

## Cross-Cutting Topics

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# Cross-Cutting Topics

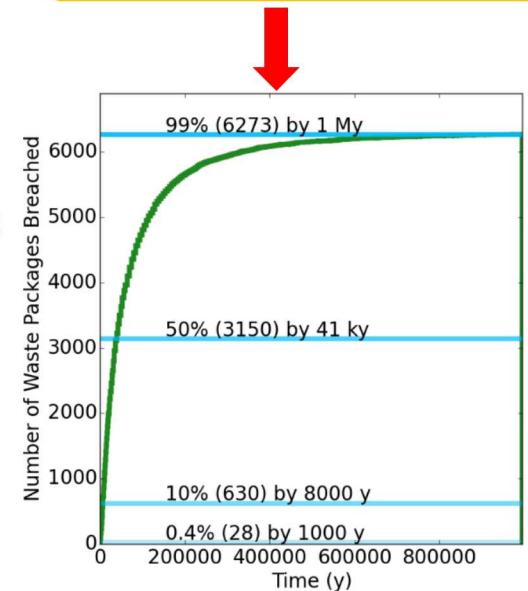
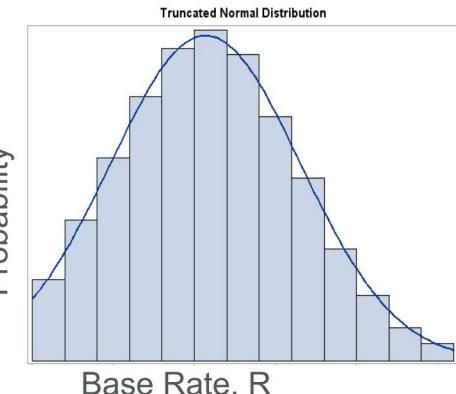
- Geologic Disposal Safety Assessment (GDSA) reference cases, modeled with the PFLOTRAN code, are based on large, higher-temperature waste packages
  - Waste package degradation model
  - Waste form degradation model
  - Effects of different geologies
  - Effect of high-temperature on engineered barriers (e.g., bentonite)
- Thermal and shielding implications for the transportation schedule

# Waste Package Degradation Model (Mariner et al. 2016)

- Waste package degradation (PFLOTRAN)
  - Current implementation for “canister vitality” is a simple probabilistic rate
    - temperature-dependent
    - can also simulate early failures
  - Future development:
    - mechanistic corrosion (general, localized)
    - effects of groundwater chemistry / redox
    - seismic, igneous (site specific)
- Dual-purpose canister (DPC) considerations
  - Elevated temperatures
  - Disposal overpack materials (Cu, alloy 22, ... ?)

