U.S. DEPARTMENT OF ENERGY | Office of NUCLEAR ENERGY

Overview of FMDM and process models

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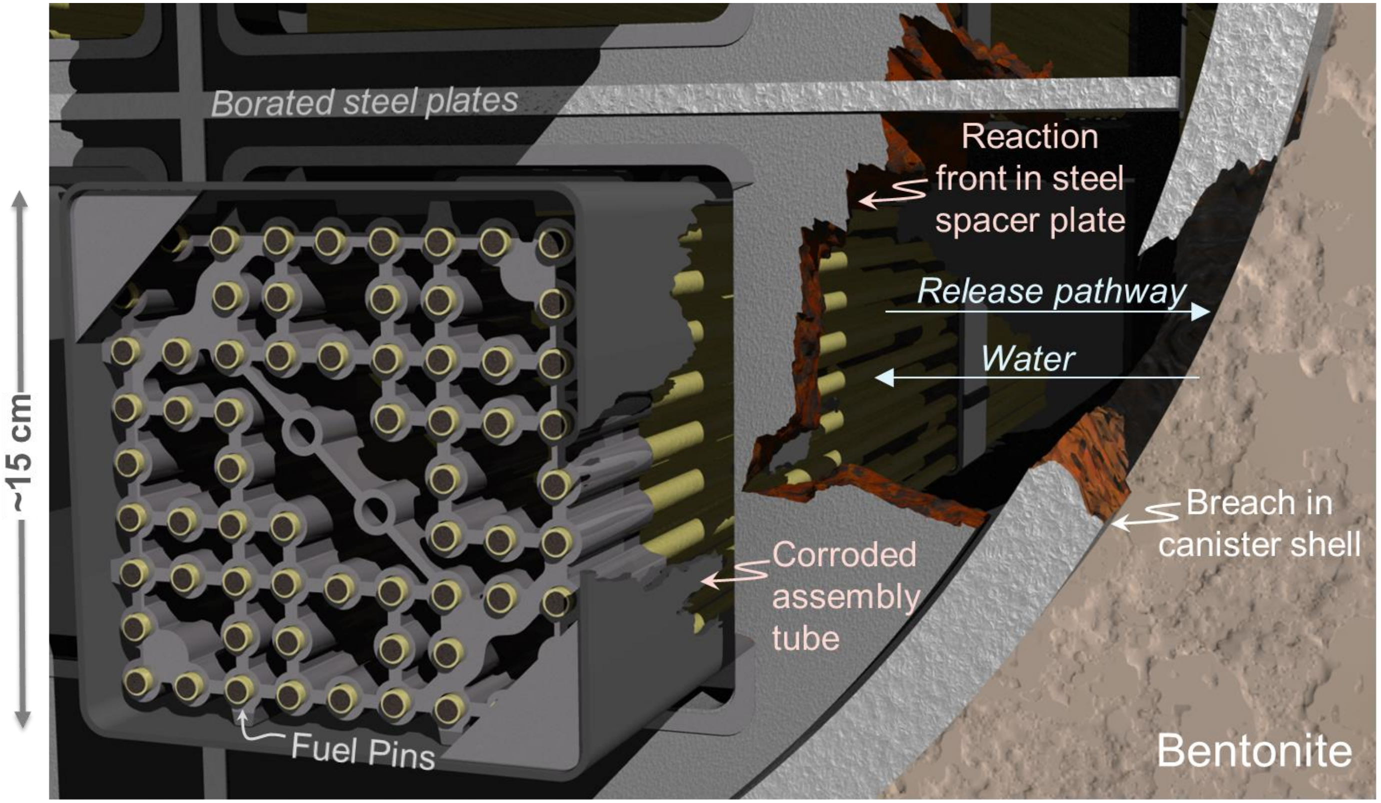
Conceptual Diagram of Breached SNF Canister in Repository



