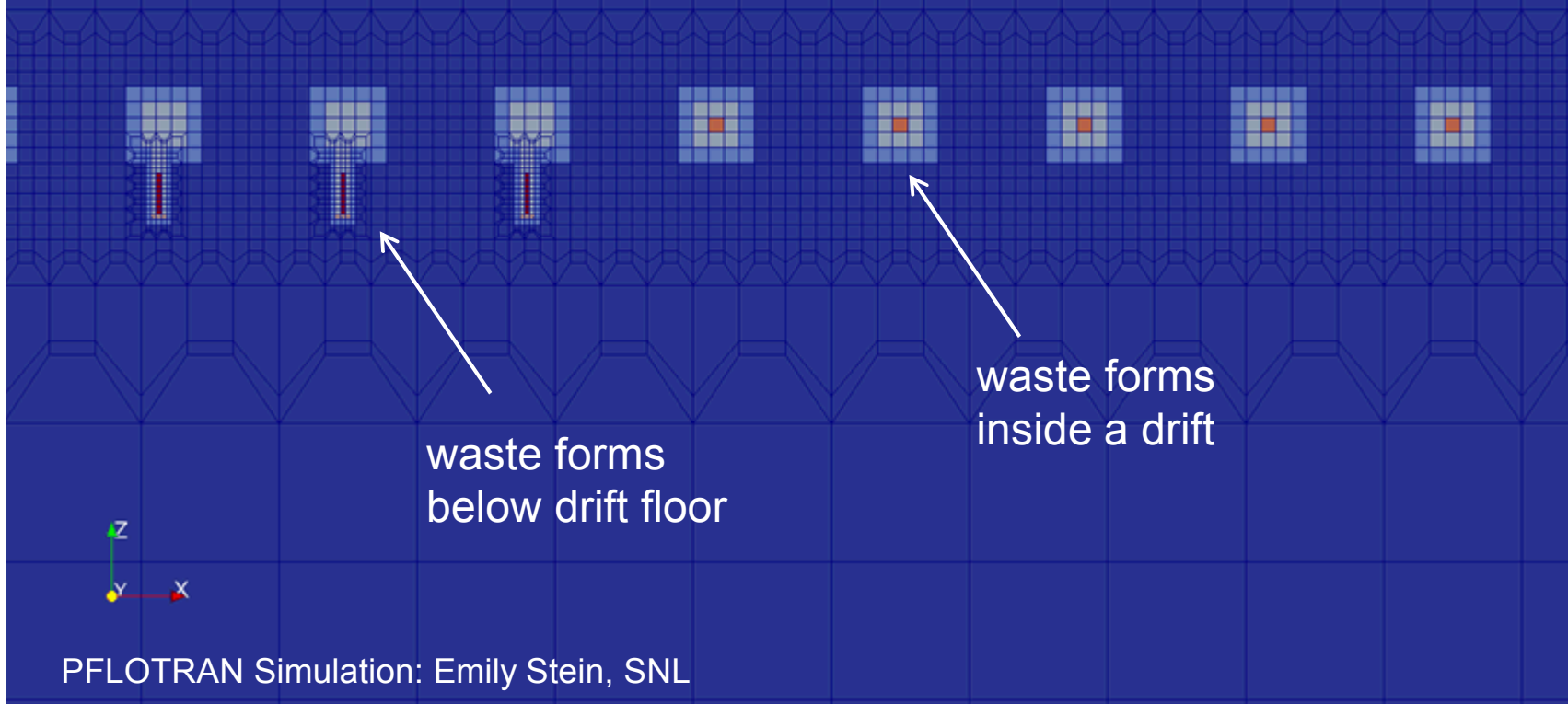


Development of a Waste Form Process Model in PFLOTRAN

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

PFLOTRAN's Waste Form Process Model

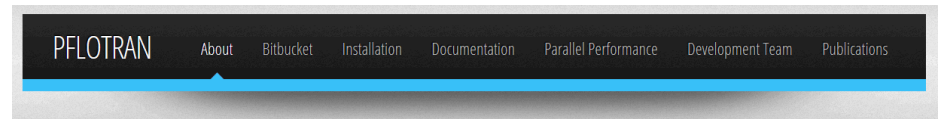
Advances in PFLOTRAN's implementation of the **radioisotope source term** due to degrading waste forms



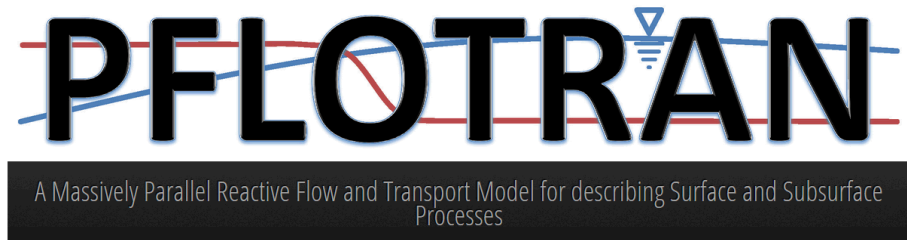
PFLOTRAN's Waste Form Process Model

- The Waste Form Process Model is used to:
 - track radioisotope decay and ingrowth inside the waste form
 - couple with a canister degradation model to determine breach time
 - track waste form dissolution and remaining volume
 - determine radionuclide source term to environment

Implemented in:



- Waste Form Process Model Development Team:
 - Jennifer M. Frederick (SNL)
 - Glenn E. Hammond (SNL)
 - Paul Mariner (SNL)