$R_{\text{eff}}$  = canister degradation rate

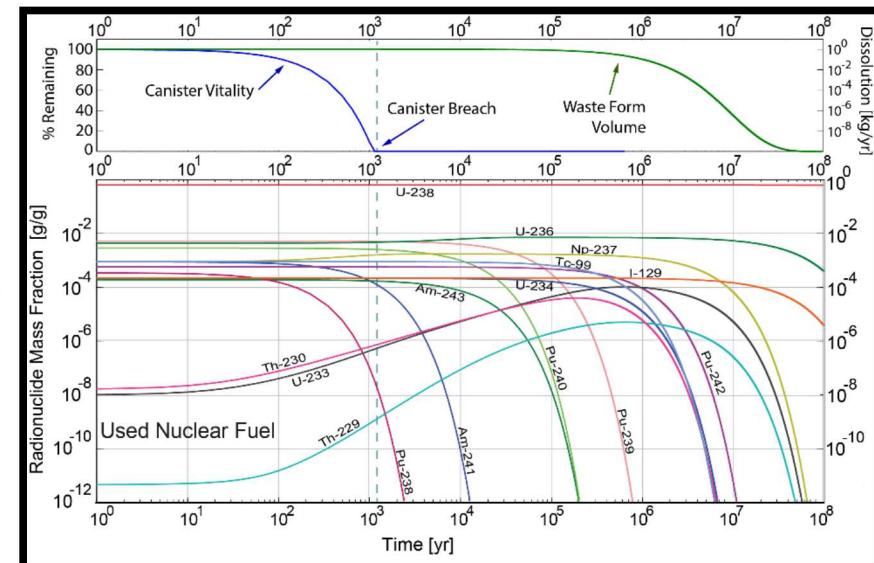
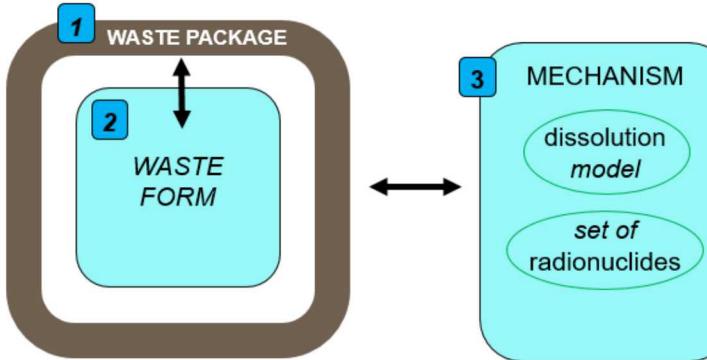
$$R_{\text{eff}} = R \cdot e^{\left[ \frac{1}{60^\circ\text{C}} - \frac{1}{T(x,t)} \right]}$$



# Waste Form Degradation Model (Mariner et al. 2016)

- Waste form degradation (PFLOTTRAN)

- Current implementation is simple spent nuclear fuel (SNF) dissolution rate that begins following waste package failure
  - Instant release fraction (specified radionuclides)
  - Fractional dissolution (e.g.,  $10^{-7}/\text{yr}$ )

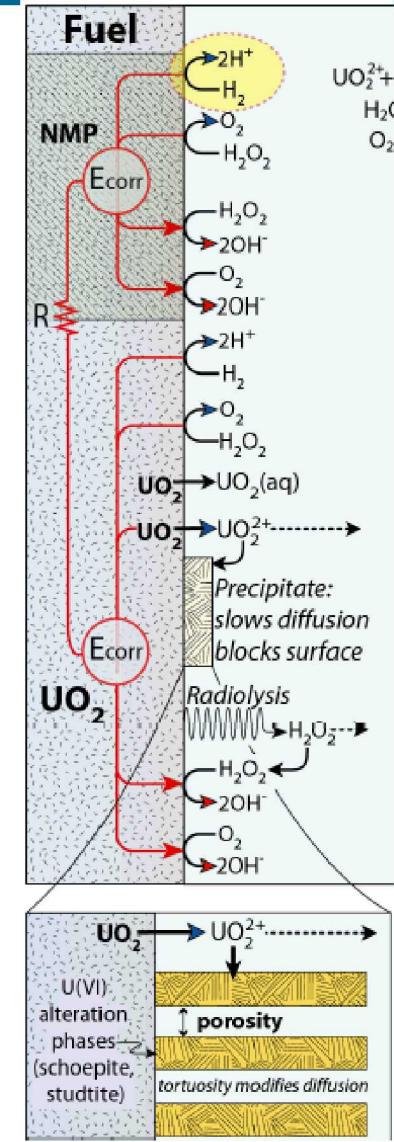


# Waste Form Degradation Model (cont.)

- Fuel Matrix Degradation Model (FMDM)
  - Radiolysis
  - Oxidation of  $H_2$  via noble metal particle (NMP) catalyst
  - 1-D reactive transport through alteration layer
  - Growth of the alteration layer
  - Diffusion of reactants/products through alteration layer

