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Securing the future of Nuclear Energy

Recent Accident Source Terms

ACRS Briefing Nov 19, 2024

Presented by Lucas I. Albright and David L. Luxat

U.S. DEPARTMENT OF ENERGY NNSA

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SAND2024-15580PE

Applicability of Source Term for Accident Tolerant Fuel, High Burn Up and Extended Enrichment – 2020 Memo (ML20126G376)

MELCOR

- ✓ HBU/HALEU/ATF PIRT – **2021**
- ✓ Additional HBU Source Term Analyses – **2023**
- ✓ Source term calculations for representative PWRs and BWRs for Cr-coated cladding – **2024**
- ✓ Source term calculations for representative PWRs and BWRs for FeCrAl cladding – **2024**

MELCOR Modeling Capabilities for ATF Concepts

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General Oxidation Model

- Parabolic Rate Kinetics

$$\frac{d\, m(T,t)^n}{dt} = K(T)$$

$m\left[\frac{kg}{m^2}\right]$ – mass per unit area of oxidized metal
T [K] – temperature
t [s] – time
n [-] – material specific exponential term
$K\left[\frac{kg^n}{m^{2n}s}\right]$ – rate constant

- Arrhenius Correlation

$$K(T) = Ae^{\frac{-B}{T}}$$

$A\left[\frac{kg^2}{m^4 s}\right]$ – experimental fit coefficient
B [K] – experimental fit coefficient

- Diffusion limited oxidation

$$\frac{dm(T_f,t)}{dt} = \frac{M_w k_c P_{ox}}{nRT_f}$$

$M_w\left[\frac{kg}{mol}\right]$ – molecular weight of the metal
$k_c\left[\frac{m}{s}\right]$ – mass transfer coefficient
P_{ox} [Pa] – partial pressure of the oxidant
n [-] – stoichiometric ratio of oxidant to metal
$R\left[\frac{m^3 Pa}{K \cdot mol}\right]$ – universal gas constant
T_f [K] – gas film temperature

User-defined Materials

- 4 Additional User-defined Material “Slots”
  - Two slots reserved for a COR package metal/oxide pair
- Tabular Material Properties
  - Density
  - Thermal Conductivity
  - Specific Heat
  - Enthalpy
- Constant Material Properties
  - Solidus Temperature
  - Latent Heat of Fusion
  - Molecular Weight
  - Viscosity
  - Thermal Expansion Coefficient

Methodological Approach

Process for Source Term Development

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1. BWR and PWR core damage accident scenario identification
2. Develop radionuclide inventory and decay heat using the SCALE code package
3. Perform accident progression and source term analyses using MELCOR
4. Develop statistically representative source term across all accident scenarios and BWR/PWR plants

Key Aspects of the Analysis

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Technology Identification

- BWR: Mark I containment (Peach Bottom) and Mark III containment (Grand Gulf)
- PWR: Ice Condenser containment (Sequoyah) and Large-dry containment (Surry)

Radionuclide Inventory and Decay Heat Development

- Core average burnup of 60GWd/MTU for enrichment of 8 wt% (peak 10 wt% for BWRs)
- Core average burnup of 80GWd/MTU for enrichment of 8 wt% (peak 10 wt% for BWRs)

Accident Scenario Identification

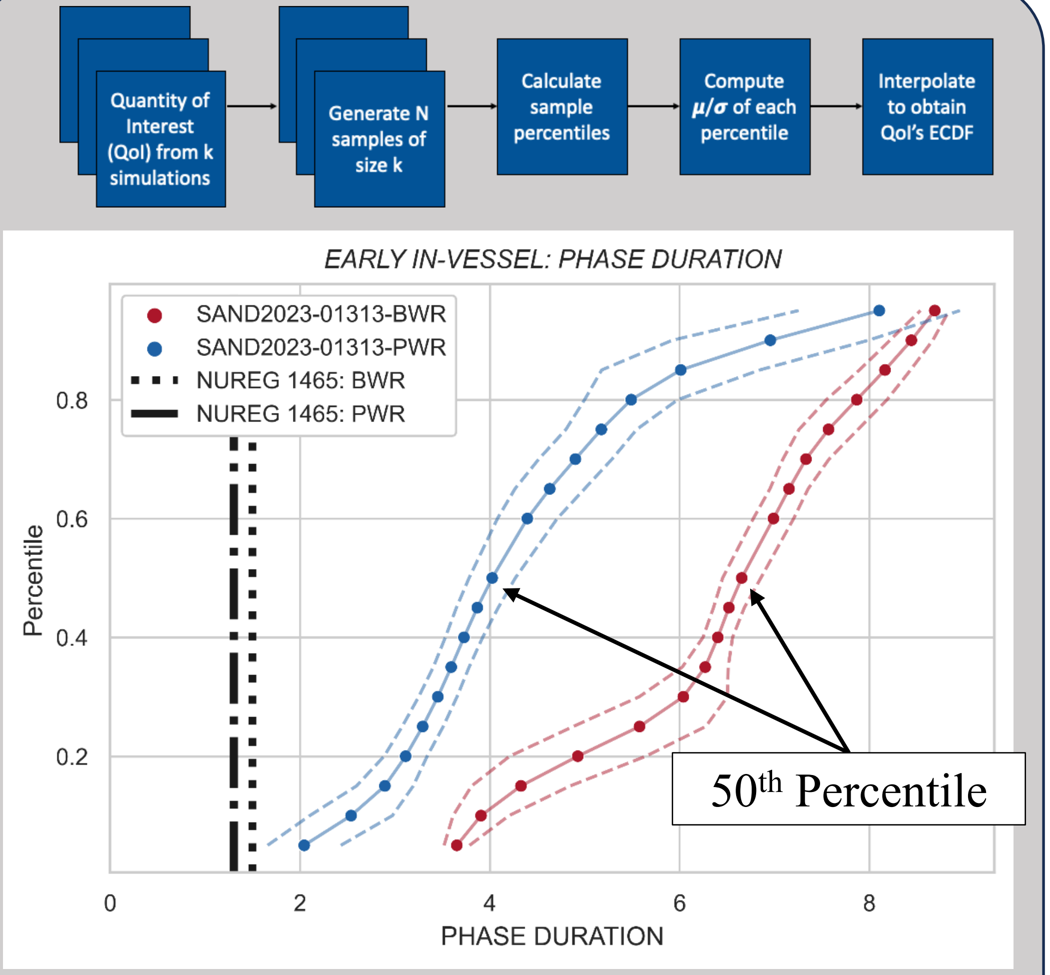
- BWR: SBLOCA, LBLOCA, STSBO, LTSBO, ATWS
- PWR: SBLOCA, LBLOCA, STSBO

*Reduced set of analyses based on SAND2023-01313 finding that there is no strong dependence

