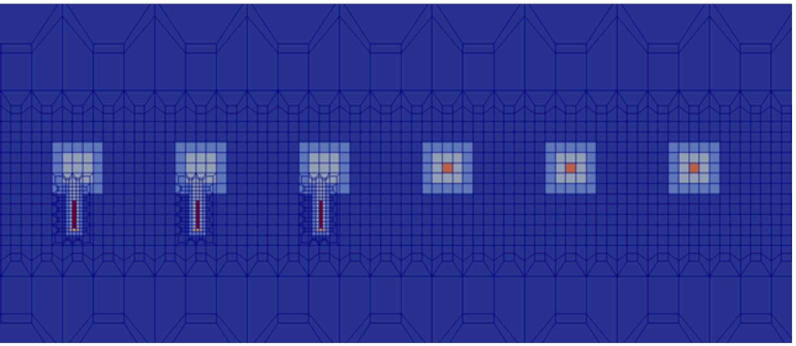
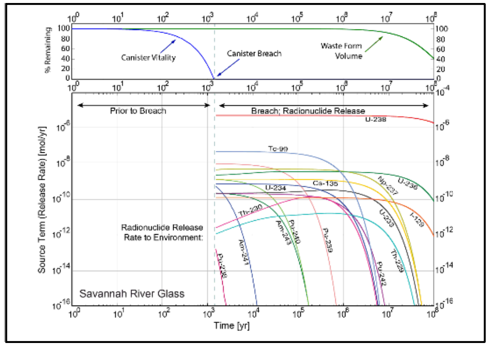
SAND2017-3430C





