

Cross-Cutting Research and Development

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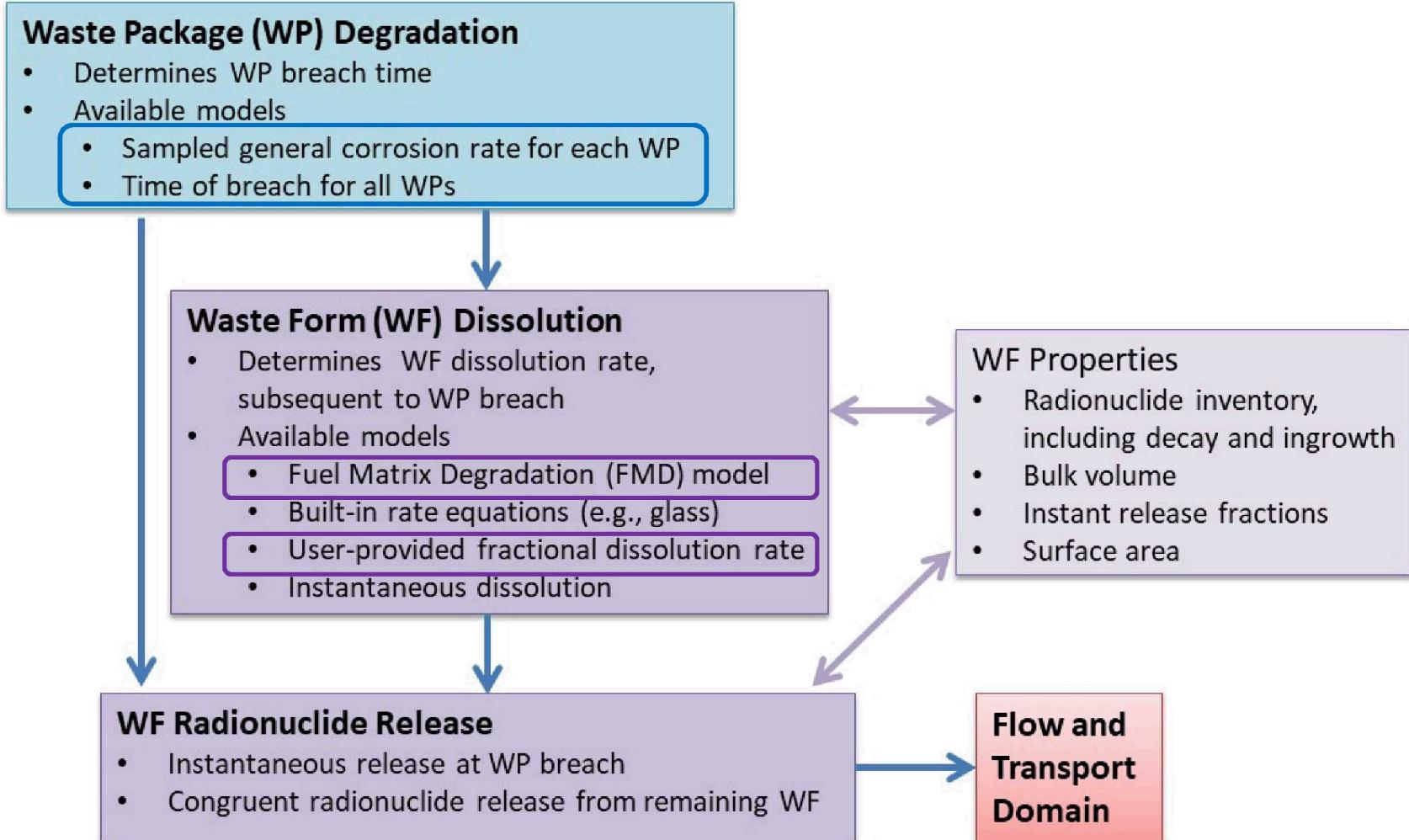
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Cross-Cutting Research and Development (R&D) Dual Purpose Canister (DPC) Considerations