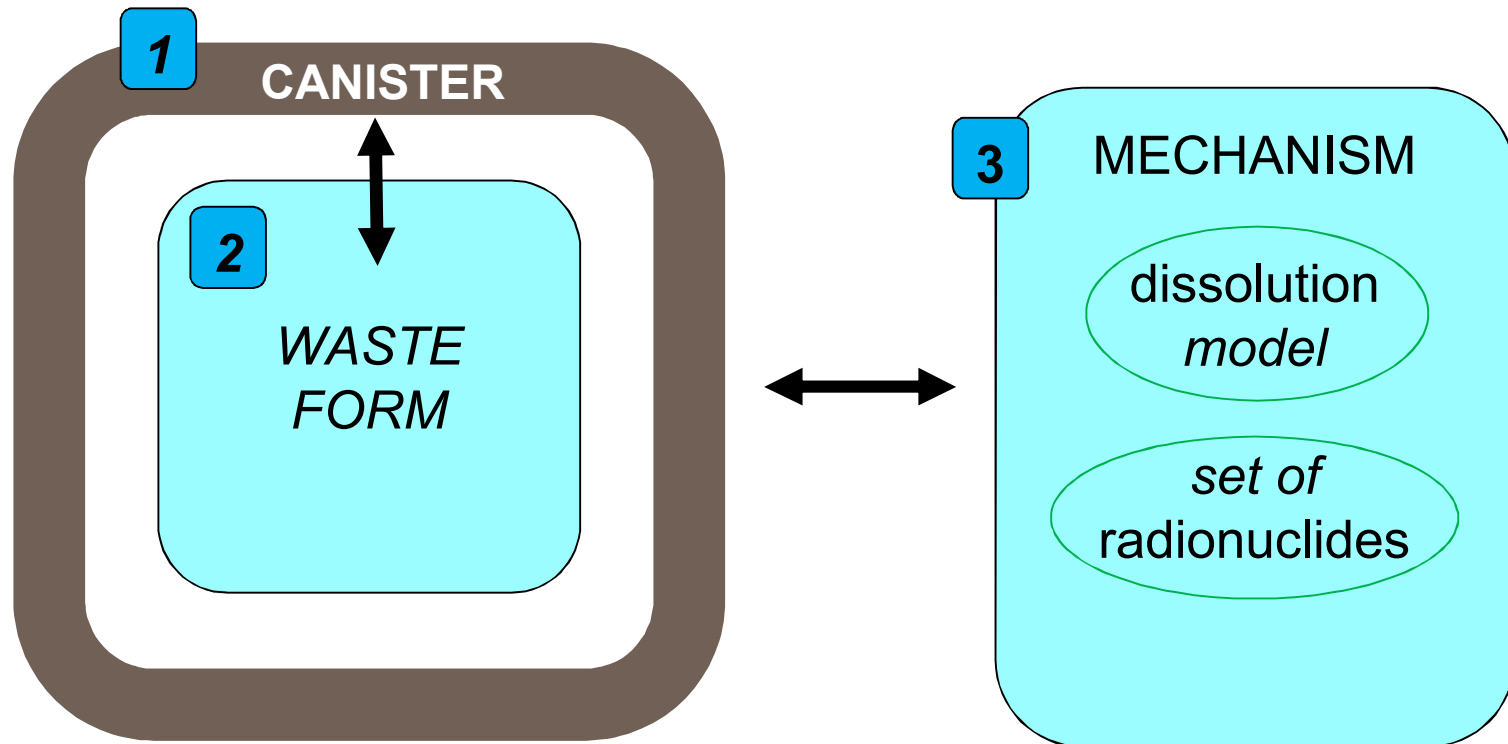
www.pflotran.org

What is PFLOTRAN?

PFLOTRAN is an open source, state-of-the-art massively parallel subsurface flow and reactive transport code. PFLOTRAN solves a system of generally nonlinear partial differential equations describing multiphase, multicomponent and multiscale reactive flow and transport in porous materials. The code is designed to run on massively parallel computing architectures as well as workstations and laptops. Parallelization is achieved through domain decomposition using the PETSc (Portable Extensible Toolkit for Scientific Computation) libraries. PFLOTRAN has been developed from the ground up for parallel scalability and has been run on up to 2¹⁸ processor cores with problem sizes up to 2 billion degrees of freedom. PFLOTRAN is written in object oriented, free formatted Fortran 2003. The choice of Fortran over C/C++ was based primarily on the need to enlist and preserve tight collaboration with experienced domain scientists, without which PFLOTRAN's sophisticated process models would not exist. The reactive transport equations can be solved using either a fully implicit Newton-Raphson algorithm or the less robust operator splitting method.

PFLOTRAN's Waste Form Process Model

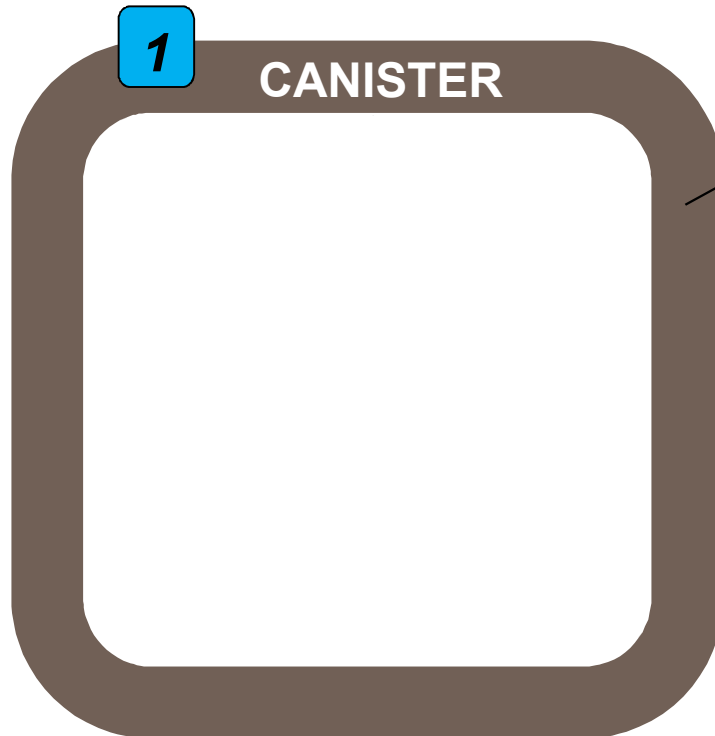
Consists of 3 Main Components:



"waste form object"
"fruit"

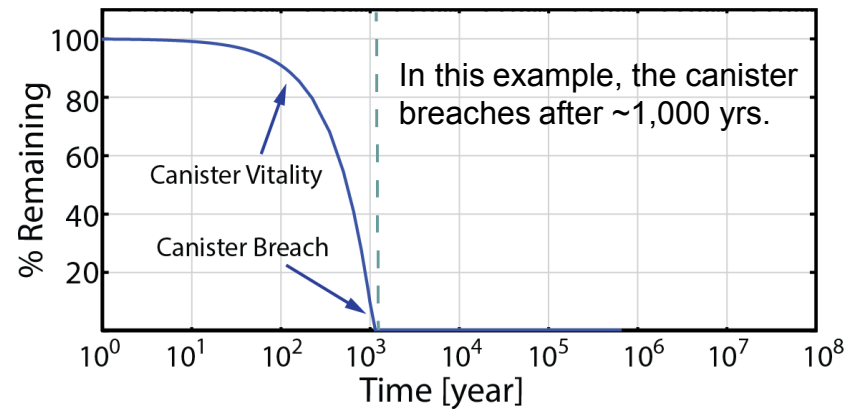
"waste form type"
"banana, apple, orange, etc."

1. Canister Degradation Model

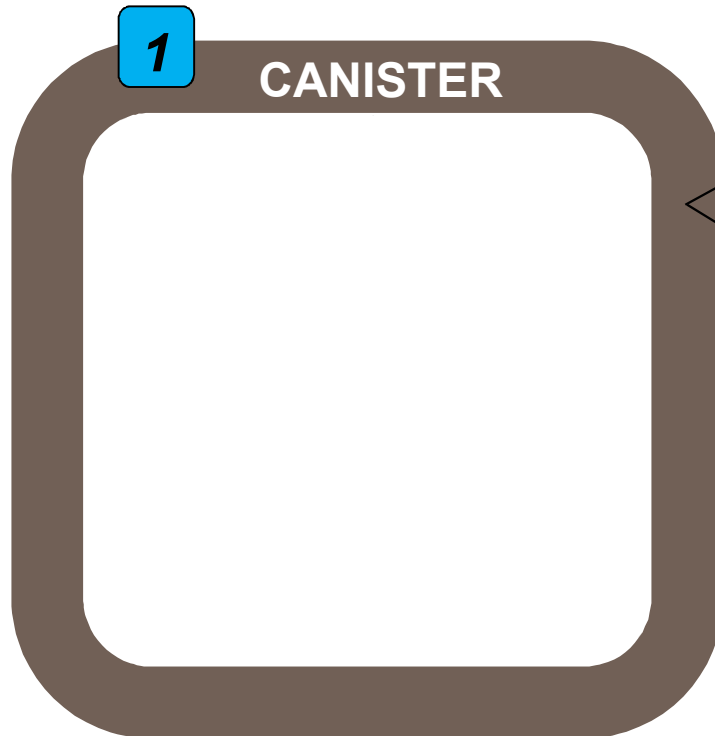


Canister Vitality

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



1. Canister Degradation Model



Canister Vitality

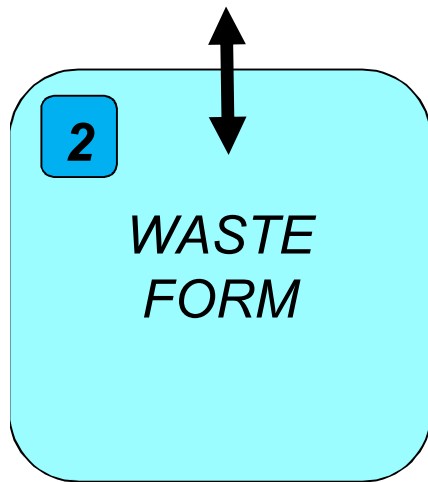
- A measure of how much 'life' the canister has remaining
- Range: 100% - 0%
- Once vitality drops to 0%, the waste form canister breaches

Canister Degradation Rate

- The rate at which canister vitality 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

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

2. Waste Form Object

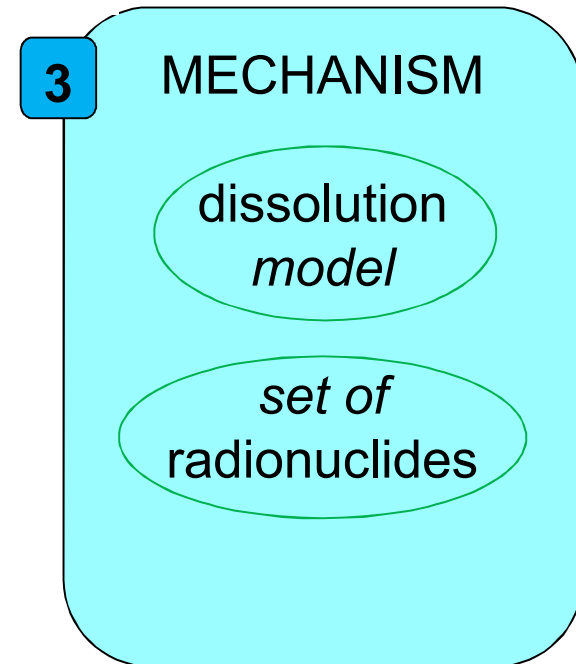


“waste form object”
“fruit”