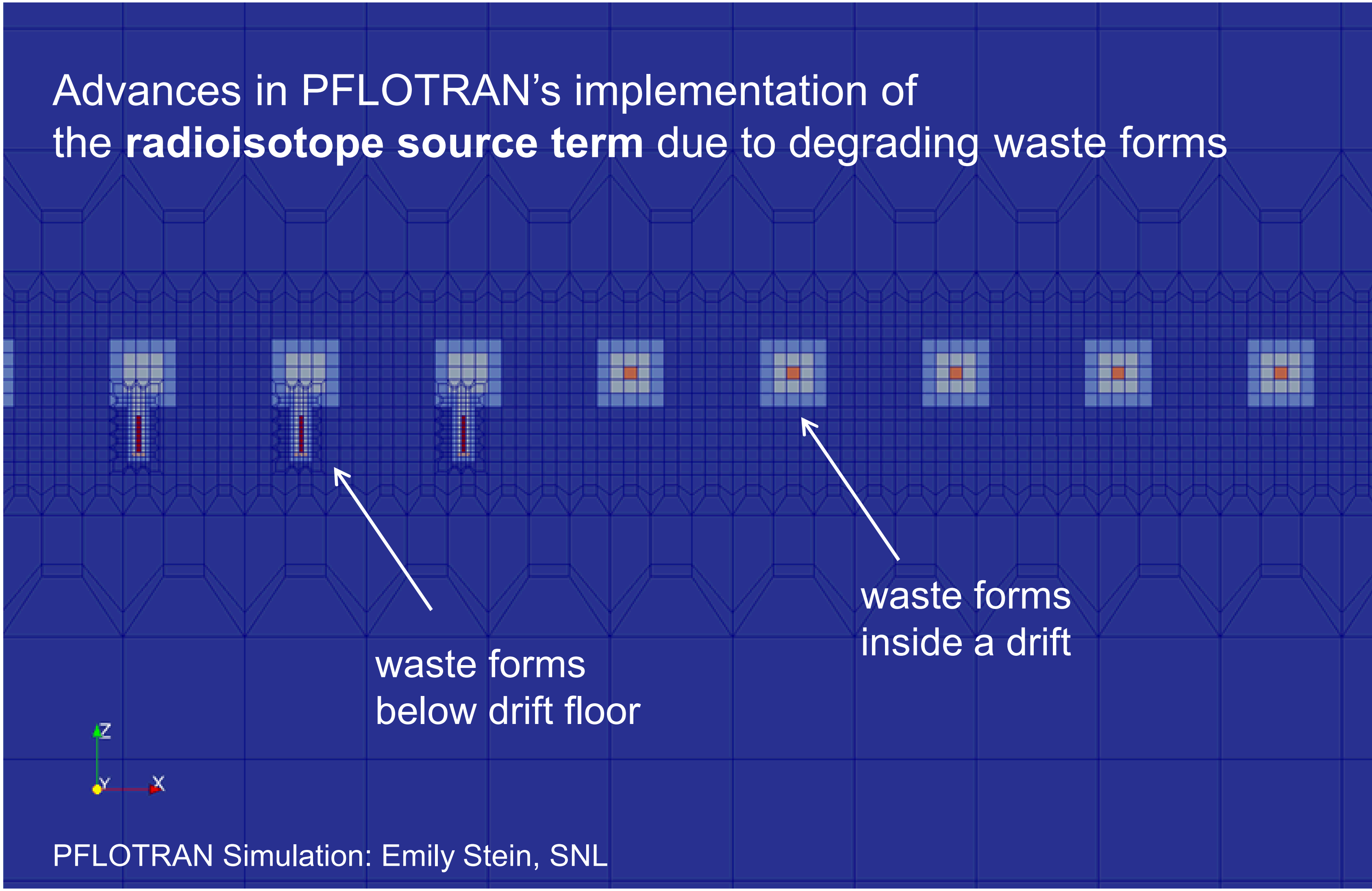

# Development of a Waste Form Process Model in PFLOTRAN

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

Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND NO. 2011-XXXXP

# 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

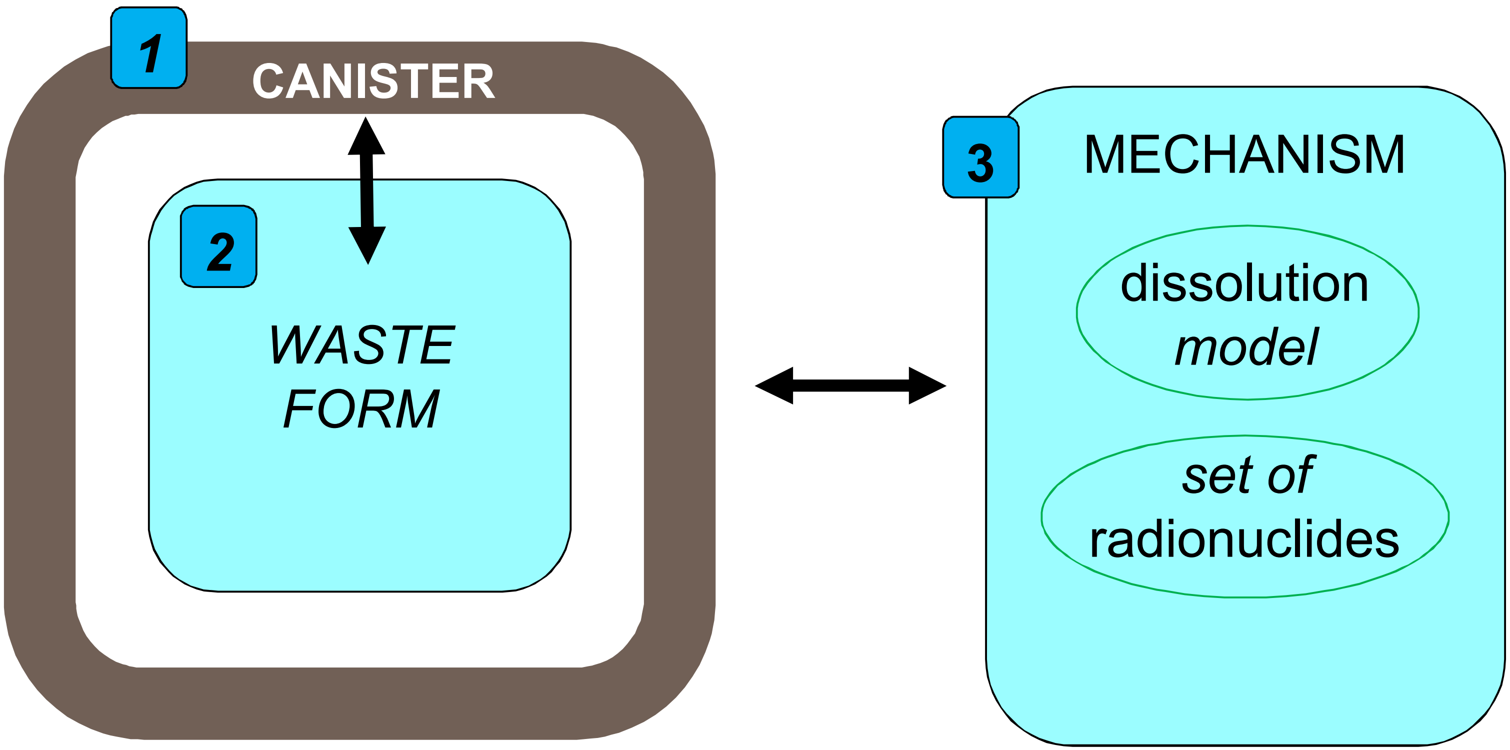
Implemented in:


www.pflotran.org

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

# PFLOTRAN's Waste Form Process Model

## Consists of 3 Main Components:

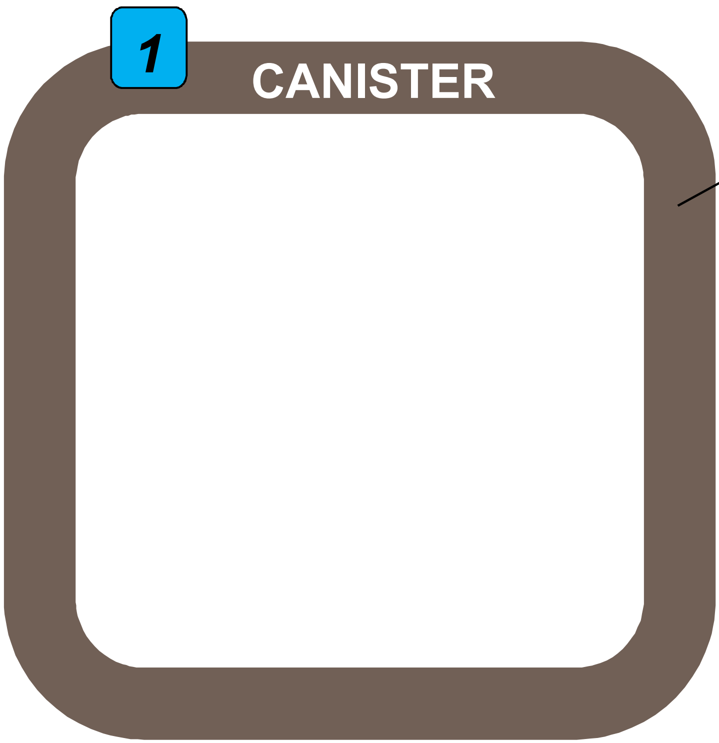



"waste form object"
"fruit"

