Used Fuel Disposition Campaign

Radioisotope Source Term Degradation and Implementation in PFLOTRAN

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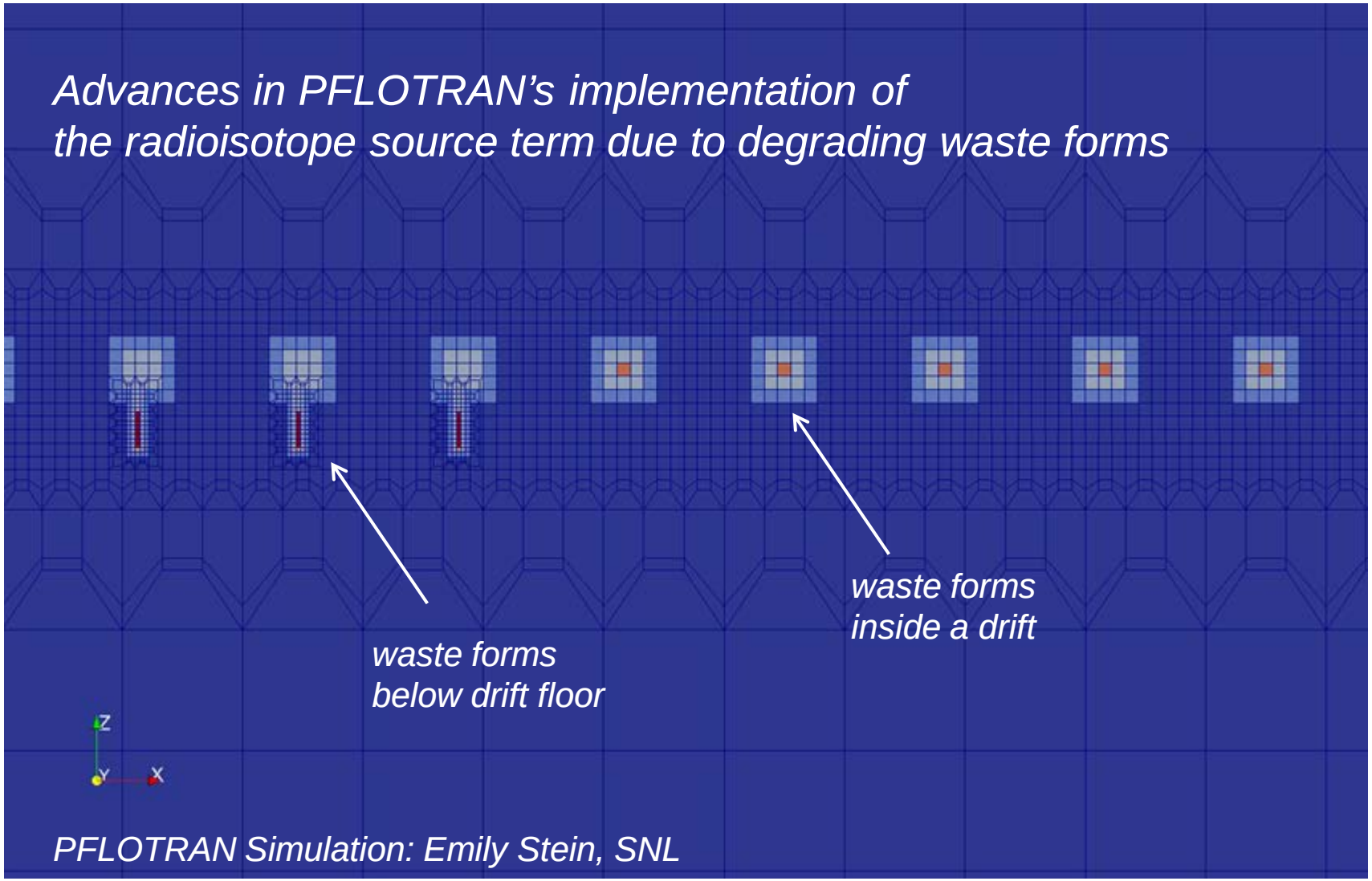
PFLOTRAN's Waste Form Process Model

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



PFLOTRAN Simulation: Emily Stein, SNL

PFLOTRAN's Waste Form Process Model

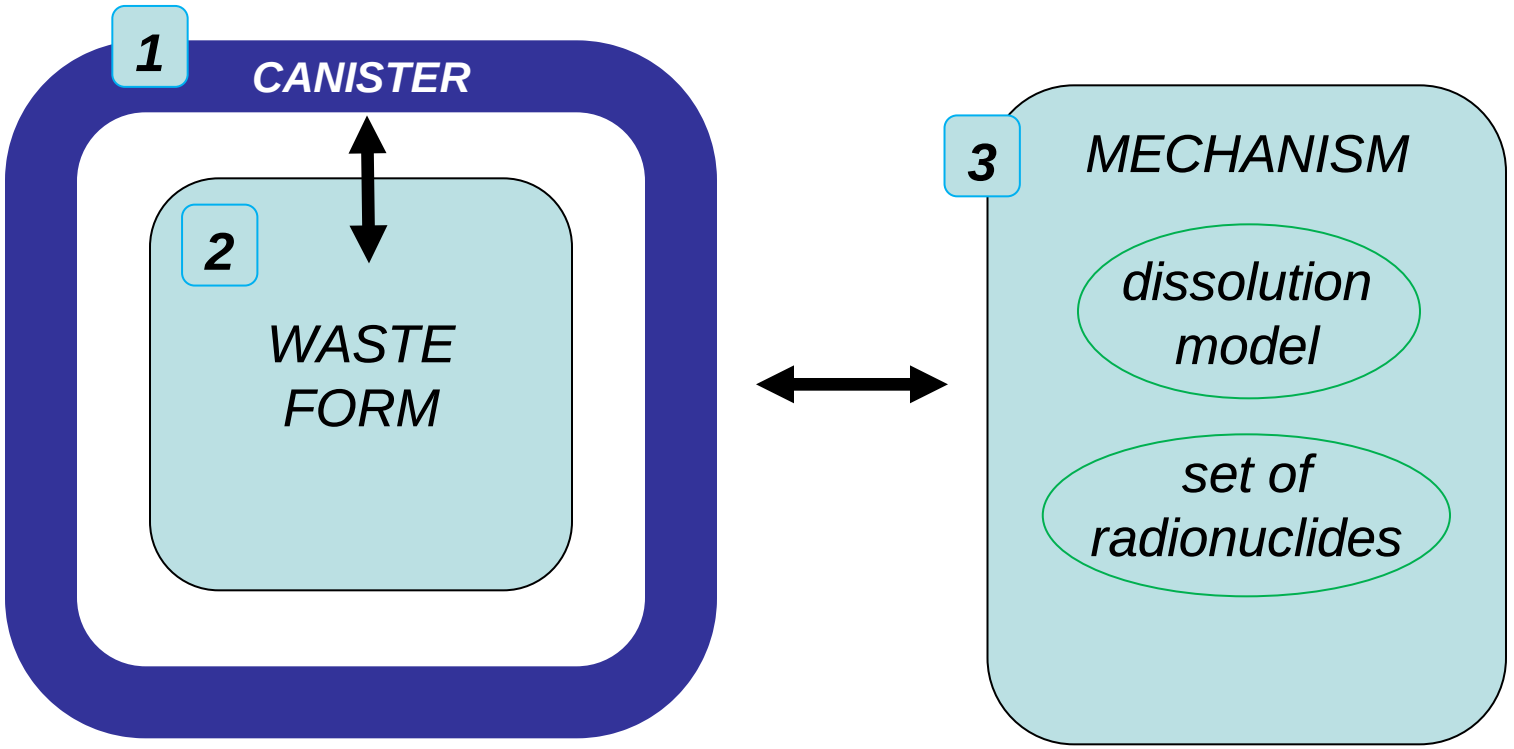
- **The Waste Form Process Model is used to:**
  - track radioisotope decay and ingrowth inside the waste form
  - couple with a canister degradation model to determine breach time
  - track waste form dissolution and remaining volume
  - determine radioisotope source term to environment

Implemented in: PFLOTRAN

- **Development Team:**
  - Jennifer M. Frederick (Sandia National Laboratories)
  - Glenn E. Hammond (Sandia National Laboratories)
  - Paul Mariner (Sandia National Laboratories)
- **Major improvements through restructuring in FY16 now allows:**
  - variable canister breach time
  - multiple waste form "types" can be run in a simulation
  - instantaneous release fraction upon canister breach

PFLOTRAN's Waste Form Process Model

Consists of 3 Main Components:

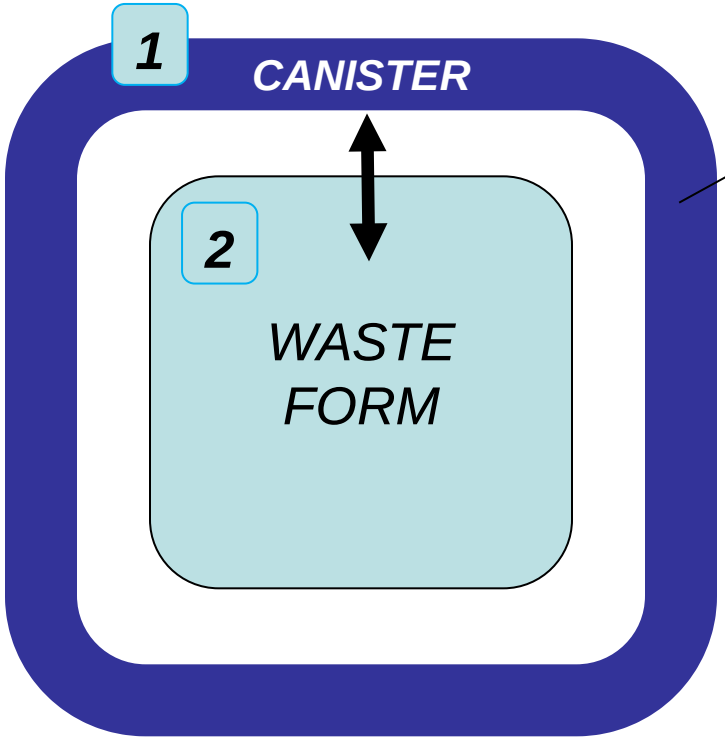


"waste form object"
"fruit"

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

PFLOTRAN's Waste Form Process Model

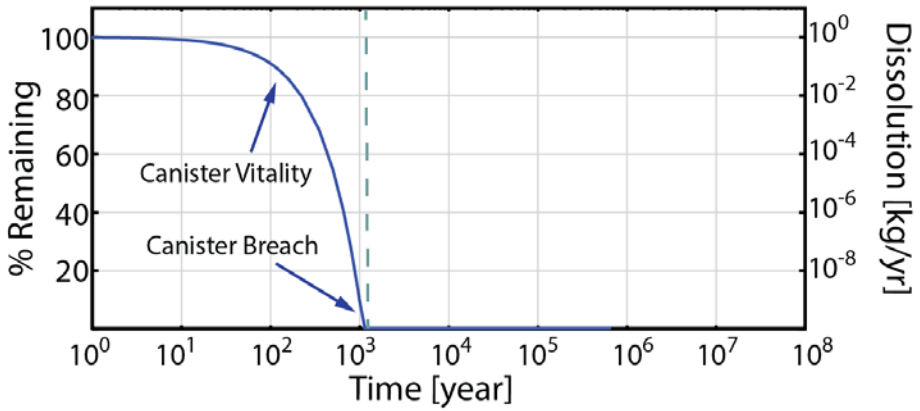
1. Canister Degradation Model



"waste form object"
"fruit"

Canister Vitality

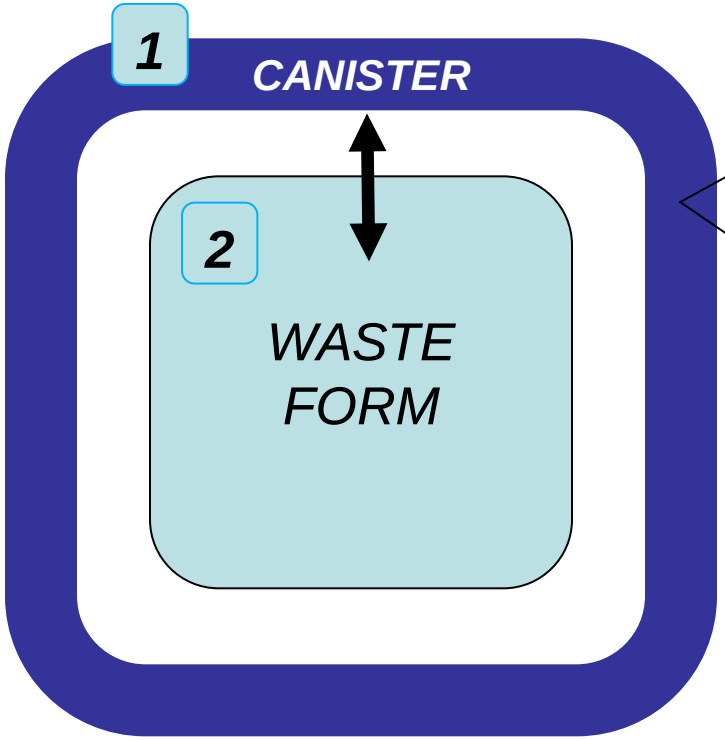
- *A measure of how much 'life' the canister has remaining*
- *Range: 100% - 0%*
- *Once vitality drops to 0%, the waste form canister breaches*



In this example, the canister breaches after ~1,000 yrs.

PFLOTRAN's Waste Form Process Model

1. Canister Degradation Model



"waste form object"
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Canister Vitality

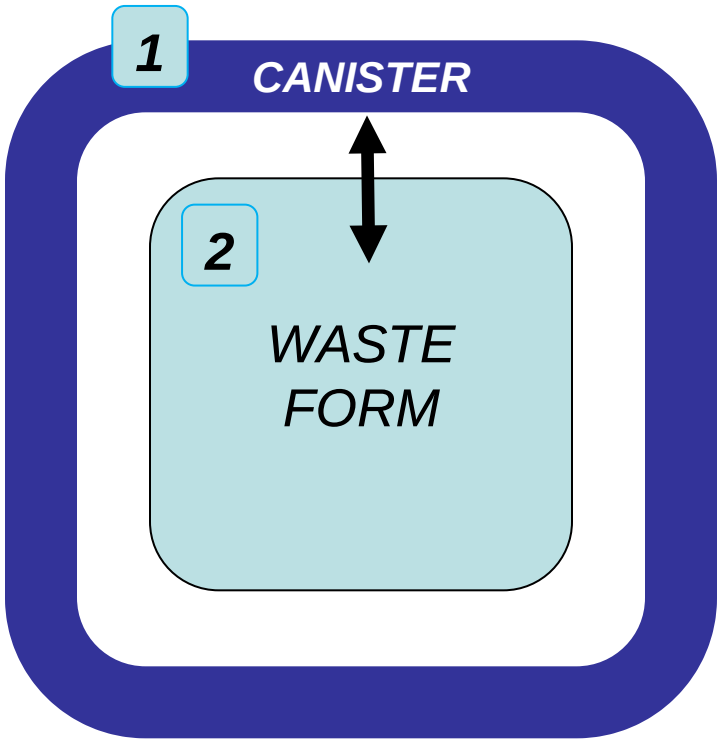
- *A measure of how much 'life' the canister has remaining*
- *Range: 100% - 0%*
- *Once vitality drops to 0%, the waste form canister breaches*

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*

PFLOTRAN's Waste Form Process Model

2. Waste Form



"waste form object"
"fruit"

Coordinate Point

- *Defines the location of a waste form*
- *Informs of local conditions (temperature, pressure, chemistry)*

Radioisotope Concentrations

- *Calculates isotope decay and ingrowth*
- *Stores isotope concentrations and mass fractions within the waste form*

determines source term

Effective Dissolution Rate

- *The rate of waste form dissolution after considering local conditions (temperature)*
- *Determines source term rate after breach*

Volume

- *Stores the remaining bulk volume*
- *Determines when source term "turns off"*

Mechanism Pointer

- *Points to the mechanism that defines the type of waste form*
- *The mechanism determines the set of radioisotopes and the waste form dissolution equation*

PFLOTRAN's Waste Form Process Model

3. Waste Form Mechanism

Mechanism GLASS

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

$$r(T) = 560e^{\frac{-7397}{T(t,\vec{x})}}$$

Mechanism FMDM

- *Assumes waste form is used nuclear fuel (UO_2)*
- *Dissolution rate via Fuel Matrix Degradation Model*

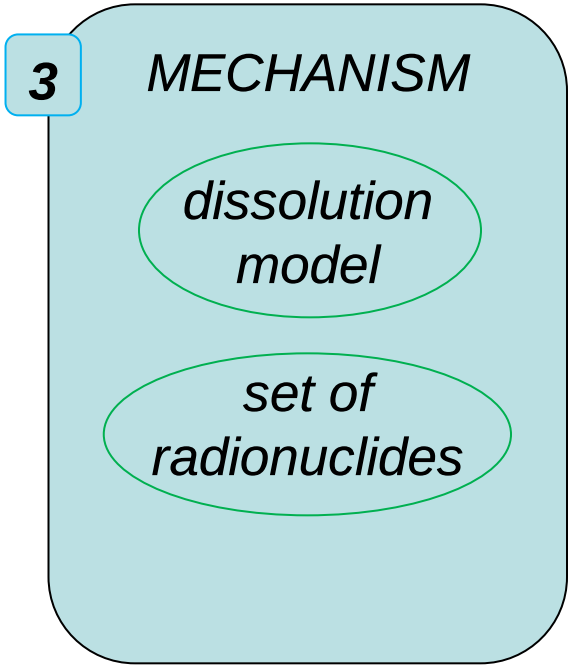
(J. Jerden et al, Argonne National Lab)