erm

PFLOTRAN's Waste Form Process Model

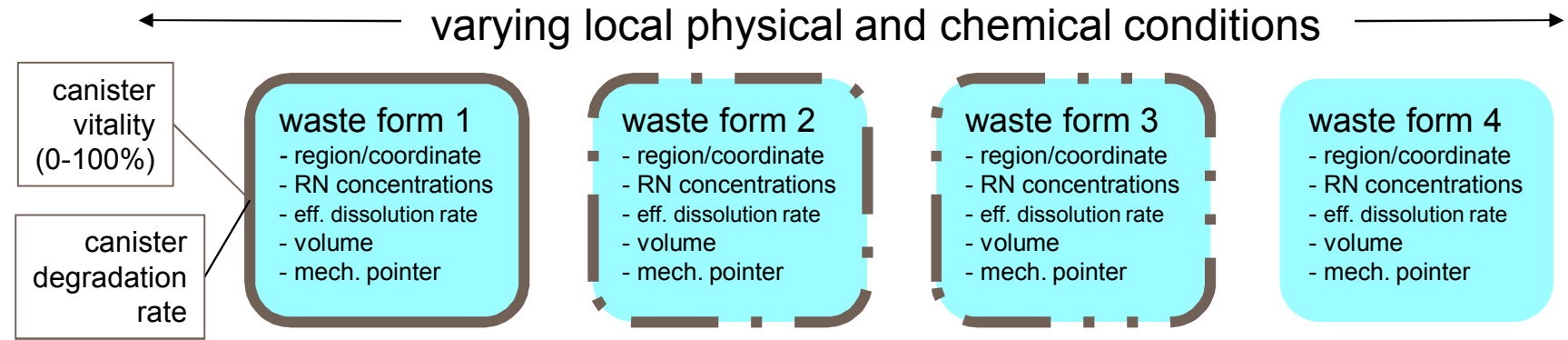
3. Waste Form Mechanism



“waste form type”

“banana, apple, orange, etc.”

PFLOTRAN's Waste Form Process Model



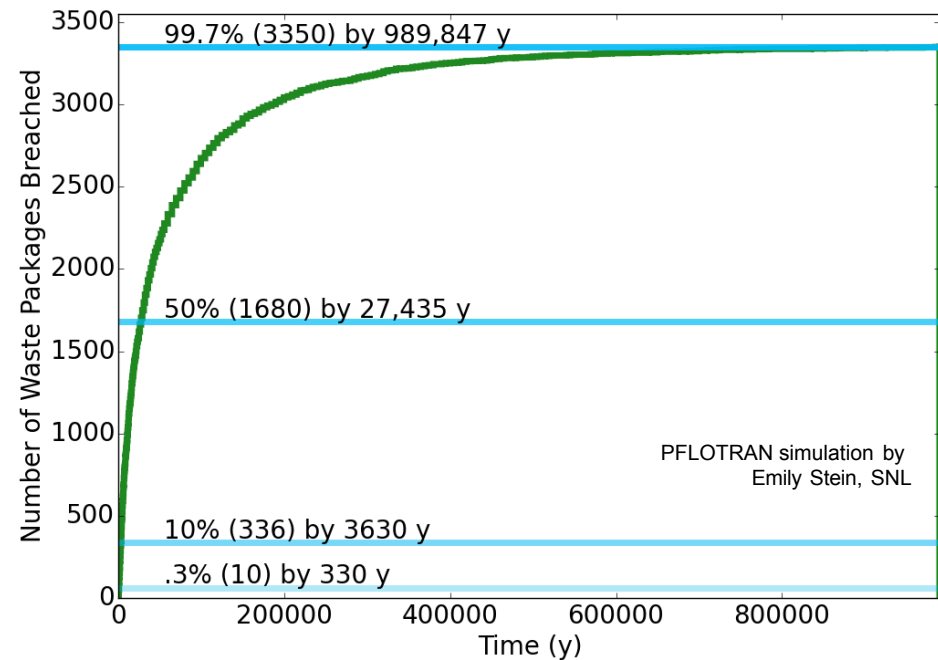
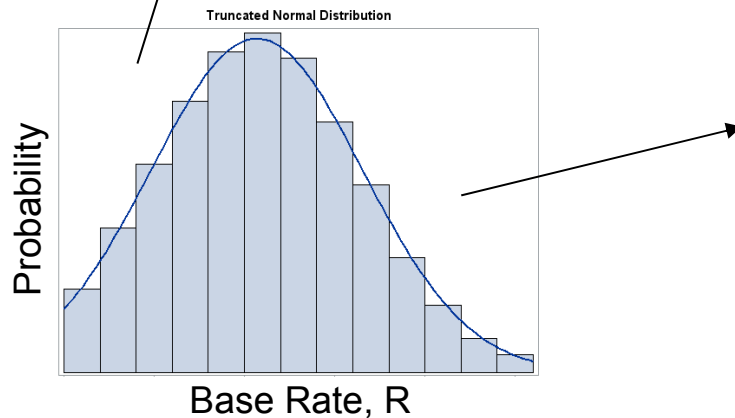
$$R_{eff} = R \cdot e^{\left[\frac{1}{60^{\circ}\text{C}} - \frac{1}{T(x,t)} \right]}$$

PFLOTRAN's Waste Form Process Model

← varying local physical and chemical conditions →

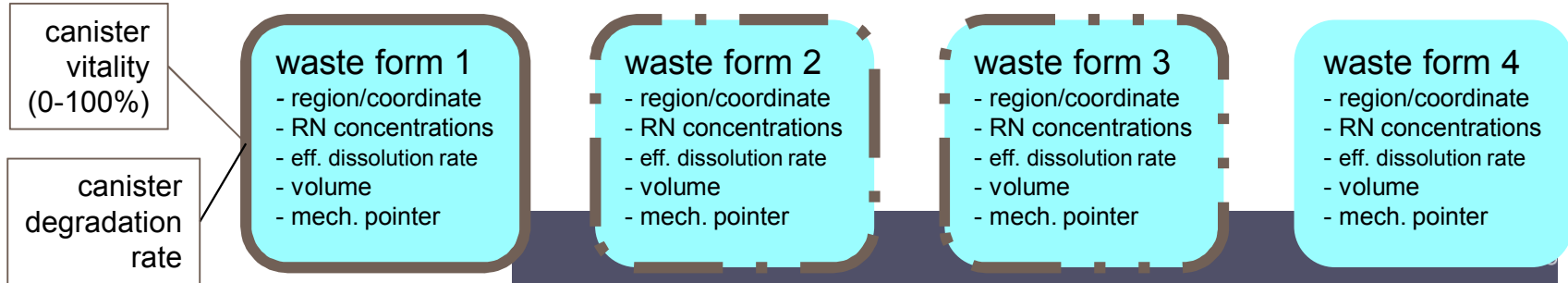


$$R_{eff} = R \cdot e^{\left[\frac{1}{60^{\circ}\text{C}} - \frac{1}{T(x,t)} \right]}$$

