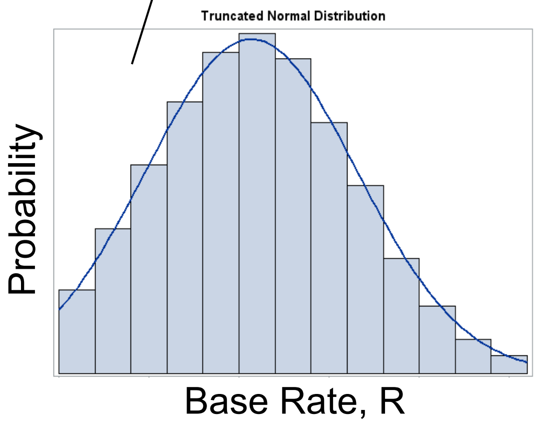
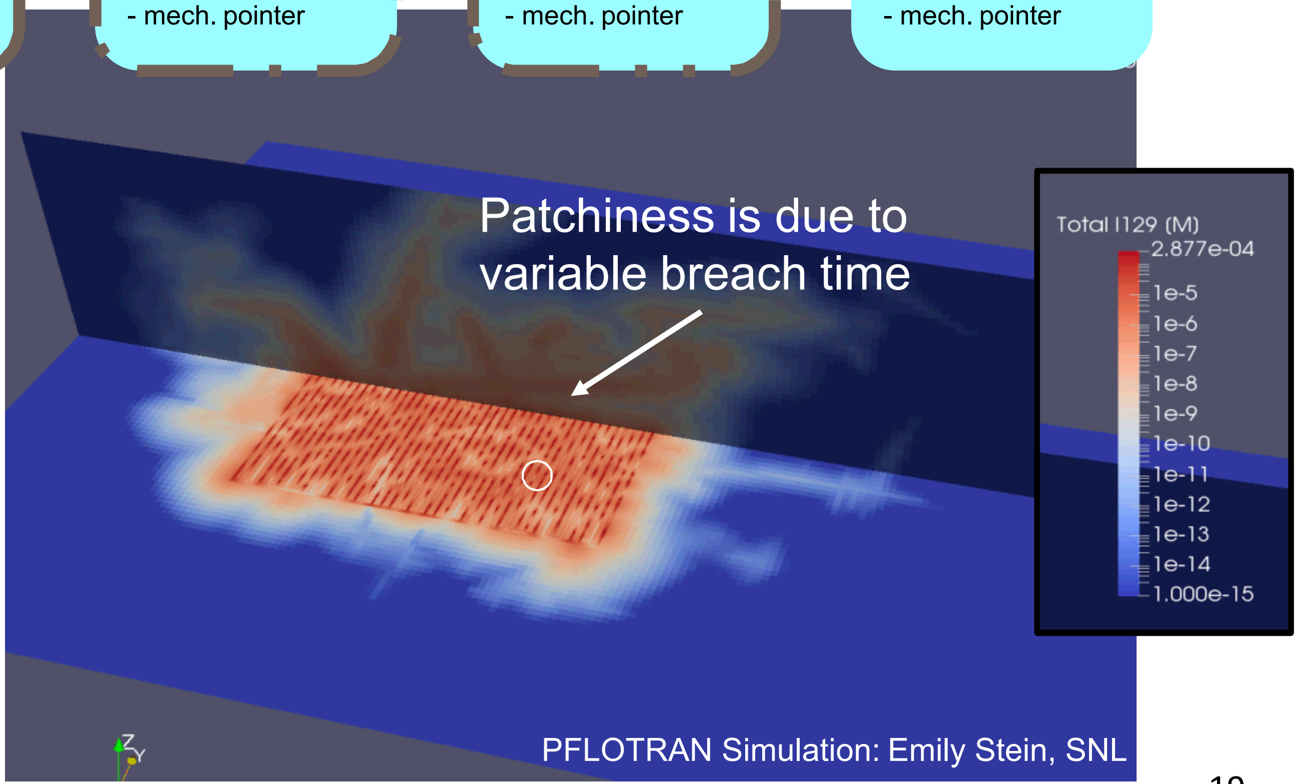
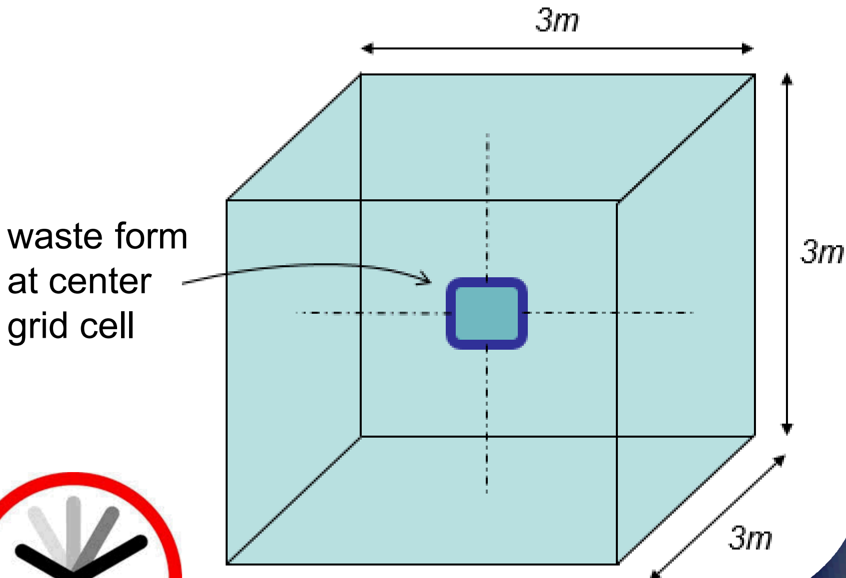