Mechanism DSNF

- *Assumes waste form DOE spent nuclear fuel*
- *Dissolution rate "instantaneous" after canister breach*

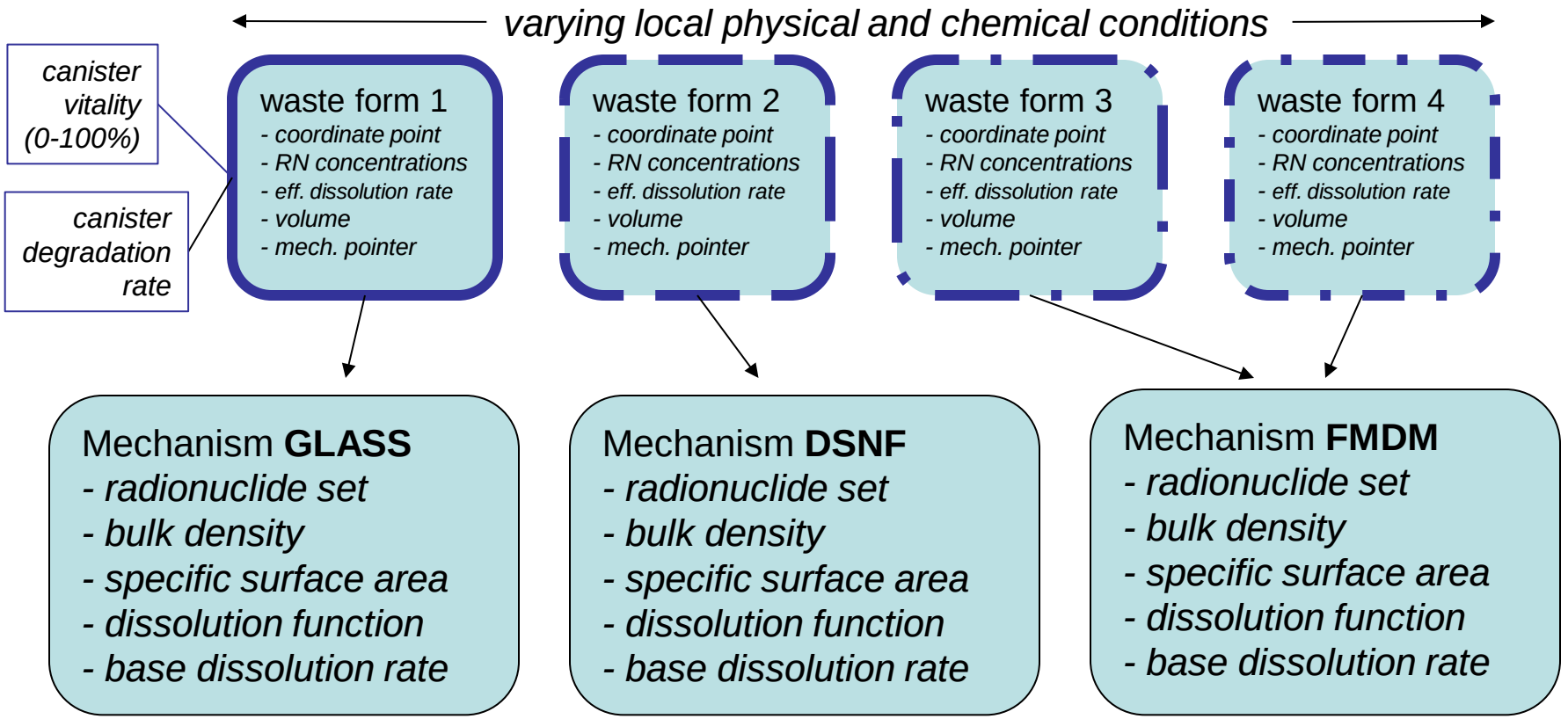
Mechanism CUSTOM

- *User-defined specific surface area and dissolution rate*
- *Allows for flexibility if you need it*



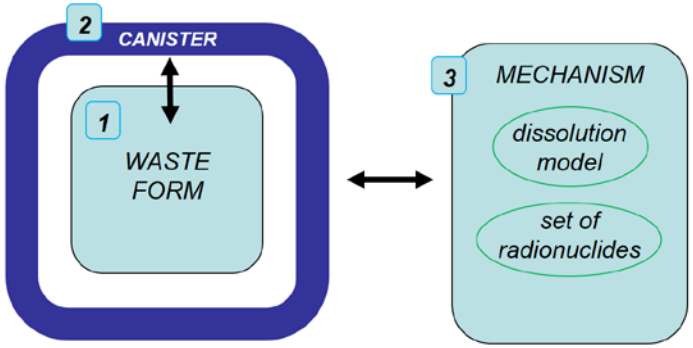
"waste form type"
"banana, apple, orange, etc."

PFLOTRAN's Waste Form Process Model

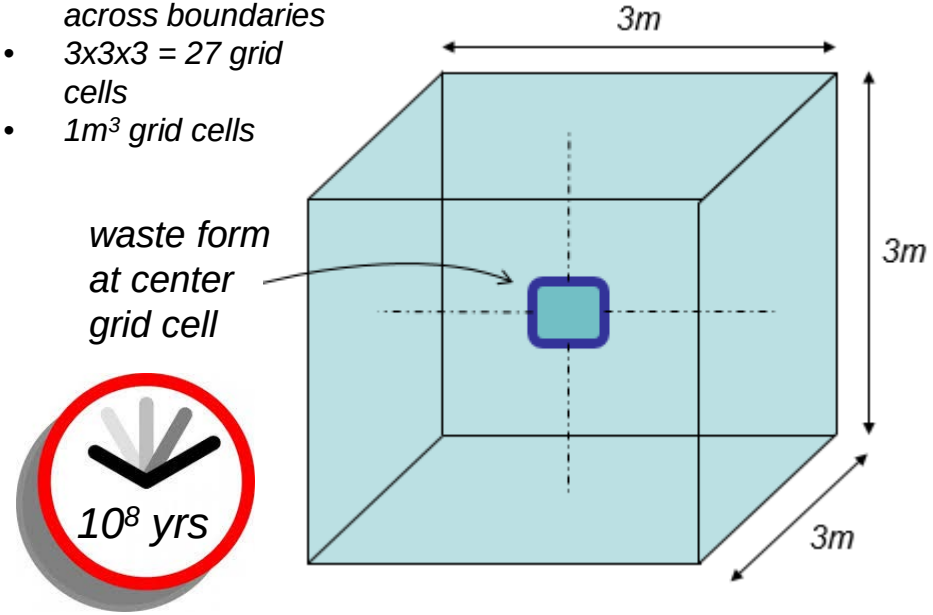


Restructuring → *More numerically efficient and modular design*
Each waste form is "independent"
Multiple waste form types; only pointers needed