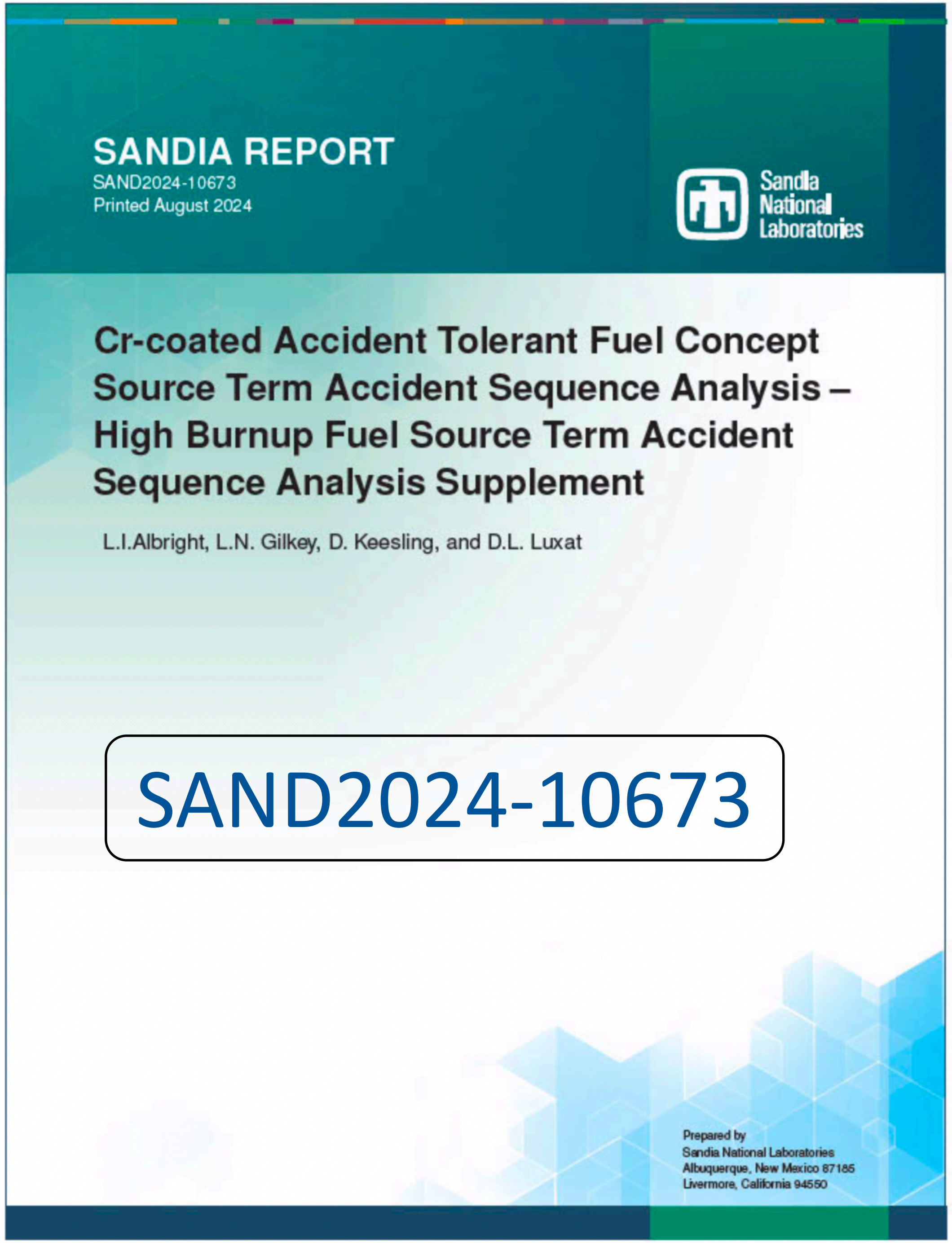
Phase	Onset Criteria	End Criteria
Gap Release	RPV water level below top of active fuel	Release of 5% of initial, total Xe inventory from fuel
Early In-Vessel	Release of 5% of initial, total Xe inventory from fuel	Lower Head Failure

Non-Parametric Statistical Analysis

- Non-parametric bootstrap methodology used to determine statistically representative source term across accident scenarios
  - Can be applied to data that follow any distribution
  - Utilizes repeated re-sampling (bootstrapping) of data
  - Estimates empirical cumulative distribution function (ECDF) of a given quantity of interest (QoI)
- Representative source term is the median (50th percentile) estimate from the ECDF
  - Equally weights all simulations
- Incorporates variability due to different plants and accident scenarios in representative source term
  - Bounds on empirical cumulative distribution function (ECDF) characterize sampling uncertainty



*Dashed colored lines illustrate confidence intervals spanning ± standard deviation (σ) at each percentile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Cr-coated Accident Tolerant Fuel Concept Source Term Accident Sequence Analysis – High Burnup Fuel Source Term Accident Sequence Analysis Supplement

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SAND2024-10673

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Cr-Coated Accident Tolerant Fuel Source Term Analysis

- Develop alternative source term applicable to LWR cores with Cr-coated zirconium alloy cladding
  - Thin, protective chromium coating on Zircaloy fuel cladding delays exothermic Zircaloy oxidation onset
- Cr-coated analysis informed by ATF severe accident PIRT (NUREG/CR-7283) findings
- Extends SAND2023-01313 alternative source terms

