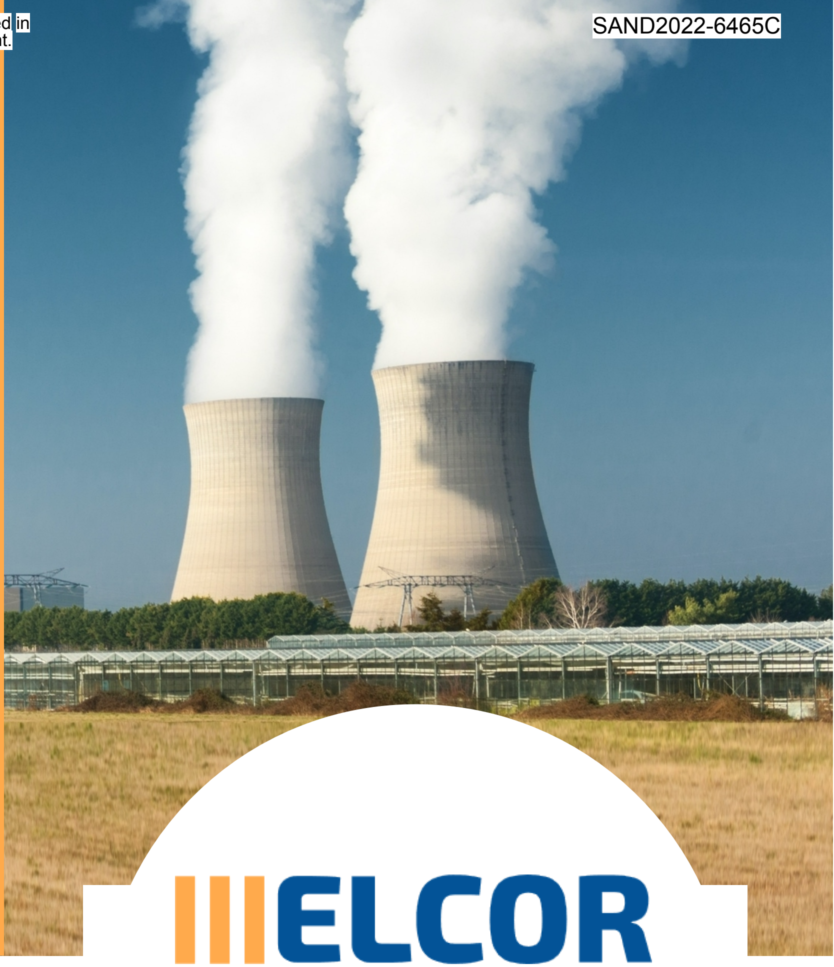
SAND2022-6465C

Sandia National Laboratories

Securing the future of Nuclear Energy



MELCOR

MELCOR Integrated Severe Accident Code Demonstration and Sensitivity Study of FHR Accident Progression

K.C. Wagner, T. Haskin, B. Beeny, F. Gelbard, and D.L. Luxat
Nuclear Energy Safety Modeling and Analysis (8852)

U.S. DEPARTMENT OF ENERGY NNSA

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Collaborations
Advancing Frontier of Nuclear Safety

ELCOR

Safety Analysis Capabilities

Naval Reactors (US & UK)

Canada
- CNSC/CNL advanced reactors
- First Nations Power Authority

Exploring collaboration with GCR Campaign (INL)

Exploring collaboration with MCRE source term needs (INL)

Advanced Reactor vendors (e.g., X-energy, TerraPower, General Atomics, Oklo)

Fusion system safety analysis (INL)

Neutronic analysis (ORNL)

Fission product transmutation (ORNL)
- Applicable to safeguards and material accounting

Multi-Scale Bridging

NEAMS (MOOSE)
- Thermochemistry (INL including Ontario Tech)
- Interfacial transport phenomena (ANL, INL)
- Multi-phase transport phenomena (ANL, INL)
- Advanced fuel performance? (INL)

Atomistic modeling
- Molten salt fission product thermochemistry (ORNL, PNNL)
- Digital twins and risk monitoring for advanced reactors (INL, ORNL, PNNL)

Safety Margin Resolution (MOOSE)
- Accident transient multi-scale bridging (INL)

Regulatory Risk Reduction

Molten salt LSTL benchmarking (ORNL)

Molten Salt and Sodium test loop benchmarking (UW-Madison)

NEAMS Source Term (ANL)

MSR Campaign Source Term/Species Transport (INL)

Regulatory LWR source term margin recovery (INL)

Accident Tolerant Fuel licensing (INL/UW-Madison)

Passive safety analysis/risk assessment methodology

Safety in autonomy (5500)

Risk-informed security

MELCOR Molten Salt Reactor Modeling

MELCOR

Added molten salt as working fluid

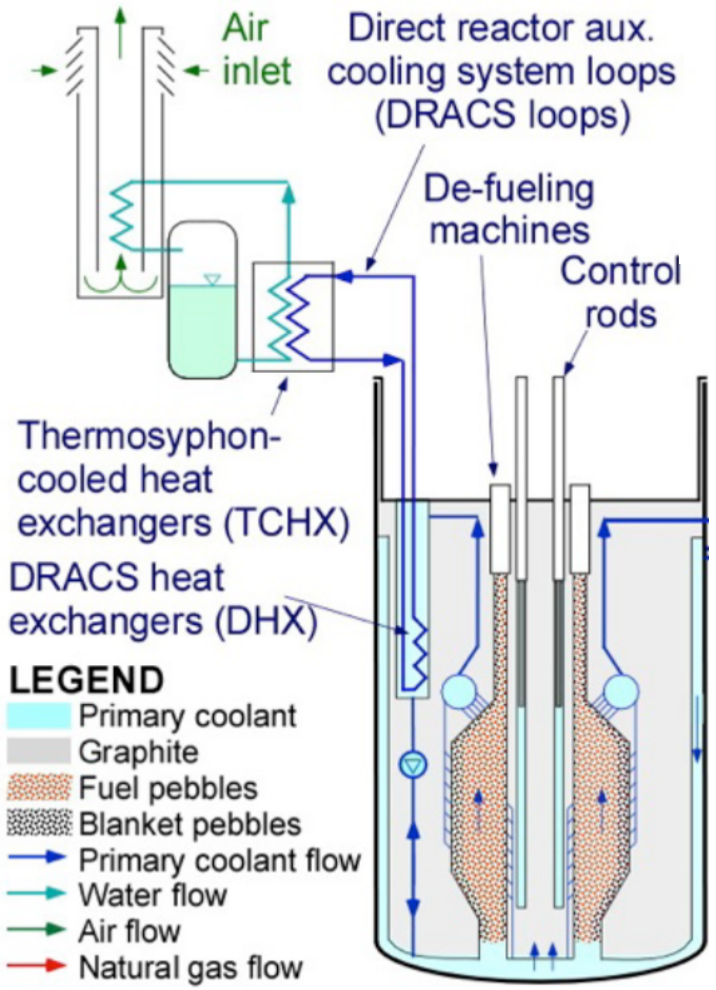
Fission product release

- Release from TRISO kernel
- Radionuclide distributions within the layers in the TRISO particle and compact
- Liquid-phase fission product chemistry and transport model

Additional core models

- Graphite oxidation
- Intercell and intracell conduction
- Convection & flow

Fluid point kinetics (liquid-fueled molten salt reactors)



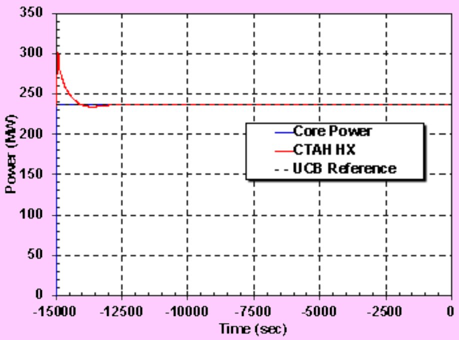
Transient/Accident Solution Methodology

Stage 0:
Normal Operation
Establish thermal state

Time constant in FHR graphite structures is very large

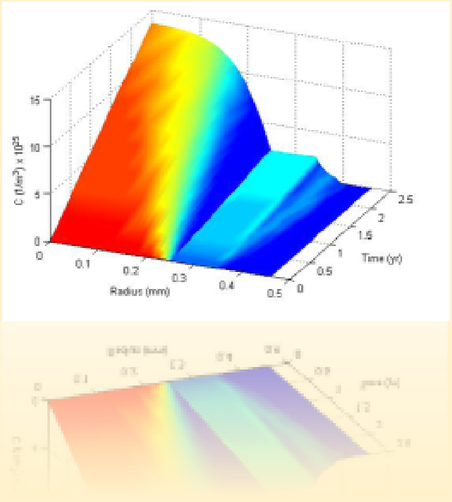
Reduce heat capacities for structures to reach steady state thermal conditions.

Reset heat capacities after steady state is achieved.