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

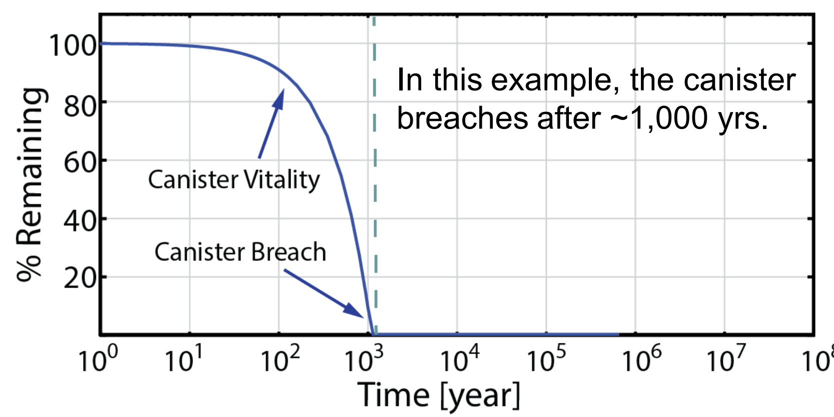
# PFLOTRAN’s Waste Form Process Model

## 1. Canister Degradation Model



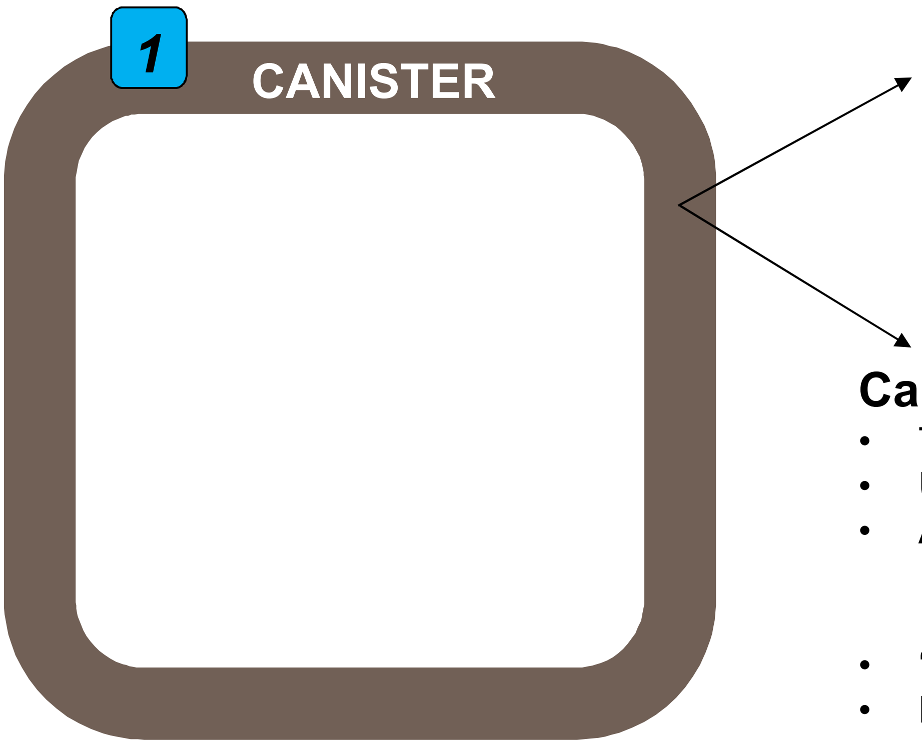

**Canister Vitality**

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



# PFLOTRAN's Waste Form Process Model

## 1. Canister Degradation Model




**Canister Vitality**

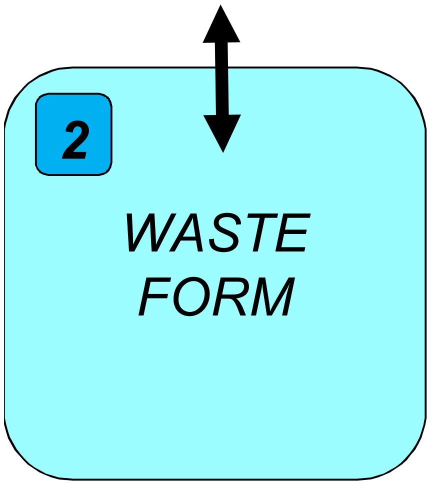
- A measure of how much 'life' the canister has remaining
- Range: 100% - 0%
- Once vitality drops to 0%, the waste form canister breaches

**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

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

## 2. Waste Form Object

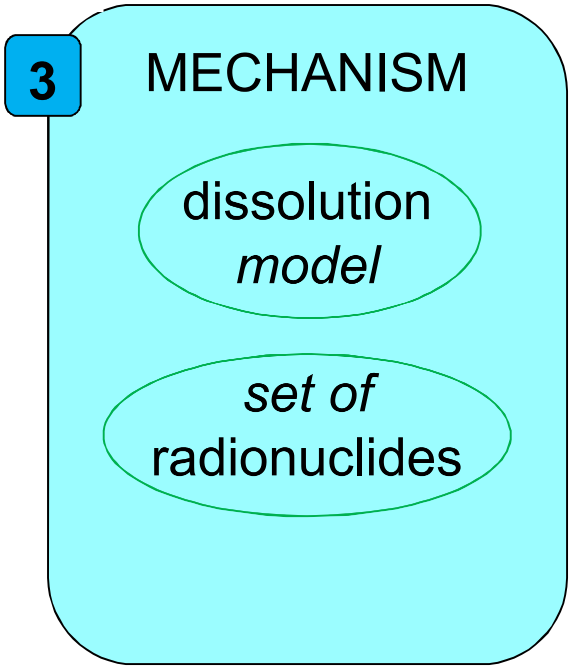



"waste form object"
"fruit"

erm

# PFLOTRAN's Waste Form Process Model

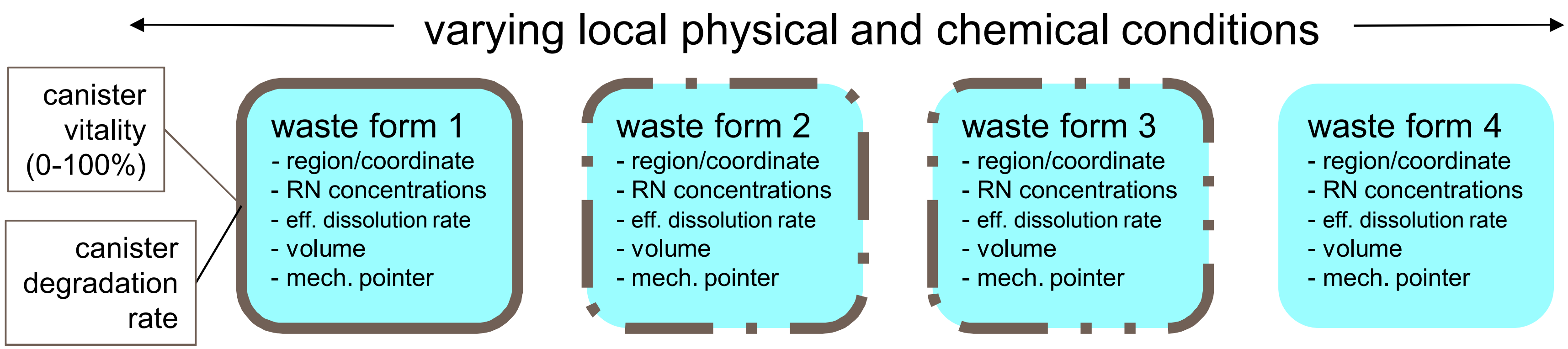
## 3. Waste Form Mechanism




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

# PFLOTRAN's Waste Form Process Model

Sandia National Laboratories




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

# PFLOTRAN's Waste Form Process Model

← varying local physical and chemical conditions →

canister vitality (0-100%)

