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Application to GEMS-HERACLES Database to MELCOR COR Degradation

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MELCOR vs. GEMS

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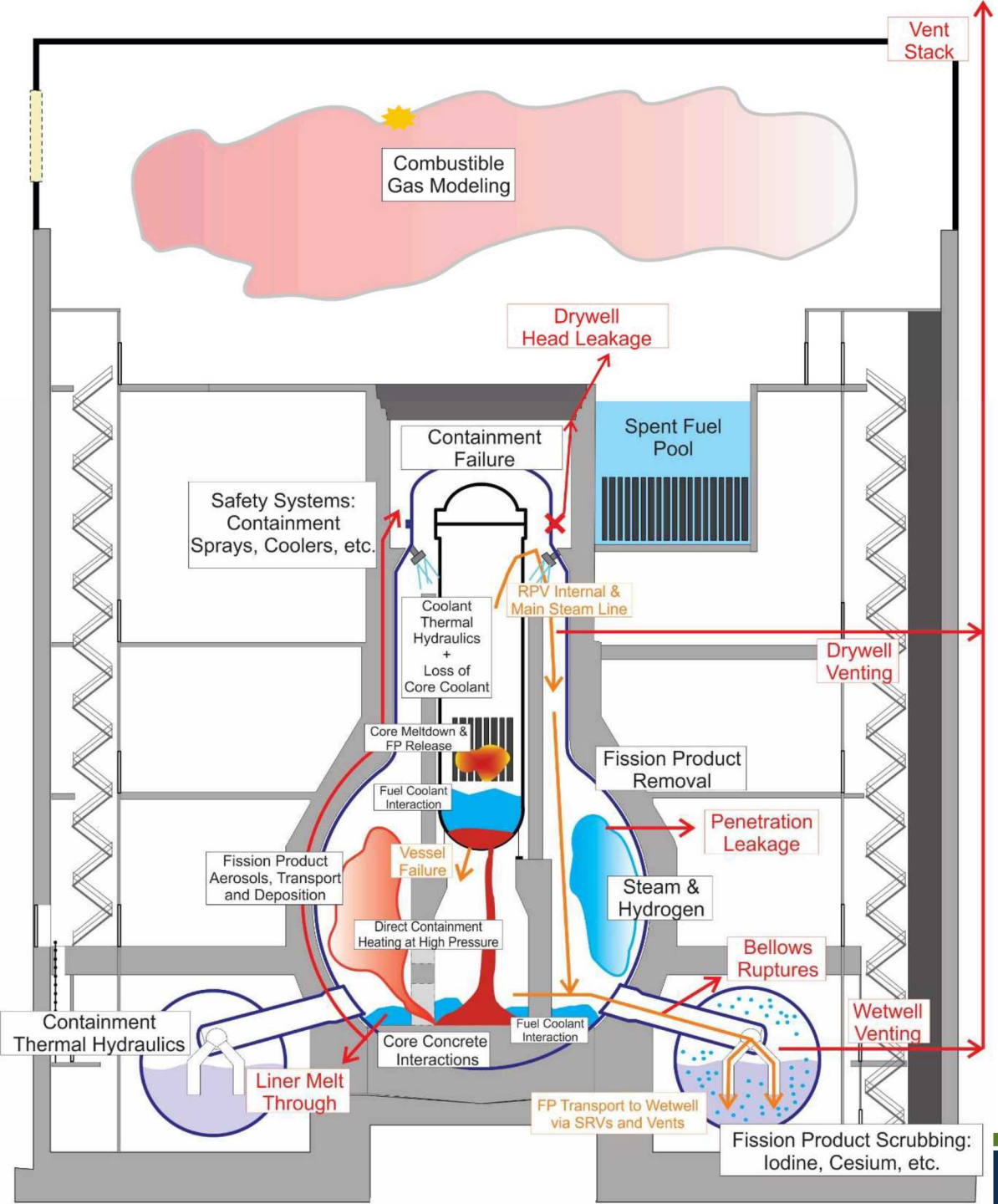
MELCOR

- Developed by SNL for NRC
- Lumped Parameter Code
- Significant number of physics packages
  - Core Degradation
  - Thermal-hydraulics
  - Materials
  - Fission Products
  - Key Systems

GEMS

- Developed by Paul Scherrer Institute
- Gibbs Energy Minimization Code
- Developed for geosciences
- Adapted for high temperature actinides
  - Part of PSI HERACLES Project
  - Focus of reprocessing



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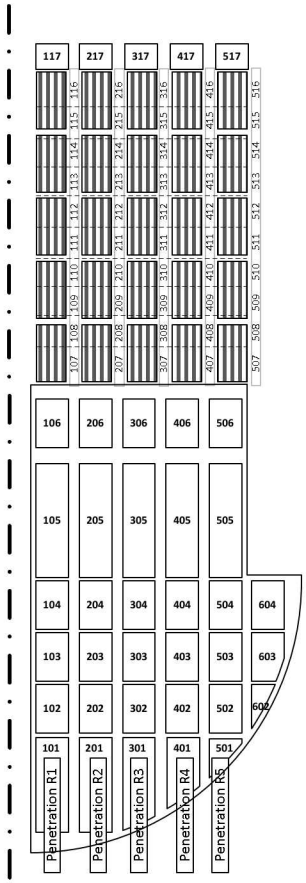
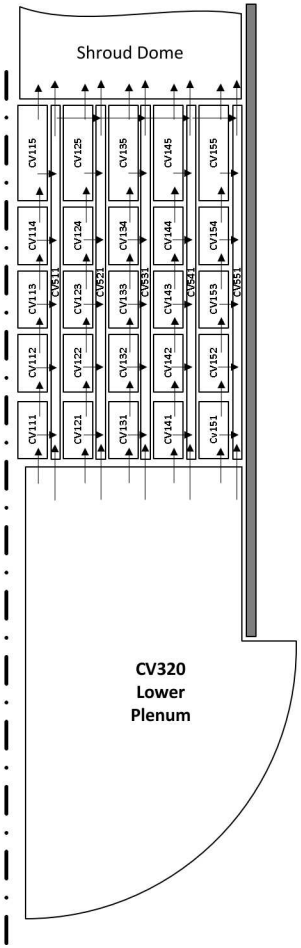
- **Reactor, Containment, Building, Venting Systems, Spent Fuel Pools**
- **Core Degradation and Severe Accident Phenomenology**
- **Operator Actions and Decisions**
- **Leakage Pathways and Component Failures**
- **Engineered Safety Features**
- **Fission Product Modeling**
- **Release and Source Terms**

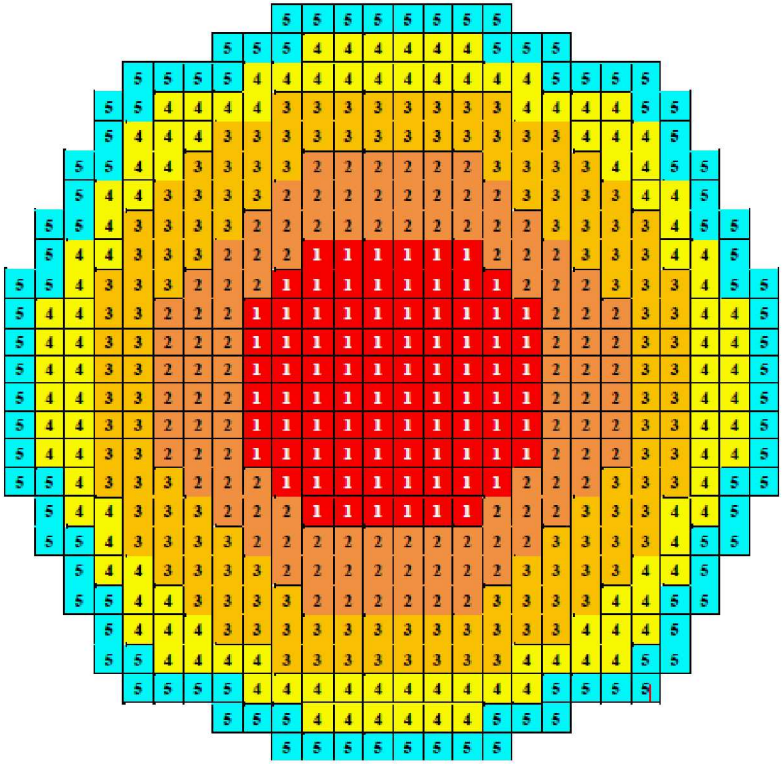
Why the comparison?