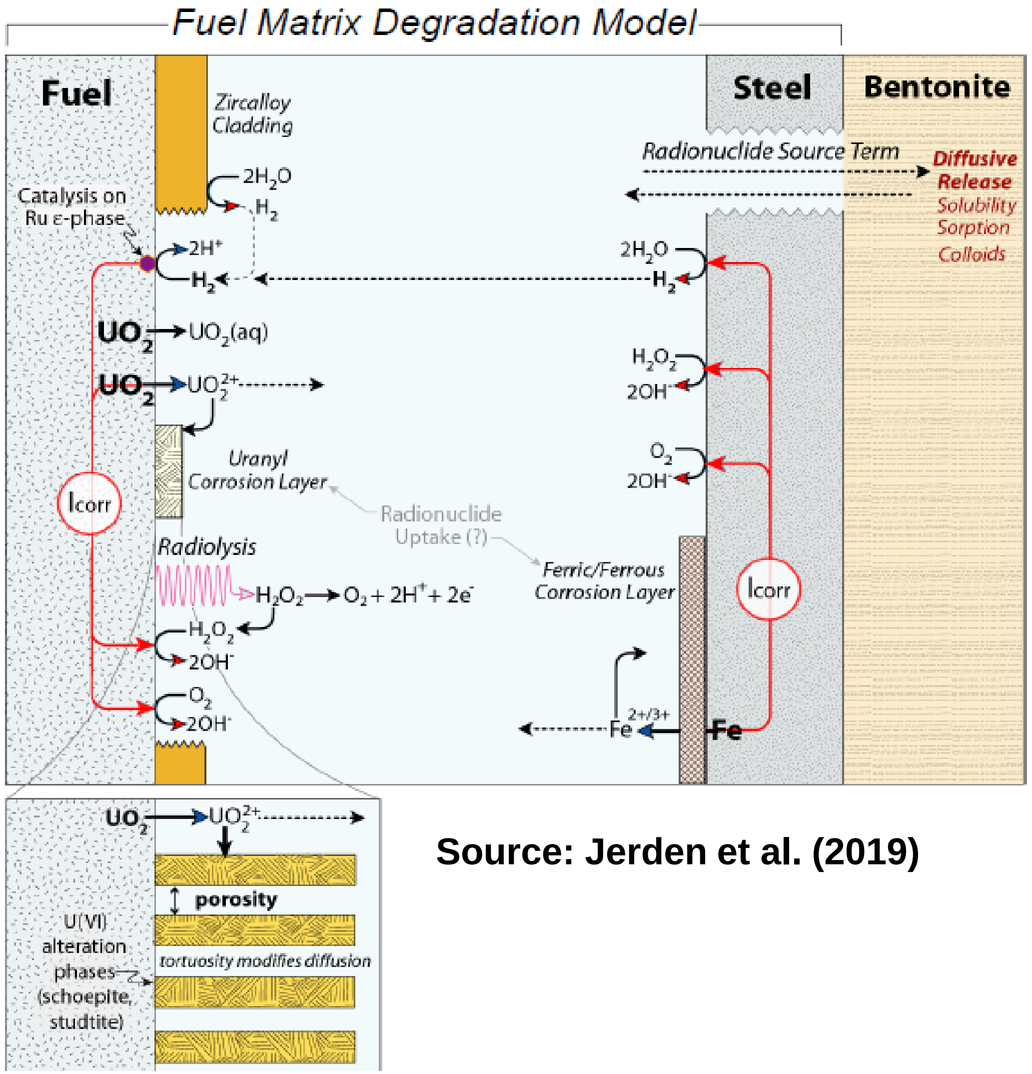
Schematic figure of a breached SNF waste canister

Waste Package Breaching

- Fluid pathways
- In-package chemistry
  - SNF corrosion
  - Metal corrosion (WP internals)
- Radionuclide (RN) release
  - Interaction with corrosion products
  - Interactions with bentonite barrier

Source: Jerden, J., Frey, K., and Ebert, W. (2016) Used Fuel Disposition (UFD) Campaign, Working Group Meeting Presentation