PFLOTRAN's Waste Form Process Model



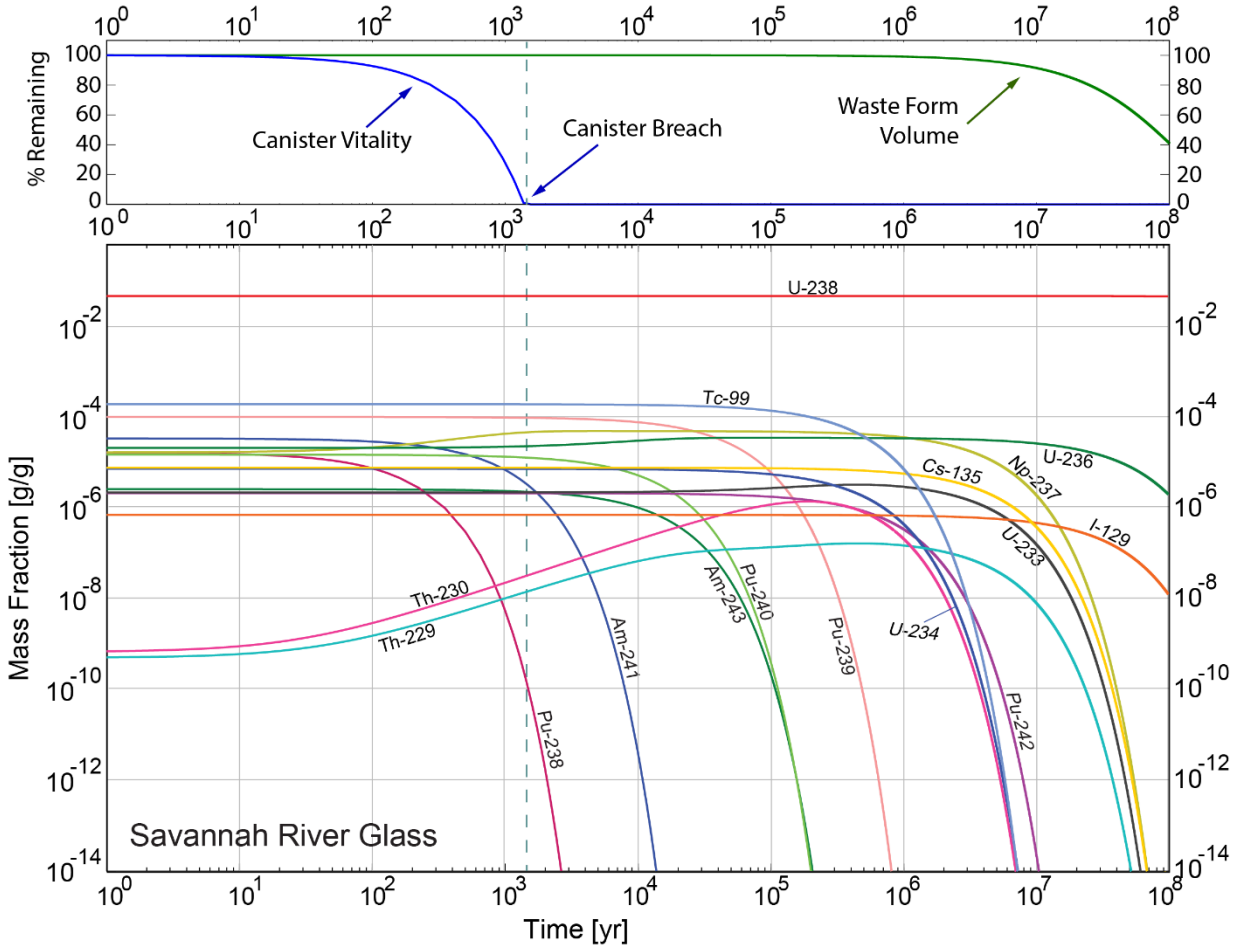
- *no fluid flow*
- *no diffusive flux across boundaries*
- *3x3x3 = 27 grid cells*
- *1m³ grid cells*



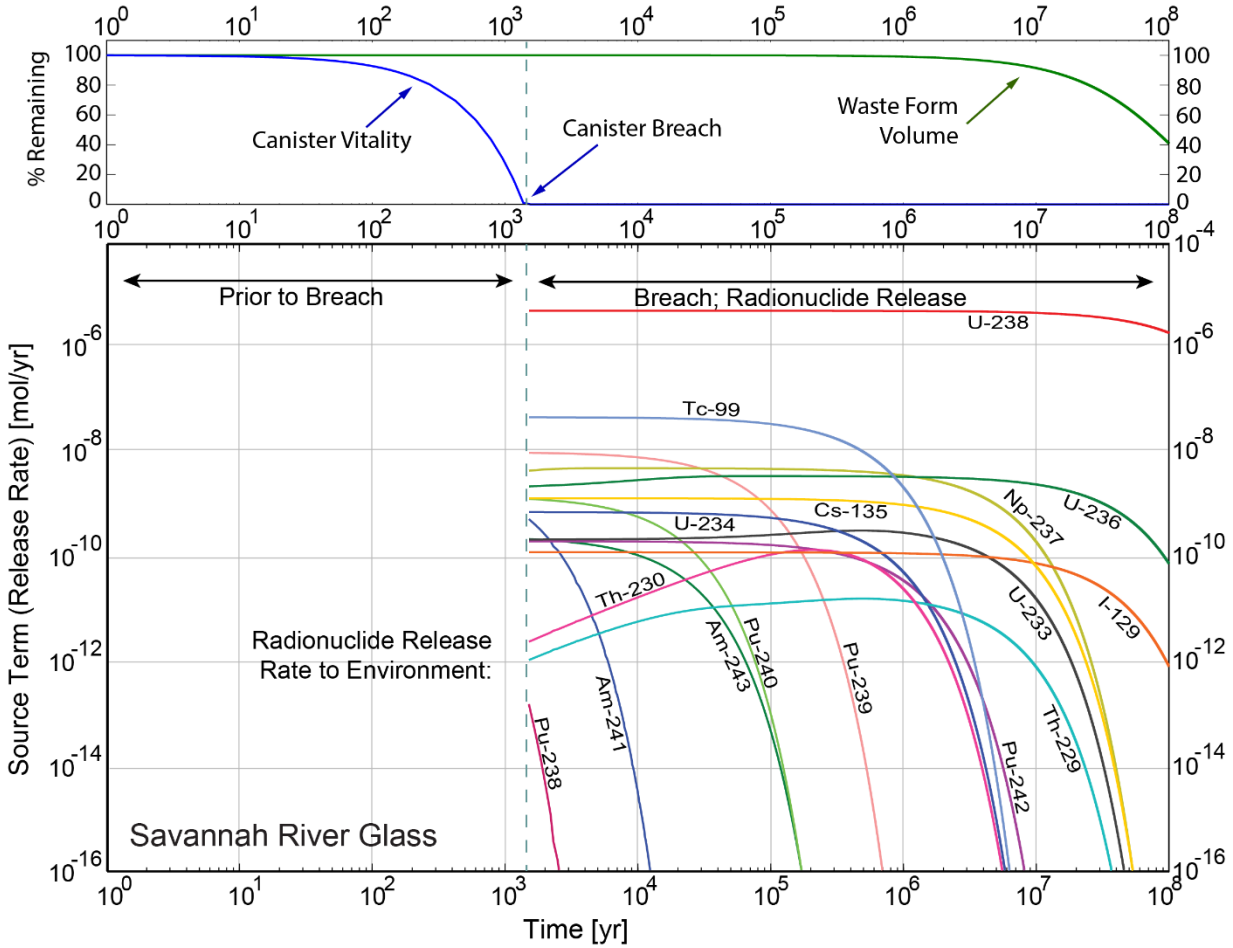
Example portion of PFLOTRAN input file:

```
#========================== waste forms =====================================
WASTE_FORM_GENERAL

  WASTE_FORM
    COORDINATE 1.5d0 1.5d0 1.5d0
    VOLUME 1.0d0 m^3
    MECHANISM_NAME fmdm_60
    CANISTER_VITALITY_RATE 0.0000042 1/day
  /

  MECHANISM FMDM
    NAME fmdm_60
    SPECIFIC_SURFACE_AREA 0.001 m^2/g
    MATRIX_DENSITY 10970. kg/m^3 #calculated assuming 100% UO2
    BURNUP 60 # MWd/MTHM
    SPECIES
     #name,   MW[g/mol],dcy[1/s], initMF,    inst_rel_frac,daughter
      Am-241  241.06d0  5.08d-11  8.7000d-4  0.0d0  Np-237
      Am-243  243.06d0  2.98d-12  1.8800d-4  0.0d0  Pu-239
      Pu-238  238.05d0  2.56d-10  3.4200d-4  0.0d0   U-243
      Pu-239  239.05d0  9.01d-13  5.1500d-3  0.0d0  #U-235 (not tracking)
      Pu-240  240.05d0  3.34d-12  2.8400d-3  0.0d0   U-236
      Pu-242  242.06d0  5.80d-14  5.6800d-4  0.0d0   U-238
      Np-237  237.05d0  1.03d-14  8.5900d-4  0.0d0   U-233
       U-233  233.04d0  1.38d-13  9.7000d-9  0.0d0  Th-229
       U-234  234.04d0  8.90d-14  2.1200d-4  0.0d0  Th-230
       U-236  236.05d0  9.20d-16  4.3300d-3  0.0d0  #Th-232 (not tracking)
       U-238  238.05d0  4.87d-18  6.3200d-1  0.0d0  #Th-234 (not tracking)
      Th-229  229.03d0  2.78d-12  4.4300d-12 0.0d0  #Ra-225 (not tracking)
      Th-230  230.03d0  2.75d-13  1.5800d-8  0.0d0  #Ra-226 (not tracking)
       I-129  128.90d0  1.29d-15  2.1800d-4  0.0d0  #Xe-129 (not tracking)
       Tc-99   98.91d0  1.04d-13  8.8700d-4  0.0d0  #Ru-99  (not tracking)
    /
    CANISTER_DEGRADATION_MODEL
      #VITALITY_LOG10_MEAN -4.5
      #VITALITY_LOG10_STDEV 0.50
      #VITALITY_UPPER_TRUNCATION -3.0
      CANISTER_MATERIAL_CONSTANT 1500.0
    /
  /

  PRINT_MASS_BALANCE

END
```