- Starting point for the eutectics model in MELCOR
- Validate the codes against one another
- Highlight key FP species that may exist but are not captured in the MELCOR framework
- Inform the thermodynamic community of key information that is needed in system-level codes such as MELCOR
- Inform the decommissioning authorities in Japan the potential species that may exist within the fuel debris
  - Cutting tools
  - FP disposition methods
  - Scrubbing of surfaces

MELCOR Core Abstraction

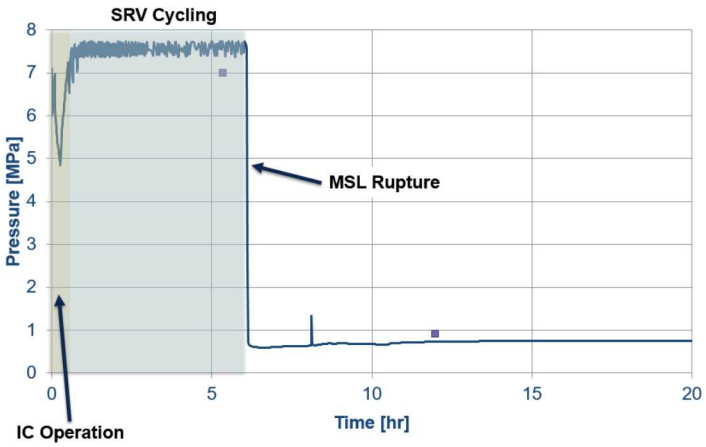


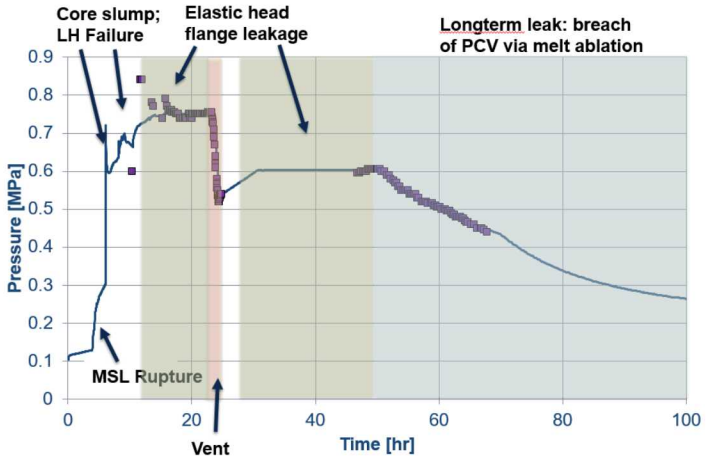




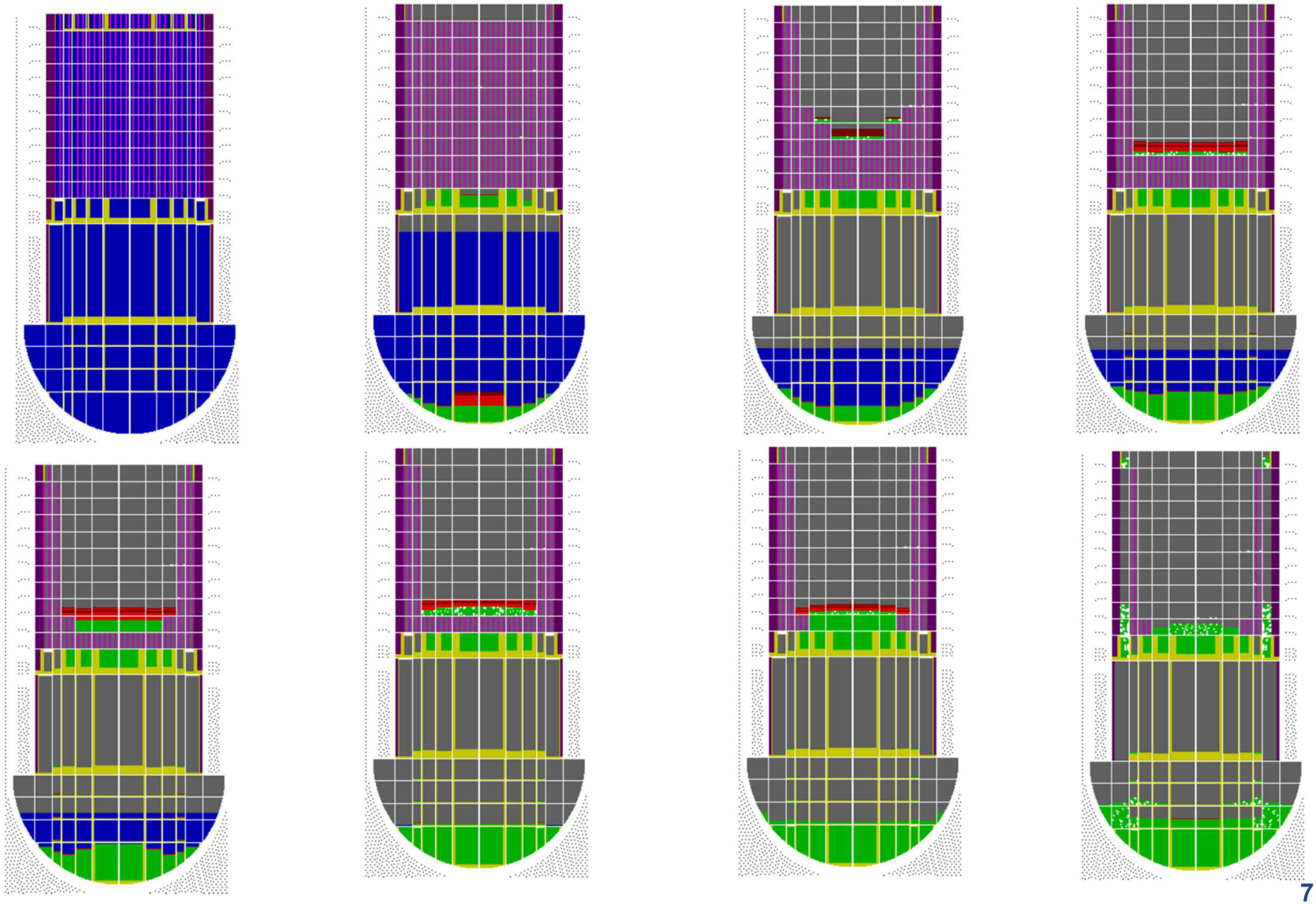
Comparison Study Parameters

- Performed a 1F1 MELCOR calculation with the deck developed for the OECD/NEA BSAF Phase II Study
  - Based on 3-week long calculations
  - However, minimal user-defined boundary conditions and sensitivity coefficients
- Compiled compositions predicted by MELCOR during the accident
  - Key elements
  - Phenomenological representations - Particulate Debris, Intact Fuel, Molten Pool
- Used the elemental compositions to serve as a input to GEMS-HERACLES
  - Returned elemental species that likely exist with given temperature and elements