Fuel Matrix Degradation Model (FMDM)



Source: Jerden et al. (2019)

The Fuel Matrix Degradation Model (FMDM)

- Based on the Canadian Mixed Potential Model for UO_2 dissolution (Shoesmith et al., 2003)
- Electrochemical transport model
- Surface potentials based on major interfacial anodic and cathodic reactions
- Reaction rates for the fuel surface reactions used to represent oxidative UO_2 dissolution
- H_2 catalysis by noble metal particles (NMPs)
- 1-D diffusive transport of chemical species
- H_2O_2 generation by radiolysis
- Surface precipitates (e.g., schoepite/studtite)
- Anoxic corrosion of steel components

Fuel Matrix Degradation Model (FMDM)

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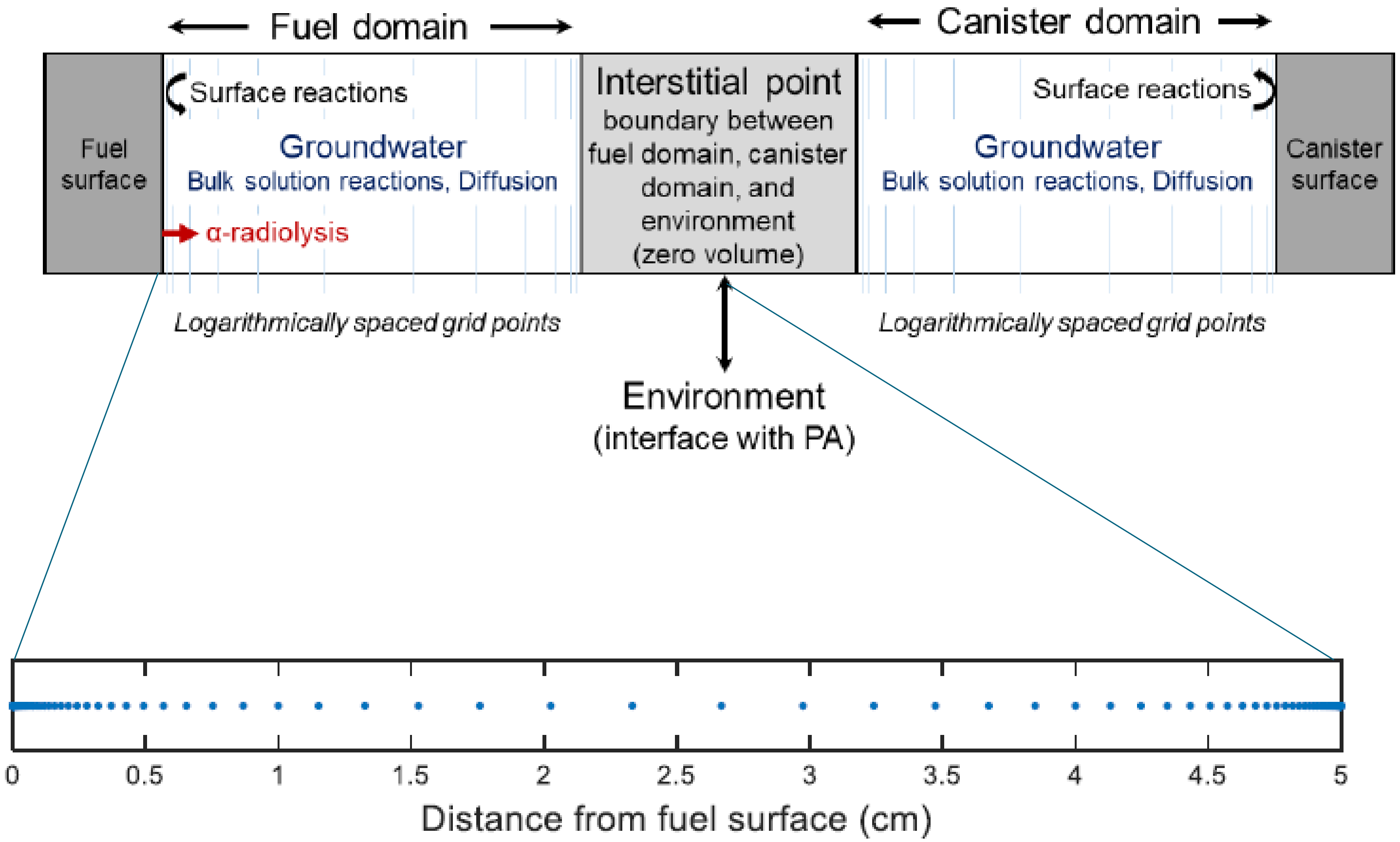