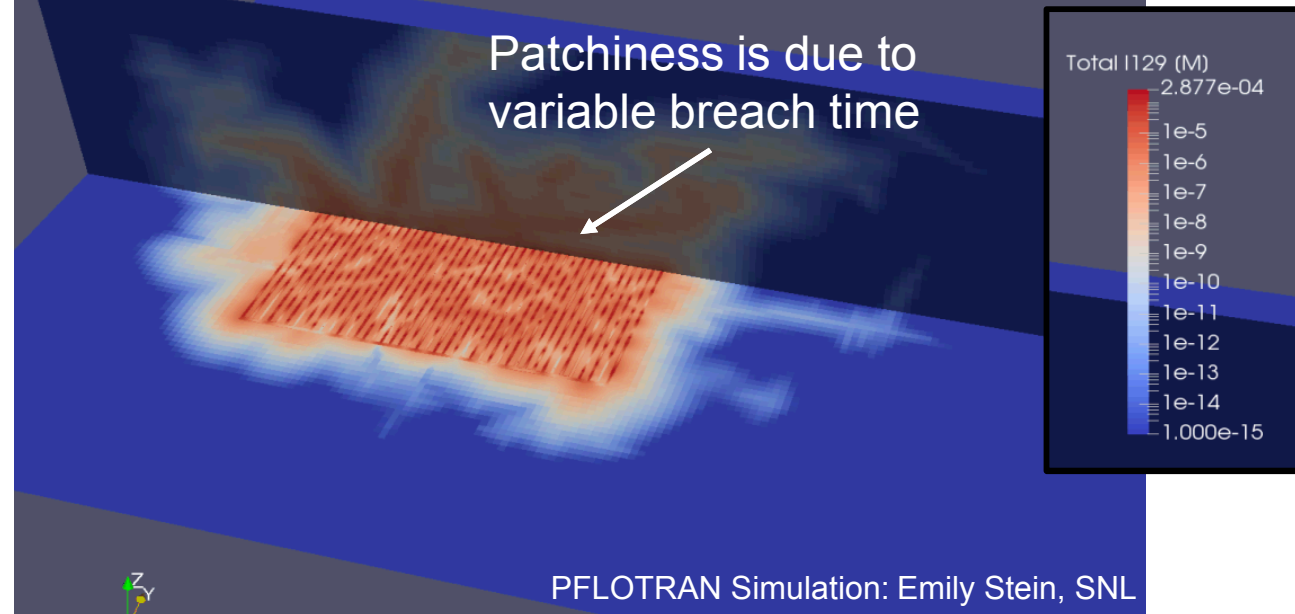
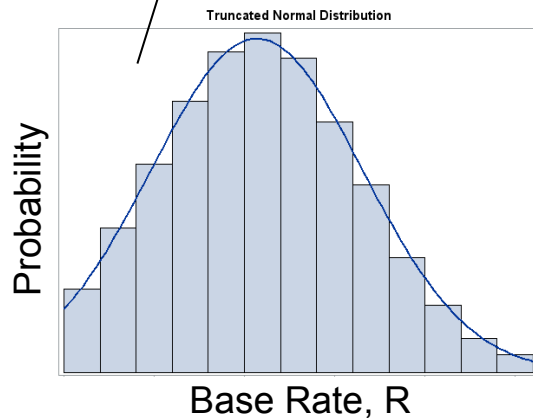


PFLOTRAN's Waste Form Process Model

← varying local physical and chemical conditions →



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



PFLOTRAN's Waste Form Process Model

← varying local physical and chemical conditions →

canister
vitality
(0-100%)