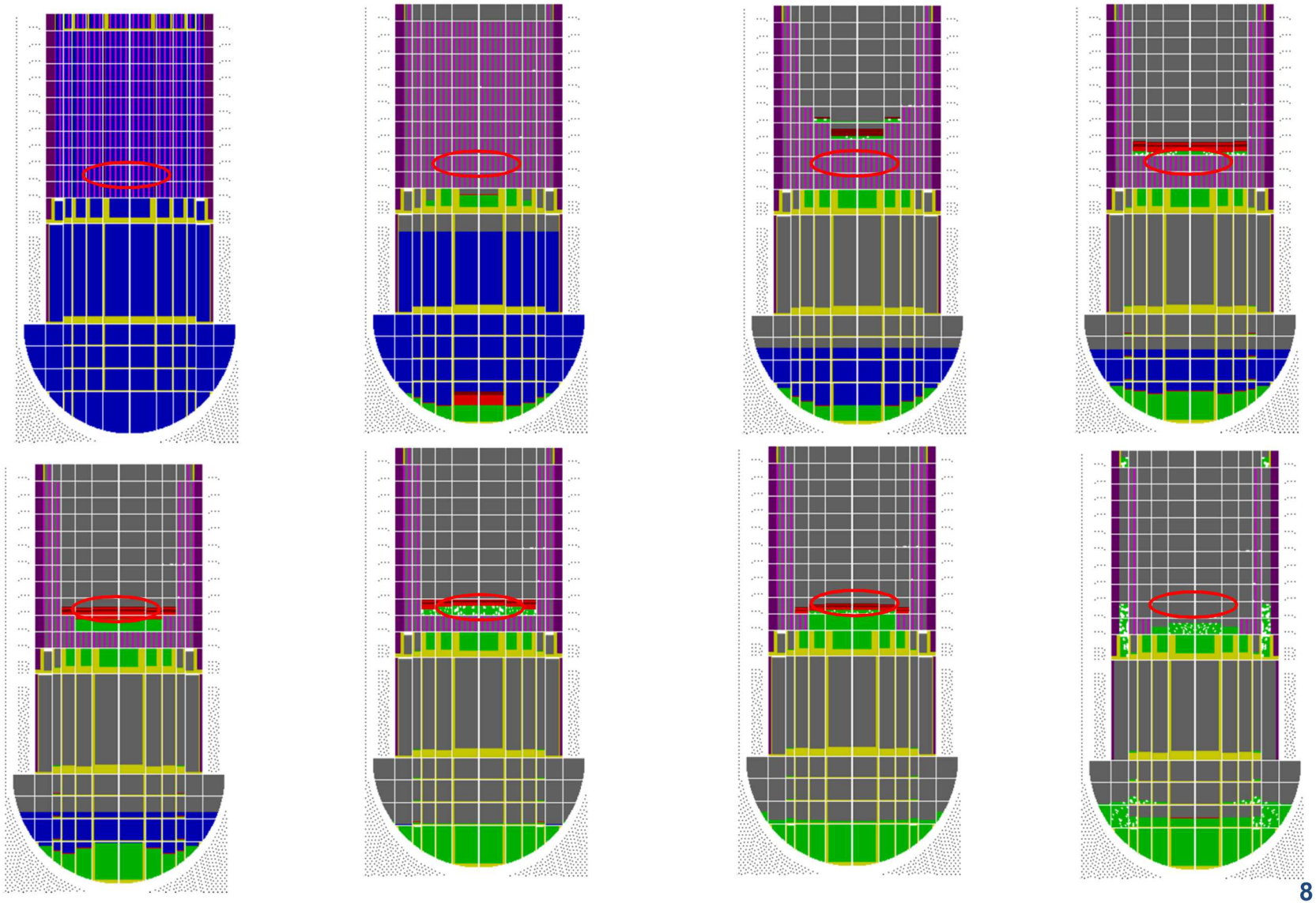




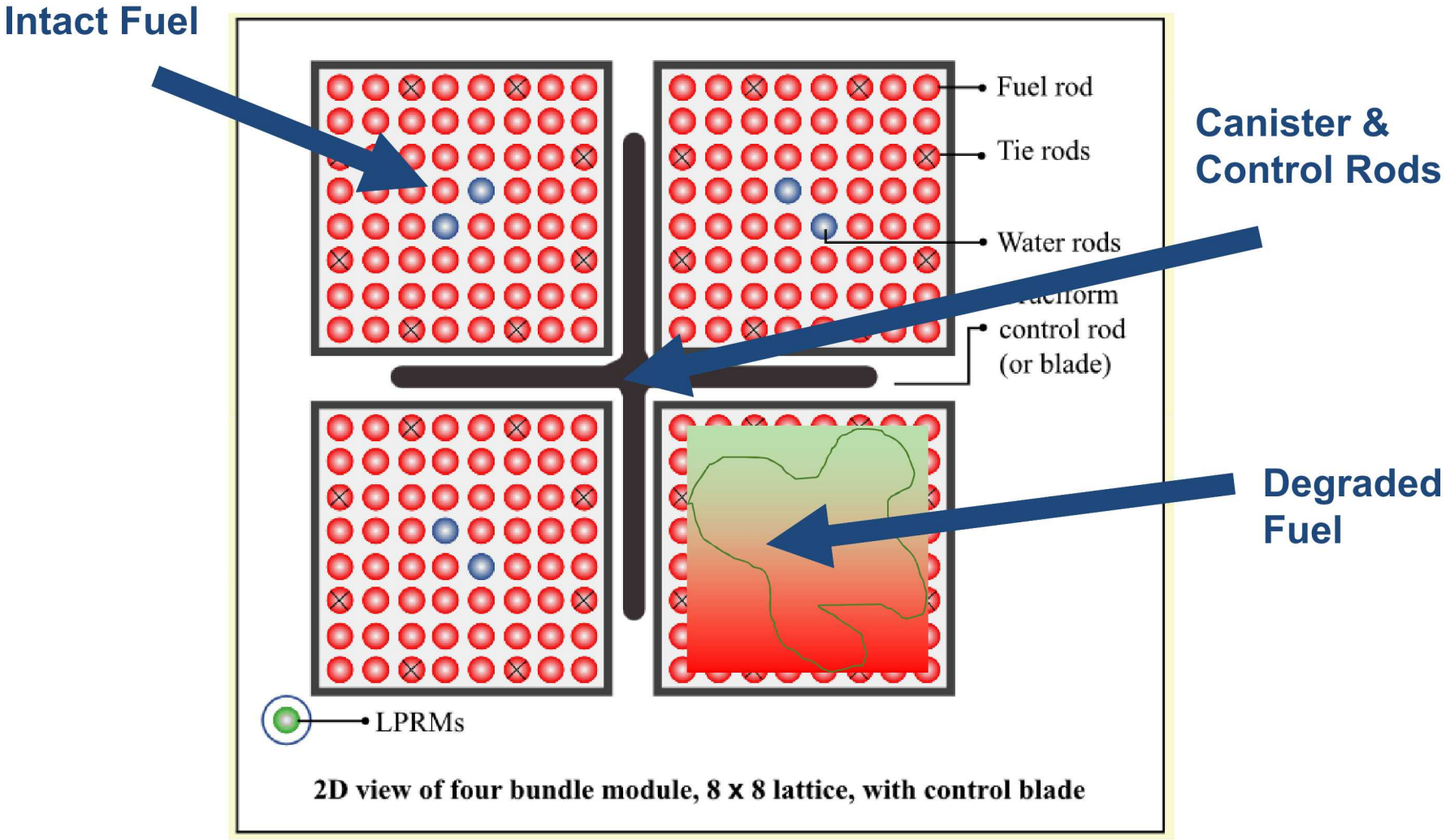
MELCOR Core Degradation Process – 1F1



MELCOR Core Degradation Process – 1F1



Core Cell Temperature