Inputs	Outputs
<ul style="list-style-type: none"> <li>• Initial concentration profiles across 1D corrosion/water layer (<math>UO_2(s)</math>, <math>UO_3(s)</math>, <math>UO_4(s)</math>, <math>H_2O_2</math>, <math>UO_2^{2+}</math>, <math>UCO_3^{2-}</math>, <math>UO_2</math>, <math>CO_3^{2-}</math>, <math>O_2</math>, <math>Fe^{2+}</math>, and <math>H_2</math>)</li> <li>• Initial corrosion layer thickness</li> <li>• Dose rate at fuel surface (= f (time, burnup))</li> <li>• Temperature ←</li> <li>• Time, time step length</li> <li>• Environmental concentrations (<math>CO_3^{2-}</math>, <math>O_2</math>, <math>Fe^{2+}</math>, and <math>H_2</math>)</li> </ul>	<ul style="list-style-type: none"> <li>• Final concentration profiles across 1D corrosion/water layer</li> <li>• Final corrosion layer thickness</li> <li>• Fuel dissolution rate</li> </ul>

- Can be coupled to PFLOTRAN



(adapted from Jerden et al. 2017)

# Waste Form Degradation Model (cont.)

- DPC considerations

- In-package chemistry and UO<sub>2</sub> degradation
  - elevated temperature, boiling?
  - reduced instant release fraction for higher burn-up fuels?
  - effects of different geologies (e.g., groundwater chemistry)
  - filler materials chemical effects
  - criticality event?
    - changes to radionuclide inventory
    - additional radiolytic oxidants from beta and gamma radiation
- Cladding degradation
  - elevated temperature?
  - criticality event?
    - intact cladding required
- Neutron absorbers
  - Boral® degradation

# Interactions with Engineered Barriers (Rutqvist 2019)

- For DPC direct disposal, a peak backfill temperature of 200°C is likely to occur, unless the SNF is aged for hundreds of years before backfilling (Hardin et al. 2015)
- For clay-based materials, a peak temperature of 100°C is often adopted to limit thermal-hydrologic-mechanical-chemical effects (e.g., chemical changes, material degradation, clay phase change, smectite swelling)
  - FEBEX: bentonite heated to 100°C in 18-year test at Grimsel Test Site
  - Backfill peak temperature >100°C is currently being evaluated
    - Mont Terri: ongoing in-situ heater test up to 140°C in Opalinus Clay (Rutqvist et al. 2018; 2019)
    - HotBENT: planned heater test at 150°C to 200°C at Grimsel Test Site
  - Bentonite backfill mixtures can be engineered to increase the thermal conductivity by mixing in graphite or graphene oxide
    - Jobmann and Buntebarth 2009; Chen et al. 2018

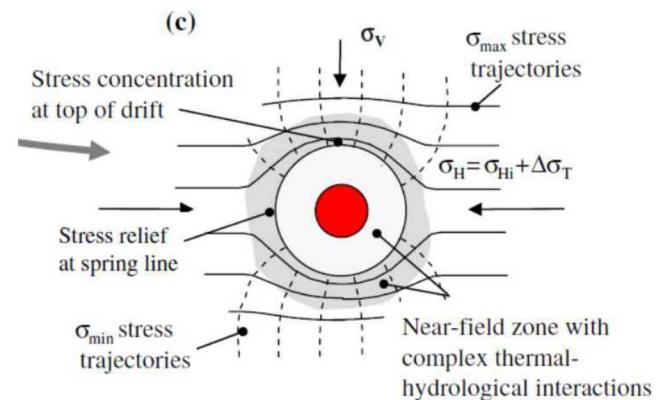
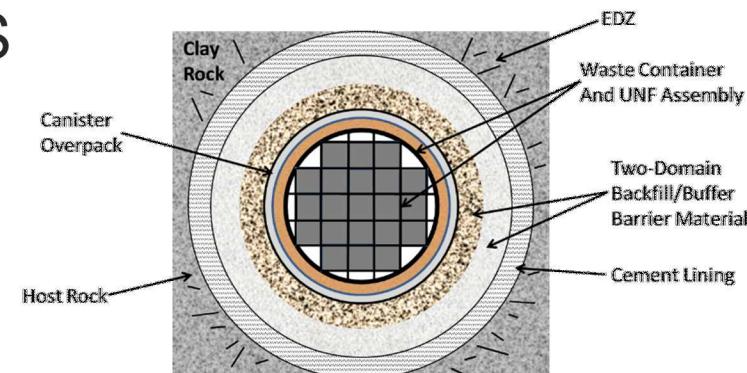
# Interactions with Engineered Barriers (cont.)