canister
degradation
rate

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

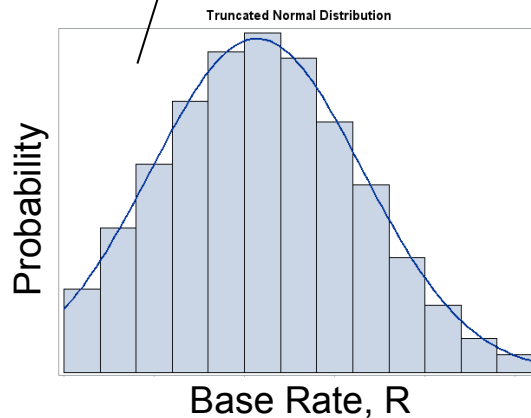
waste form 3

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

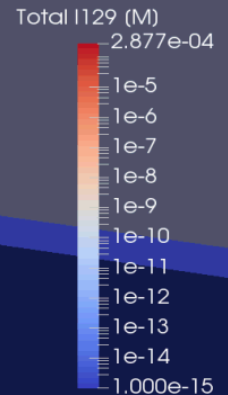
waste form 4

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

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

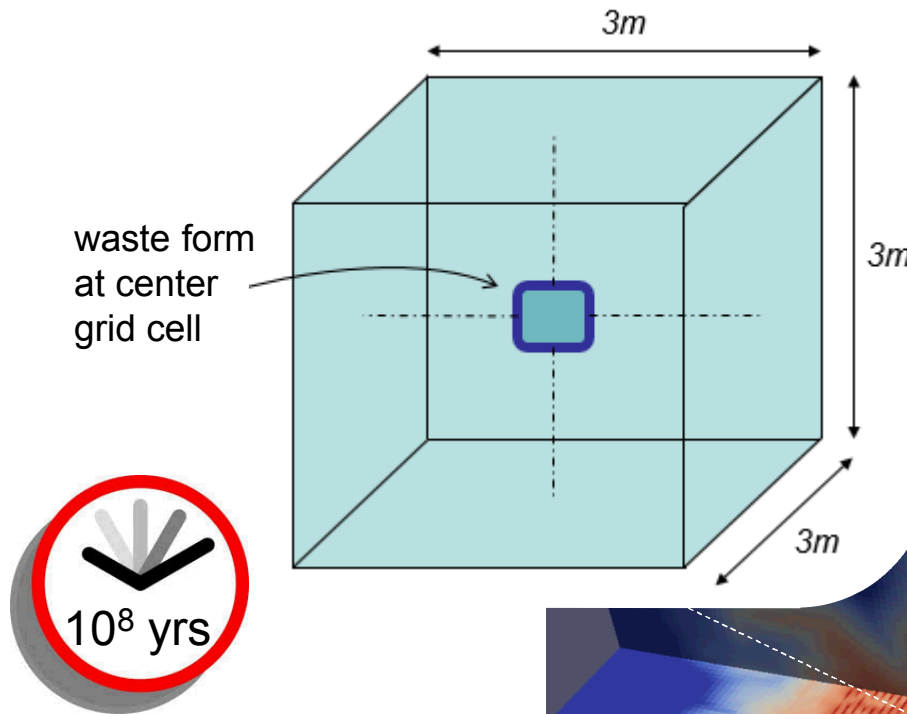


Patchiness is due to