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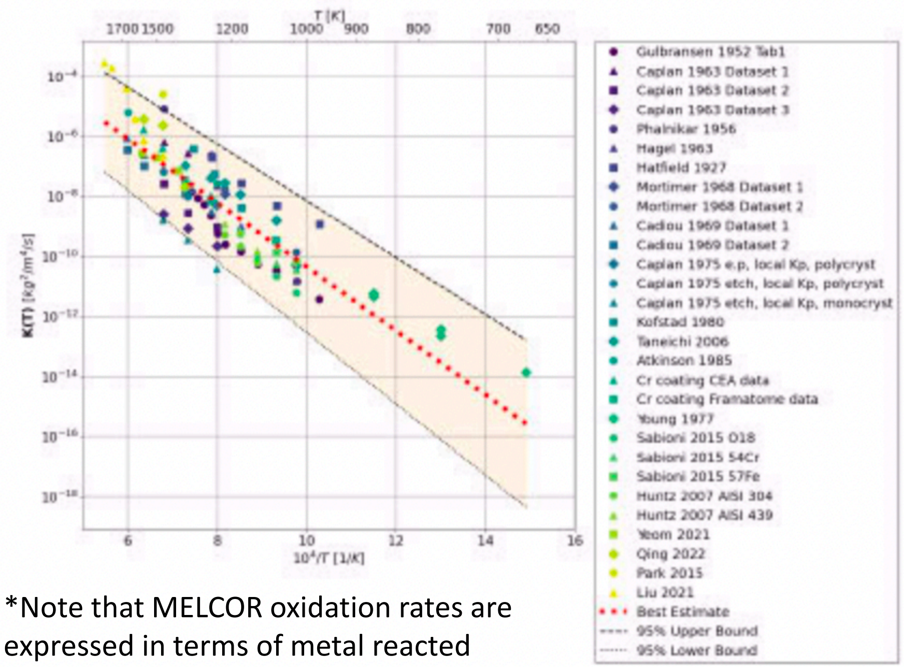
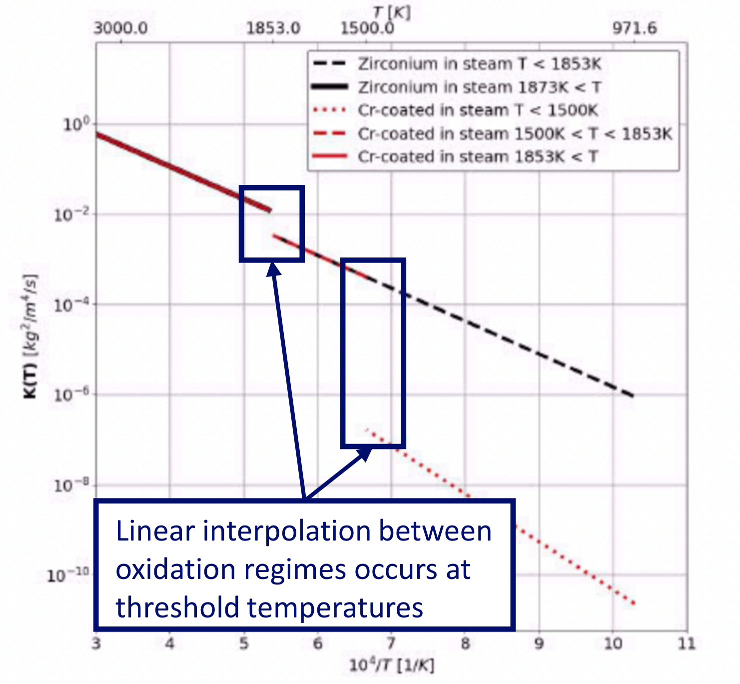
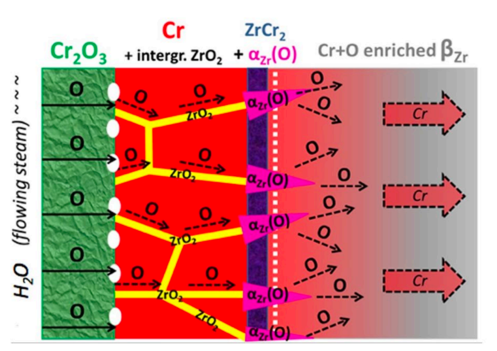
Cr-Coated Cladding Modeling



*Note that MELCOR oxidation rates are expressed in terms of metal reacted



- Oxidation correlation is based on previous Cr and Cr-coated zirconium oxidation experiments
- Transition from a protective Cr-coating to non-protective coating occurs at elevated temperatures (1500K – 1600K)



J.-C. Brachet, E. Rouesne, J. Ribis, T. Guilbert, S. Urvoy, G. Nony, C. Toffolon-Masclet, M. Le Saux, N. Chaabane, H. Palancher, A. David, J. Bischoff, J. Augereau, and E. Pouillier, *Corrosion Science* **167**, 108537 (2020).

- Assumed thin Cr-coating (10 microns) on cladding and canister (for BWRs) structures
  - Tens to hundreds kg additional Cr mass
- Temperature-based oxidation rate
  - Loss of protective coating assumed at 1500K
- Cr mass-based heat of reaction

Cr-Coating BWR Source Term

	Gap Release			Early In-vessel		
Report	2024 Cr-coated	2023 HBU/HALEU	NUREG-1465	2024 Cr-coated	2023 HBU/HALEU	NUREG-1465
Phase Duration [h]	0.80	0.70	0.5	5.9	6.7	1.5
Noble Gases	0.019	0.016	0.05	0.94	0.95	0.95
Halogens	0.007	0.005	0.05	0.73	0.71	0.25
Alkali Metals	0.006	0.005	0.05	0.29	0.32	0.20
Te Group	0.005	0.003	0.0	0.55	0.56	0.05
Ba/Sr Group	0.0009	0.0006	0.0	0.004	0.005	0.02
Ru Group	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0	0.004	0.006	0.003
Mo Group	1.9×10^{-5}	2×10^{-5}	0.0	0.093	0.12	0.003
Lanthanides	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0002
Ce Group	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0005

- Gap release phase duration is slightly increased, but within 2023 HBU/HALEU study uncertainties
- Release fractions observed during the gap release phase are within 2023 HBU/HALEU study uncertainties
- Early in-vessel phase duration is decreased
- Smaller release fractions (compared to 2023 HBU/HALEU) are generally observed during the early in-vessel phase
- Larger halogen release fractions observed during the early in-vessel phase are within 2023 HBU/HALEU study uncertainties