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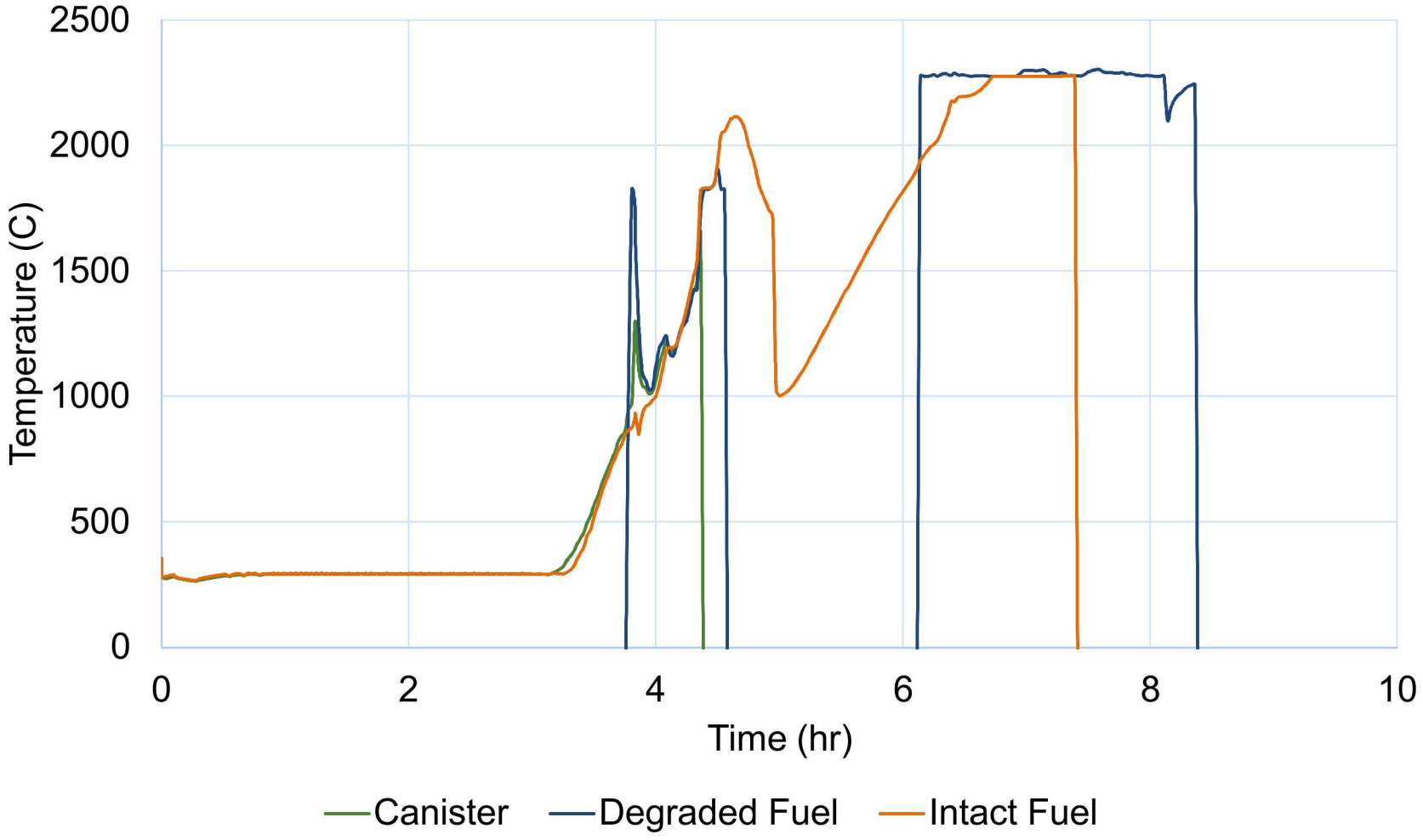
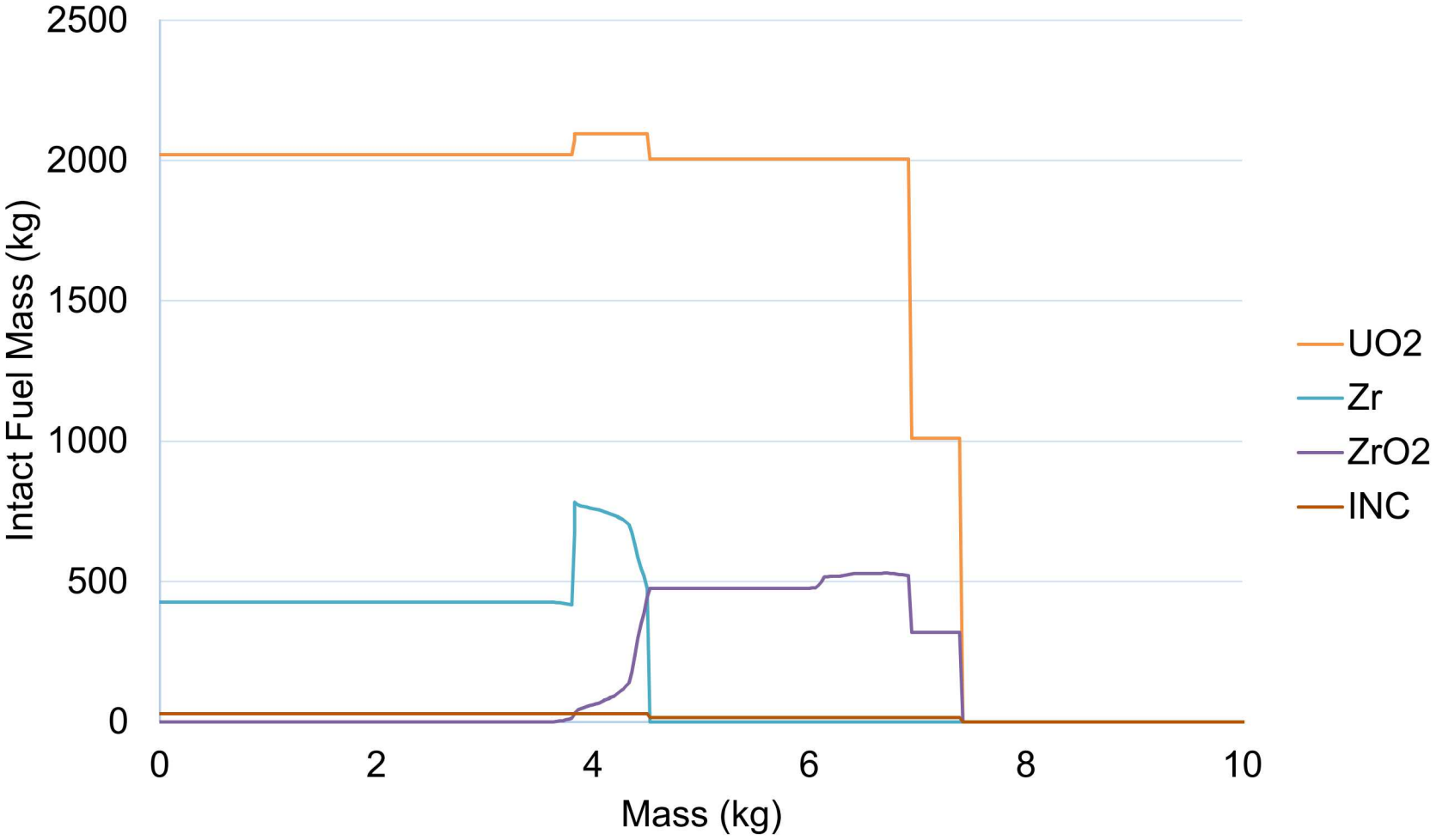
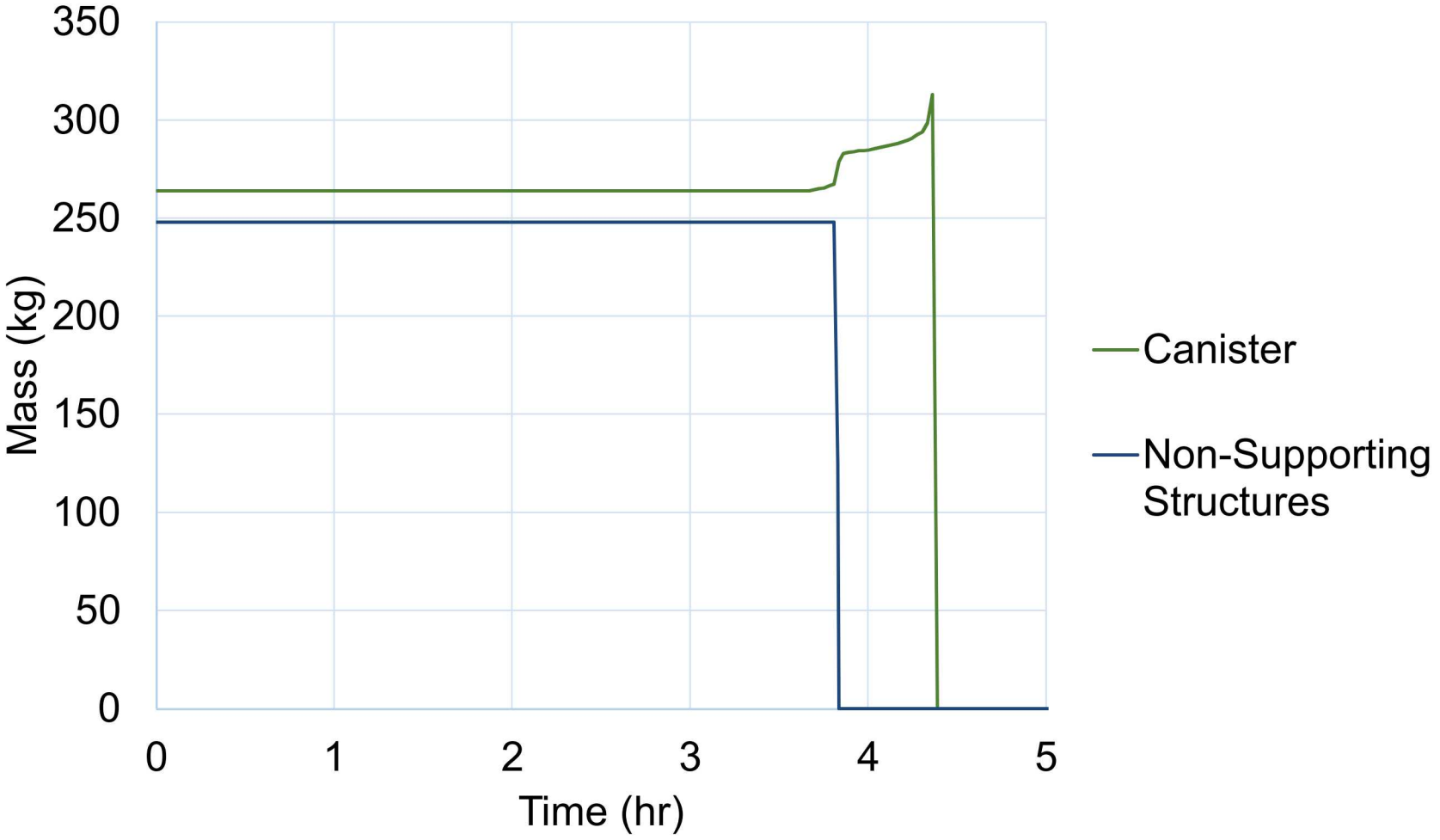