Savannah River Glass



Savannah River Glass



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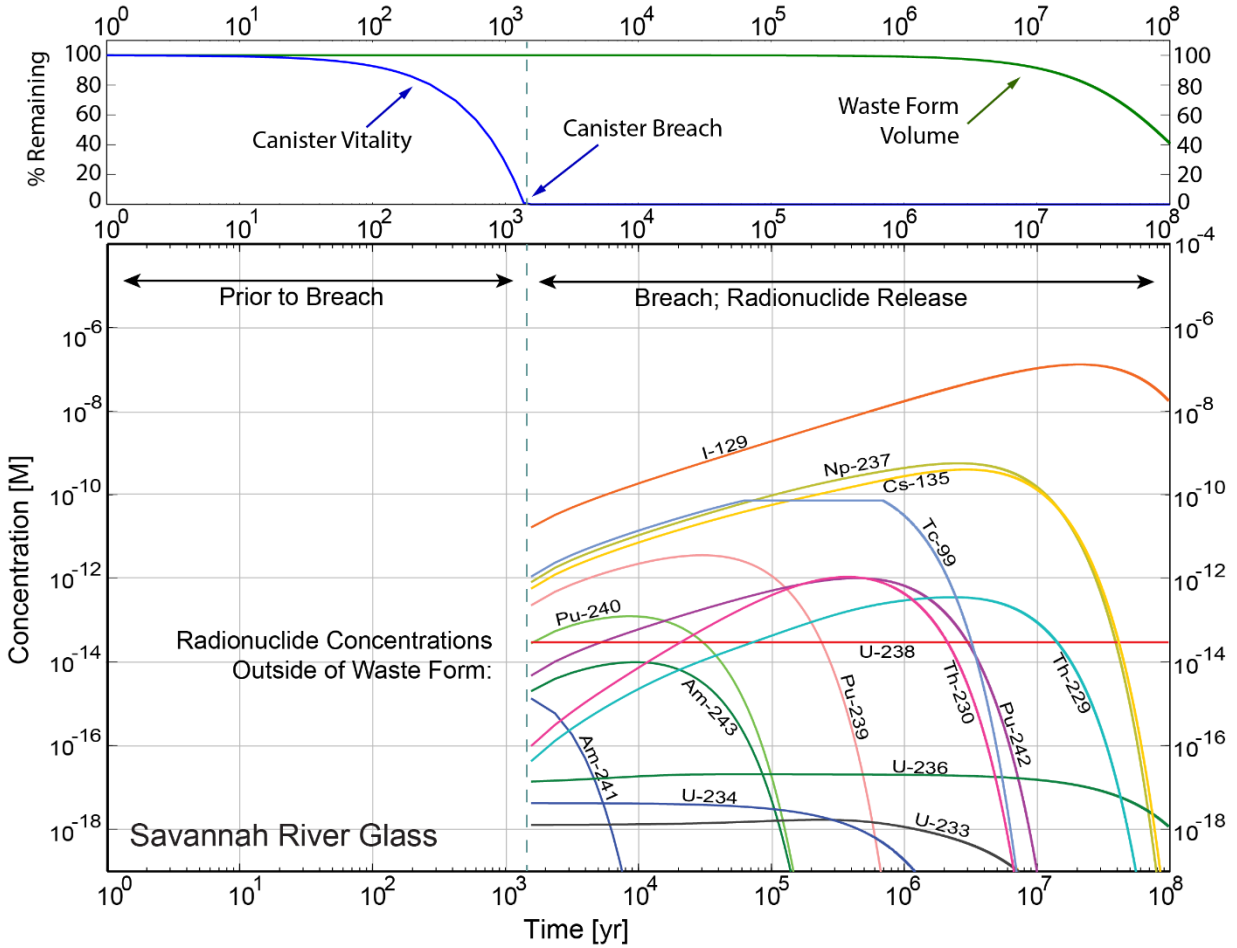
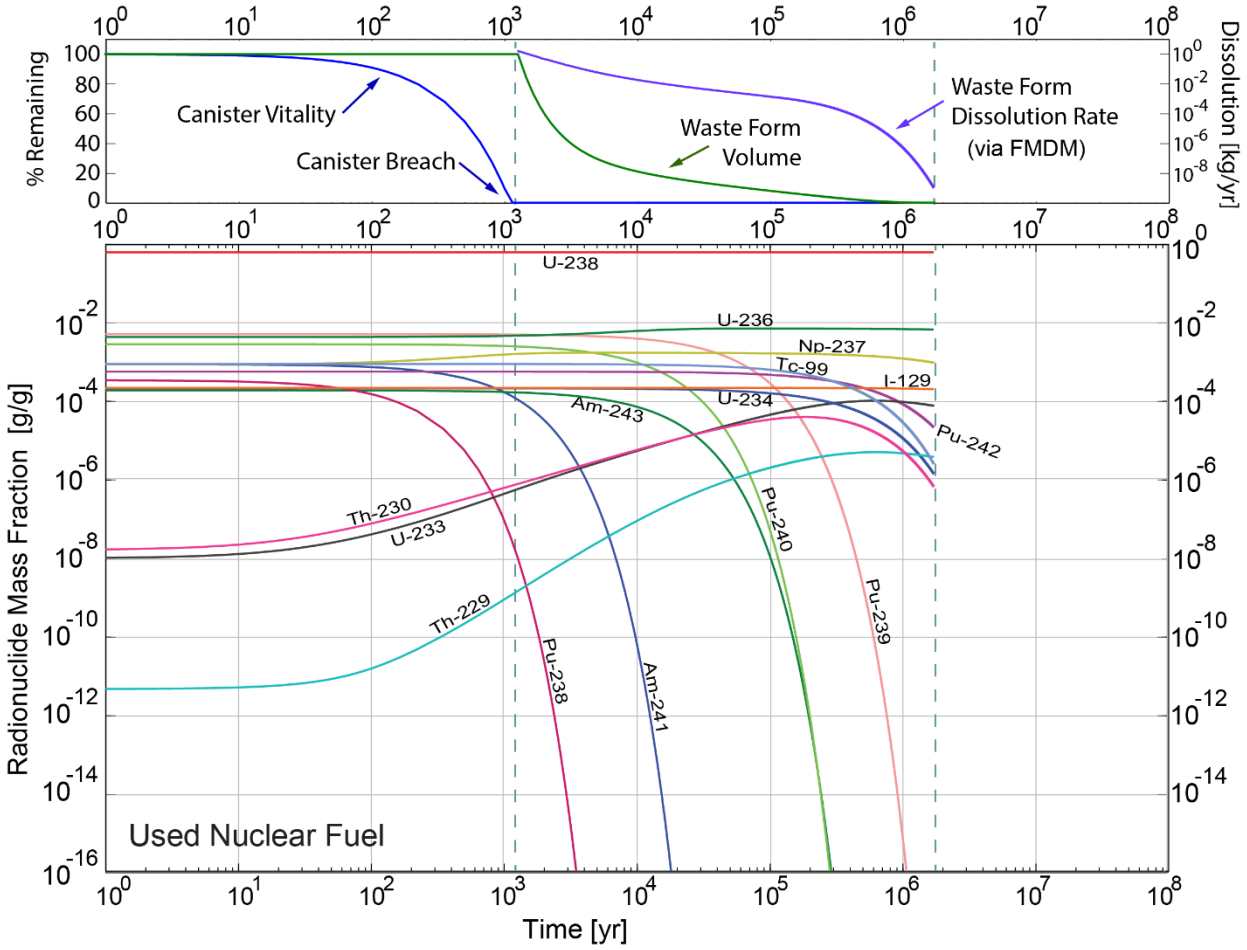


Used Nuclear Fuel (FMDM)