canister degradation rate

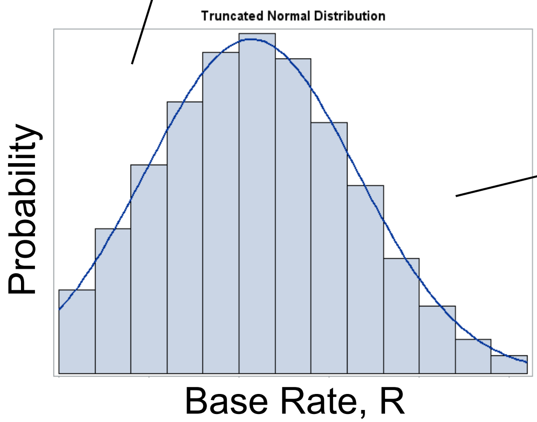
**waste form 1**
- region/coordinate
- RN concentrations
- eff. dissolution rate
- volume
- mech. pointer

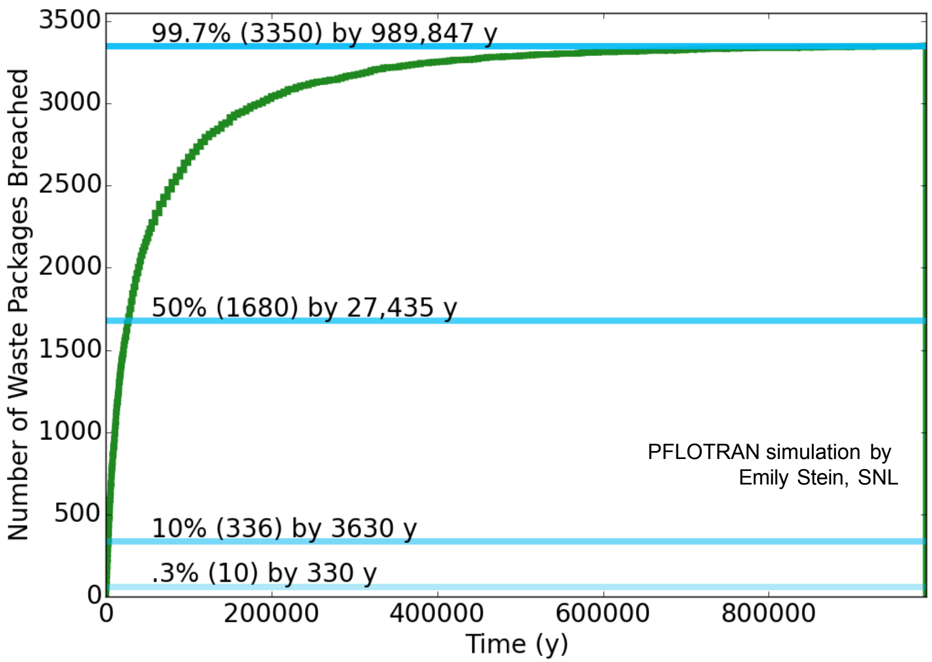
**waste form 2**
- region/coordinate
- RN concentrations
- eff. dissolution rate
- volume
- mech. pointer

**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

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



# PFLOTRAN's Waste Form Process Model

← varying local physical and chemical conditions →

canister vitality (0-100%)

canister degradation rate

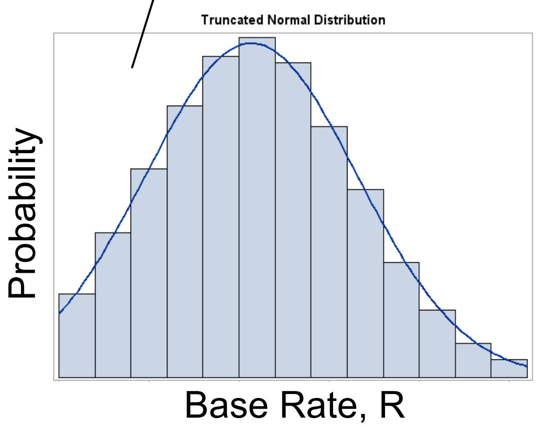
**waste form 1**
- region/coordinate
- RN concentrations
- eff. dissolution rate
- volume
- mech. pointer