Source: Thomas (2024), Fuel Matrix Degradation Process Model Documentation, in prep.

FMDM Domain Description

- **Two chemical domains**
  - **Fuel domain**
  - **Canister domain**
- **Interstitial domain**
  - **Interface between fuel and canister domains**
  - **Environment domain is the interface with performance assessment (PA)**
- **Species concentrations and mass fluxes**
  - **Calculated at each node within each domain**
  - **Diffusive fluxes calculated at the fuel surface**

Fuel Matrix Degradation Model (FMDM)

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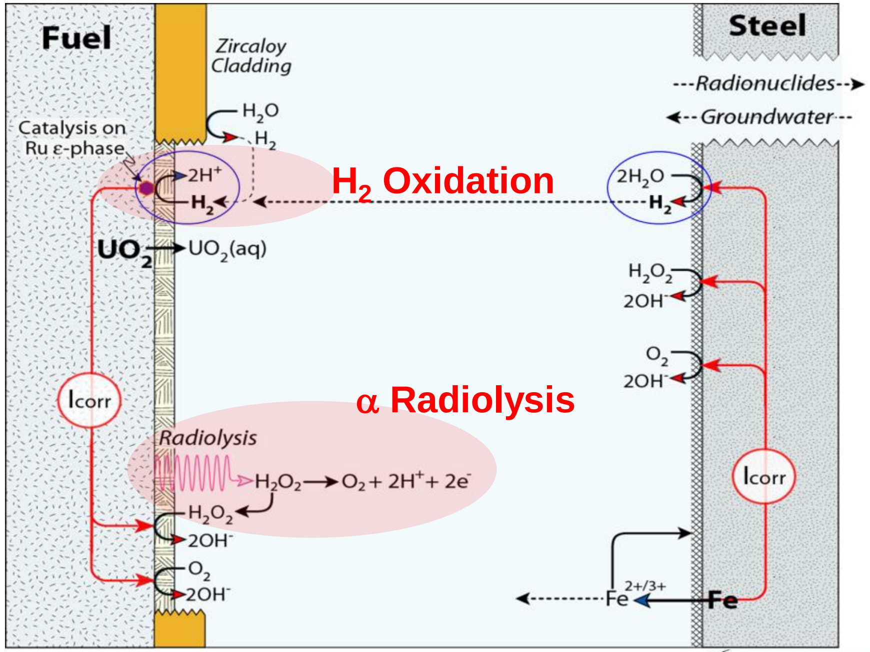
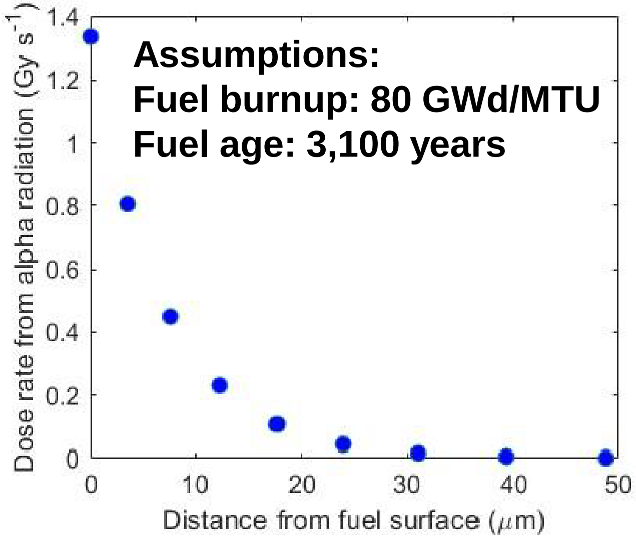
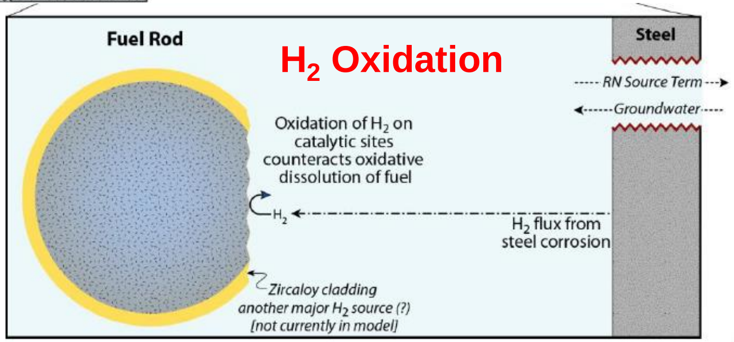