PFLOTRAN's Waste Form Process Model

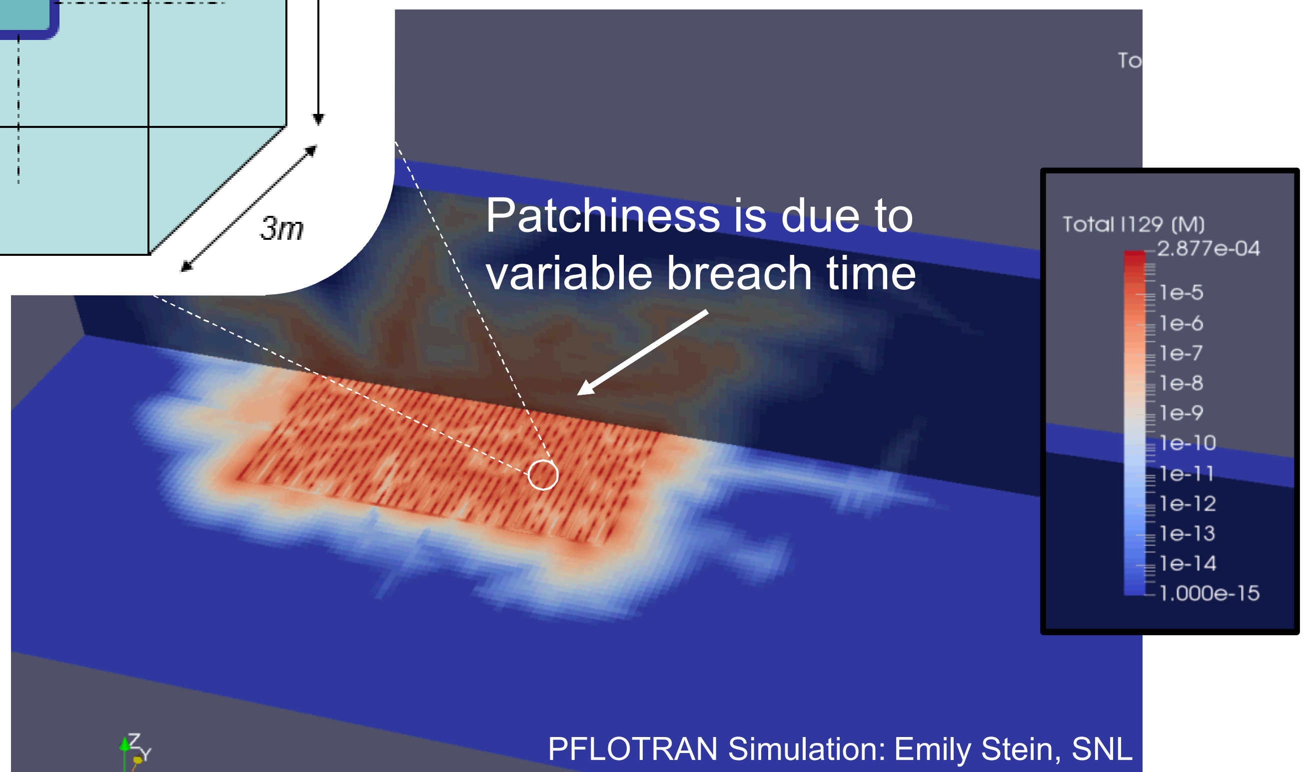


Mechanism GLASS

- Assumes waste form is a glass log type
- Dissolution equation (Kienzler et al. 2012):

$$R_g = 560e^{-7397/T(t,\mathbf{x})}$$

- no fluid flow
- no diffusive flux across boundaries
- 3x3x3 = 27 grid cells
- $1m^3$ grid cells