variable breach time



PFLOTRAN Simulation: Emily Stein, SNL

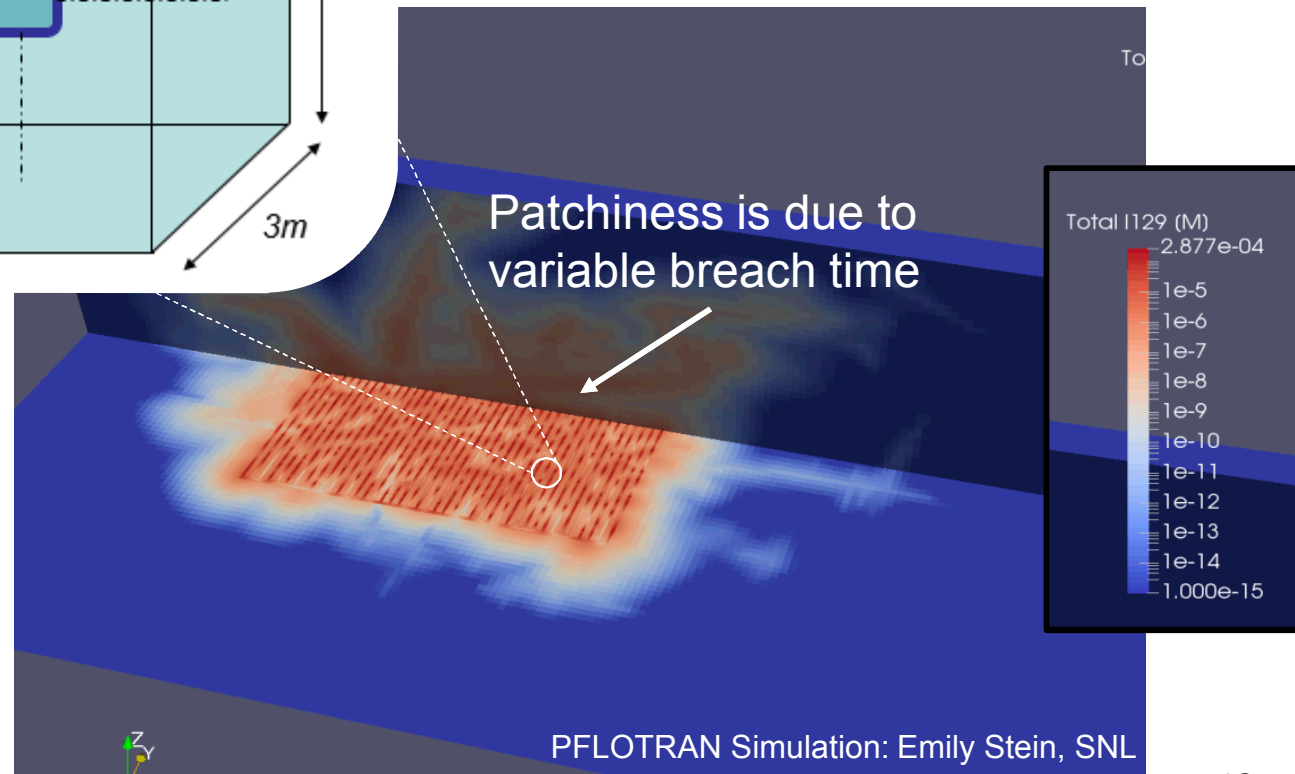
PFLOTRAN's Waste Form Process Model



Mechanism GLASS

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

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

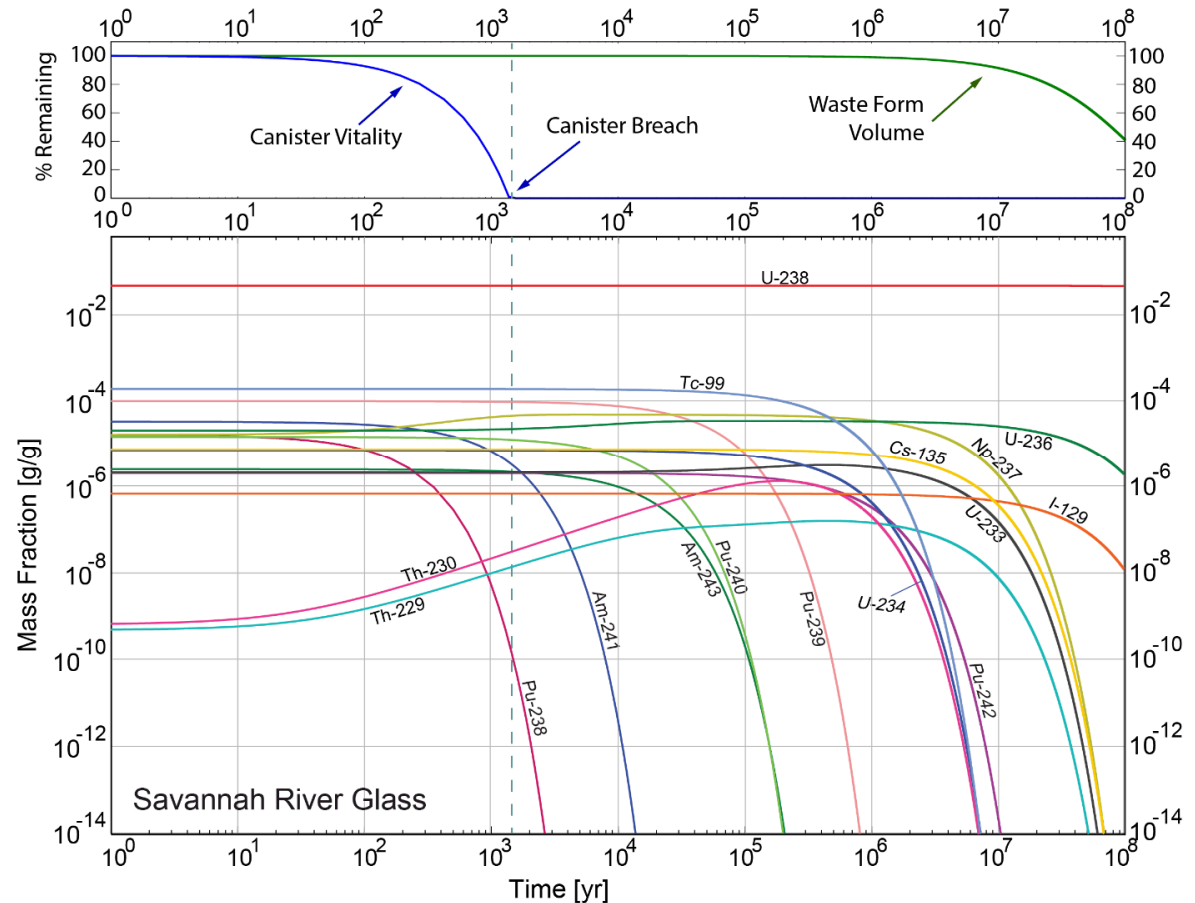


- no fluid flow
- no diffusive flux across boundaries
- 3x3x3 = 27 grid cells
- 1m³ grid cells