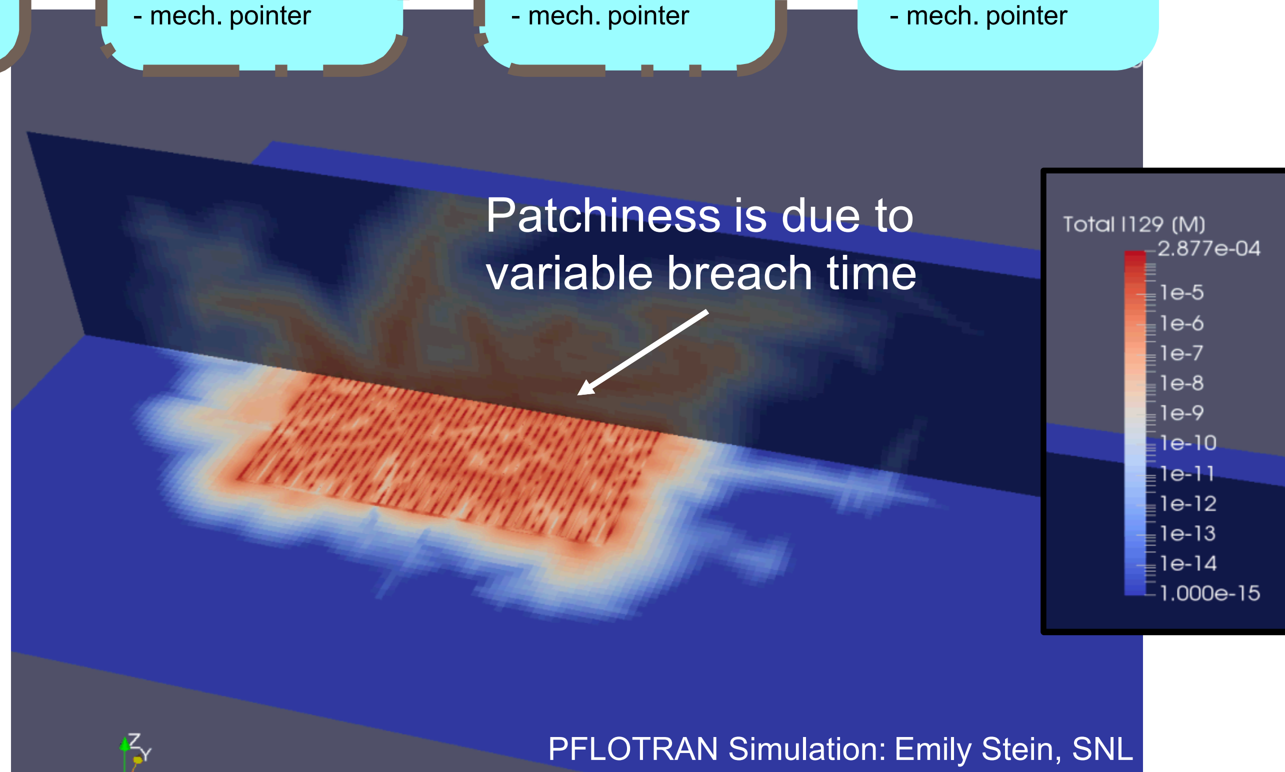
**waste form 2**
- region/coordinate
- RN concentrations
- eff. dissolution rate
- volume
- mech. pointer

**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

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



# PFLOTRAN's Waste Form Process Model

varying local physical and chemical conditions

canister vitality (0-100%)

canister degradation rate

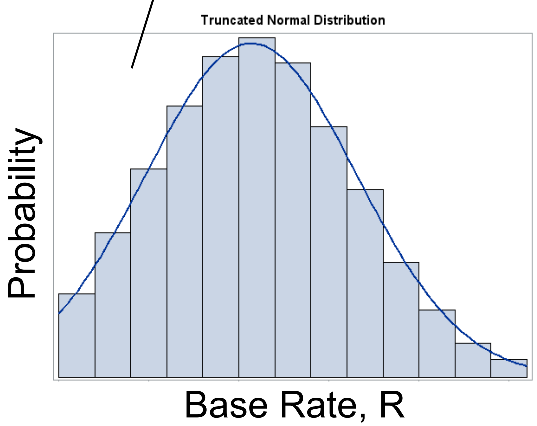
**waste form 1**
- region/coordinate
- RN concentrations
- eff. dissolution rate
- volume
- mech. pointer

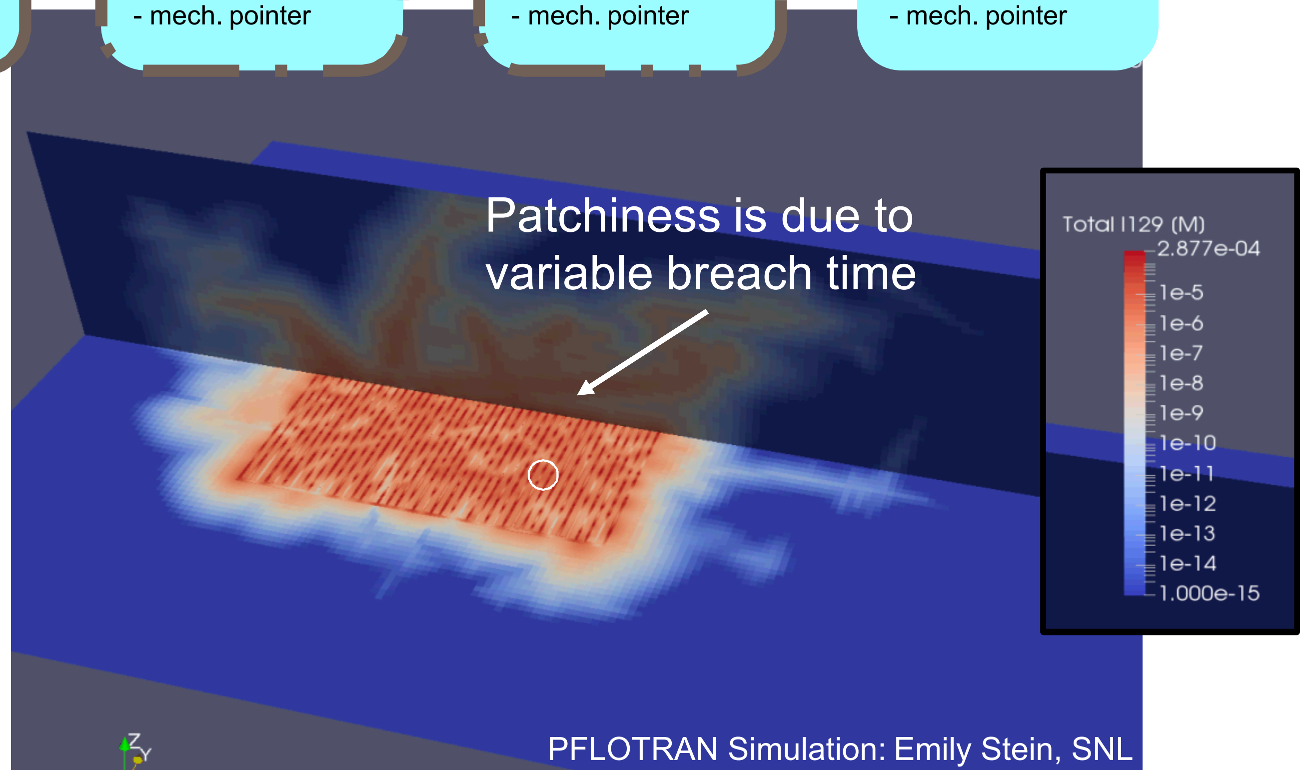
**waste form 2**
- region/coordinate
- RN concentrations
- eff. dissolution rate
- volume
- mech. pointer