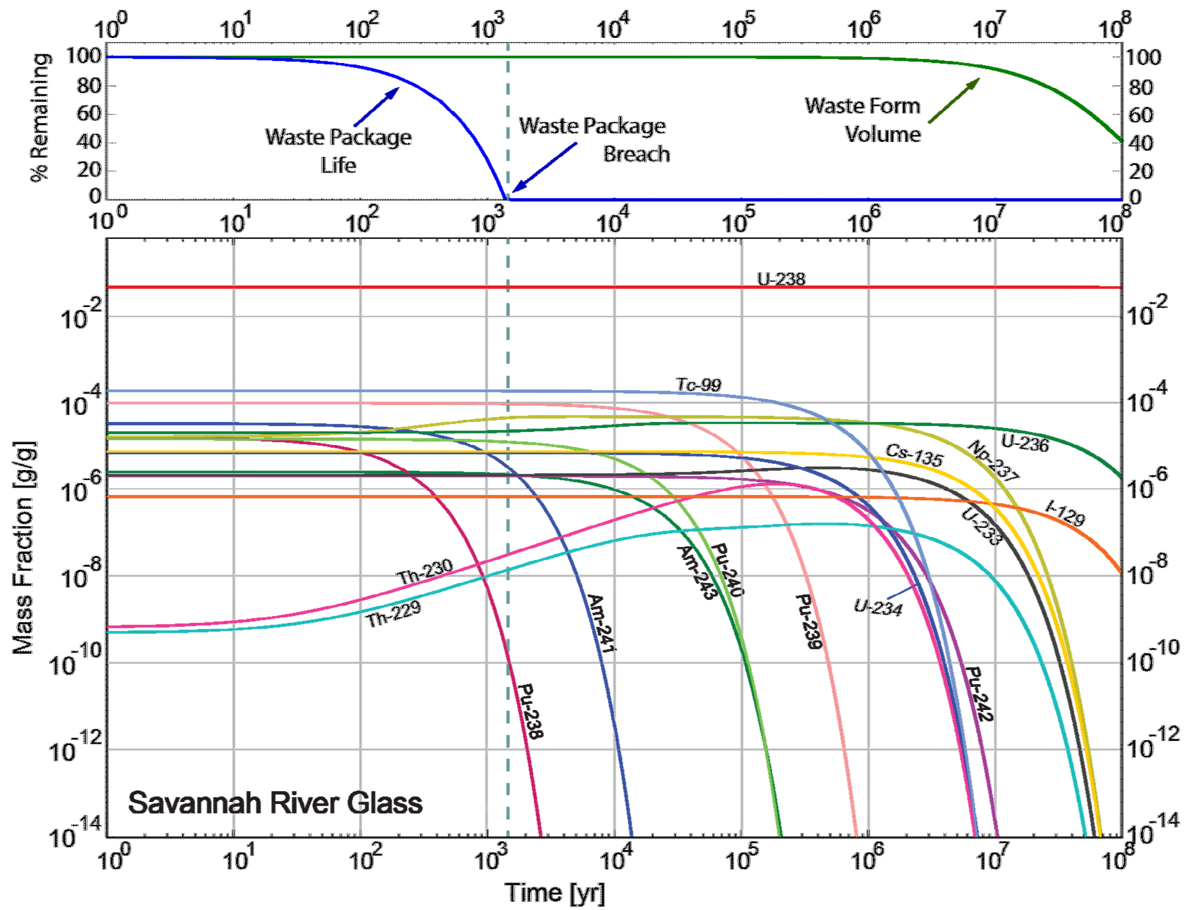
PFLOTRAN's Waste Form Process Model

- Waste package breach occurs at 1,000 yrs
- Waste form volume slowly decreases after breach

- Over time, the mass fractions of radionuclides evolve due to decay and ingrowth
- Mass fraction = g-RN/g-bulk