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

Source Term Processes



Source: adapted from Mariner et al. 2019, Figure 2-4

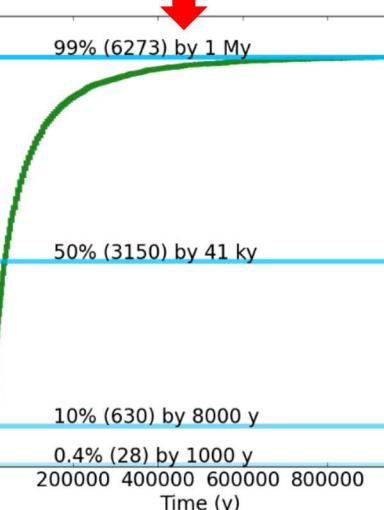
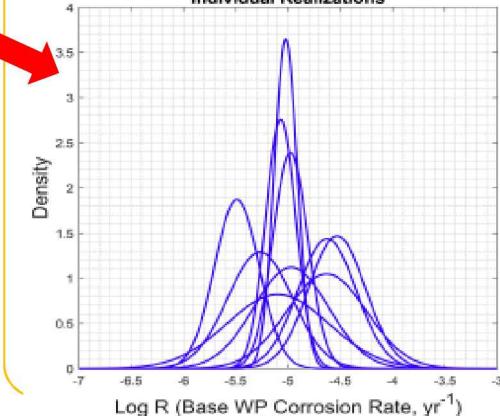
Waste Package Canister Vitality Model

- Canister vitality (wall thickness remaining) is a simple probabilistic rate (Mariner et al. 2016)
 - temperature-dependent general corrosion
 - can also define a breach time (e.g., early failures)
- Future development (Mariner et al. 2018)
 - mechanistic corrosion (general, localized)
 - DECOVALEX Task F
 - effects of groundwater chemistry / redox
 - seismic, igneous (site specific)
- Dual-purpose canister (DPC) considerations
 - Elevated temperatures
 - Disposal overpack materials (Cu, alloy 22, ... ?)

R_{eff} = canister degradation rate

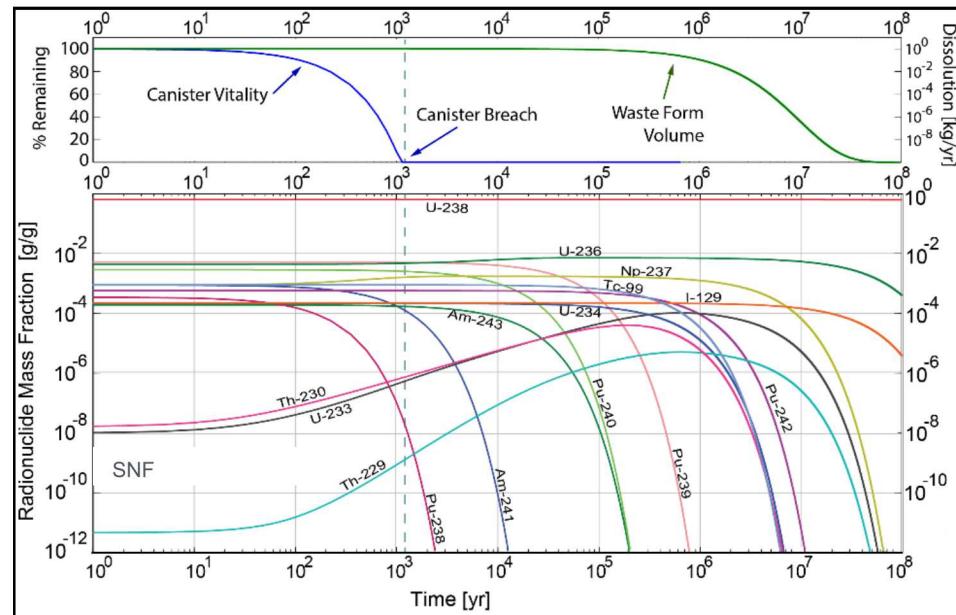
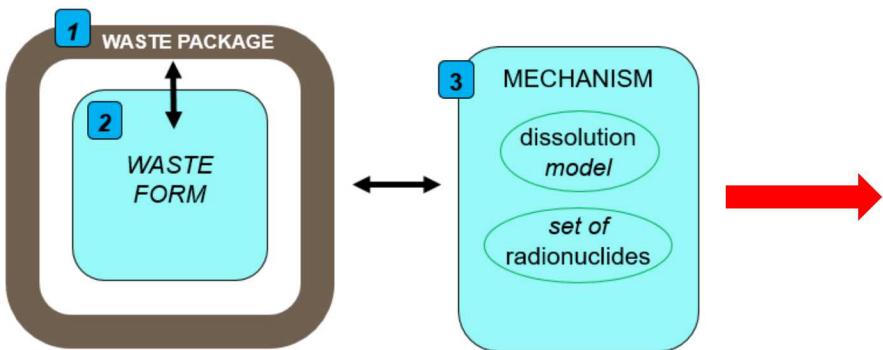
$$R_{\text{eff}} = R \cdot e^{\left[\frac{1}{60^\circ\text{C}} - \frac{1}{T(x,t)} \right]}$$