Cr-Coating PWR Source Term

	Gap Release			Early In-vessel		
Report	2024 Cr-coated	2023 HBU/HALEU	NUREG-1465	2024 Cr-coated	2023 HBU/HALEU	NUREG-1465
Phase Duration [h]	1.5	1.3	0.5	3.6	4.0	1.3
Noble Gases	0.036	0.026	0.05	0.89	0.93	0.95
Halogens	0.010	0.007	0.05	0.56	0.58	0.35
Alkali Metals	0.005	0.003	0.05	0.49	0.50	0.25
Te Group	0.008	0.006	0.0	0.54	0.55	0.05
Ba/Sr Group	0.001	0.001	0.0	0.003	0.002	0.02
Ru Group	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0	0.009	0.008	0.003
Mo Group	0.0001	$< 2 \times 10^{-5}$	0.0	0.16	0.15	0.003
Lanthanides	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0002
Ce Group	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0005

- Gap release phase duration is slightly increased, but within 2023 HBU/HALEU study uncertainties
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- Smaller release fractions (compared to 2023 HBU/HALEU) are generally observed during the early in-vessel phase
- Larger release fractions observed during the early in-vessel phase are within 2023 HBU/HALEU study uncertainties (Ru and Mo Group) or smaller than NUREG-1465 (Ba/Sr Group)

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NUREG/CR-7282
ERI/NRC 21-203

Review of Accident Tolerant Fuel Concepts with Implications to Severe Accident Progression and Radiological Releases

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ERI/NRC 21-204

Phenomena Identification Ranking Tables for Accident Tolerant Fuel Designs Applicable to Severe Accident Conditions

HBU/HALEU/ATF PIRT

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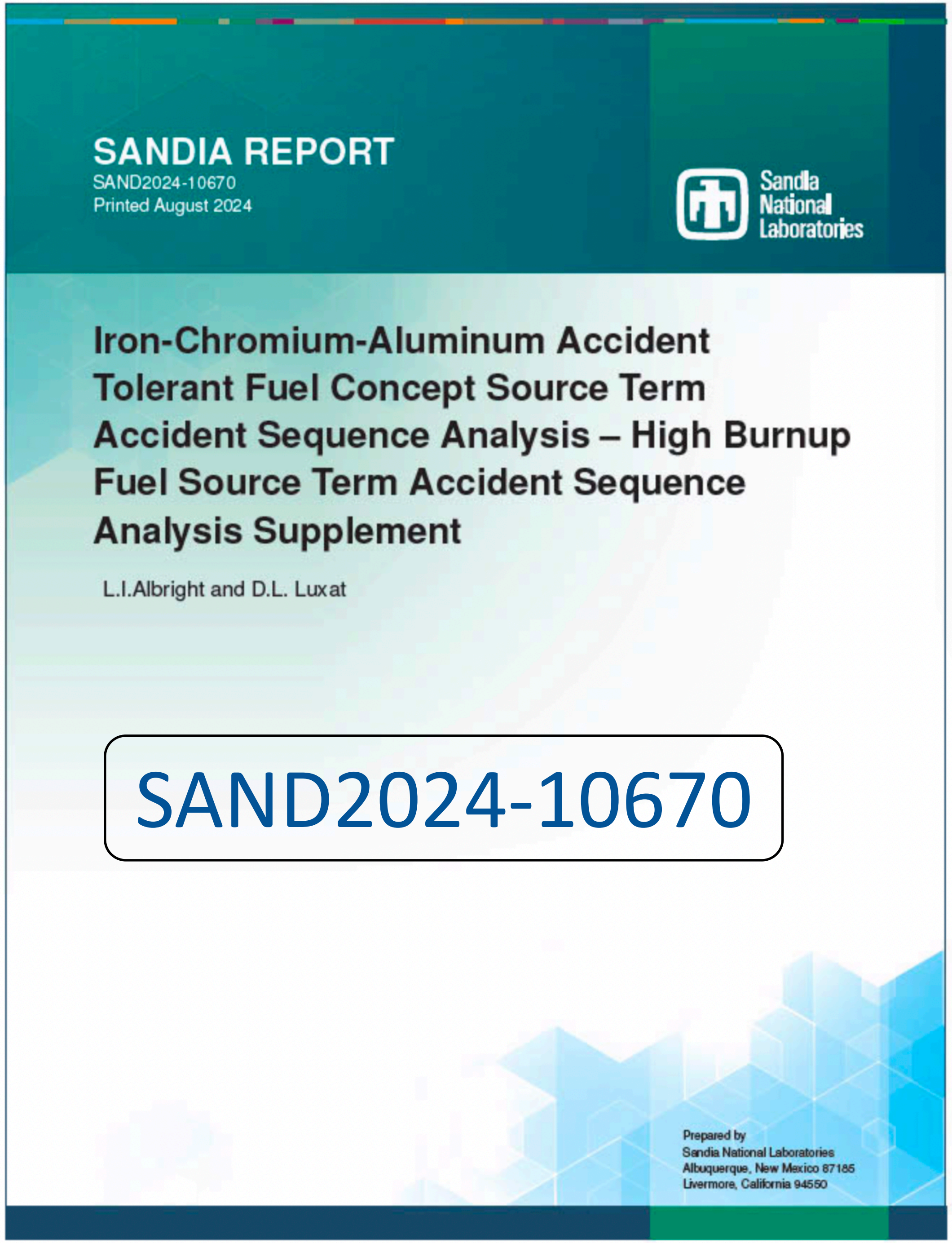
- **Cr-coated cladding severe accident behavior**
  - Behavior of oxidized cladding under severe accident conditions – *The protective Cr oxide does not survive to severe accident temperatures; underlying conventional zircaloy is exposed*
  - Alteration of the thermophysical properties of the fuel and cladding – *explored in SAND2023-01313*
  - Solid debris particle size and porosity – *explored in SAND2023-01313*
  - Formation of Hexavalent Cr – *Cr is a standard material in LWR structures (MELCOR assumes 20% Cr in steel structures). Thin Cr coatings change the Cr mass in the reactor by <1%*

Cr-Coated Source Term Summary (SAND2024-10673)

1. Results from this analysis are consistent with those reported in SAND2023-01313 demonstrating that alternative oxidation kinetics, do not significantly change accident source terms
2. Due to the similarity between conventional cladding and Cr-coated cladding identified in the ATF/HBU/HALEU PIRT (NUREG/CR-7283), in-pile experiments are not expected to identify new, significant primary drivers of in-containment source term (e.g., fuel failure mechanisms).
3. The source terms presented in SAND2023-01313 are considered applicable to Cr-coated cladding given the current state-of-knowledge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Iron-Chromium-Aluminum Accident Tolerant Fuel Concept Source Term Accident Sequence Analysis – High Burnup Fuel Source Term Accident Sequence Analysis Supplement