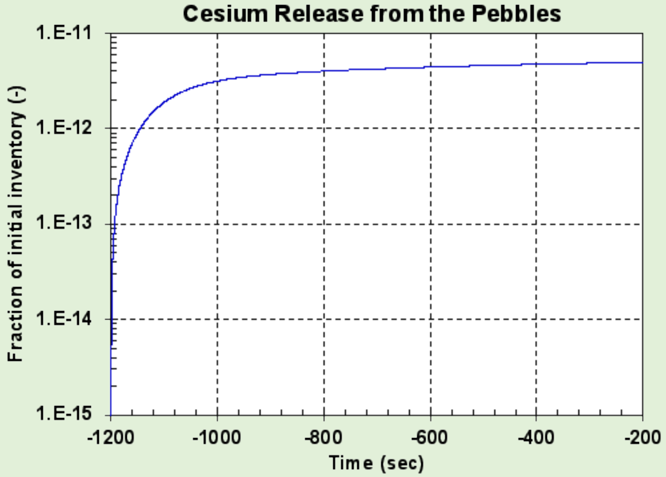
Stage 1:
Normal Operation
Diffusion Calculation

Establish steady state distribution of radionuclides <u>in TRISO particles, and matrix</u>



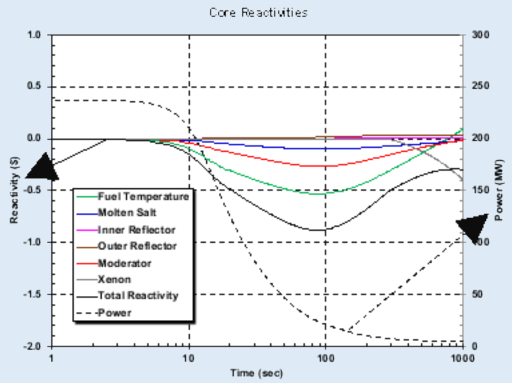
Stage 2:
Normal Operation
Transport Calculation

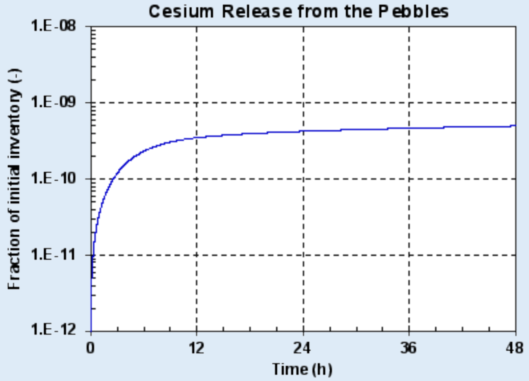
Calculate steady state distribution of radionuclides <u>into the molten salt</u> (formation of soluble, colloidal fission products, deposition on surfaces, convection through flow paths)



Stage 3:
Accident
Diffusion & Transport calculation

Calculate accident progression and radionuclide release

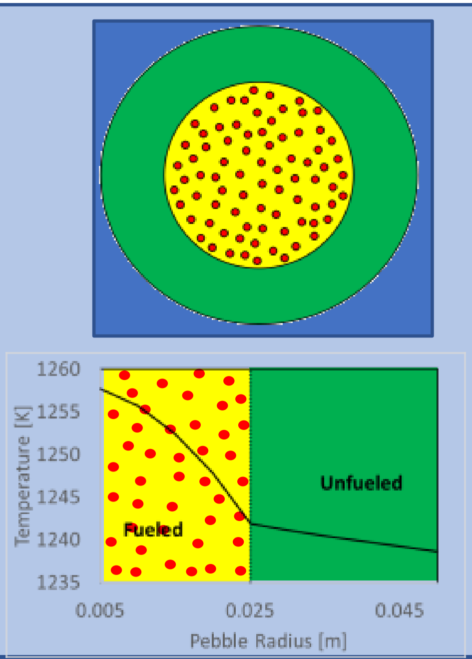




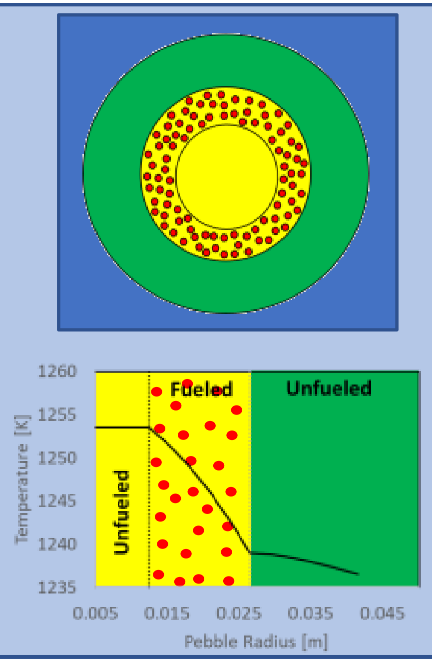
Core components

- Pebble Bed Reactor Fuel/Matrix Components
  - Fueled part of pebble
  - Unfueled shell (matrix) is modeled as separate component
  - Fuel radial temperature profile for sphere

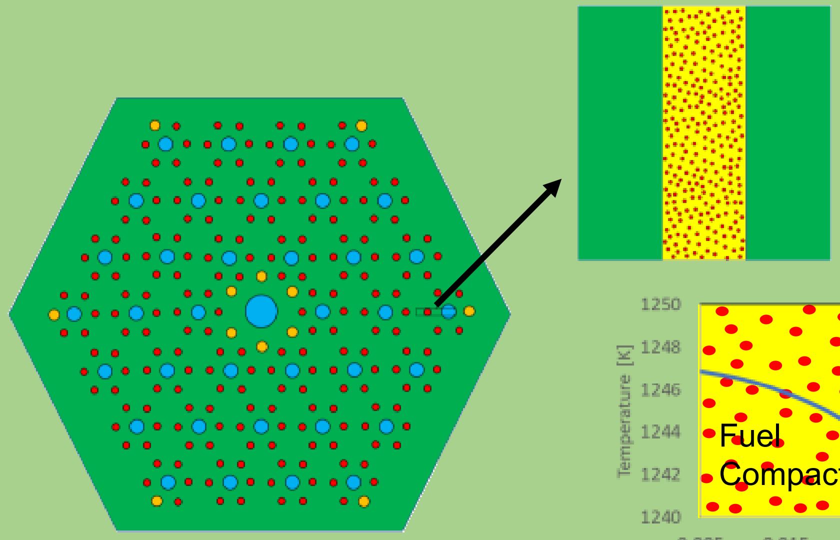
Fueled pebble core

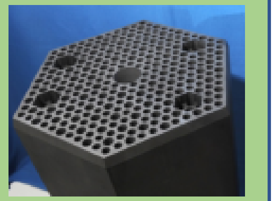


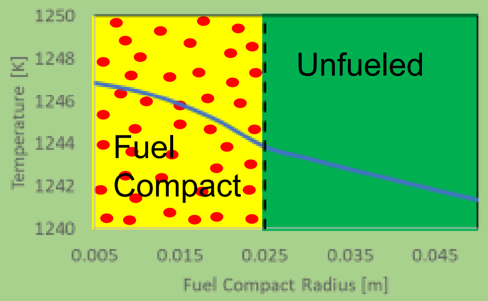
Unfueled pebble core



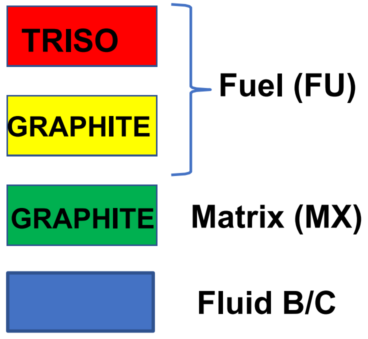
- Prismatic Modular Reactor Fuel/Matrix Components
  - “Rod-like” geometry
  - Part of hex block associated with a fuel channel is matrix component
  - Fuel radial temperature profile for cylinder

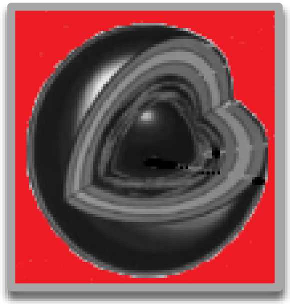






Legend





TRISO (FU)

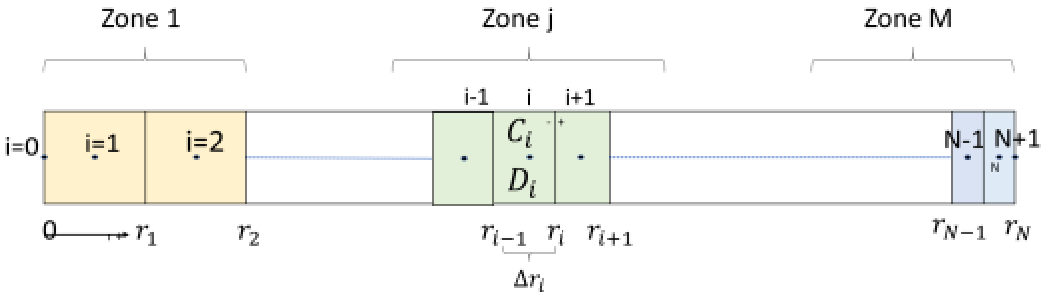
Sub-component model for zonal diffusion of radionuclides through TRISO particle