- The THMC effects of high-temperature on bentonite and near-field host rock are being examined in multiple SFWST Work Packages

- Argillite Disposal R&D
- Engineered Barrier System (EBS) R&D
- International Collaborations Research

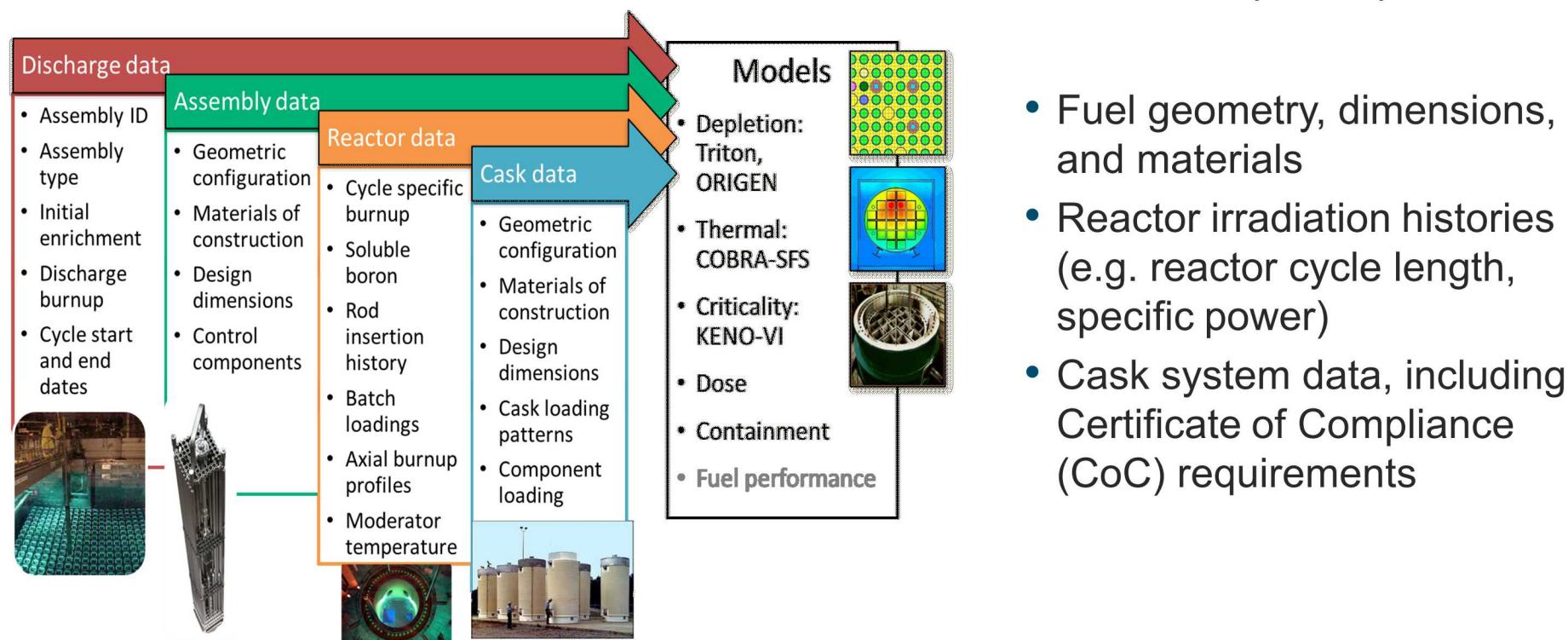
- These effects will be captured in GDSA reference cases