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SAND2024-10670

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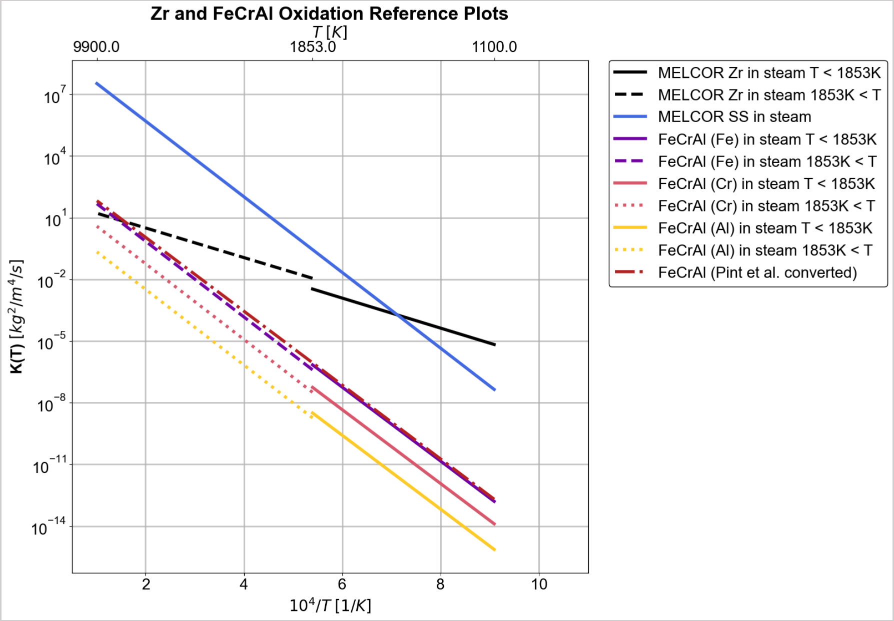
FeCrAl Accident Tolerant Fuel Source Term Analysis

- Develop alternative source term applicable to LWR cores with FeCrAl cladding
  - Substitution of Zr-based alloy with an FeCrAl alloy
  - Intended to reduce both oxidation in the core and associated hydrogen production
- FeCrAl analysis informed by ATF severe accident PIRT (NUREG/CR-7283) findings
  - Sensitivity analyses deployed to interrogate FeCrAl cladding knowledge uncertainties
- Extends SAND2023-01313 alternative source terms

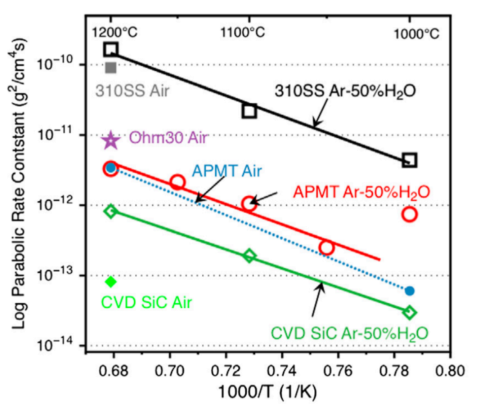
FeCrAl Cladding Modeling

- Assumed replacement of Zr-based cladding with FeCrAl (Fe:74, Cr: 21, Al:5)
  - Zr-based canister in BWR remained Zr-based
- Temperature based oxidation
- Assumed conventional Zr-based clad fuel failure
  - Default Fuel Rod Lifetime
  - Conventional Fuel Melting and Collapse Temperatures (2479K)



- FeCrAl oxidation rate and material properties are extrapolated from available data

Parameter	FeCrAl	FeCrAl-Oxide
Density [kg/m^3]	7100	5180
Solidus temperature [K]	1773	1901
Latent Heat of Fusion [J/kg]	270000	687463
Thermal Expansion Coefficient [1/K $\cdot$ cm^3]	3.1×10^{-5}	3.1×10^{-5}
Empirical Dynamic Viscosity Coefficients [1/K] and [Pa $\cdot$ s]	N/A	3313 and 1.076×10^{-3}



- Oxidation correlation is based on prior work by INL/ORNL (Pint et al.) – conversion from mass of oxygen consumed to mass of metal reacted

B.A.Pint,etat.,"HighTemperatureOxidationofFuelCladdingCandidateMaterialsinSteam-Hydrogen Environments,"JournalofNuclearMaterials440,pp.420-427,2013.

FeCrABWR Source Term

	Gap Release			Early In-vessel		
Report	2024 FeCrAl	2023 HBU/HALEU	NUREG-1465	2024 FeCrAl	2023 HBU/HALEU	NUREG-1465
Phase Duration [h]	0.84	0.70	0.5	6.1	6.7	1.5
Noble Gases	0.019	0.016	0.05	0.91	0.95	0.95
Halogens	0.007	0.005	0.05	0.65	0.71	0.25
Alkali Metals	0.006	0.005	0.05	0.37	0.32	0.20
Te Group	0.005	0.003	0.0	0.52	0.56	0.05
Ba/Sr Group	0.001	0.0006	0.0	0.009	0.005	0.02
Ru Group	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0	0.003	0.006	0.003
Mo Group	2×10^{-5}	2×10^{-5}	0.0	0.088	0.12	0.003
Lanthanides	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0002
Ce Group	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0005

- Gap release phase duration is slightly increased, but within 2023 HBU/HALEU study uncertainties
- Release fractions observed during the gap release phase are within 2023 HBU/HALEU study uncertainties
- Early in-vessel phase duration is decreased
- Smaller release fractions (compared to 2023 HBU/HALEU) are generally observed during the early in-vessel phase
- Larger release fractions observed during the early in-vessel phase are within 2023 HBU/HALEU study uncertainties (alkali metals) or smaller than NUREG-1465 (Ba/Sr Group)