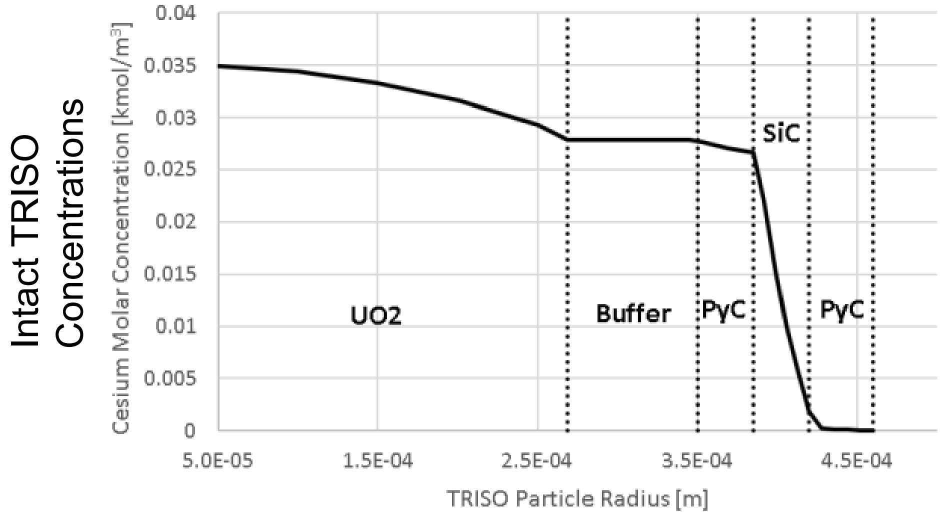
Radionuclide Diffusion Release Model

Intact TRISO Particles

- One-dimensional finite volume diffusion equation solver for multiple zones (materials)
- Temperature-dependent diffusion coefficients (Arrhenius form)

$$\frac{\partial C}{\partial t} = \frac{1}{r^n}\frac{\partial}{\partial r}\left(r^n D \frac{\partial C}{\partial r}\right) - \lambda C + \beta \qquad D(T) = D_0 e^{-\frac{Q}{RT}}$$





Diffusivity Data Availability

Radionuclide	UO_2	UCO	PyC	Porous Carbon	SiC	Matrix Graphite	TRISO Overall
Ag	Some	Not investigated	Some	Not found	Extensive	Some	Extensive
Cs	Some		Some		Extensive	Some	Some
I	Some		Some		Some	Not found	Not found
Kr	Some		Some		Not found	Some	Some
Sr	Some		Some		Extensive	Some	Some
Xe	Some		Some		Some	Some	Not found

Data used in the demo calculation

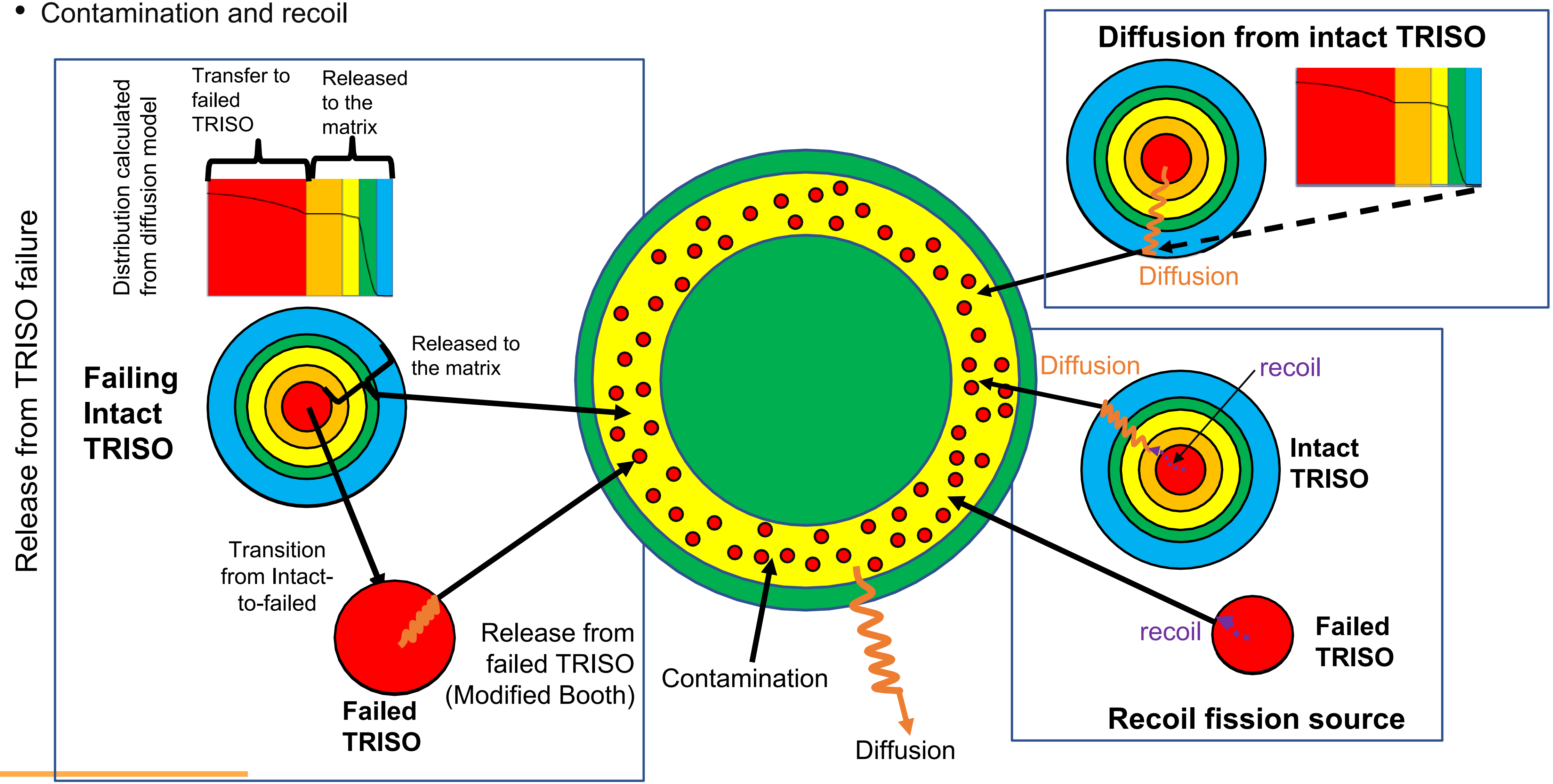
[IAEA TECDOC-0978]

	FP Species							
	Kr		Cs		Sr		Ag	
Layer	D (m^2/s)	Q (J/mole)	D (m^2/s)	Q (J/mole)	D (m^2/s)	Q (J/mole)	D (m2/s)	Q (J/mole)
Kernel (normal)	1.3E-12	126000.0	5.6-8	209000.0	2.2E-3	488000.0	6.75E-9	165000.0
Buffer	1.0E-8	0.0	1.0E-8	0.0	1.0E-8	0.0	1.0E-8	0.0
PyC	2.9E-8	291000.0	6.3E-8	222000.0	2.3E-6	197000.0	5.3E-9	154000.0
SiC	3.7E+1	657000.0	7.2E-14	125000.0	1.25E-9	205000.0	3.6E-9	215000.0
Matrix Carbon	6.0E-6	0.0	3.6E-4	189000.0	1.0E-2	303000.0	1.6E00	258000.0
Str. Carbon	6.0E-6	0.0	1.7E-6	149000.0	1.7E-2	268000.0	1.6E00	258000.0

Iodine assumed to behave like Kr

Radionuclide Release Models

- Recent failures – particles failing within latest time-step (burst release, diffusion release in time-step)
- Previous failures – particles failing on a previous time-step (time history of diffusion release)
- Contamination and recoil



Graphite Oxidation

Existing capability introduced with High-Temperature Gas-cooled Reactors (HTGRs)

Steam oxidation

$$R_{OX,steam} = \frac{k_4 P_{H_2O}}{1 + k_5 P_{H_2}^{0.5} + k_6 P_{H_2O}}$$

Reactions

$C + H_2O(g) \rightarrow CO(g) + H_2(g)$
$CO(g) + H_2O(g) \rightarrow CO_2(g) + H_2(g)$

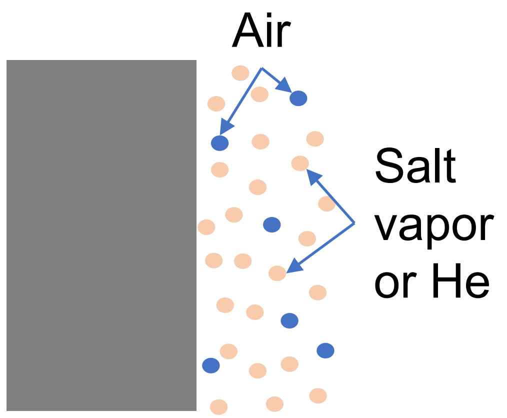
Air oxidation

$$R_{OX} = 1.7804x10^4 \exp\left(-\frac{20129}{T}\right)\left(\frac{P}{0.21228x10^5}\right)^{0.5}$$

Reactions

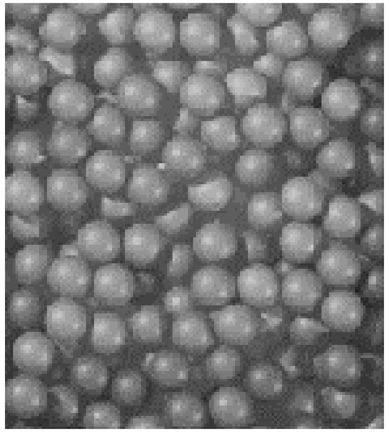
1. $C + O_2 \rightarrow CO_2(g)$
2. $C + \frac{1}{2}O_2 \rightarrow CO(g)$
3. $CO(g) + \frac{1}{2}O_2(g) \rightarrow CO_2(g)$
4. $C + CO_2(g) \rightarrow 2CO(g)$