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

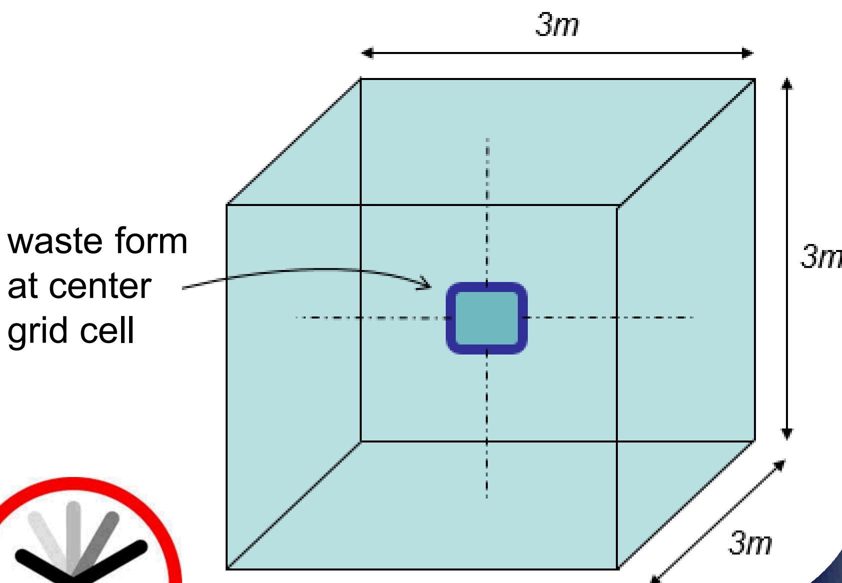
**waste form 4**
- region/coordinate
- RN concentrations
- eff. dissolution rate
- volume
- mech. pointer

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



# PFLOTRAN's Waste Form Process Model



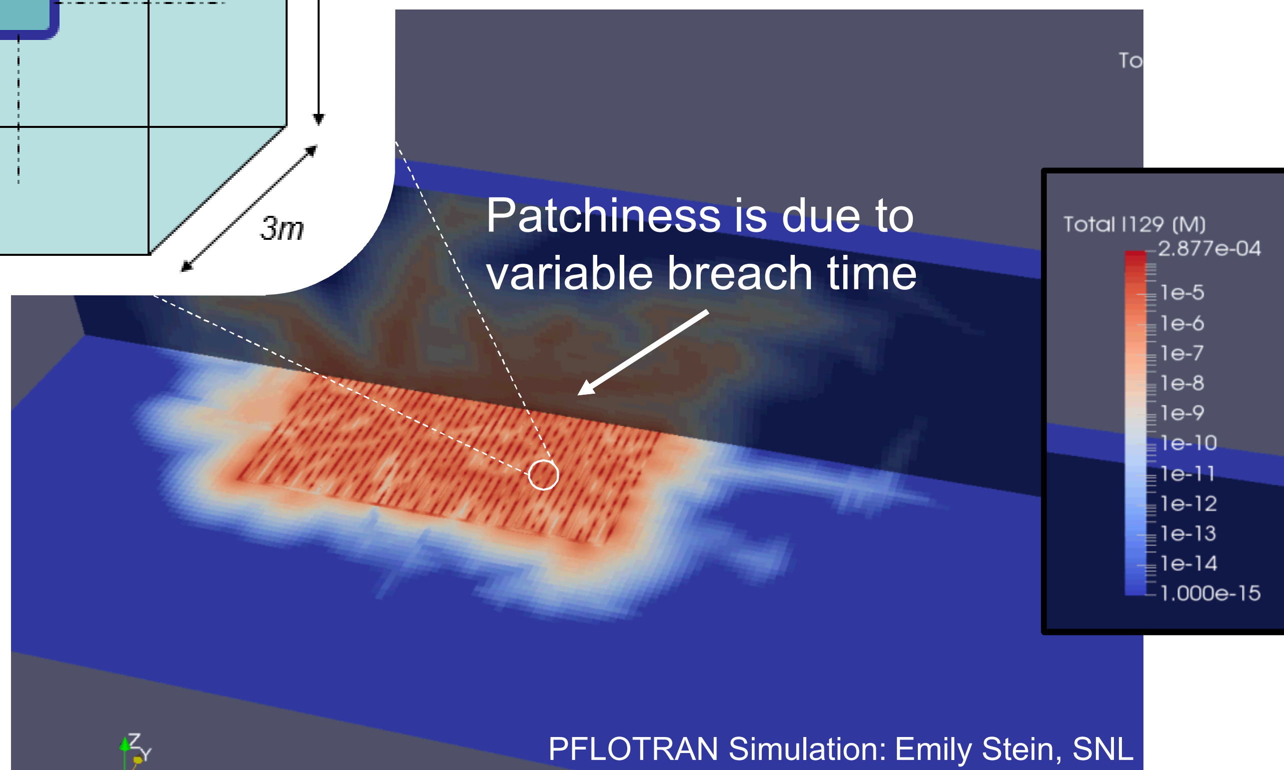


- no fluid flow
- no diffusive flux across boundaries
- 3x3x3 = 27 grid cells
- $1m^3$ grid cells