- The remaining mass fraction of each radionuclide and the glass dissolution rate determines its release rate

$$R_g = 560e^{-7397/T(t,\mathbf{x})}$$



Savannah River Glass Log Waste Form

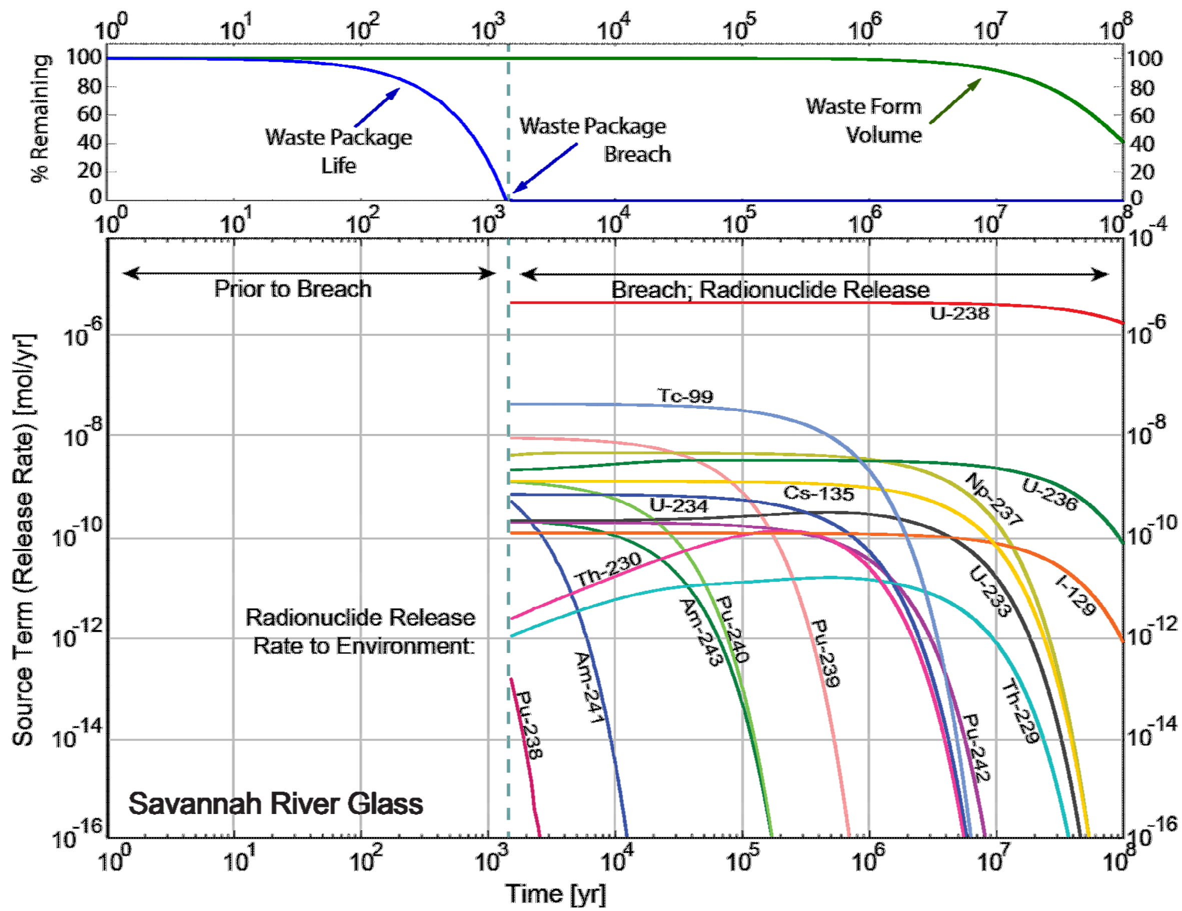
PFLOTRAN's Waste Form Process Model

- Waste package breach occurs at 1,000 yrs
- Waste form volume slowly decreases after breach

- Upon breach, radionuclides are released to the surroundings
- The source terms decrease over time, proportionally to the remaining inventory

- The remaining mass fraction of each radionuclide and the glass dissolution rate determines its release rate