Example Log R Distribution among WPs in Individual Realizations



Waste Form Dissolution Rate Model

- Spent nuclear fuel (SNF) dissolution rate that begins following waste package failure (Mariner et al. 2016)
 - Instant release fraction (specified radionuclides)
 - Fractional dissolution (e.g., $10^{-5}/\text{yr}$)
- Directly implemented in PFLTRAN

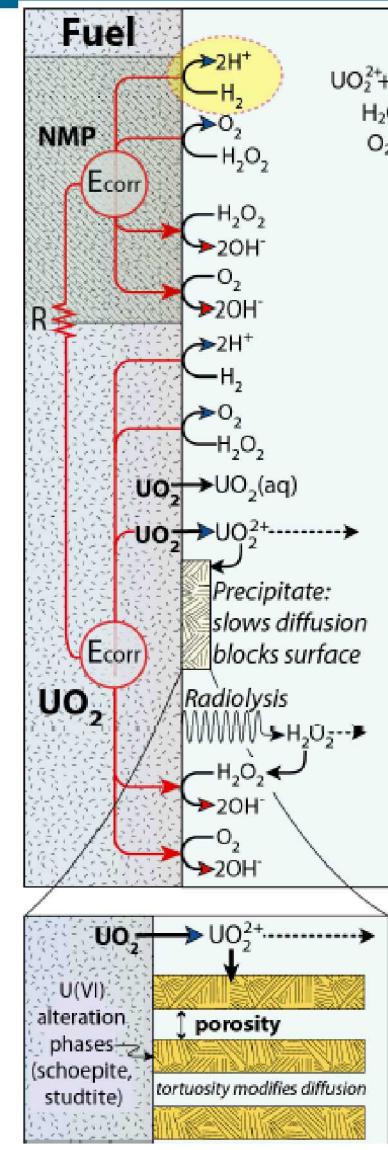


Electrochemical Fuel Matrix Degradation (FMD) Model

- 1-D reactive transport model to simulate diffusion of chemical species (Jerdon et al. 2017)
- SNF dissolution rate is a function of (Mariner et al. 2018)
 - Radiolysis
 - Growth of alteration layer on UO_2 surface
 - Diffusion of reactants through the alteration layer
 - Interfacial corrosion potential

Inputs	Outputs
<ul style="list-style-type: none">• Initial concentration profiles across 1D corrosion/water layer ($\text{UO}_2(s)$, $\text{UO}_3(s)$, $\text{UO}_4(s)$, H_2O_2, UO_2^{2+}, UCO_3^{2-}, UO_2, CO_3^{2-}, O_2, Fe^{2+}, and H_2)• Initial corrosion layer thickness• Dose rate at fuel surface (= f (time, burnup))• Temperature• Time, time step length• Environmental concentrations (CO_3^{2-}, O_2, Fe^{2+}, and H_2)	<ul style="list-style-type: none">• Final concentration profiles across 1D corrosion/water layer• Final corrosion layer thickness• Fuel dissolution rate

- Mechanistic model and emulators coupled to PFLOTRAN (Mariner et al. 2019)



(adapted from Jerden et al. 2017)

Waste Form Degradation Model for DPCs

- DPC considerations

- In-package chemistry and UO₂ degradation
 - elevated temperature, boiling?
 - reduced instant release fraction for higher burn-up fuels?
 - effects of different geologies (e.g., groundwater chemistry)
 - chemical effects from filler materials
 - criticality event?
 - changes to radionuclide inventory
 - additional radiolytic oxidants from beta and gamma radiation
- Cladding degradation
 - elevated temperature?
 - criticality event?
 - intact cladding assumed
- Neutron absorbers
 - degradation of aluminum-based materials
 - e.g., BoralTM, MetamicTM