- DPC disposal in unsaturated alluvium
- DPC disposal in saturated argillite



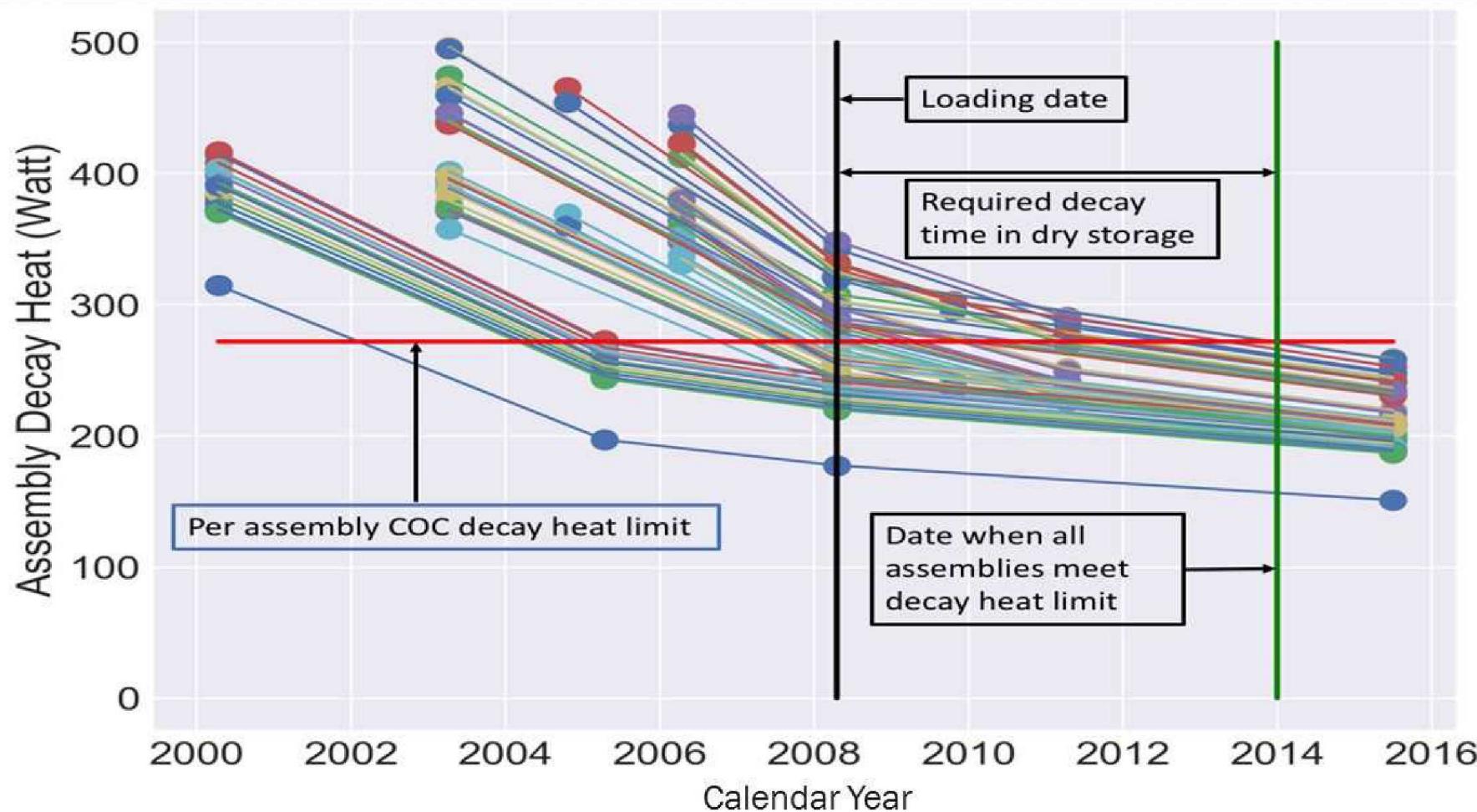
# Implications for Transportation

- The same tools and specific data that are used to evaluate criticality margin for the direct disposal of DPCs can also be used to evaluate the thermal and shielding criteria to determine when the DPC is transportable –
  - UNF-ST&DARDS and the Unified Database (UDB)