FeCrAPWR Source Term

	Gap Release			Early In-vessel		
Report	2024 FeCrAl	2023 HBU/HALEU	NUREG-1465	2024 FeCrAl	2023 HBU/HALEU	NUREG-1465
Phase Duration [h]	1.4	1.3	0.5	4.4	4.0	1.3
Noble Gases	0.028	0.026	0.05	0.95	0.93	0.95
Halogens	0.007	0.007	0.05	0.6	0.58	0.35
Alkali Metals	0.003	0.003	0.05	0.52	0.50	0.25
Te Group	0.006	0.006	0.0	0.58	0.55	0.05
Ba/Sr Group	0.001	0.001	0.0	0.004	0.002	0.02
Ru Group	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0	0.008	0.008	0.003
Mo Group	$< 3 \times 10^{-5}$	$< 2 \times 10^{-5}$	0.0	0.17	0.15	0.003
Lanthanides	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0002
Ce Group	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0	$< 1 \times 10^{-6}$	$< 1 \times 10^{-6}$	0.0005

- Gap release phase duration is slightly increased, but within 2023 HBU/HALEU study uncertainties
- Release fractions observed during the gap release phase are within 2023 HBU/HALEU study uncertainties
- Early in-vessel phase duration is increased and within 2023 HBU/HALEU study uncertainties
- Smaller release fractions (compared to 2023 HBU/HALEU) are generally observed during the early in-vessel phase
- Larger release fractions observed during the early in-vessel phase are within 2023 HBU/HALEU study uncertainties (halogens, alkali metals, Te group, and Mo Group) or smaller than NUREG-1465 (Noble Gases and Ba/Sr Group)

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Review of Accident Tolerant Fuel Concepts with Implications to Severe Accident Progression and Radiological Releases

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Phenomena Identification Ranking Tables for Accident Tolerant Fuel Designs Applicable to Severe Accident Conditions

HBU/HALEU/ATF PIRT

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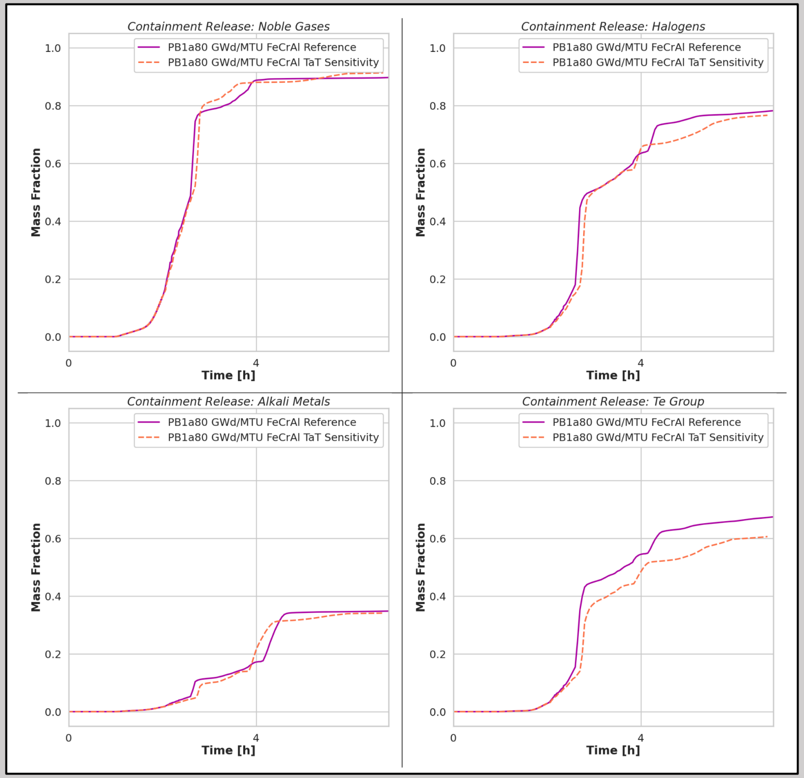
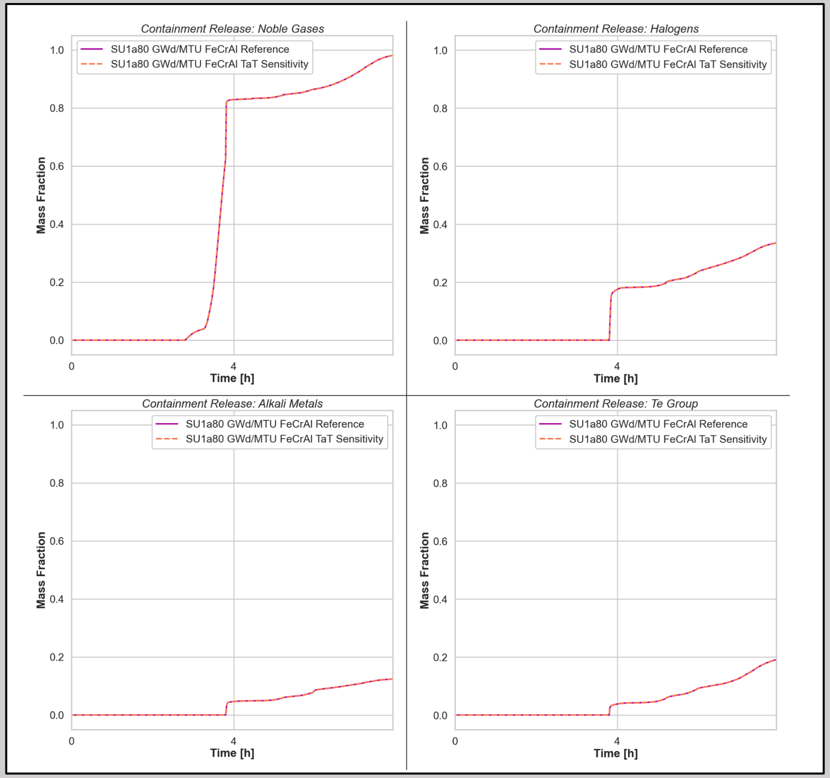
- **FeCrAl clad fuel severe accident behavior**
  - The present analysis focused on primary uncertainties impacting fission product releases from the fuel
    - Early Fuel Rod Failure – *Uncertainty explored through fuel relocation temperature and fuel rod lifetime sensitivity calculations*
    - Tellurium Retention – *Uncertainty explored through CORSOR-Booth class scaling sensitivity*
  - Other identified uncertainties
    - Foaming potential of FeCrAl Cladding
    - Formation of Hexavalent Chromium
    - Fission Product Speciation and Chemistry
    - Fission Product Retention and Revaporization