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

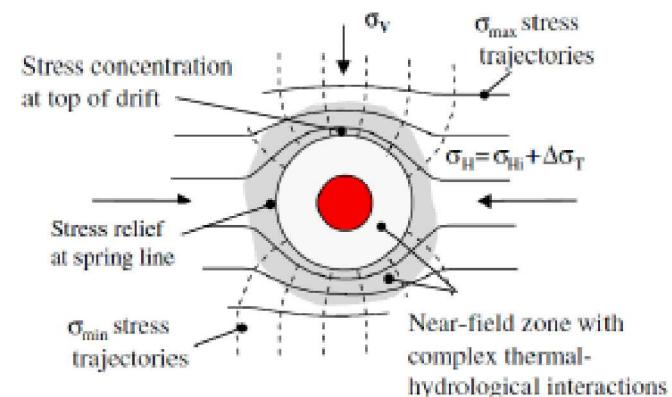
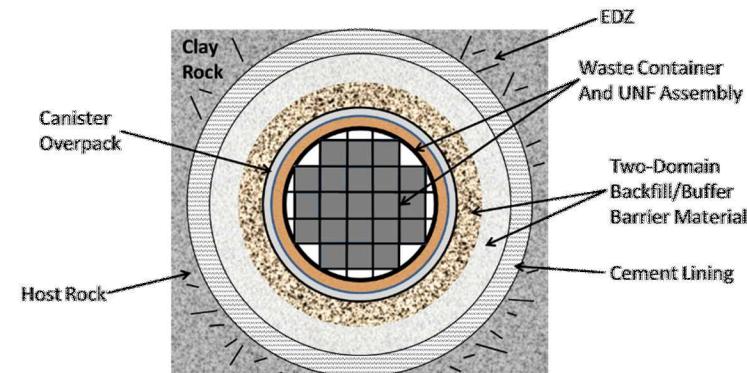
Interactions with Engineered Barriers (cont.)

- The thermal-hydrologic-mechanical-chemical (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

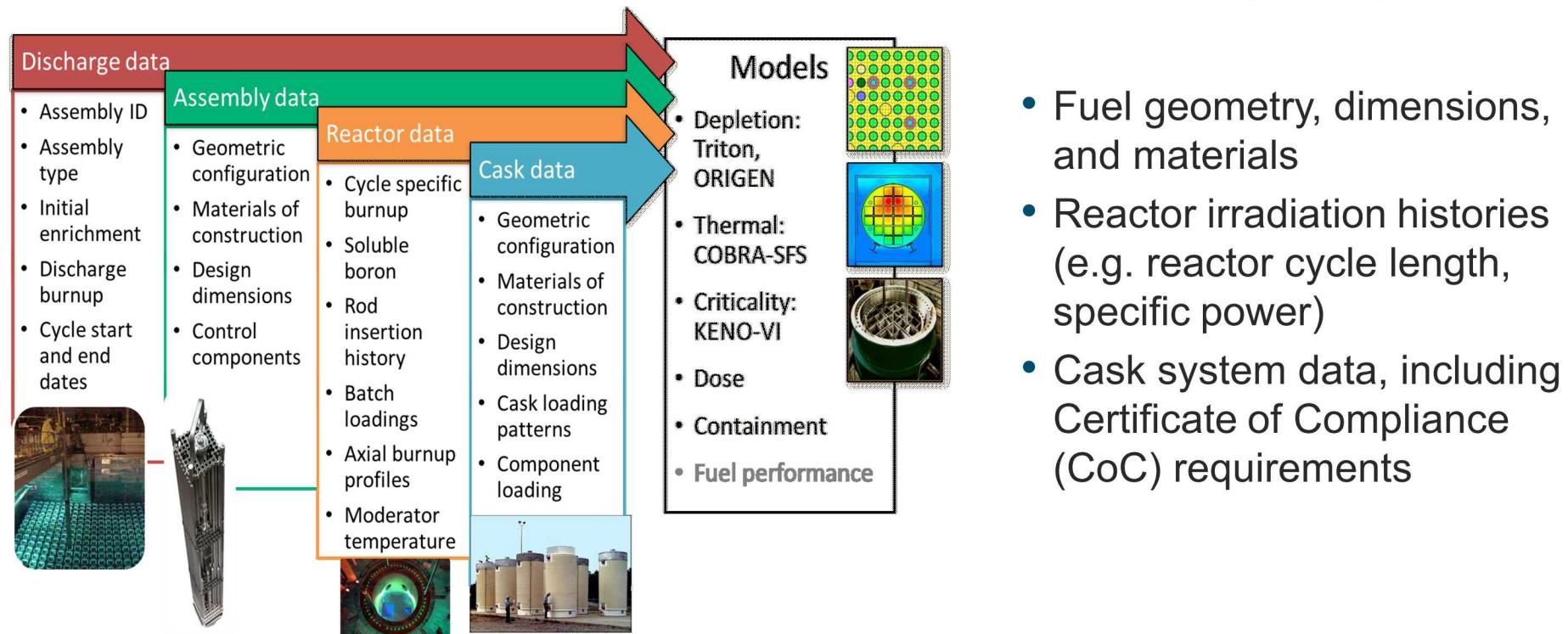
- DPC disposal in unsaturated alluvium
- DPC disposal in saturated argillite