Source: Thomas (2024), Fuel Matrix Degradation Process Model Documentation, in prep.



Radiolysis

- H_2O_2 is the only radiolytically-produced oxidant
- H_2O_2 generated by α irradiation field (extends to ~35 microns from fuel surface)
- α dose irradiation decreases exponentially from the fuel surface
- No hydroxy radical generation
- G_{H2O2} value per alpha dose rate is assumed to be constant

Catalysis

- H_2 oxidation at the fuel surface catalyzed by NMPs (ε-phases)
- Protects fuel from oxidative dissolution by decreasing E_{CORR}

FMDM Electrochemical (E-chem) Reactions at the SNF Surface

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SNF Surface Half Reactions

Number	Reaction	Type
1	$UO_2 \rightarrow UO_2^{2+} + 2e^-$	Anodic
2	$UO_2 + 2CO_3^{2-} \rightarrow UO_2(CO_3)_2^{2-} + 2e^-$	Anodic
3	$UO_2 \rightarrow UO_{2(aq)}$	Chemical
4	$H_2 + 2OH^- \rightarrow 2H_2O + 2e^-$	Anodic
5	$H_2O_2 + 2OH^- \rightarrow O_2 + 2H_2O + 2e^-$	Anodic
6	$H_2O_2 + 2e^- \rightarrow 2OH^-$	Cathodic
7	$O_2 + 2H_2O + 4e^- \rightarrow 4OH^-$	Cathodic

NMP Surface Half Reactions

Number	Reaction	Type
8	$H_2 + 2OH^- \rightarrow 2H_2O + 2e^-$	Anodic
9	$H_2O_2 + 2e^- \rightarrow 2OH^-$	Cathodic
10	$H_2O_2 + 2OH^- \rightarrow O_2 + 2H_2O + 2e^-$	Anodic
11	$O_2 + 2H_2O + 4e^- \rightarrow 4OH^-$	Cathodic

The Fuel Matrix Degradation Model (FMDM)

- **Anodic/cathodic e-chem reactions applied to UO_2 and NMP surfaces**
- **UO_2 oxidative dissolution rate is represented by the net current densities of e-chem reactions**
- **E-chem reaction rates determine the current densities**
- **SNF degradation rate is calculated from total U flux into solution**

Source: Thomas (2024), Fuel Matrix Degradation Process Model Documentation, in prep.