R_{OX} is the rate term in the parabolic oxidation equation [1/s]



Air diffusion towards oxidation surface is rate limited due to mass transfer limitations in presence of salt vapor

Energy Transport between Discrete Core Volumes



Effective conductivity prescription for pebble bed (bed conductance)

- Zehner-Schlunder-Bauer, without radiation heat transfer

$$k_{eff} = \left(1 - \sqrt{1-\varepsilon}\right)k_f + \left(\sqrt{1-\varepsilon}\right)k_c\left(T, \varepsilon, k_f, k_s\right)$$

where:

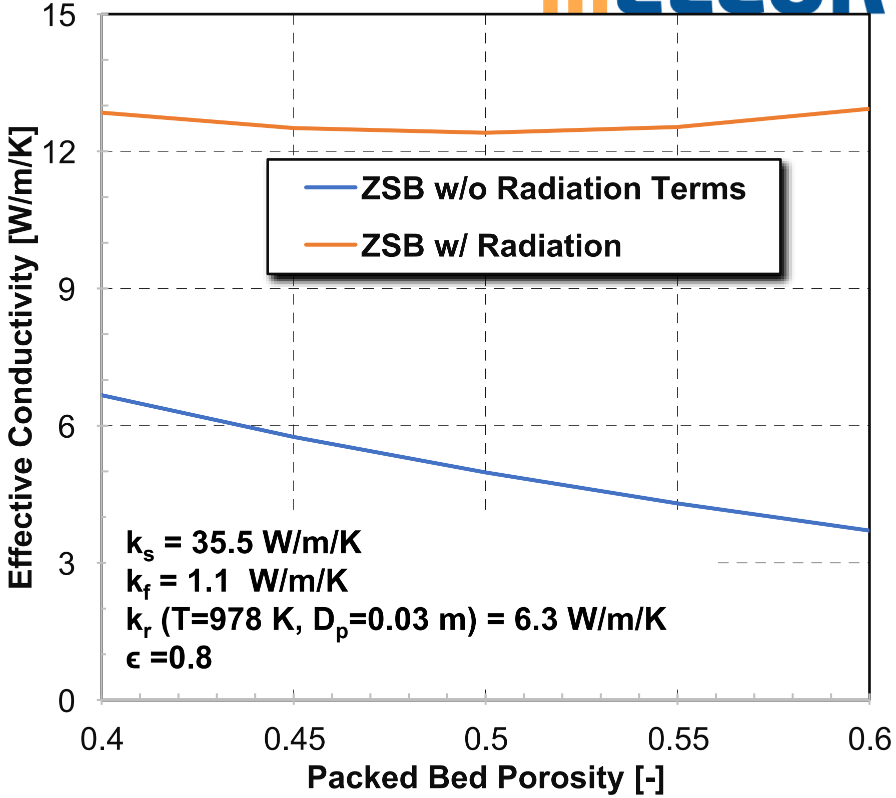
ε = Bed porosity [-]

k_f = Fluid (FLiBe) conductivity [W/m/K]

k_c = Effective bed conductivity [W/m/K], used with zero radiative conductivity

k_s = Solid conductivity [W/m/K]

T = Solid temperature [K]



- Effective fluid conductivity combines liquid and vapor contributions according to vapor fraction
- Radiative conductivity is combined by vapor fraction and used in ZSB model with radiation terms

$$k_{eff} = \left(1 - \sqrt{1-\varepsilon}\right)k_r + \left(1 - \sqrt{1-\varepsilon}\right)k_f + \left(\sqrt{1-\varepsilon}\right)k_c\left(T, D_p, \varepsilon, k_f, k_s, k_r\left(X_{Vapor}\right)\right)$$

$$k_r = 4\varepsilon\sigma T^3 D_p X_{Vapor}$$

Interface Between Thermal Hydraulics and Reactor Core Structures

Heat transfer coefficient (Nusselt number) correlations for pebble bed convection:

- Isolated, spherical particles
- Use T_{film} to evaluate non-dimensional numbers, use maximum of forced and free Nu

$$Nu_{Free} = 2.0 + 0.6\, Gr_f^{1/4}\, Pr_f^{1/3} \qquad Nu_{Forced} = 2.0 + 0.6\, Re_f^{1/2} Pr_f^{1/3}$$

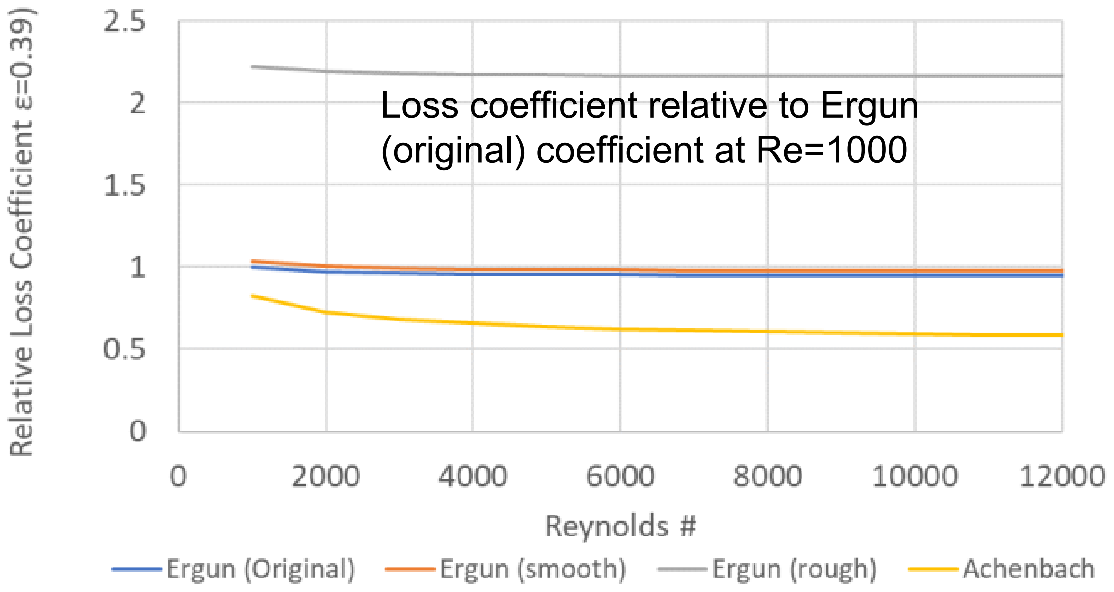
- Constants and exponents accessible by sensitivity coefficient

Flow resistance

- Packed bed pressure drop

$$K_L(\varepsilon, Re) = \left[C_1 + C_2\frac{1-\varepsilon}{Re} + C_3\left(\frac{1-\varepsilon}{Re}\right)^{C_4}\right]\frac{(1-\varepsilon)}{\varepsilon D_p}L$$

Correlation	C_1	C_2	C_3	C_4
Ergun (original)	3.5	300.	0.0	-
Modified Ergun (smooth)	3.6	360.	0.0	-
Modified Ergun (rough)	8.0	360.	0.0	-
Achenbach	1.75	320.	20.0	0.4