PFLOTRAN's Waste Form Process Model

- Canister 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

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

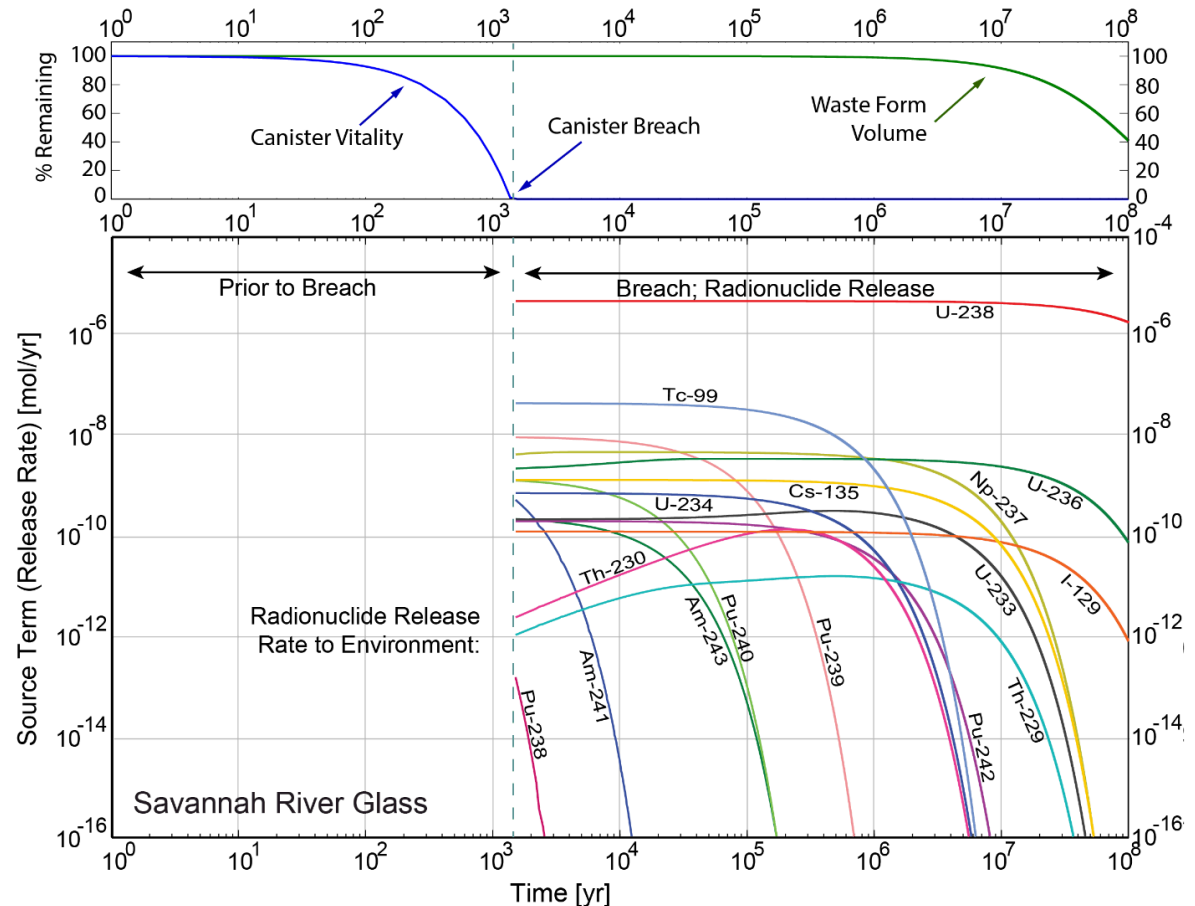


Savannah River Glass Log Waste Form

PFLOTRAN's Waste Form Process Model

- Canister 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

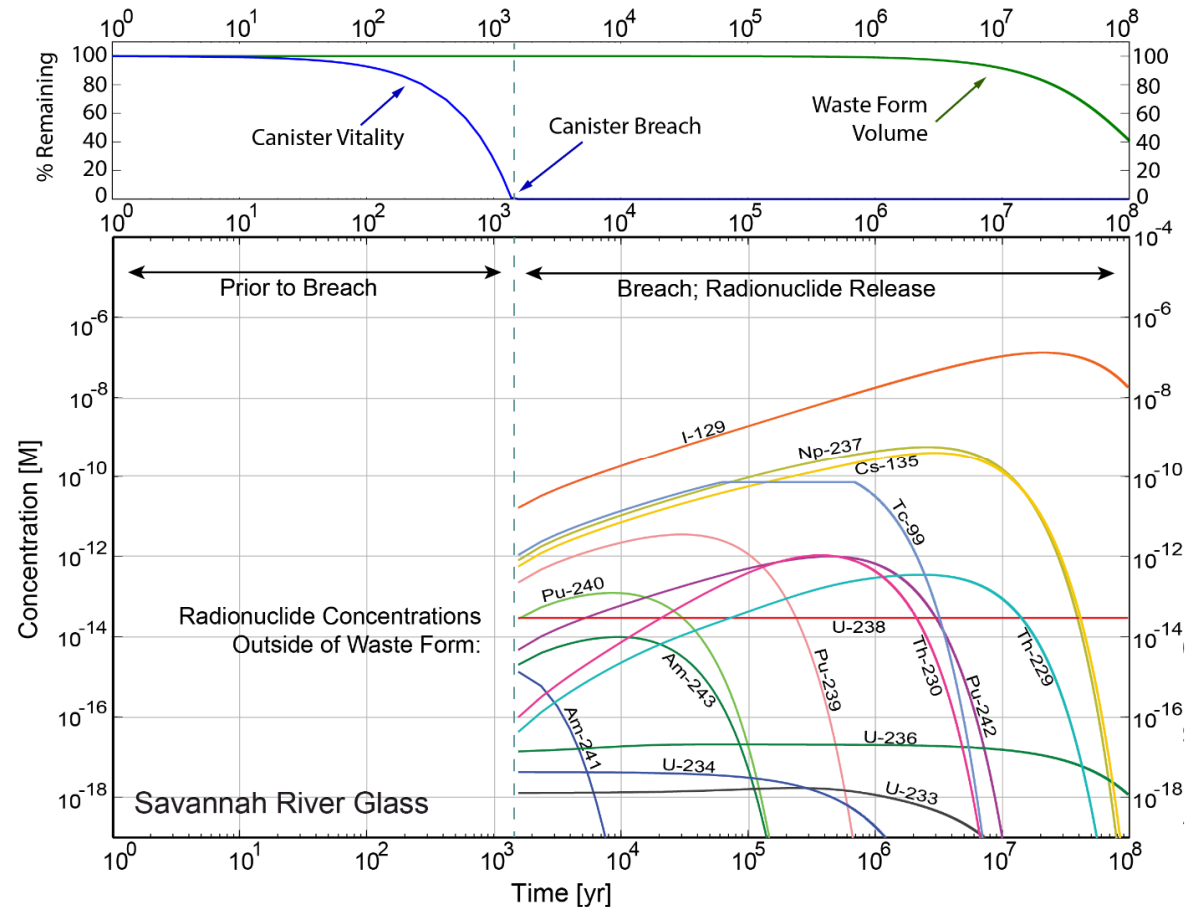
$$R_g = 560e^{-7397/T(t,x)}$$



Savannah River Glass Log Waste Form

PFLOTRAN's Waste Form Process Model

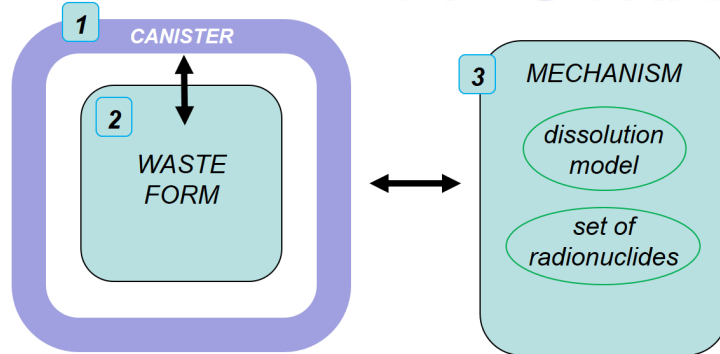
- Canister breach occurs at 1,000 yrs
- Waste form volume slowly decreases after breach
- The radionuclide concentrations outside of the waste form are influenced by:
 - Solubility
 - Sorption to host rock
 - Diffusion/advection
 - Decay and ingrowth



Savannah River Glass Log Waste Form

PFLOTRAN's Waste Form Process Model

Future Development



- **Isotope decay and ingrowth algorithm:**
 - Fully implicit solution rather than 3-generation explicit
- **4D Waste Forms:**
 - Allows ultra-refinement in a 4th spatial dimension (think nested) spaces
- **PFLOTRAN's waste form process model is open-source and modular**
 - We invite collaboration to create new type of waste forms, mechanisms, etc.
 - We will work with you to get your functionality implemented
- **Waste form mechanisms:**
 - Add more mechanism types
 - Make dissolution models more mechanistic and interactive
- **Canister degradation model:**
 - Include canister degradation mechanisms like corrosion and damage models