Core Cell Composition - Intact



Core Cell Compositions: Canister



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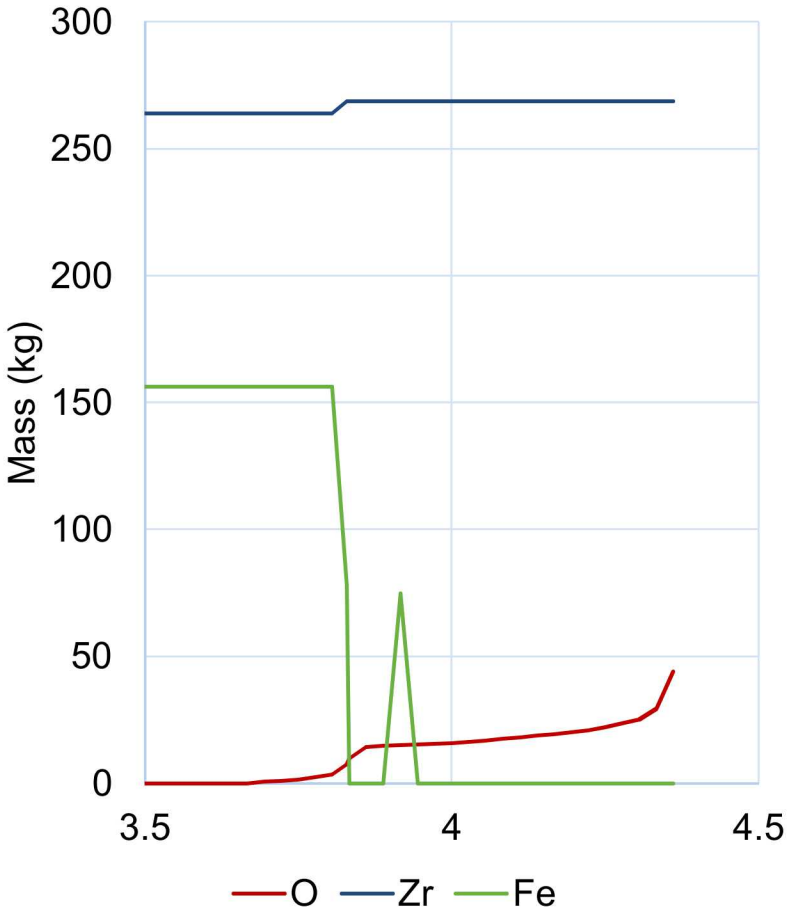