Point Kinetics Modeling

ELCOR

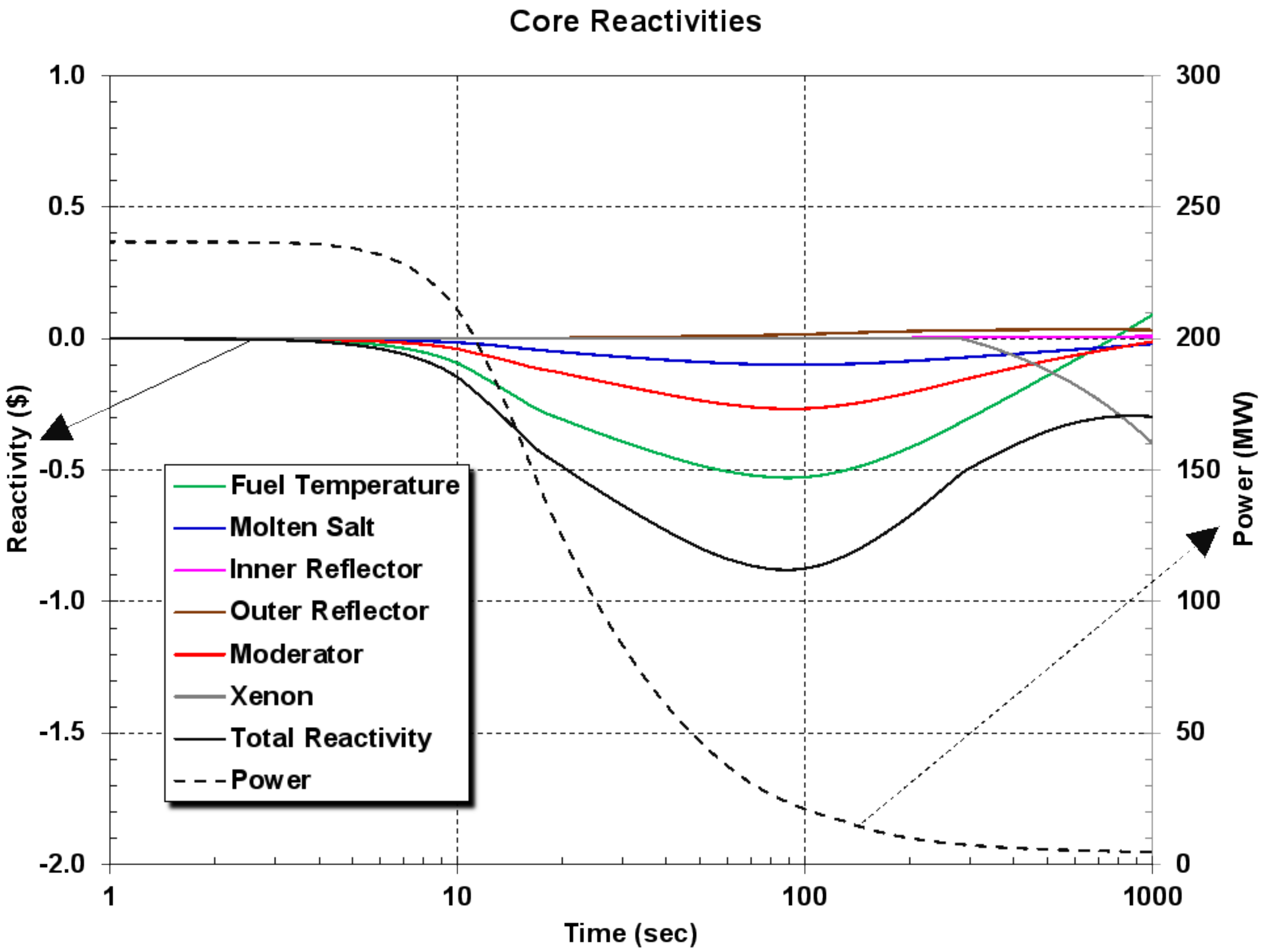
Standard treatment

$$\frac{dP}{dt} = \left(\frac{\rho - \beta}{\Lambda}\right) P + \sum_{i=1}^{6} \lambda_i Y_i + S_0$$

$$\frac{dY_i}{dt} = \left(\frac{\beta_i}{\Lambda}\right) P - \lambda_i C_i, \qquad for\ i = 1 \ldots 6$$

Feedback models

- User-specified external input
- FHR example includes multiple feedbacks
  - Fuel
  - Molten salt around the fuel
  - Inner reflector
  - Outer reflector and unfueled pebbles
  - Moderator (matrix around fueled pebbles)



Point Kinetics Modeling (MSR)

MELCOR

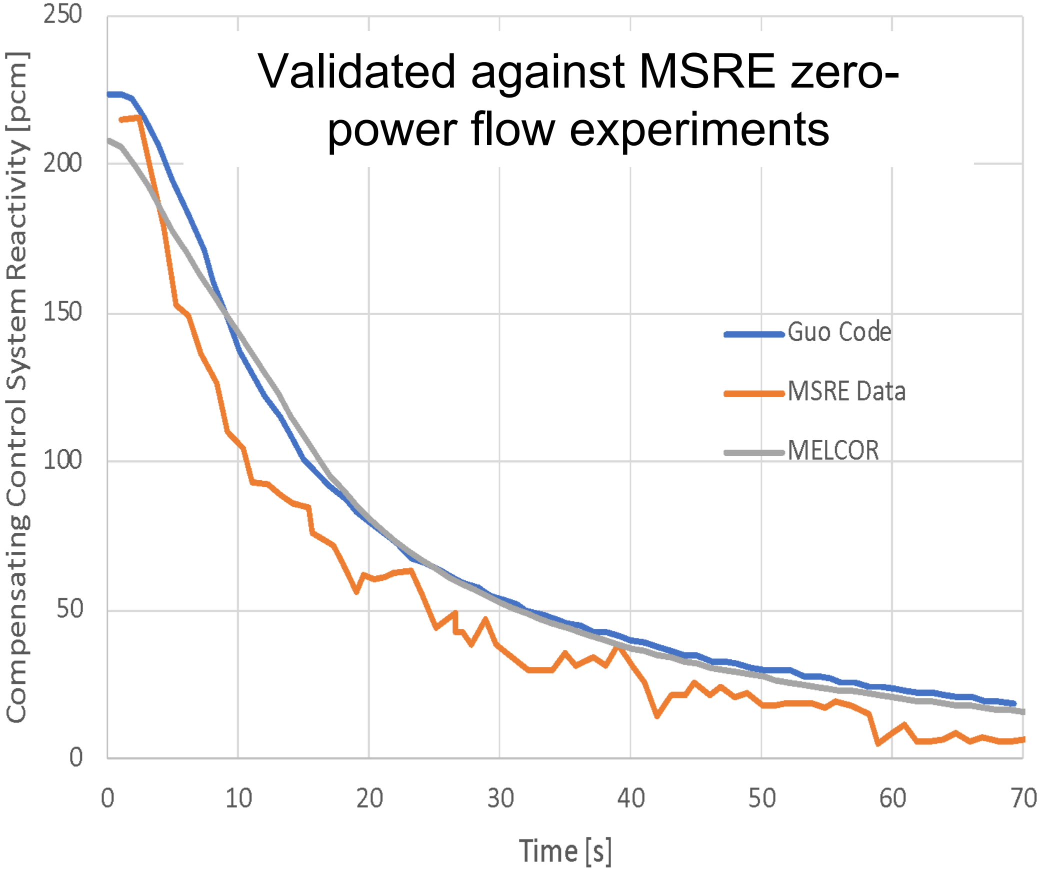
Derived from standard PRKEs and solved similarly

$$\frac{dP(t)}{dt} = \left(\frac{\rho(t) - \bar{\beta}(t)}{\Lambda}\right) P(t) + \sum_{i=1}^{6} \lambda_i C_i^C(t) + S_0$$

$$\frac{dC_i^C(t)}{dt} = \left(\frac{\beta_i}{\Lambda}\right) P(t) - \left(\lambda_i + {}^2/_{\tau_C}\right) C_i^C(t) + \left(\frac{V_L}{V_C}\right)\left(\lambda_i + {}^2/_{\tau_L}\right) C_i^L(t), \qquad i = 1 \ldots 6$$

$$\frac{dC_i^L(t)}{dt} = \left(\frac{V_C}{\tau_C V_L}\right) C_i^C(t) - \left(\lambda_i + {}^1/_{\tau_L}\right) C_i^L(t), \qquad i = 1 \ldots 6$$

$$\bar{\beta}(t) = \beta - \beta(t)_{lost} = \beta - \left(\frac{\Lambda}{P(t)}\right) \sum_{i=1}^{6} \lambda_i C_i^L(t)$$



Feedback models

- User-specified external input
- Doppler
- Fuel and moderator density
- Flow reactivity feedback effects integrated into the equation set

Molten Salt Chemistry and Radionuclide Release

MELCOR

Model Scope

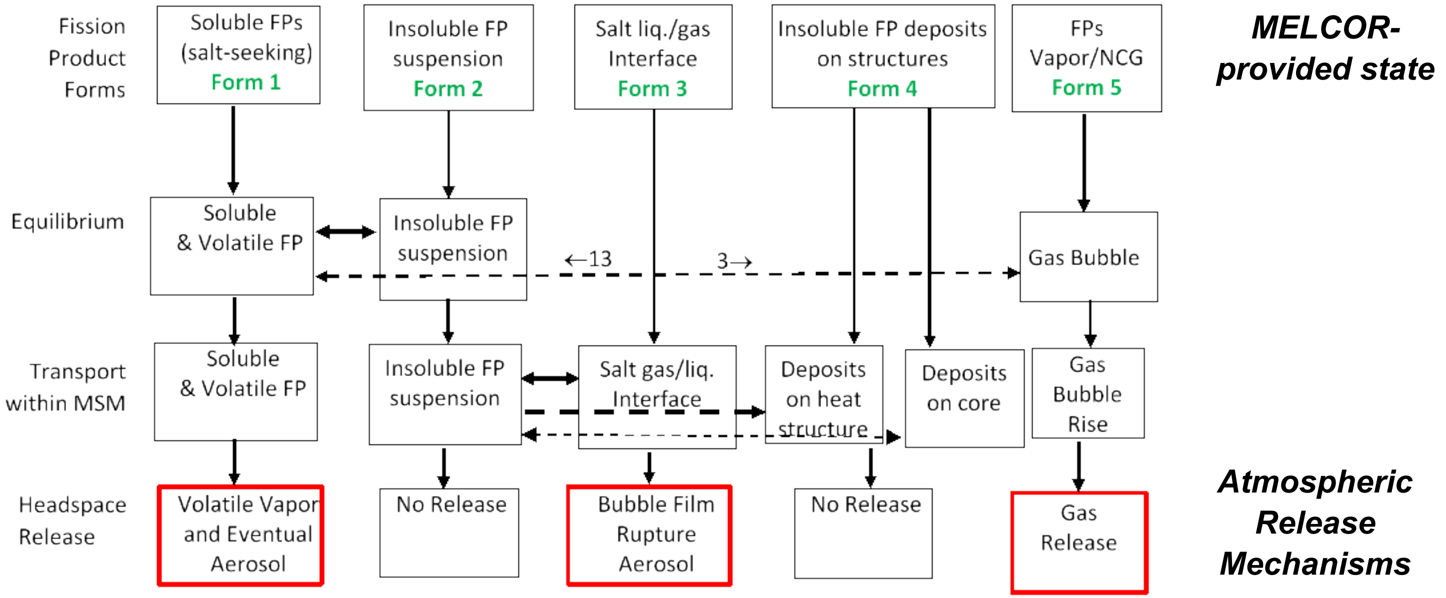
Evaluation of thermochemical state

- Gibbs Energy Minimization with Thermochimica
- Provides solubilities and vapor pressures