Fuel Rod Lifetime Sensitivity



Peach Bottom



Surry

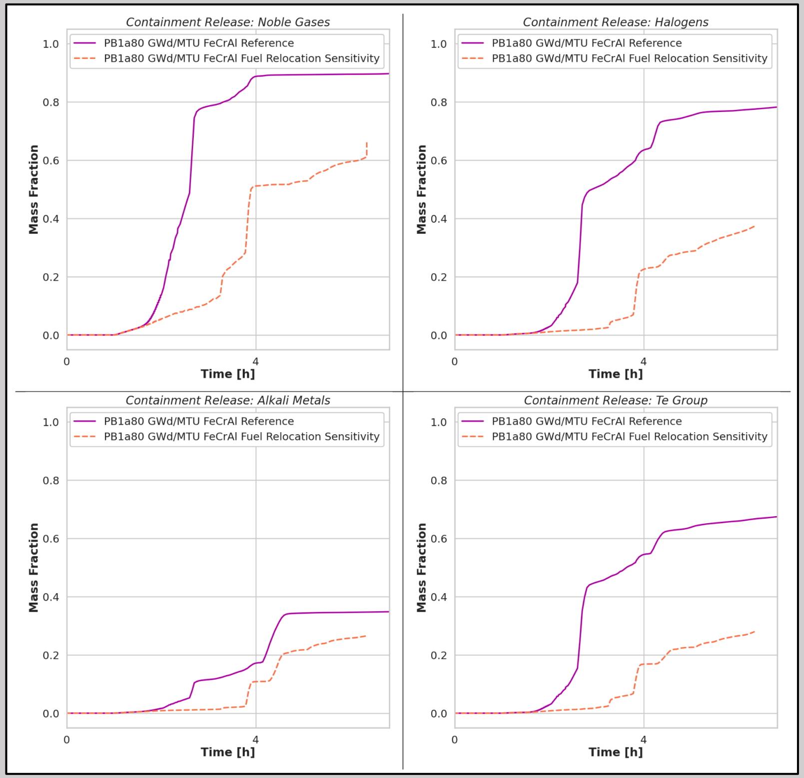
- Minimal variation is observed in the in-containment source term
- Early fuel failure by damage accrual models may reduce in-containment source terms
- Variations observed are small relative to the variability observed across the accident scenario set

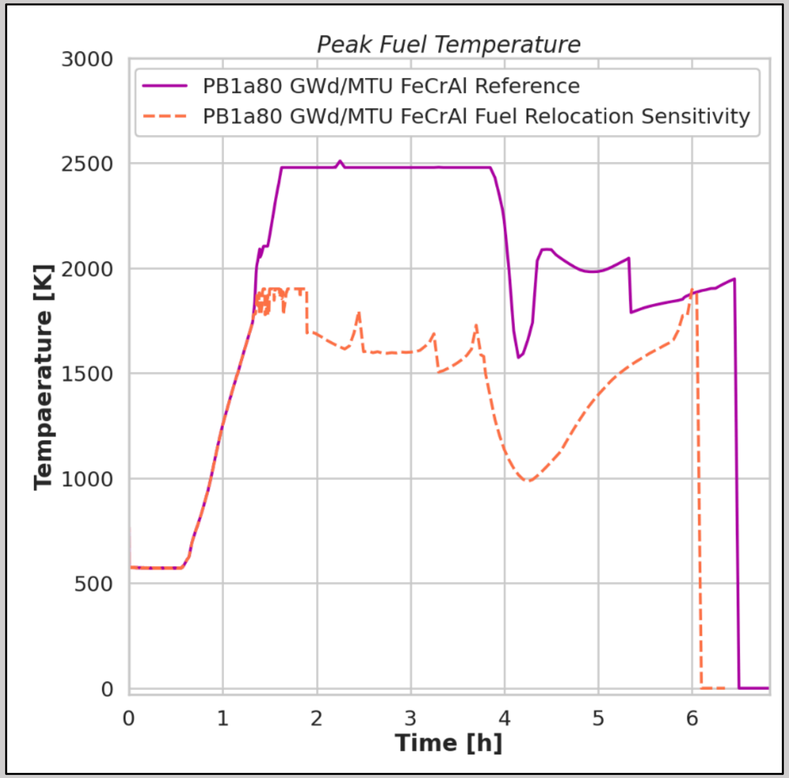
- Reference Fuel Rod Lifetime – default time-at-temperature model
  - Assumes damage accrual is similar to conventional fuels
- Reduced Fuel Rod Lifetime – shorter tabulated fuel rod lifetimes
  - Assumes accelerated damage accrual and shorter time to failure at high temperatures