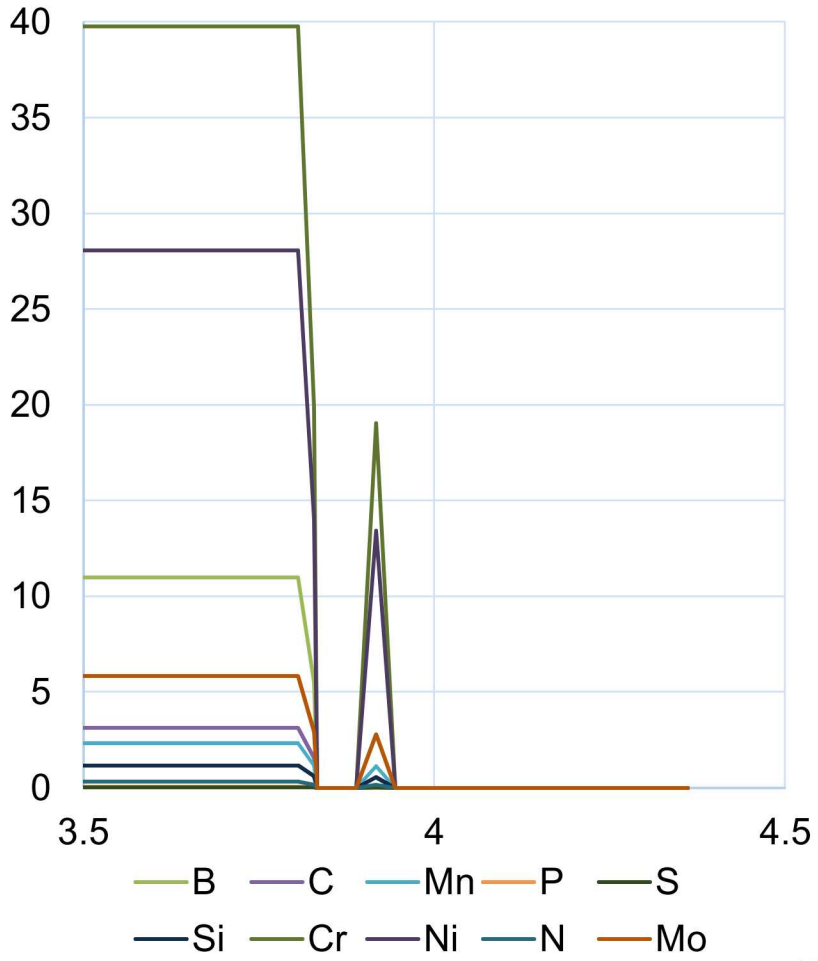
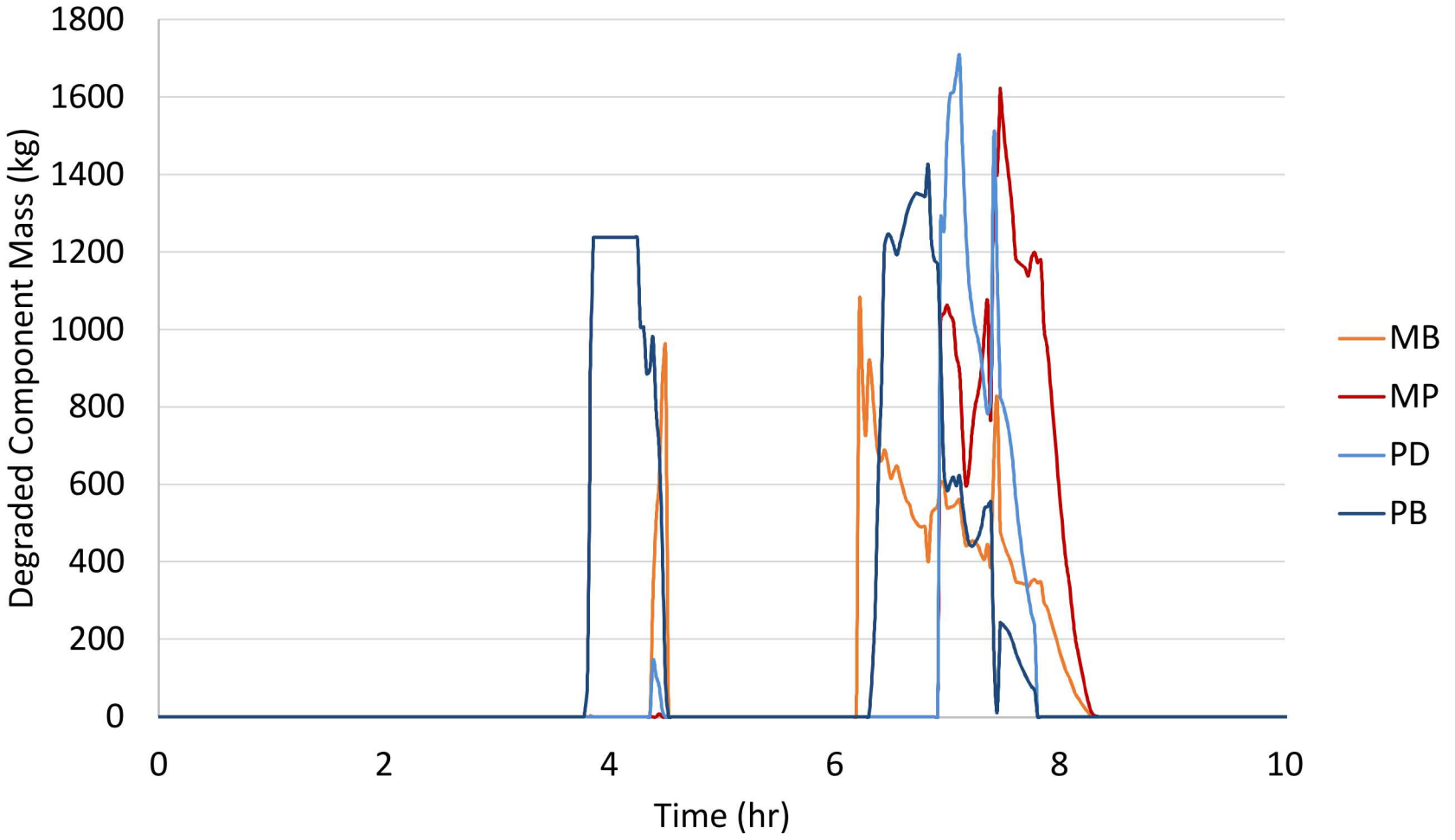
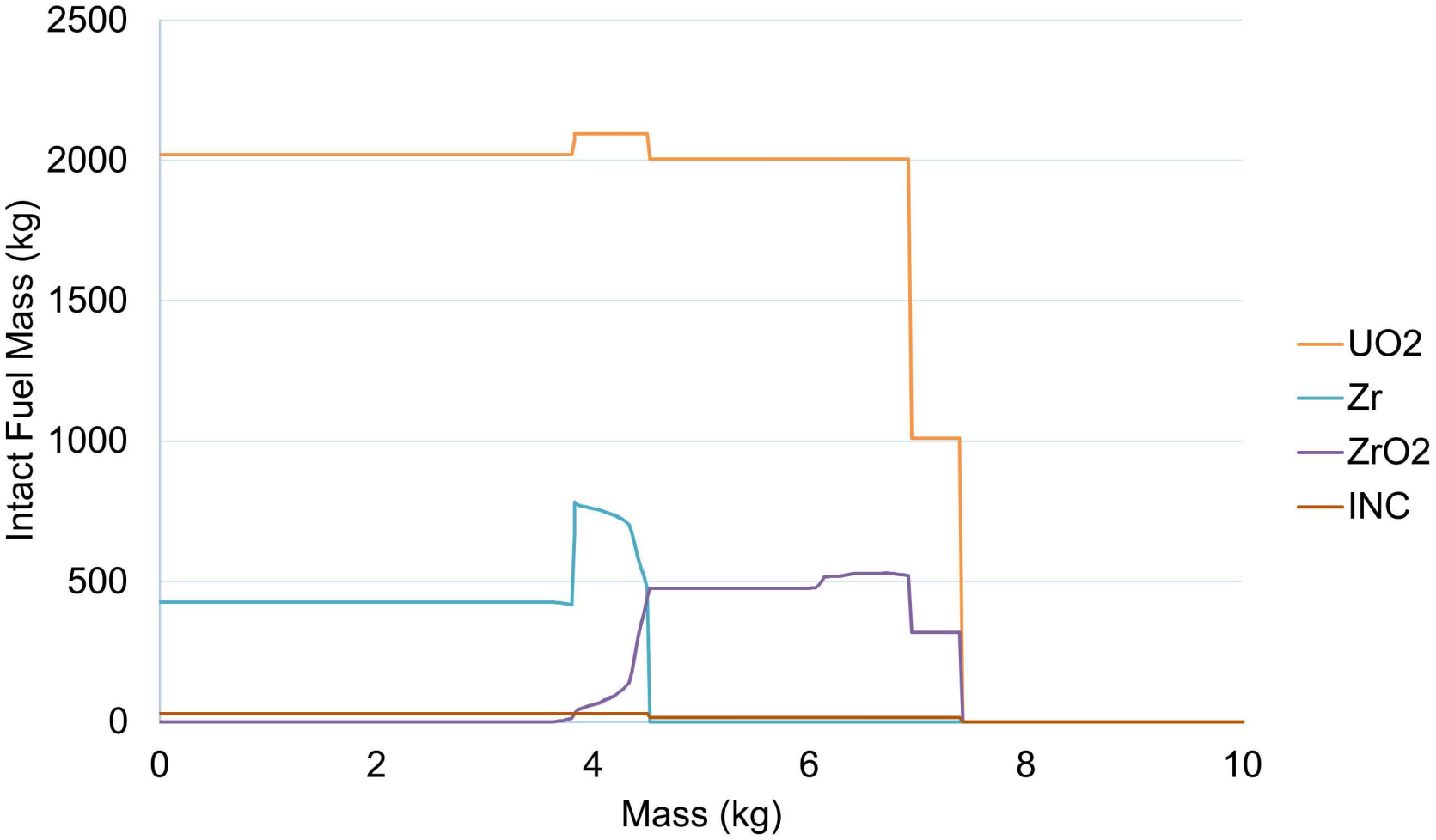