Thermodynamic database

- Generalized approach to utilize any thermodynamic database
- An example is the Molten Salt Thermal Database
  - FLiBe-based systems
  - Chloride-based systems

Radionuclides grouped into forms found in the Molten Salt Reactor Experiment



Initial Model Form

Solubility determined from empirical evidence (P. Britt ORNL 2017)

Solubilities mapped to 17 MELCOR fission product classes

Insoluble MELCOR classes are assigned to be colloidal

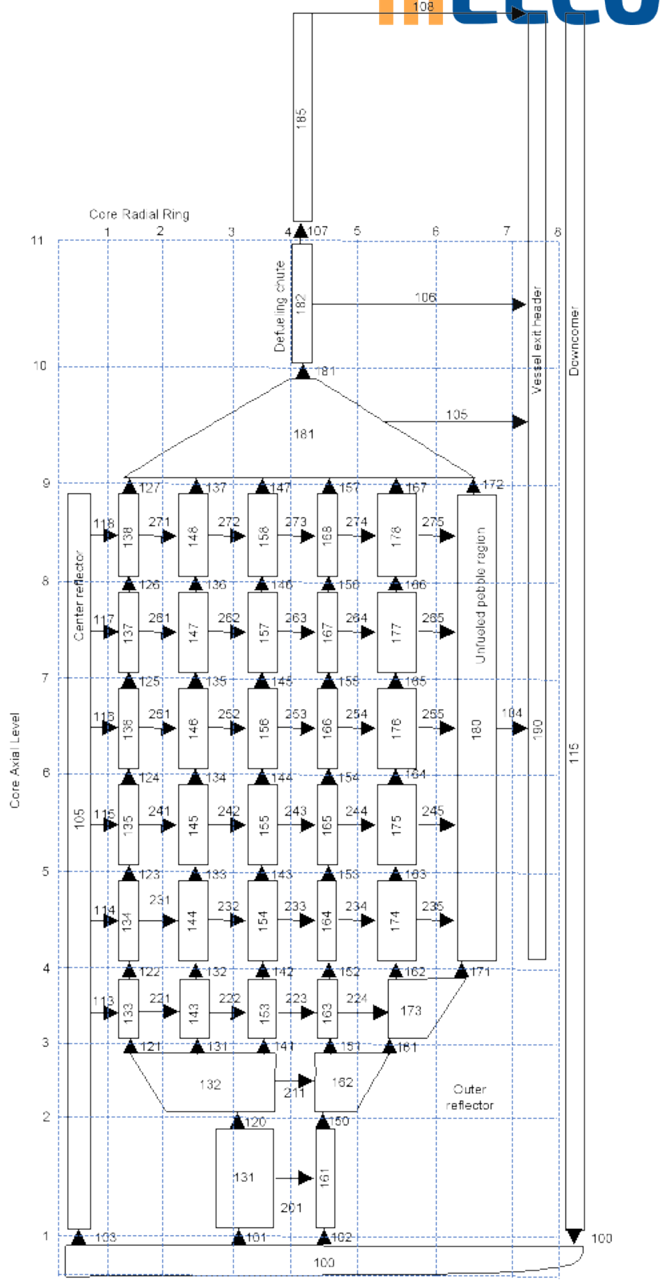
Core and reactor vessel

Core nodalization – light blue lines

- Assumes azimuthal symmetry
- Subdivided into 11 axial levels and 8 radial rings
- Core cells model molten salt fluid volume, reflector structures, the pebble-bed core, and the pebbles in the defueling chute

Fluid flow nodalization – black boxes

- Molten salt enters through the downcomer and flows into the center reflector and into the bottom of the pebble bed
- Molten salt leaves through the periphery of the core and upwards through the refueling chute
- Unfueled graphite pebbles in box labeled “180”



Recirculation loops

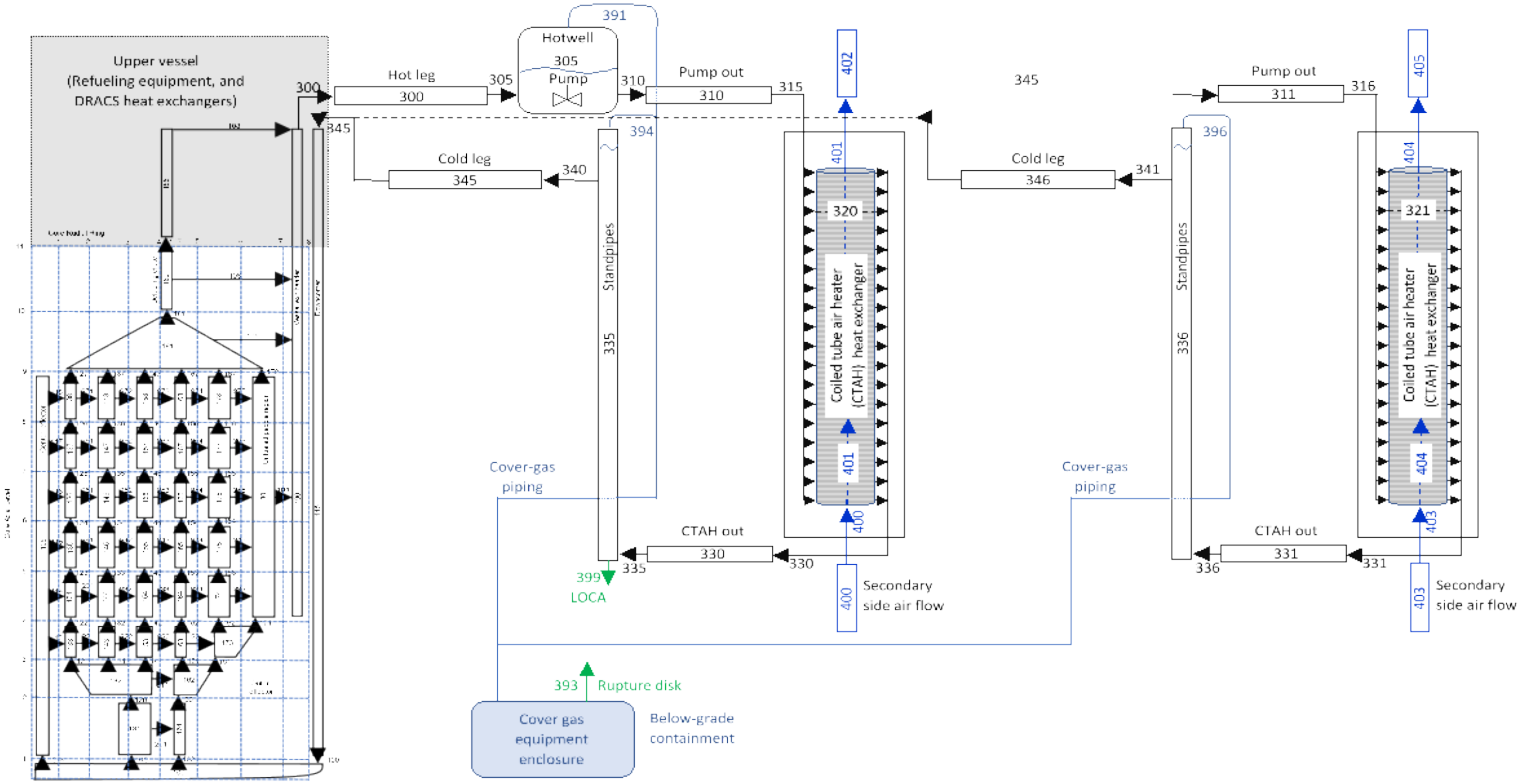
Each loop has a pump, a heat exchanger, and a standpipe

Molten salt has free surface in the hotwell and the standpipes

Argon gas above the free surfaces with connection to the cover-gas system

- Over-pressurization relief passes through the cover gas system
- Cover gas enclosure leaks into the containment when over-pressurized

Secondary-side air cools primary -side molten salt



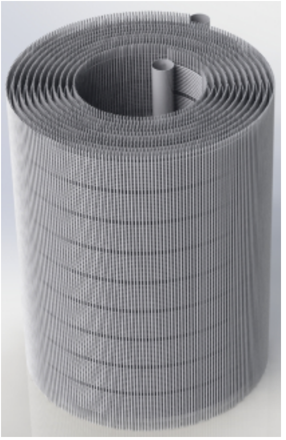
Direct Reactor Auxiliary Cooling System (DRACS)