(Source: Rutqvist 2019, Figure 1-1)

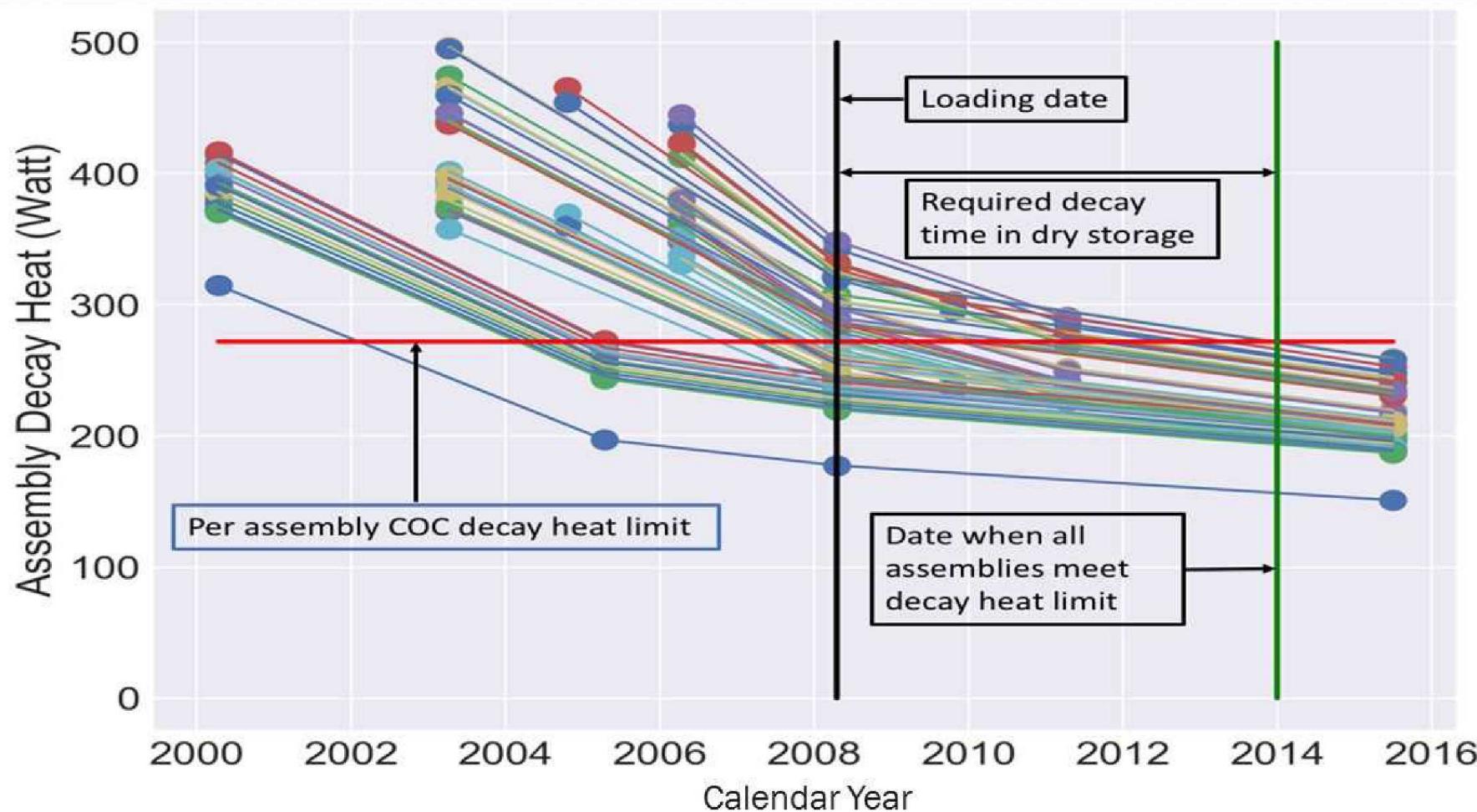
Implications for Transportation

- 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)