$$R_g = 560e^{-7397/T(t,x)}$$

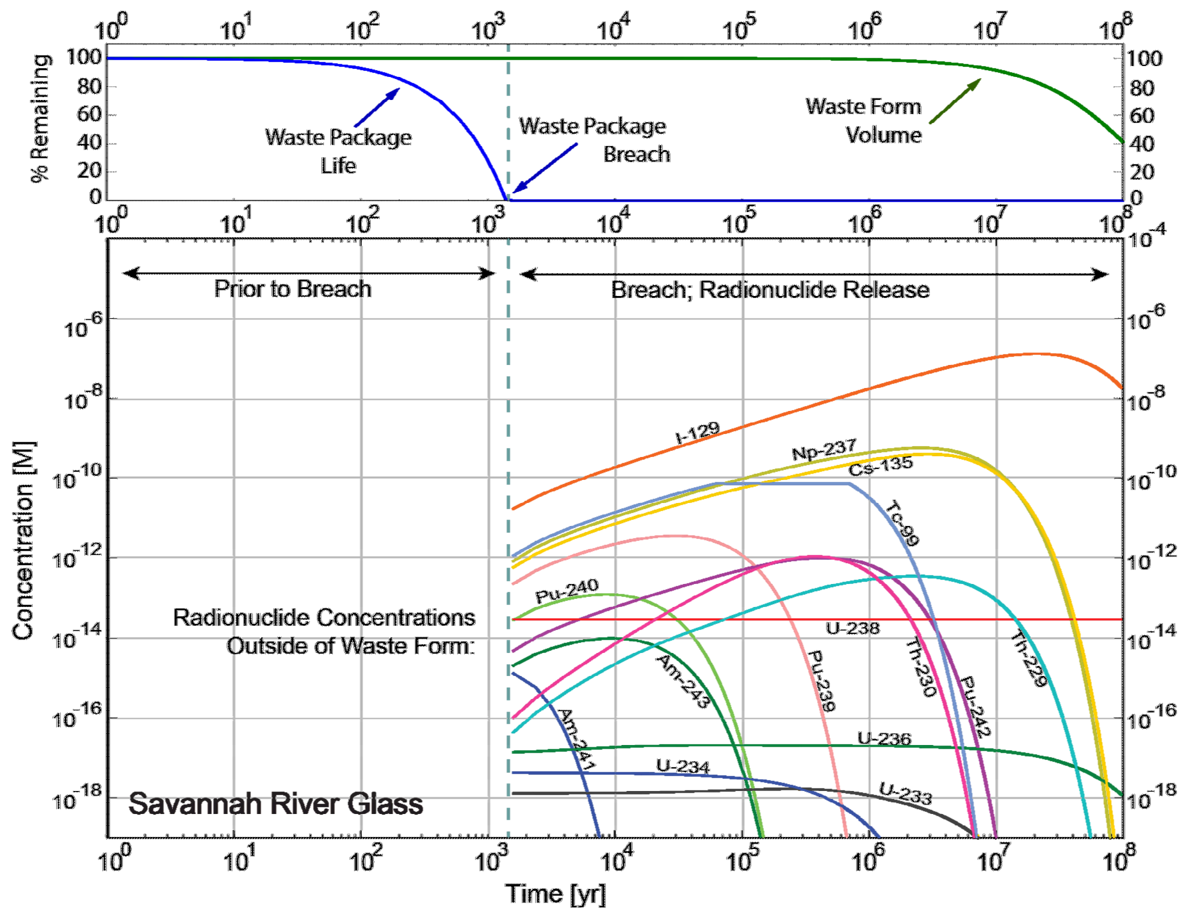


Savannah River Glass Log Waste Form

PFLOTRAN's Waste Form Process Model

- Waste package breach occurs at 1,000 yrs
- Waste form volume slowly decreases after breach

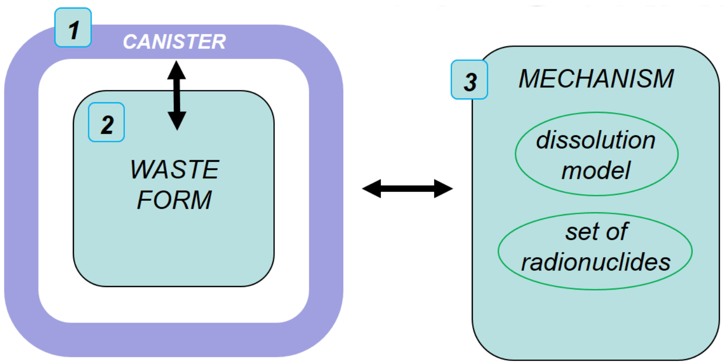
- The radionuclide concentrations outside of the waste form are influenced by:
  - Solubility
  - Sorption to host rock
  - Diffusion/advection
  - Decay and ingrowth



Savannah River Glass Log Waste Form

PFLOTRAN's Waste Form Process Model

Future Development



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GDSA Framework

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- **Waste form mechanisms:**
  - Add more mechanism types
  - Make dissolution models more mechanistic and interactive
- **Waste package degradation model:**
  - Include waste package degradation mechanisms like corrosion and damage models
- **PFLOTRAN's waste form process model is <u>open-source</u> and <u>modular</u>**
  - We invite collaboration to create new type of waste forms, mechanisms, etc.
  - We can work with you to get your functionality implemented