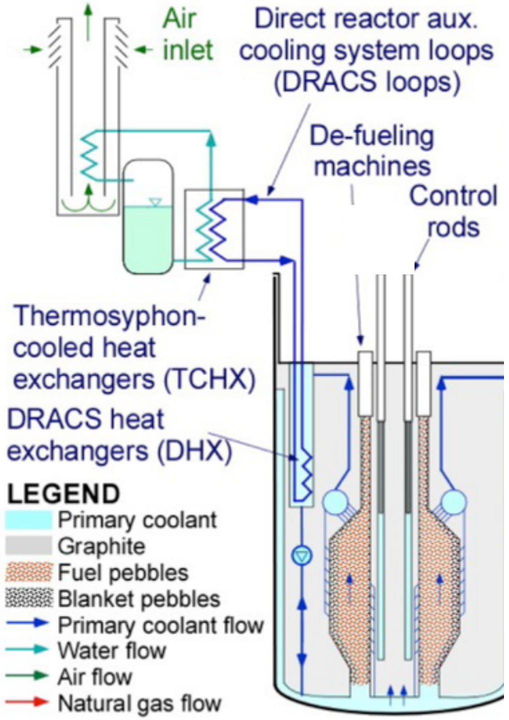
3 trains – 2.36 MW/train
- 236 MWt reactor

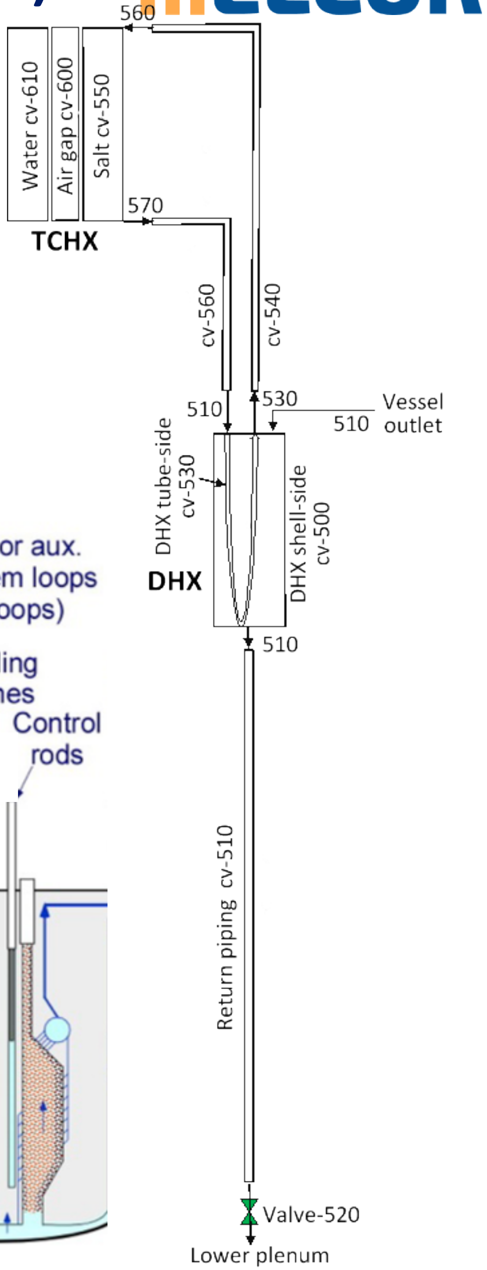
Each train has 4 loops in series
- Primary coolant circulates to DRACS heat exchanger
- Molten-salt loop circulates to the thermosyphon-cooled heat exchangers (TCHX)
- Water circulates adjacent to the secondary salt tube loop in the TCHX
- Natural circulation air circuit cools and condenses steam

Start-up: RCS-pump trip causes ball in valve to drop

Additional system information
- DHXs are in the reactor vessel
- TCHXs are in the shield building







Containment

Shield dome

- Protection against aircraft and natural gas detonations (co-fired turbine concept)
- Contains water for DRACS and RCCS
- DRACS air natural circulation chimneys connected to the shield dome

Reactor cavity

- Fire-brick insulation
- Low free volume
- Low-leakage bellows between reactor cavity and adjacent cavities

Separate compartments for the other RCS components

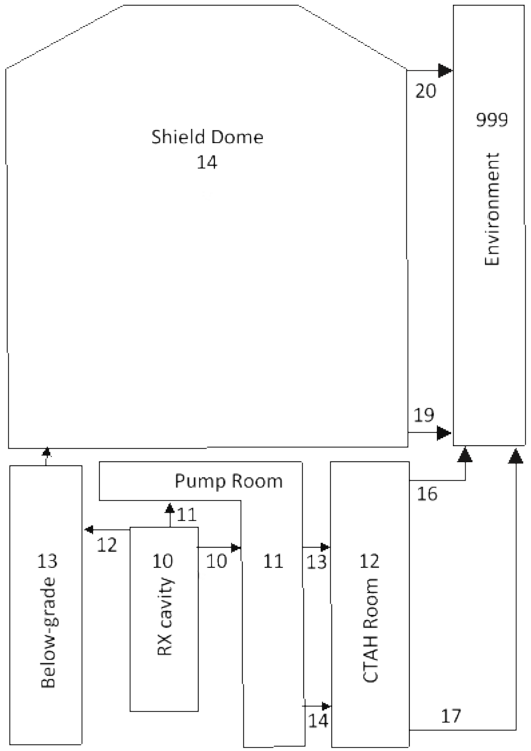
- Below-grade compartment includes the cover-gas enclosure for reactor cavity over-pressurization

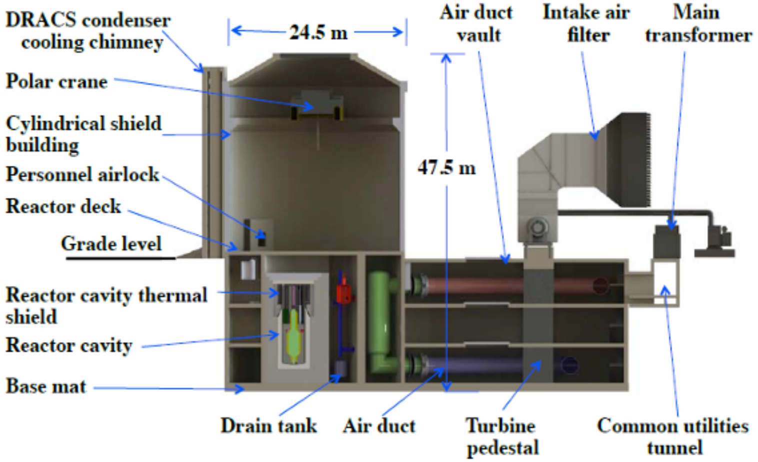
Reactor cavity cooling subsystem in reactor cavity wall

- Water circulation
- Cooling tubes affixed to reactor cavity steel liner
- Cools concrete during normal operation

Leak rate assumed consistent with BWR Mark 1 reactor building

- 100% vol/day at 0.25 psig



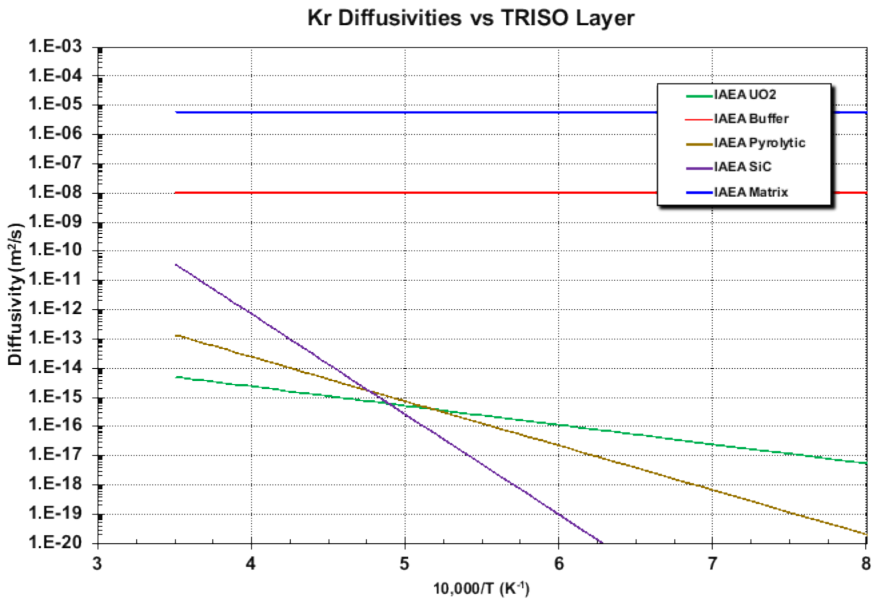


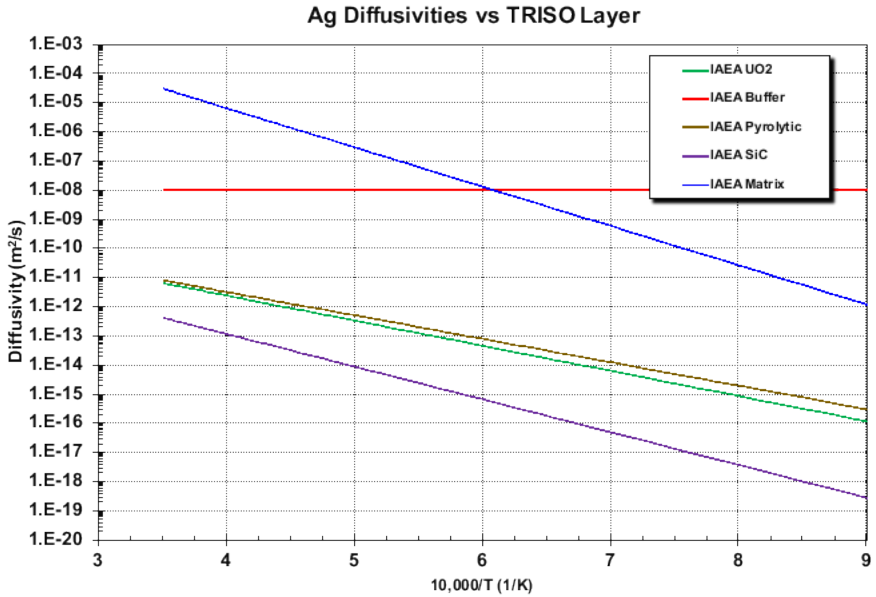
MELCOR model inputs (1/2)