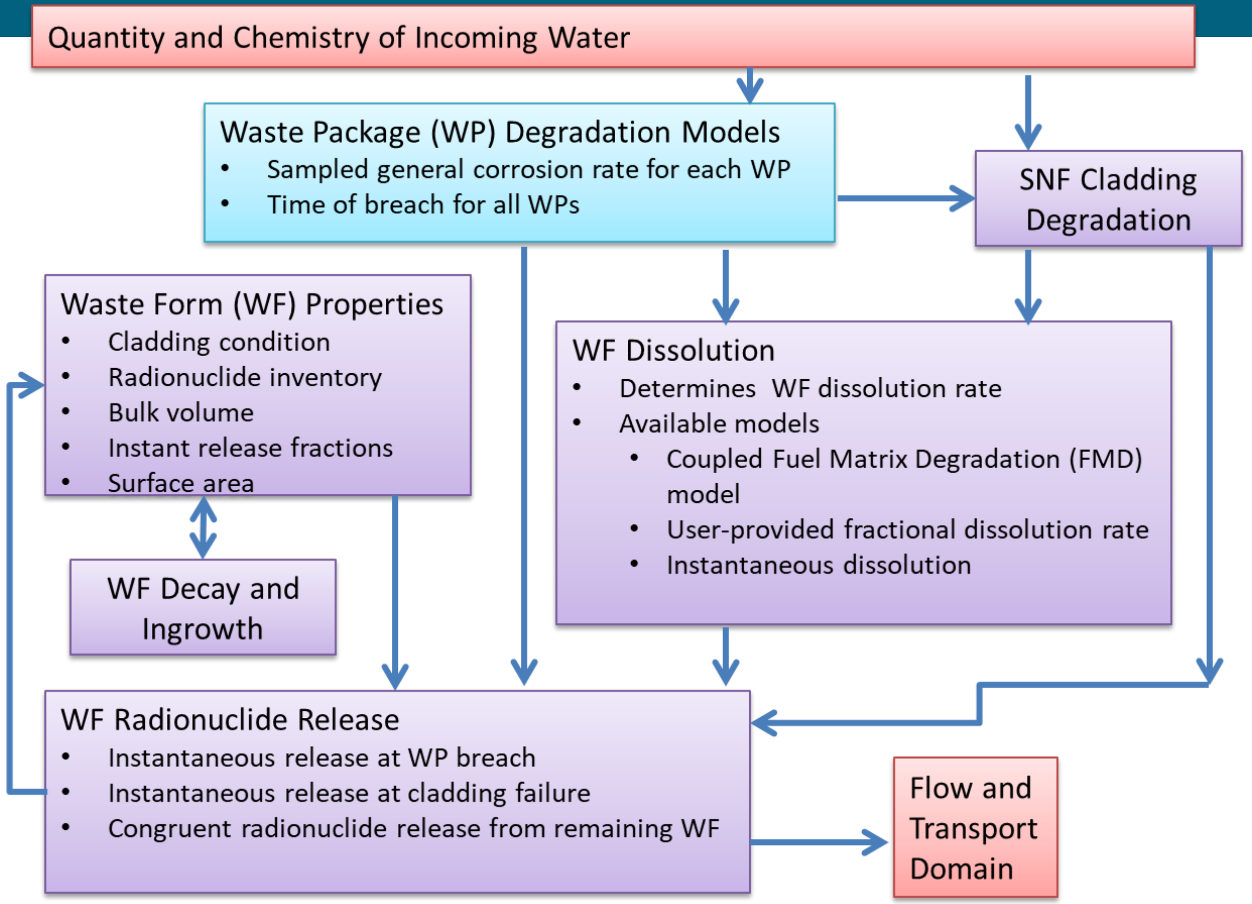
Ongoing and Future R&D Activities (SNL)

Summary:

- FMDM describes SNF degradation including effects of NMP catalysis, radiolysis, and steel corrosion
- Development considers literature and experimental SNF degradation data

Ongoing/Future Activities:

- FMDM coupling to the Geologic Disposal Safety Assessment (GDSA) framework
- Gap analysis and prioritization of testing activities for SNF degradation



Conceptual Framework for Source Term Processes in GDSA (Adapted from Mariner, et al., 2019)