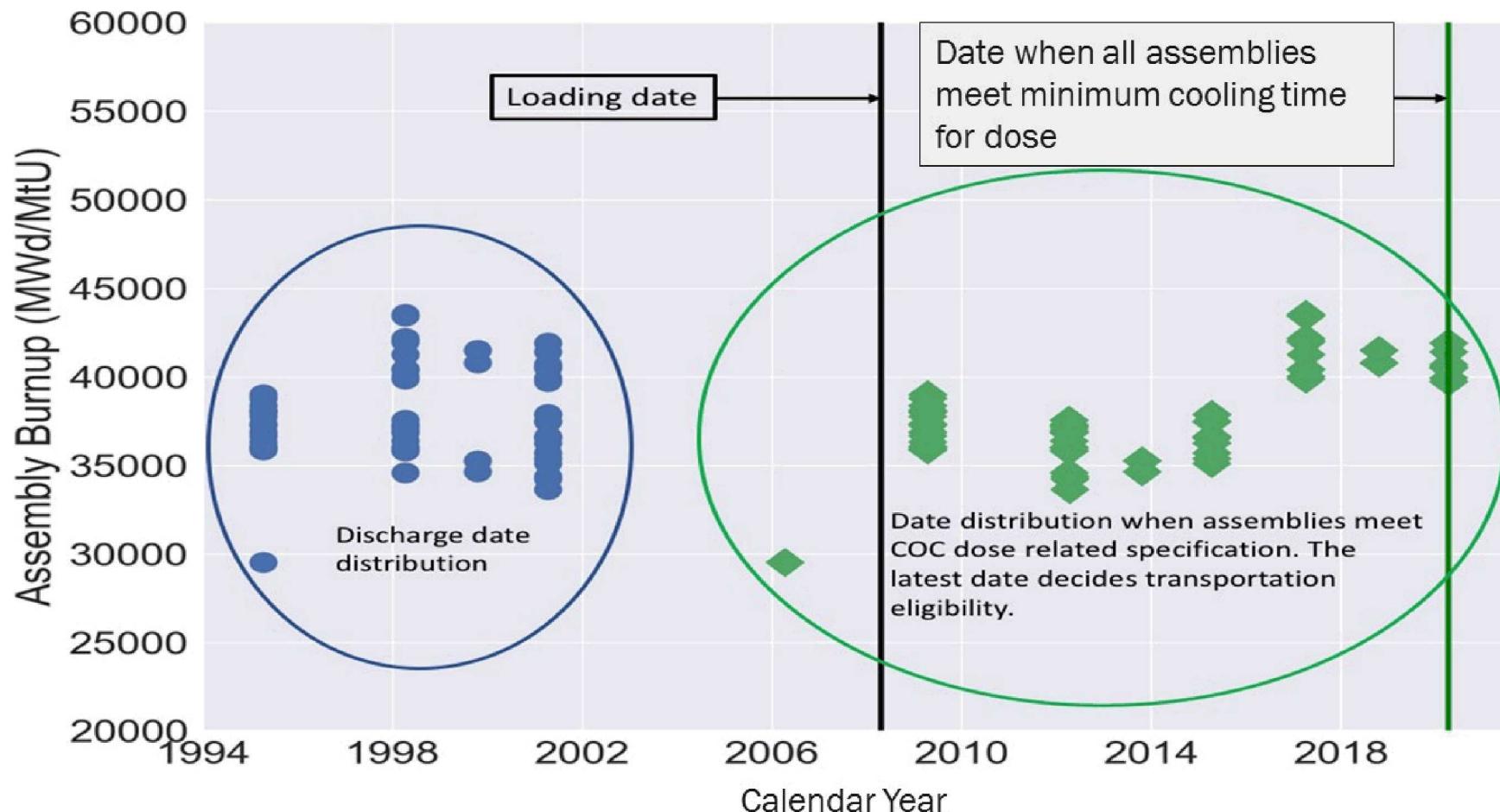
Unified Database (UDB) checks against transportation Certificate of Compliance (CoC) limits can be used to determine dates when SNF could be shipped

### Assembly Decay Heat Example



Unified Database (UDB) checks against transportation Certificate of Compliance (CoC) limits can be used to determine dates when SNF could be shipped

### Assembly Minimum Cooling Time Example (Dose Related)



# References

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# Questions?