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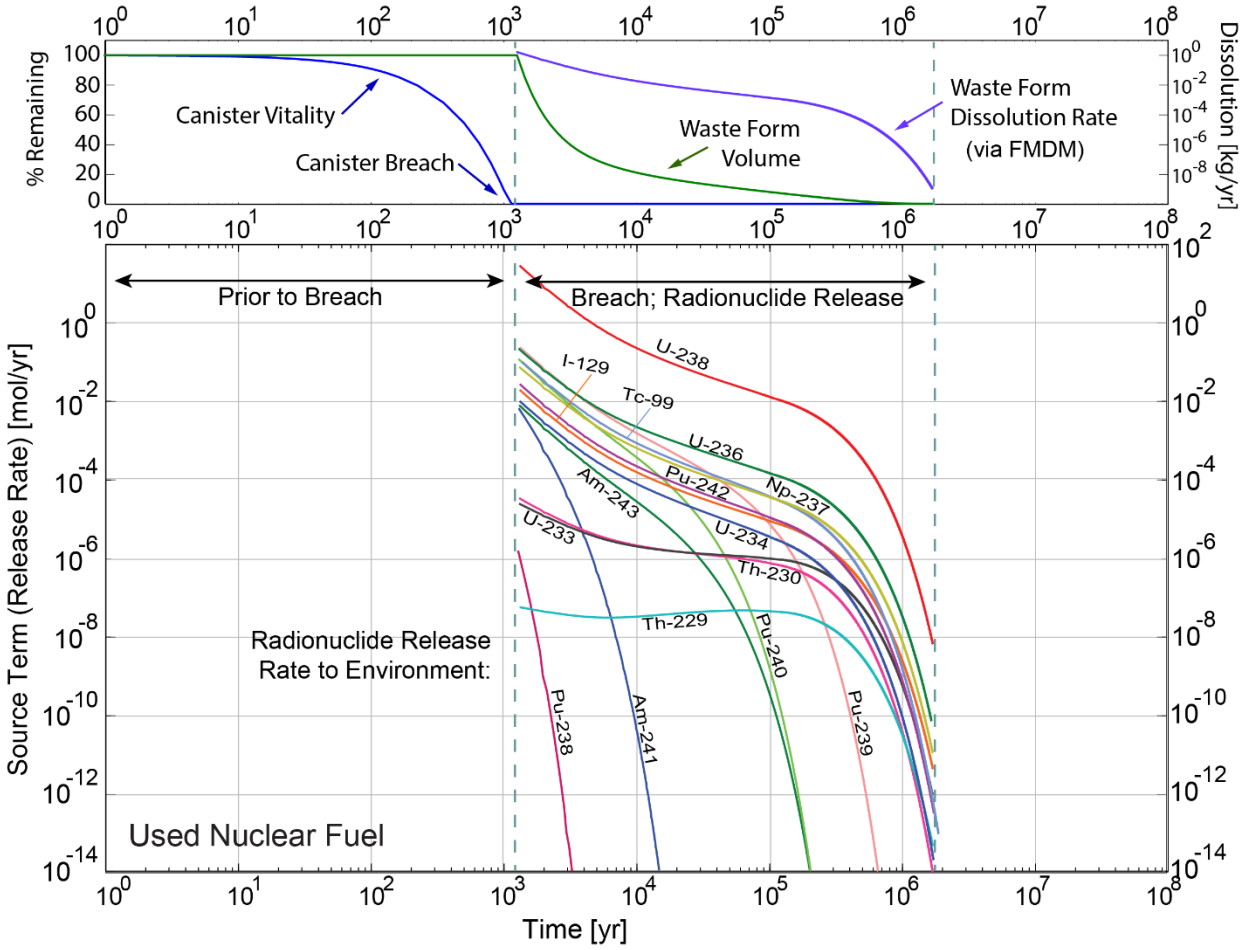

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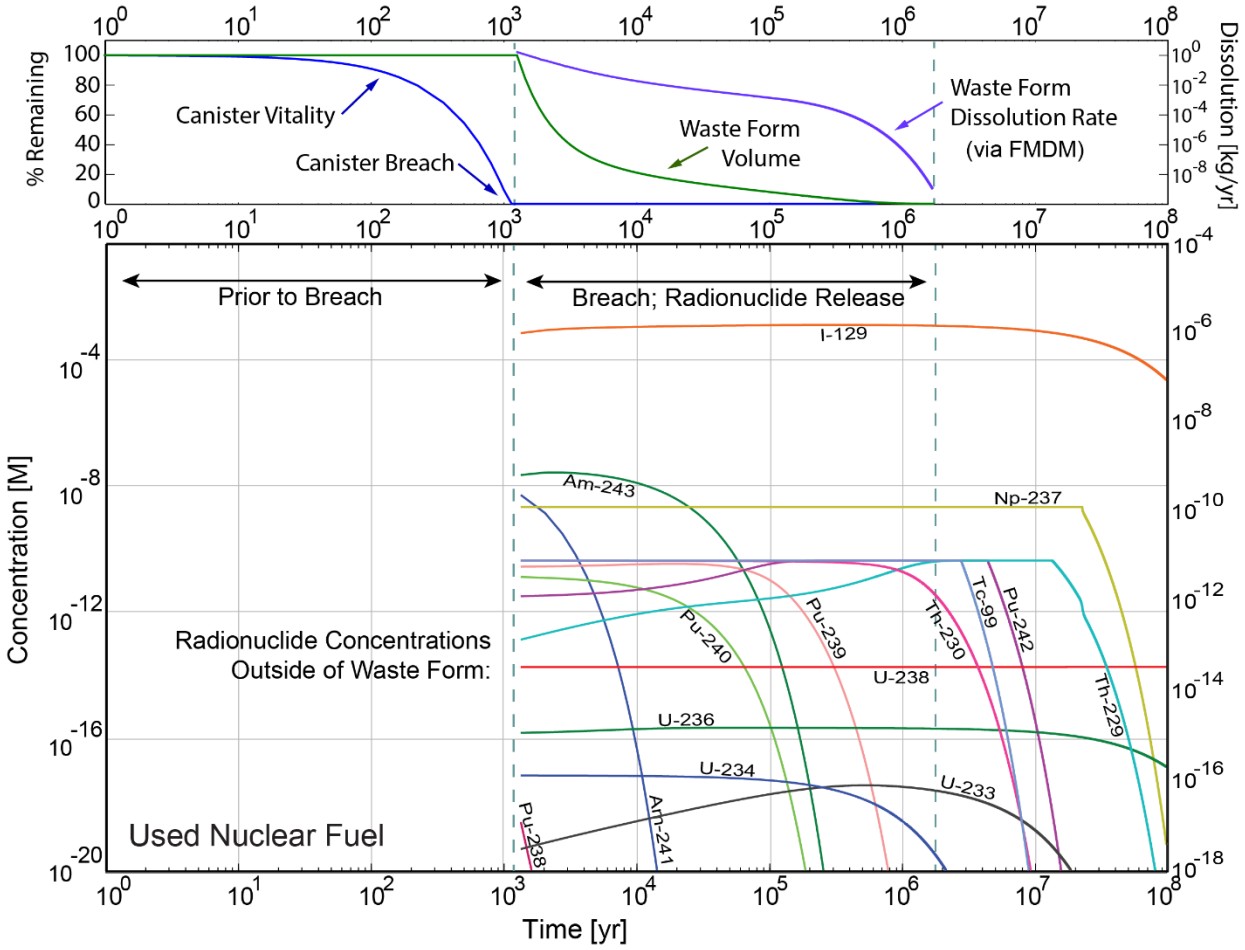
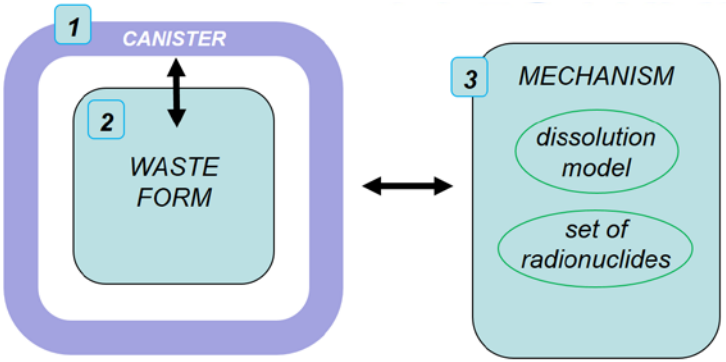