**Mechanism GLASS**

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

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



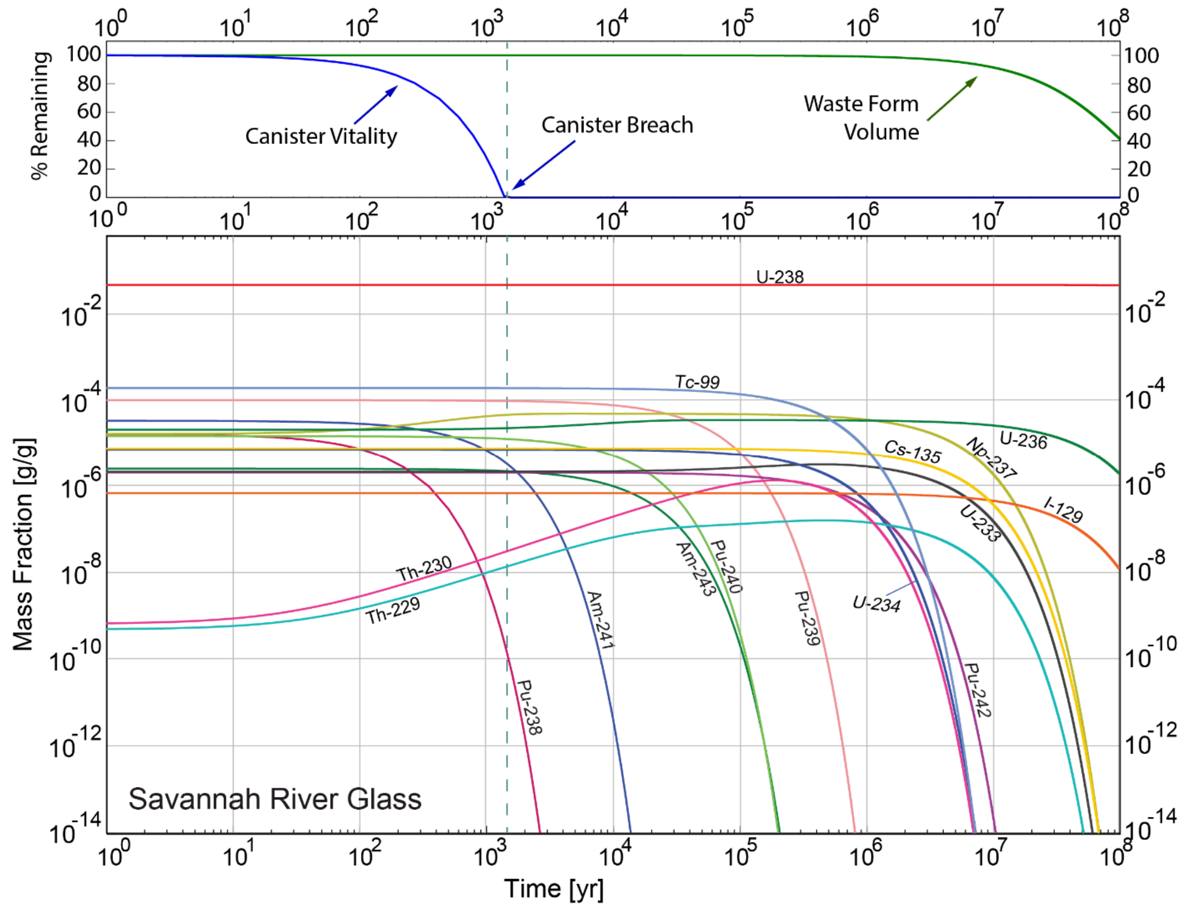
# PFLOTRAN's Waste Form Process Model

- 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

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




Savannah River Glass Log Waste Form

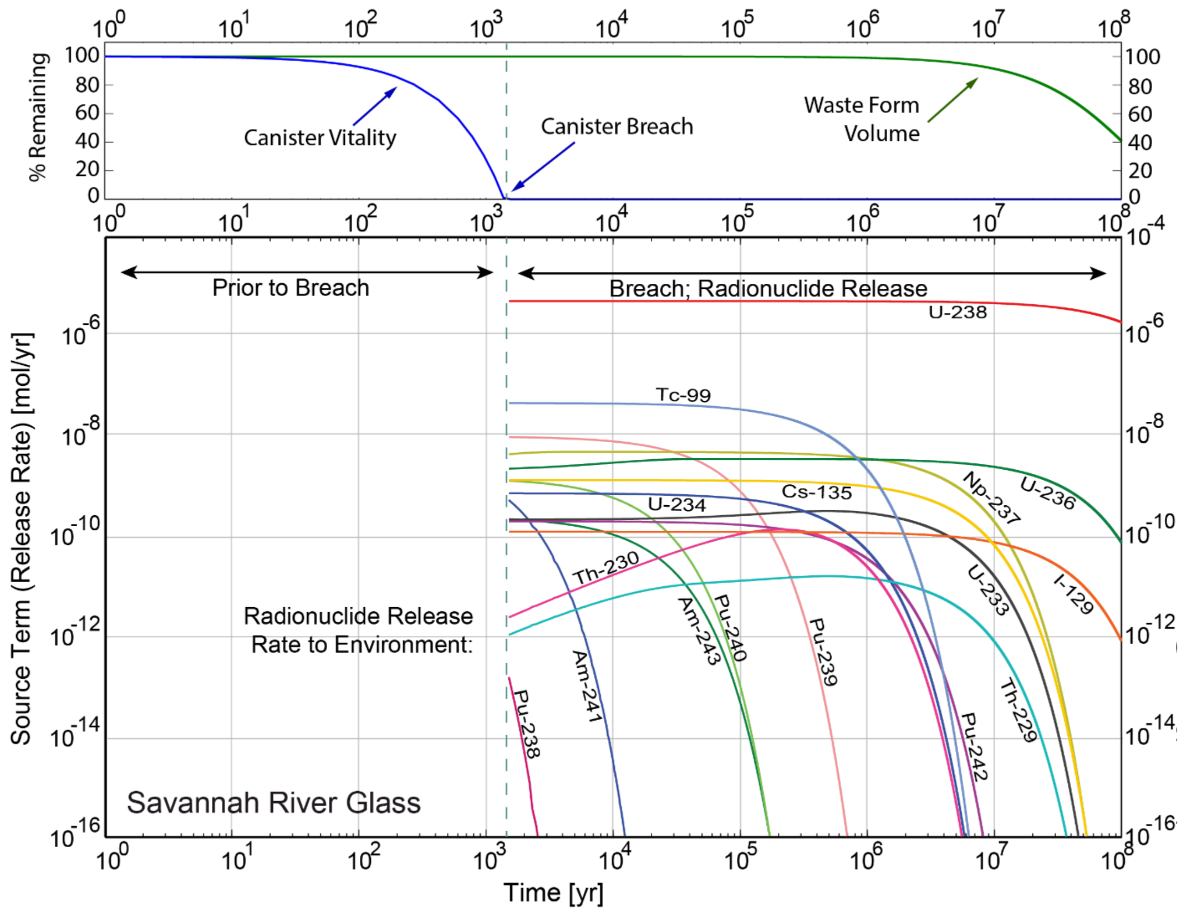
# PFLOTRAN's Waste Form Process Model

- 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

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

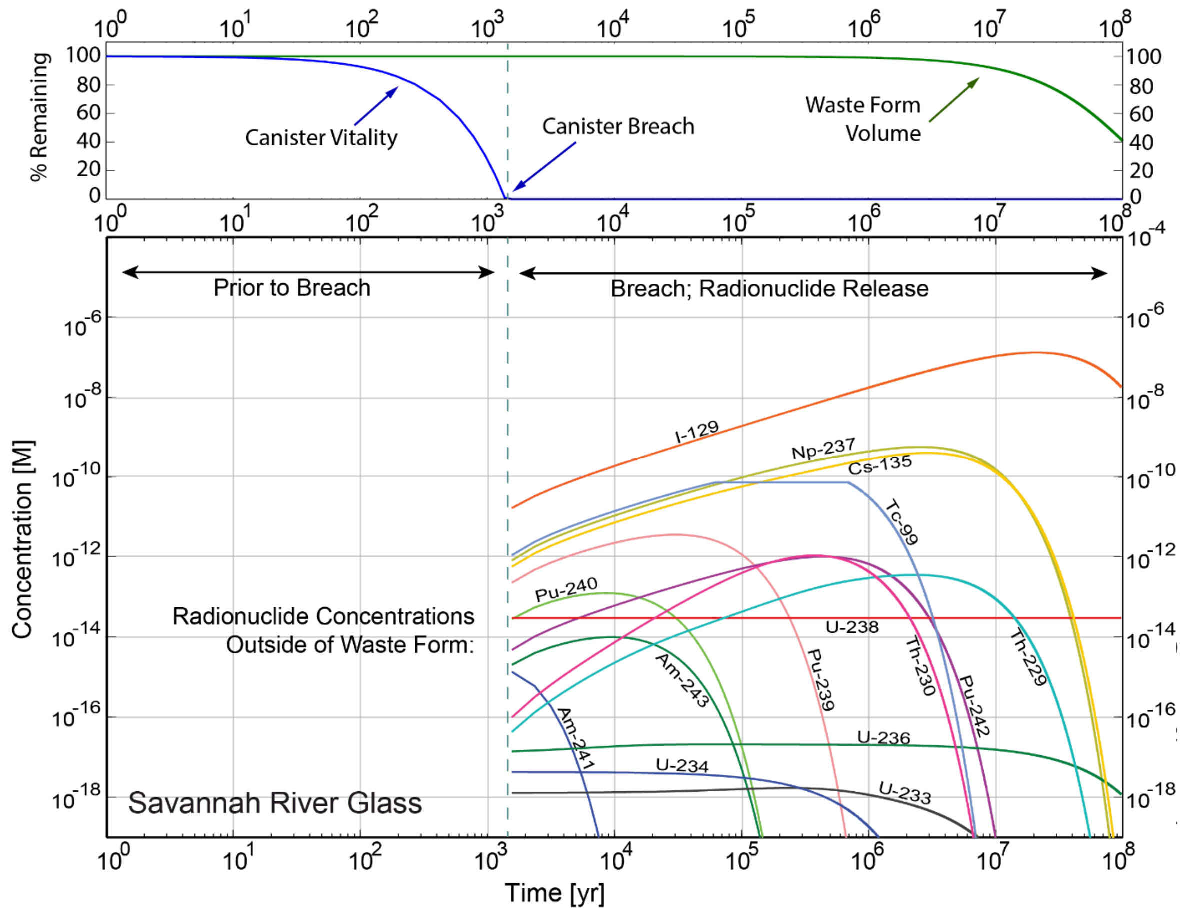



Savannah River Glass Log Waste Form

# PFLOTRAN's Waste Form Process Model

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