Temperature [K]	Lifetime [s]
<2090	Infinite
2100	6000
2500	600
2600	200

Reduced Tabular Fuel Rod Lifetime

Fuel Relocation Temperature Sensitivity



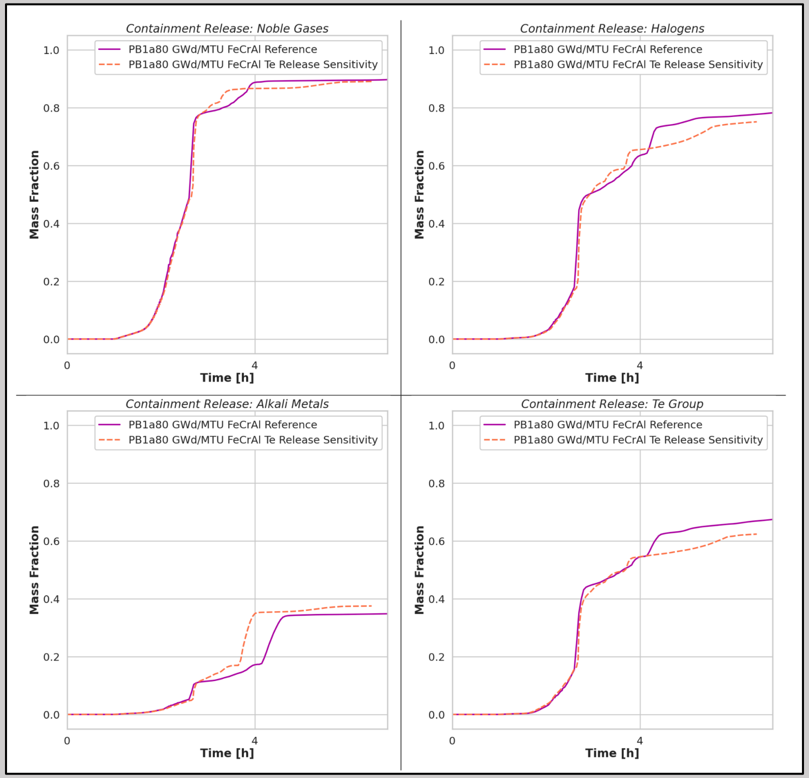


Peach Bottom

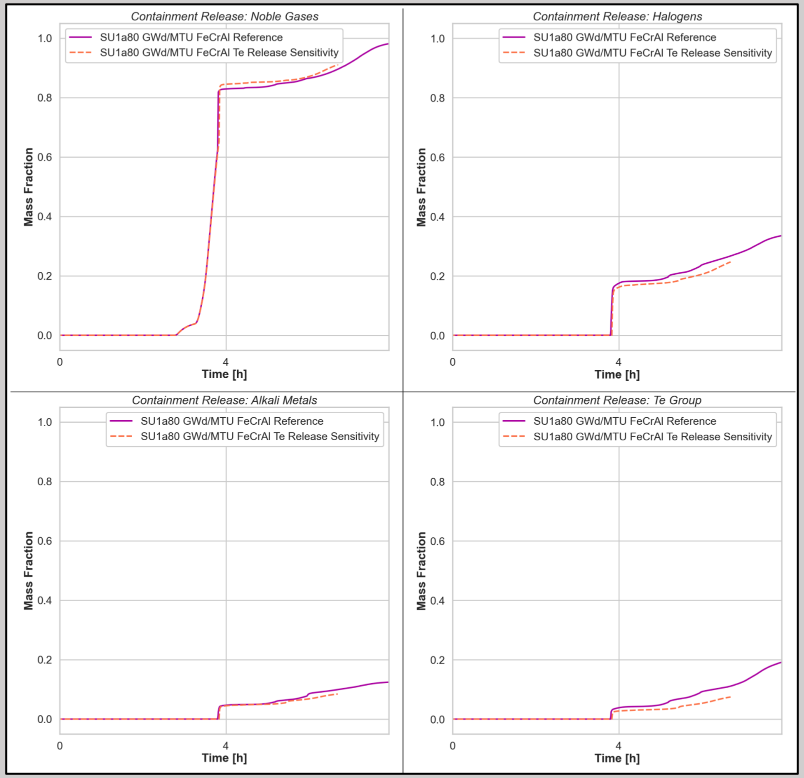
- Reference Fuel Relocation Temperature – 2479K
  - Assumes fuel collapse and melting is similar to conventional fuels
- Reduced fuel relocation temperature – 1901K
  - Assumes fuel collapse and melting occurs at lower temperatures near the constituent material melting points

- Reduced fuel relocation temperatures are strongly correlated to smaller in-containment source terms for each radionuclide class considered in the present analysis
- Simulations that assume higher fuel relocation temperatures are observed to be conservative and bounding – SAND2023-01313 in-containment source terms is applicable to FeCrAl clad fuel.

Te Release Sensitivity



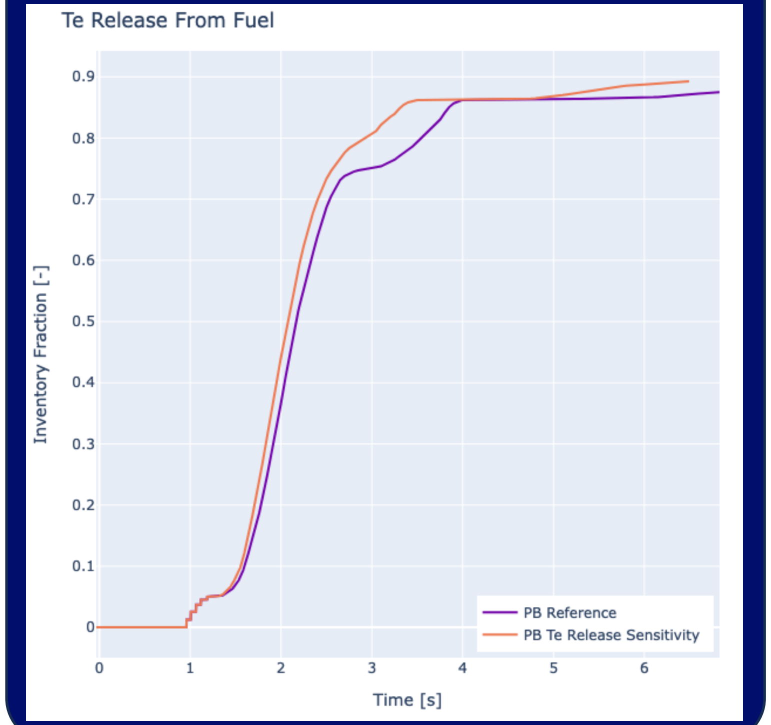
Peach Bottom



Surry

- Reference Te Release Rate – Default CORSOR-BOOTH class scaling
  - Te release rate is approximately 2/3 the Cs release rate
- Enhanced Te Release Rate – Increased Te CORSOR-Booth class scaling
  - Te releases commensurate to Cs

- Enhanced Te release rates exhibit minimal impact on the in-containment source term due to rapid release from the fuel during core heatup by nature of the unmitigated scenarios.



FeCrAl Source Term Summary (SAND2024-10670)

1. Results from this analysis are consistent with those reported in SAND2023-01313 demonstrating that alternative oxidation kinetics in FeCrAl, do not significantly change accident source terms
2. FeCrAl clad fuel is expected to exhibit earlier melt formation and loss of rod-like geometry relative to conventional clad fuels, which could reduce the in-containment source term based on the present analysis
   - The ATF/HBU/HALEU PIRT (NUREG/CR-7283) identifies differences between conventional cladding and FeCrAl cladding that may require in-pile experiments to reduce uncertainties
3. The source terms presented in SAND2023-01313 are considered applicable to FeCrAl cladding given the current state-of-knowledge

Thank you for your attention!

MELCOR