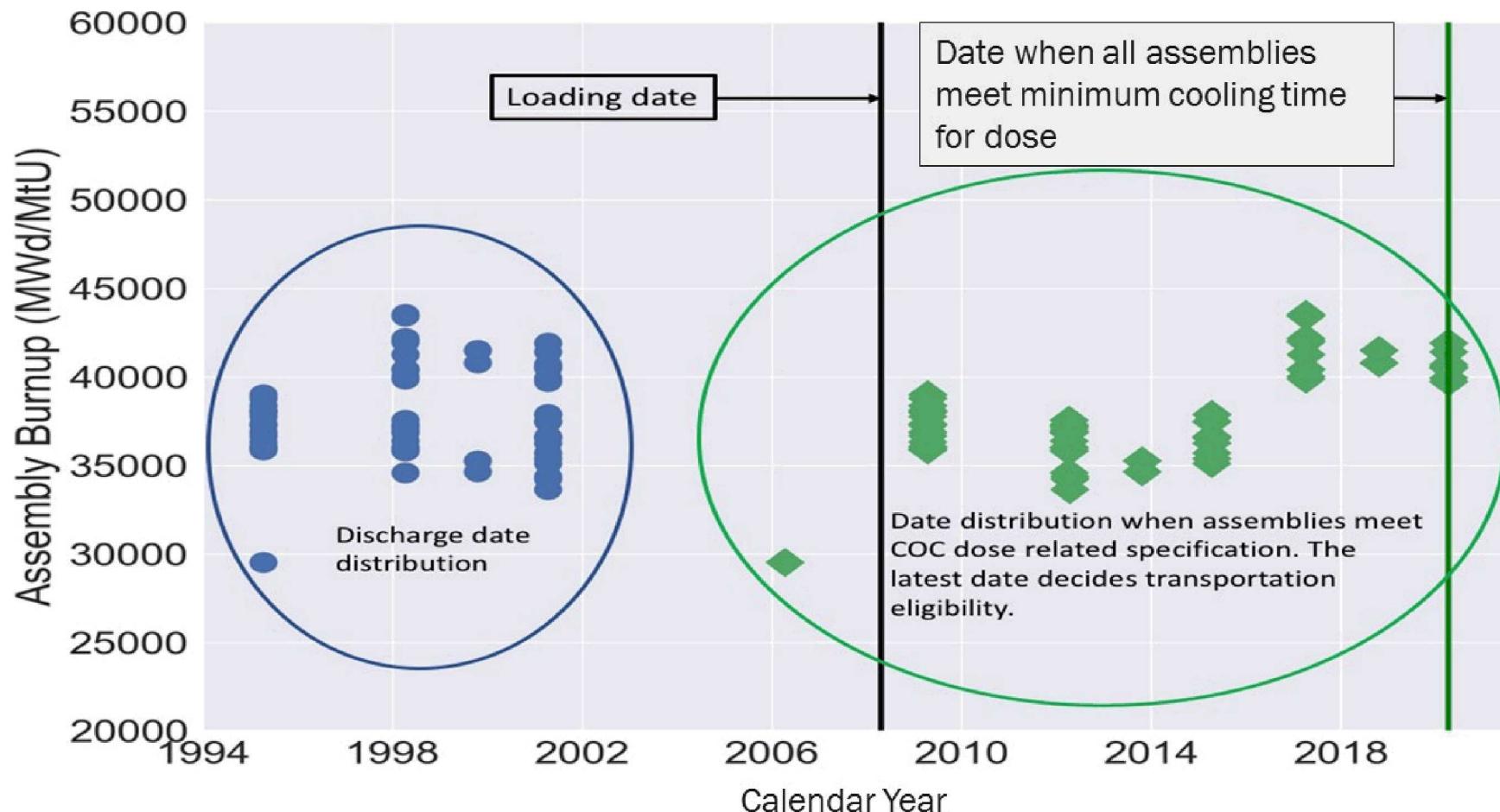
Unified Database (UDB) checks against transportation Certificate of Compliance (CoC) limits can be used to determine dates when SNF could be shipped

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)



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Questions?