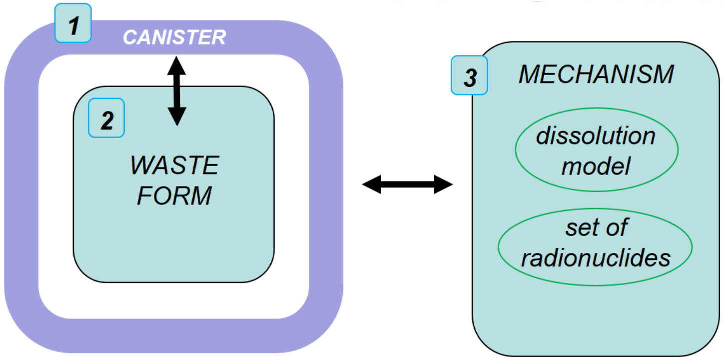
- The radionuclide concentrations outside of the waste form are influenced by:
  - Solubility
  - Sorption to host rock
  - Diffusion/advection
  - Decay and ingrowth




Savannah River Glass Log Waste Form

# PFLOTRAN's Waste Form Process Model

## Future Development




PFLOTRAN

pflotran.org

- **Isotope decay and ingrowth algorithm:**
  - Fully implicit solution rather than 3-generation explicit
- **4D Waste Forms:**
  - Allows ultra-refinement in a 4$^{th}$ spatial dimension (think nested) spaces

- **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

- **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 will work with you to get your functionality implemented