PFLOTRAN's Waste Form Process Model

Future Development

PFLOTRAN
pflotran.org



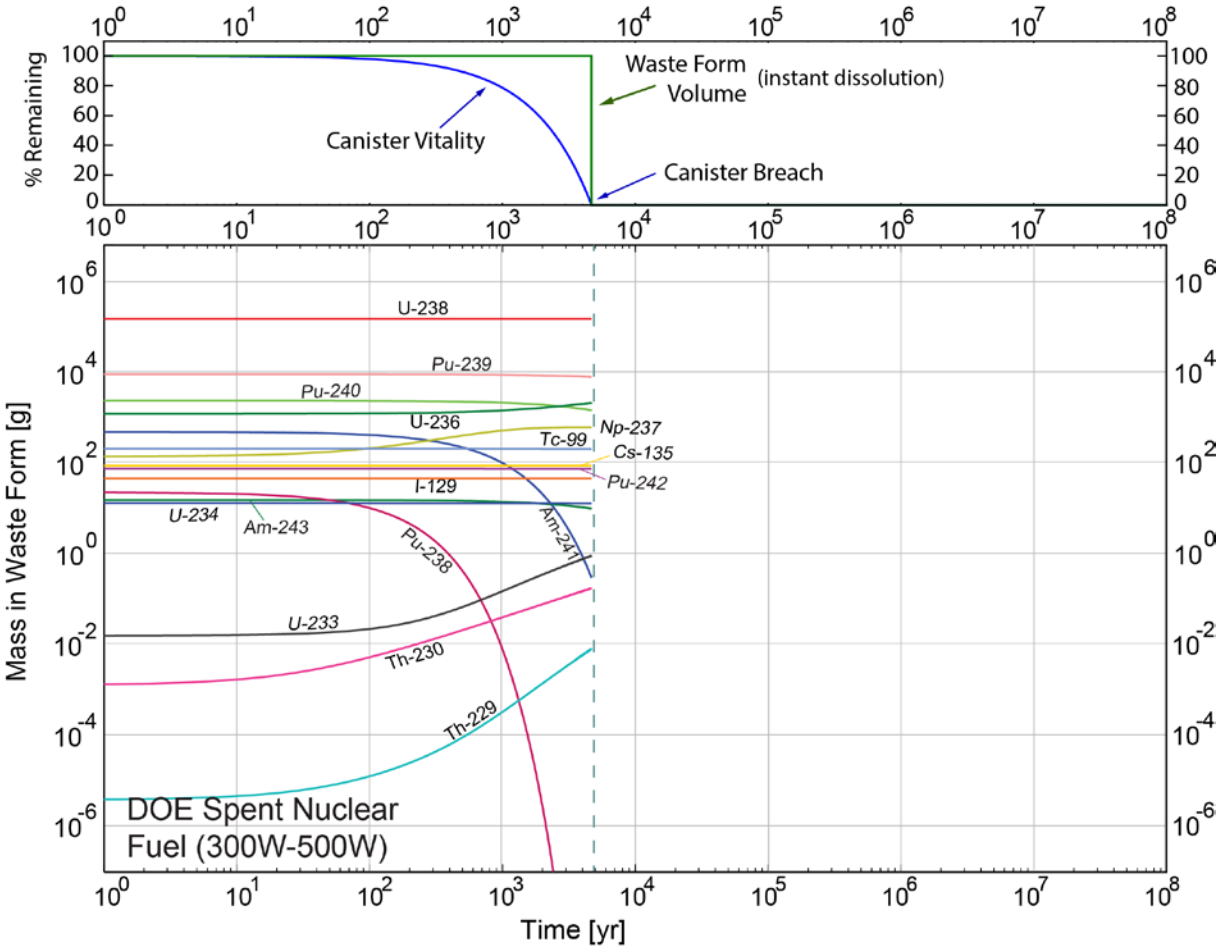
- ***Waste form mechanisms:***
  - *Add more mechanism types*
  - *Make dissolution models more mechanistic and interactive*
- ***Canister degradation model:***
  - *Include canister degradation mechanisms like corrosion and damage models*

- **Isotope decay and ingrowth algorithm:**
  - Fully implicit solution rather than 3-generation explicit

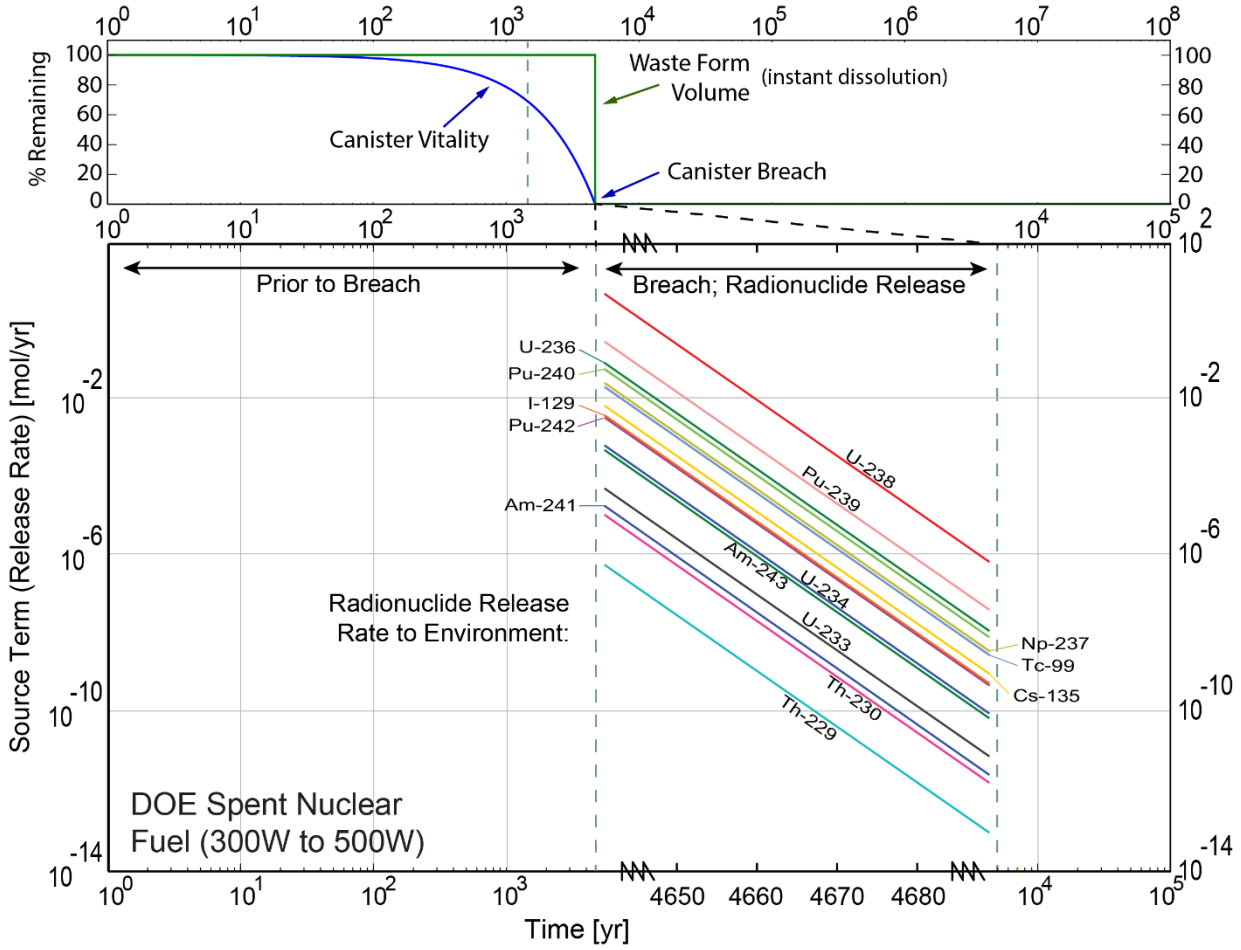
- **PFLOTRAN's waste form process model is <u>open-source</u> and <u>modular</u>**
  - We invite collaboration to create new type of waste forms, mechanisms, etc.
  - We will work with you to get your functionality implemented