Degraded Material Composition



Core Cell Composition - Intact



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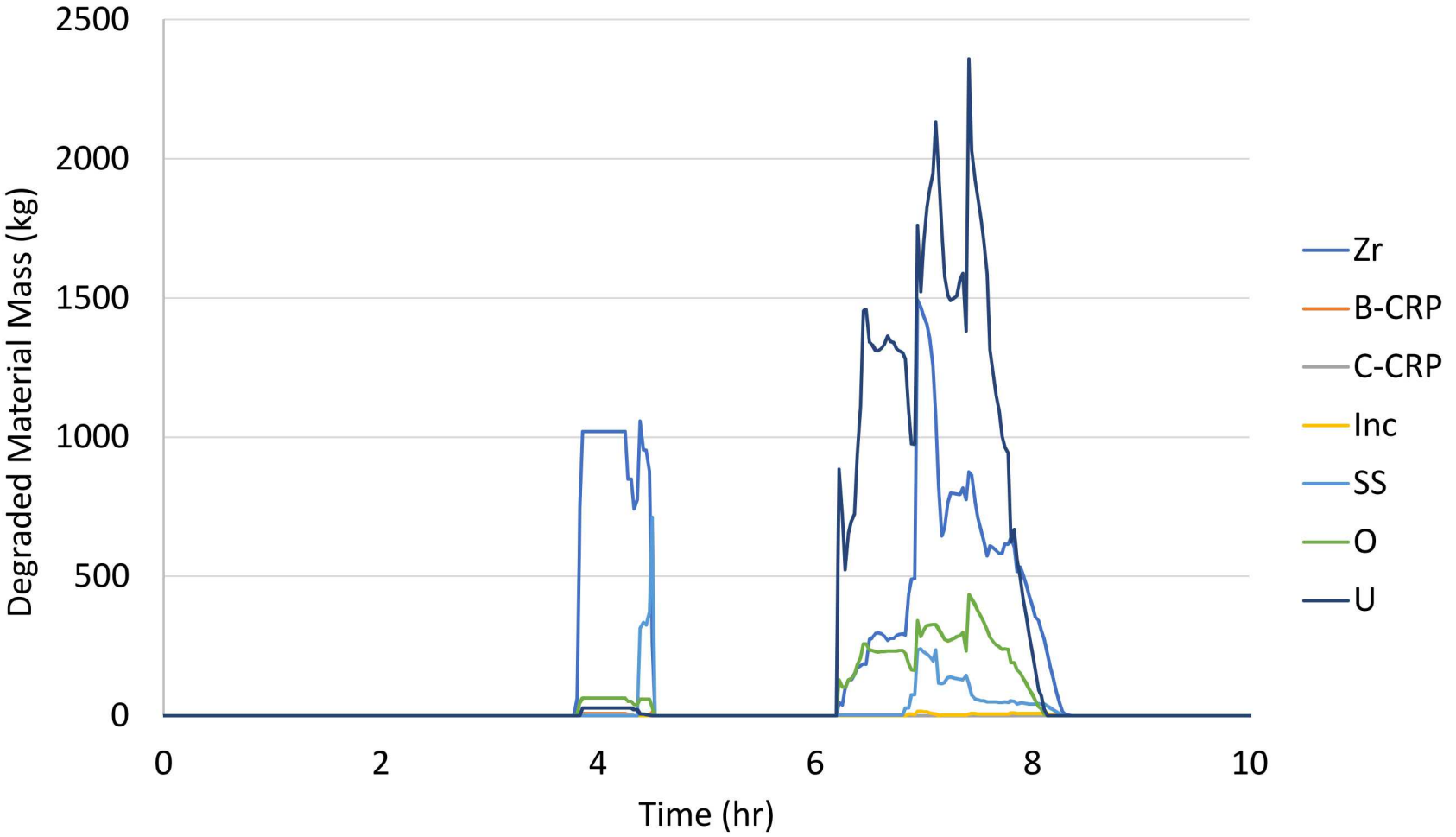
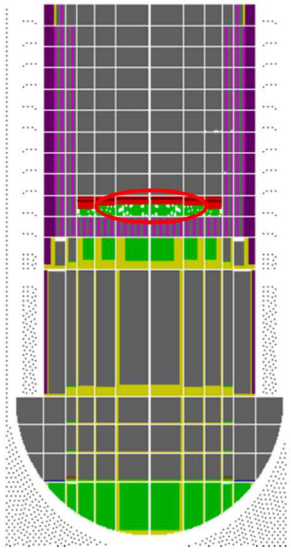


COMPARISON OF DEGRADED MATERIALS TO GEMS

GEMS-HERACLES Analyses Performed

- Degraded material comparison
  - Imported elements predicted by MELCOR
  - Added representative FPs
    - Bases on MELCOR RN classes
  - Returned key speciation information
  - Gas generation was predicted in all cases
    - CsI and other volatile FPs predicted to leave system
- Impact of additional elemental species
  - Added key elements neglected in 1st pass
  - Demonstrate the number of additional species that need to be tracked as all elements are taken into account
- Solidified material prediction
  - Took the predicted MELCOR comparison and lowered the temperature to 50 C
  - First level of insight into what may be there during decommissioning

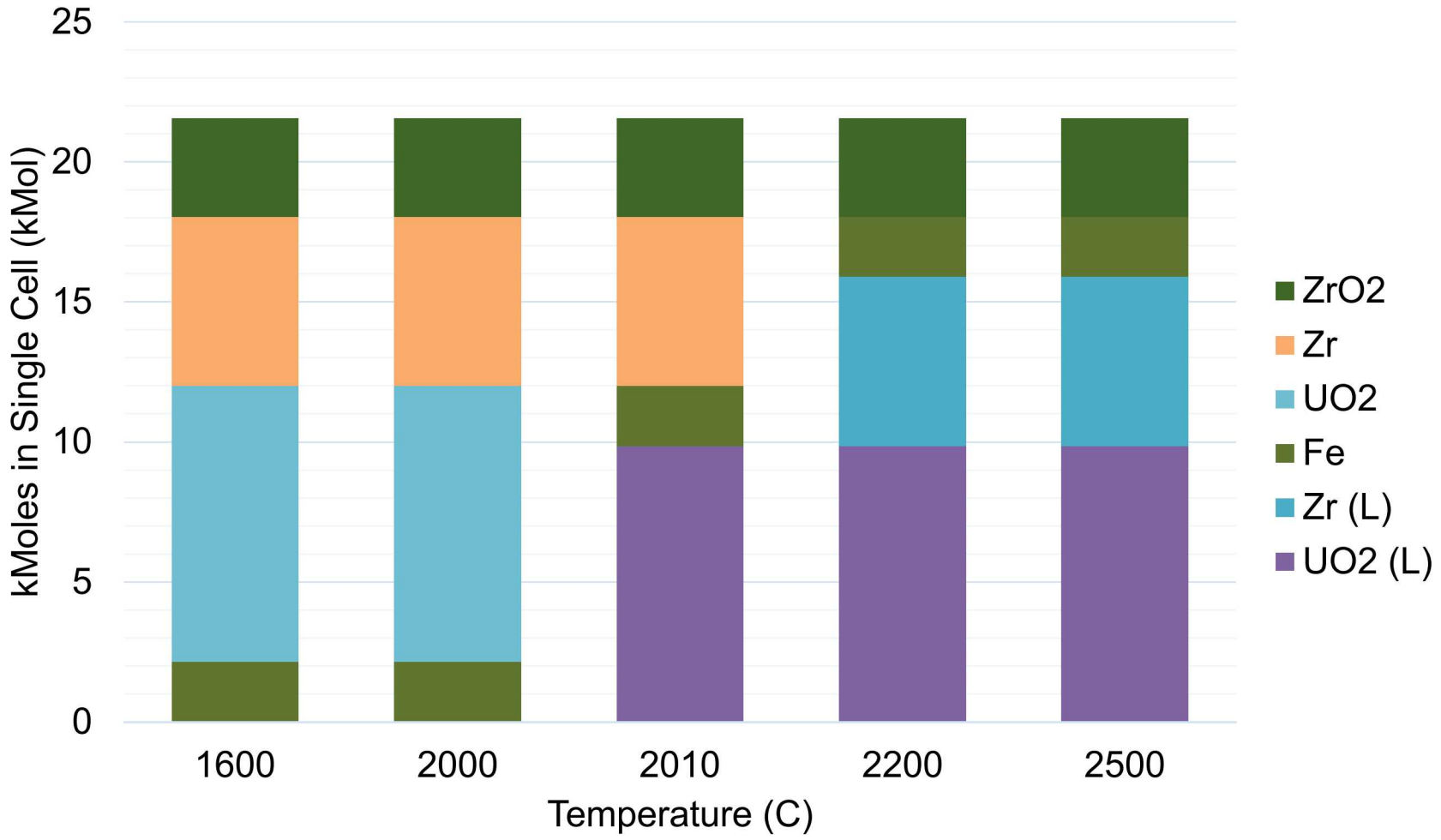
GEMS Input Parameters



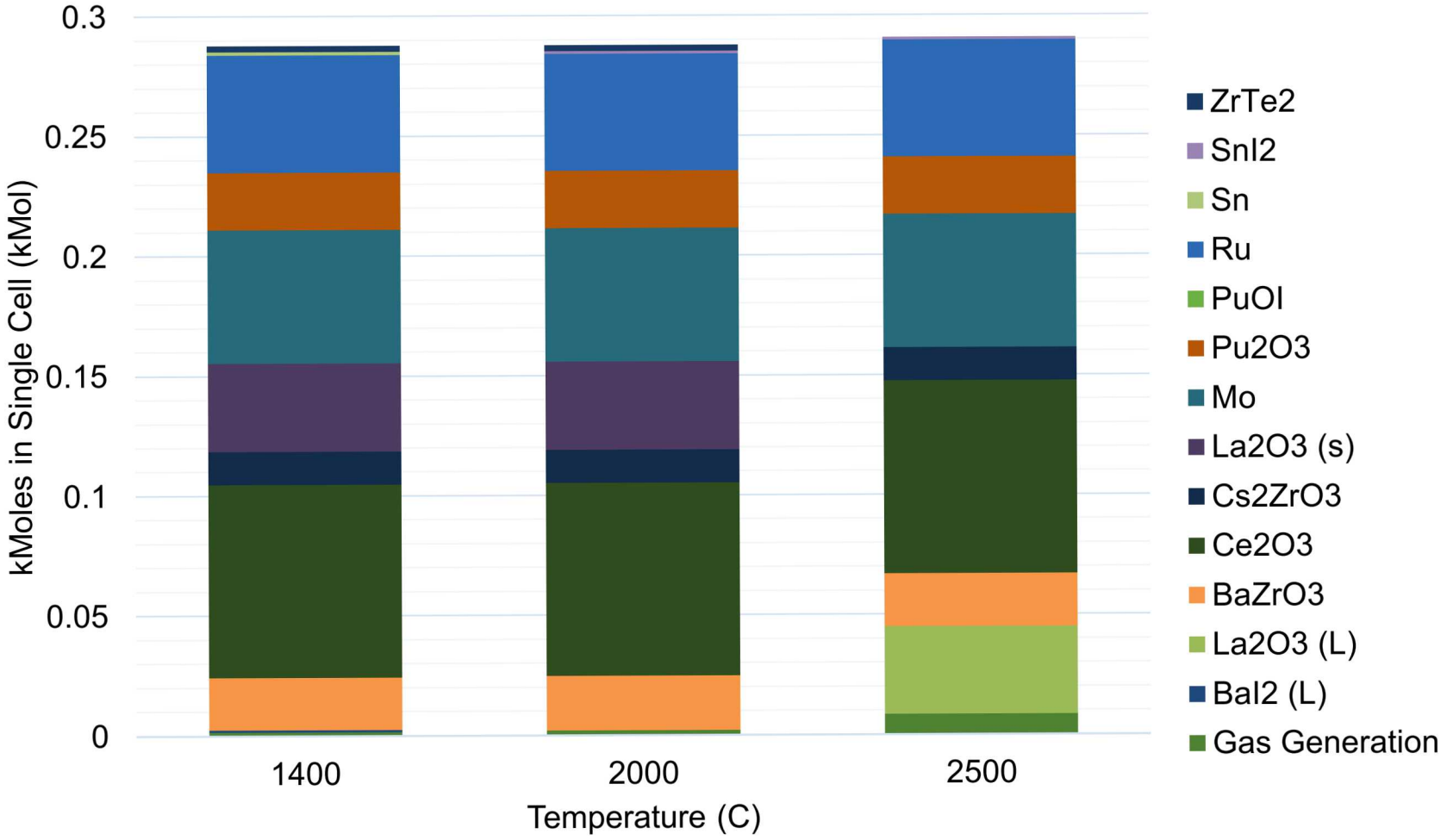
Element	Moles
Ba	22.9
Cd	1.5
Ce	160.9
Cs	27.9
Fe	2148.8
I	2.2
La	73.4
Mo	55.6
O	27299.4
Pu	47.9
Ru	48.9
Sn	1.4
Te	5.5
U	9860.1
Zr	9602.7

- Obtained input elemental compositions for degraded fuel geometry from (Ring 1, Level 2)
- Examined several different temperatures
  - 1000 – 2500 C
- FP compositions are informed by inventory calculation performed for 1F1 analysis
- Key differences
  - UO2 transition from solid to liquid
  - No models for molten Fe
  - Not all elements/species are accounted for (Cr, Ni, B, etc.)

Phase Description of Degraded Materials – Major Constituents



Phase Description of Degraded Materials – Minor Constituents



Impact of Minor Elements

- Presence of a small amount of minor elements can drastically impact chemistry for decommissioning
  - Impurities in structural materials
  - Non-radioactive fission products
- Elements of interest
  - Si, C, Sb, Sn, Ce, Nb, Mn, P, S, minor actinides, etc.
- Not modeled in MELCOR, since any impacts of these elements can be accounted for by altering bulk properties of structures
- Including the above elements of interest in the previous equilibrium calculation results in:
  - NbO2, Si, CeB6, MnO, Sn, SnI2, UC, UP, Usb, ZrN, ZrS2
  - Would be additional species if treatment of Fe, Ni and Cr were more robust

Re-solidified Molten Debris

Species	kMol	Species	kMol
Cd(l)	0.001468	NbO2	0.01
BaZrO3	0.022865	Pu2O3	0.023969
CeB6	0.066667	Ru	0.048877
Ce2O3	0.042098	Si	0.1
CeS	0.01	Sn	0.01
CsI	0.002232	U	5.877658
Cs2Te	0.005	UC	0.1
Cs2ZrO3	0.007844	UO2	3.872442
Fe	2.148805	USb	0.01
La2O3	0.036714	ZrN	0.01
MnO	0.01	ZrO2	9.562027
Mo	0.055561		

- Physical composition of degraded molten fuel
  - MELCOR molten pool and particulate debris
  - Cooled from ~2000 C to 50 C
- Decommissioning authorities are unsure of the composition of solidified molten debris
- MELCOR can inform the final location of the debris
- Thermodynamic database can then be used to determine the final end state of the debris and physical characteristics

What MELCOR Needs

- Information on key eutectic pairs not currently examined in MELCOR
  - Ni, Cr, Al, Fe
- Simple representations for ternary systems
  - U-ZR-O
  - Fe-Cr-Ni
  - B-C-Fe
- Fission product retention under MCCI conditions
  - Species of FPs is not well characterized in MELCOR for MCCI
- Core degradation insight
  - Breakdown between molten components and solid components during degradation

QUESTIONS OR COMMENTS?