EXTRA SLIDES FOLLOW

DOE Spent Nuclear Fuel



DOE Spent Nuclear Fuel



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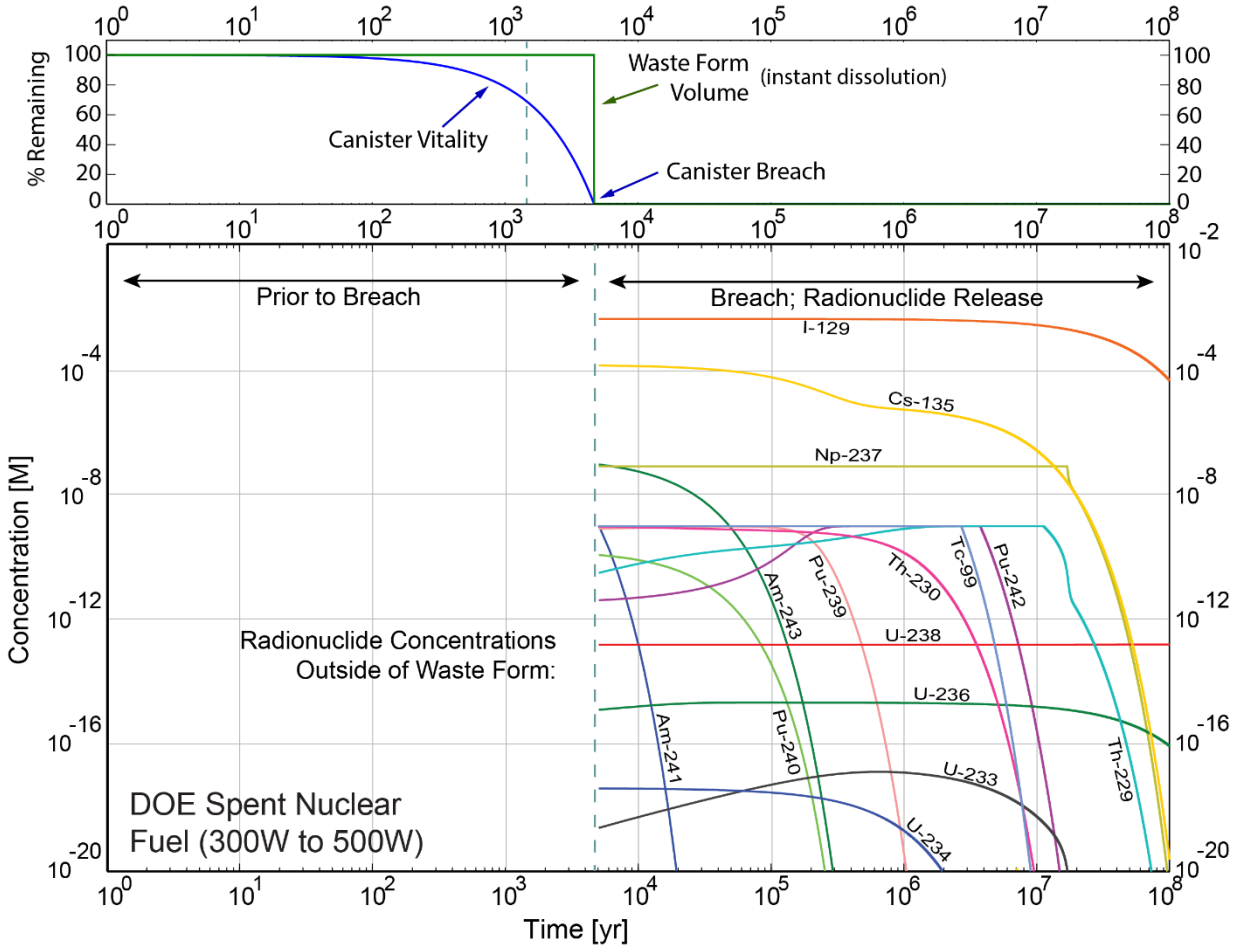
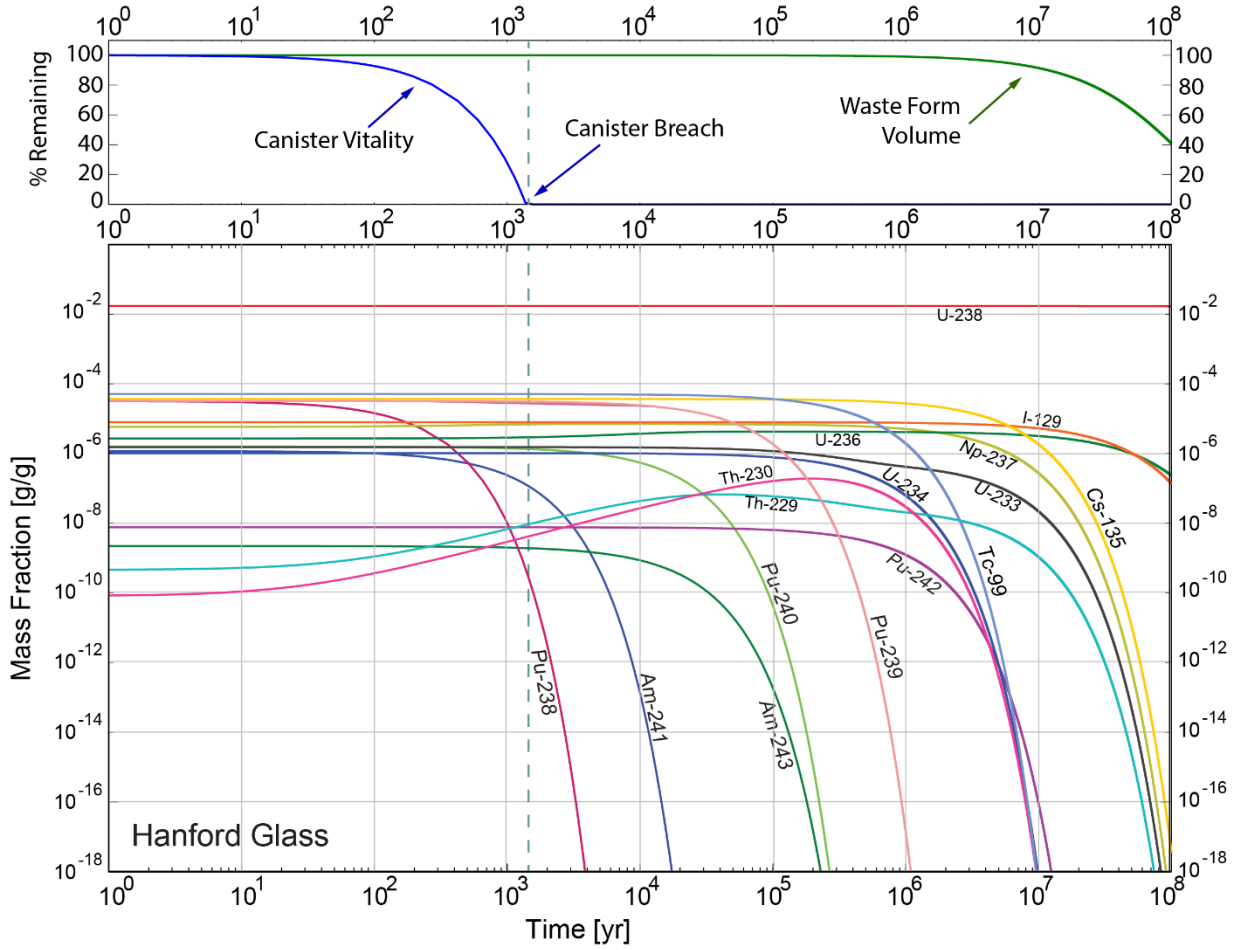


Hanford Glass



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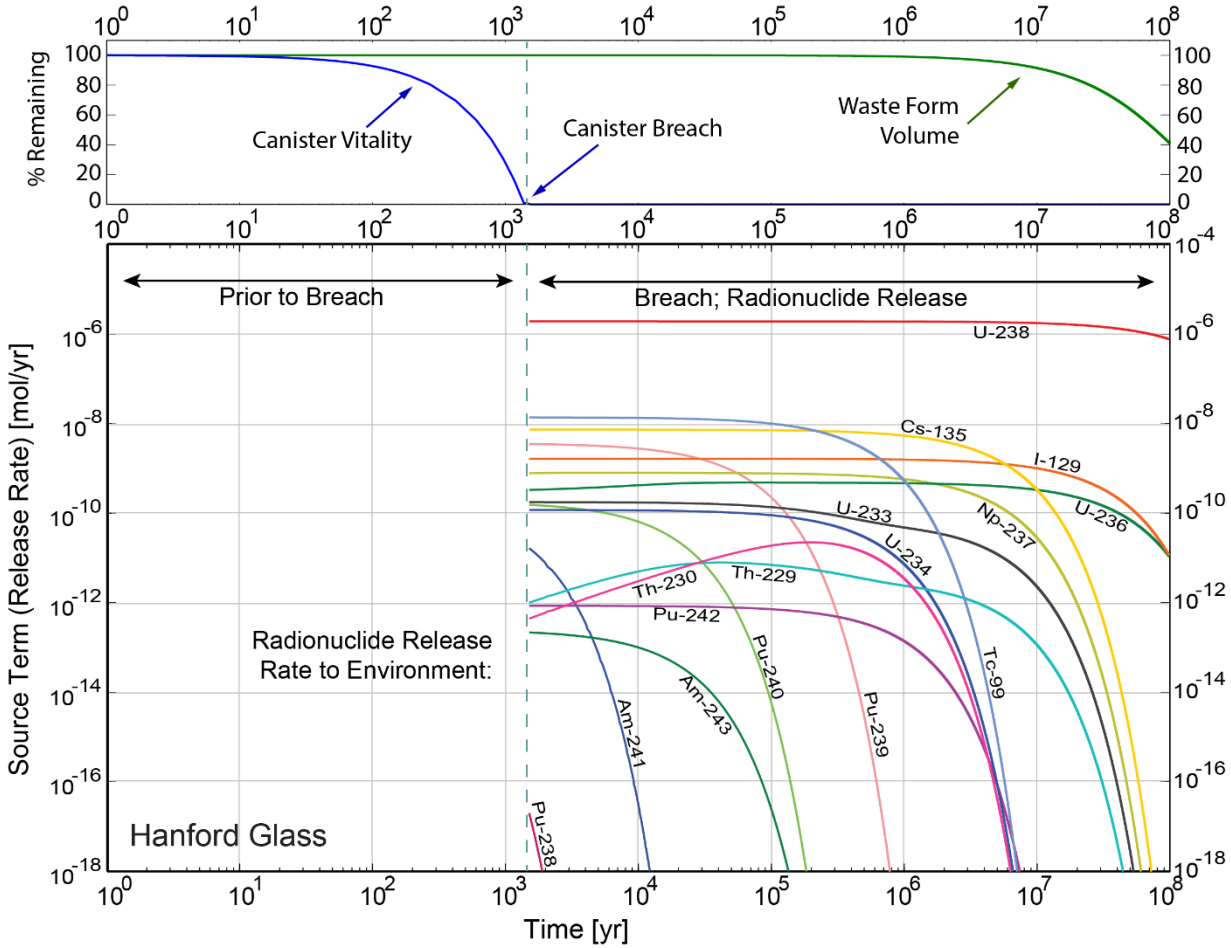

Hanford Glass