MELCOR model inputs **(2/2)**

Fission product diffusivities through the TRISO and the pebble matrix from IAEA-TECDOC-978, Appendix A

- Primarily based on values from German experiments with UO_2 TRISO pebbles
  - UO_2 data can be easily updated to UCO data*
- Limited data based on nuclides of Xe, Cs, Sr, and Ag
- Iodine assumed to behave like Kr





* UCO TRISO thermal failure characteristics were not available, so UO_2 TRISO diffusivity and UO_2 failure data were used. Both are changeable through user input with design-specific data.

Scenarios

ELCOR

Three scenarios with a loss of secondary heat removal

- ATWS – Anticipated transient without SCRAM
- SBO – Station blackout
- LOCA – Loss-of-coolant accident

Sensitivity calculations included

- DRACS performance
- Alternate cover-gas system interconnections (LOCA only)

ATWS

MELCOR

Loss-of-onsite power with failure to SCRAM

- Salt pumps shut off
- Reactor fails to SCRAM
- Secondary heat removal ends
- 0 to 3 trains of DRACS operating

Includes preliminary analysis with xenon transient

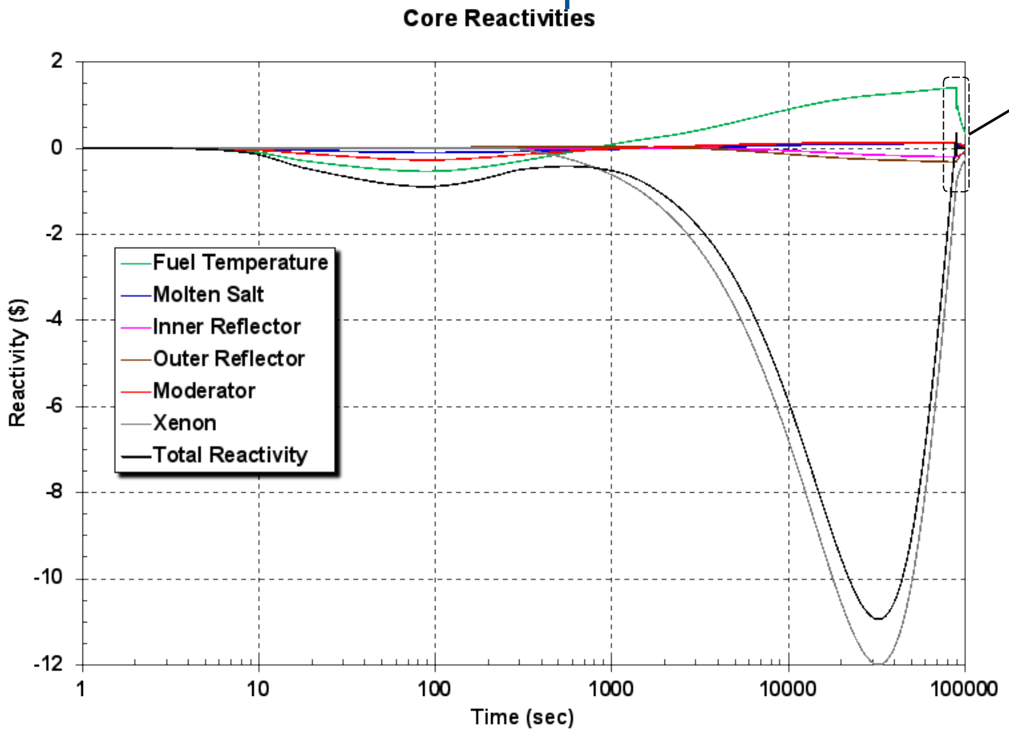
- Guided by ORNL calculations
- Xenon reactivity feedback model being implemented into MELCOR

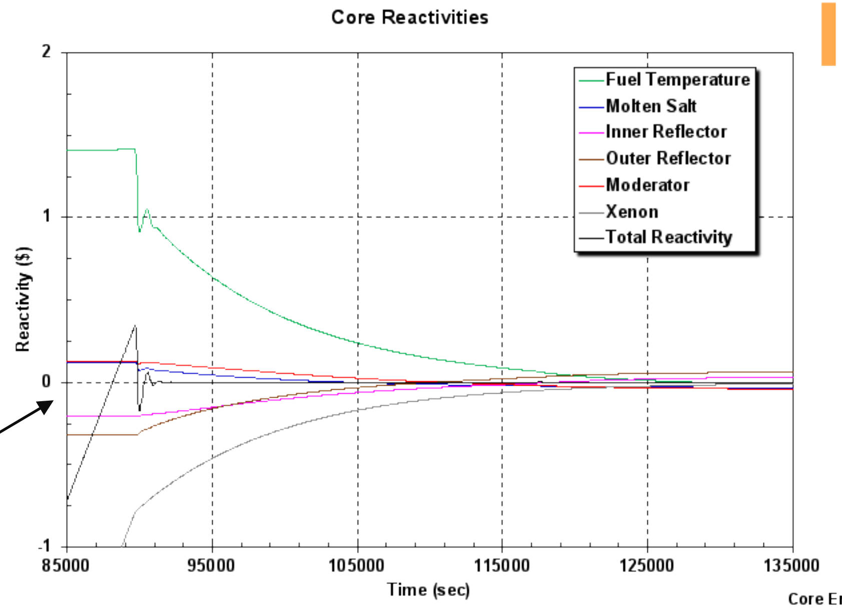
ATWS with 3xDRACS

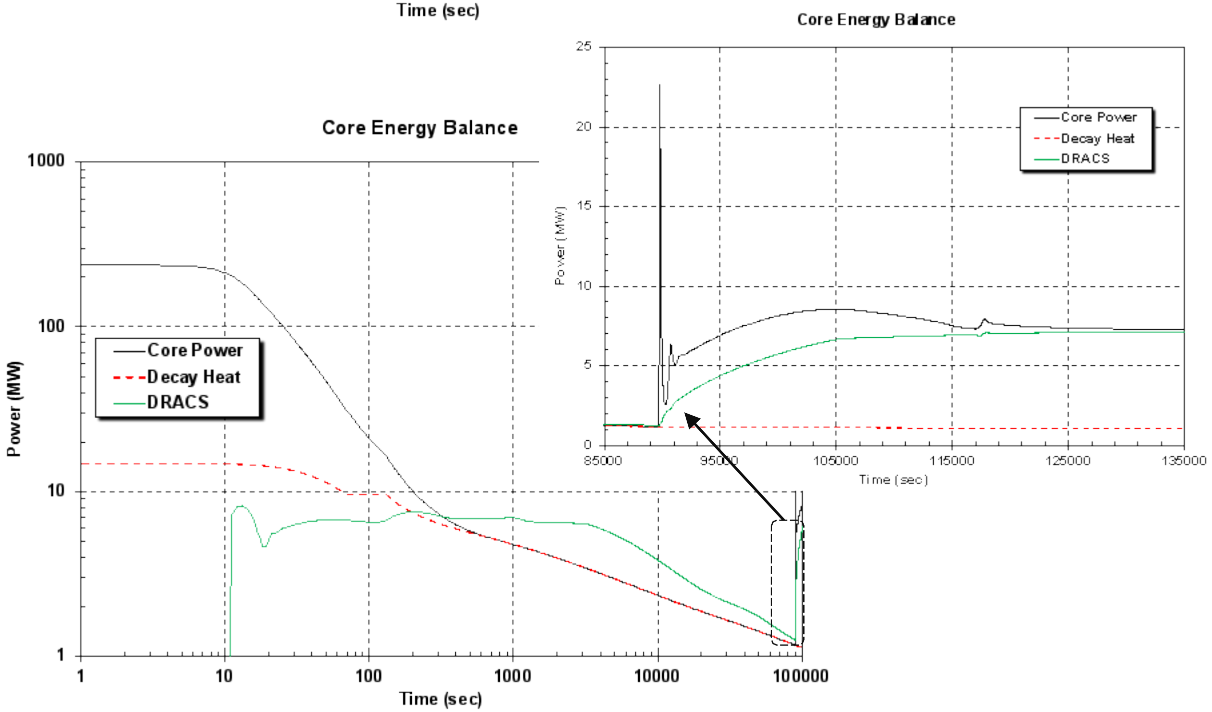
Initial fuel heatup has strong negative fuel and moderator feedback that offsets positive reflector feedbacks

Strong negative xenon transient feedback *

3xDRACS exceeds core power after 330 s







* Xenon transient approximated.

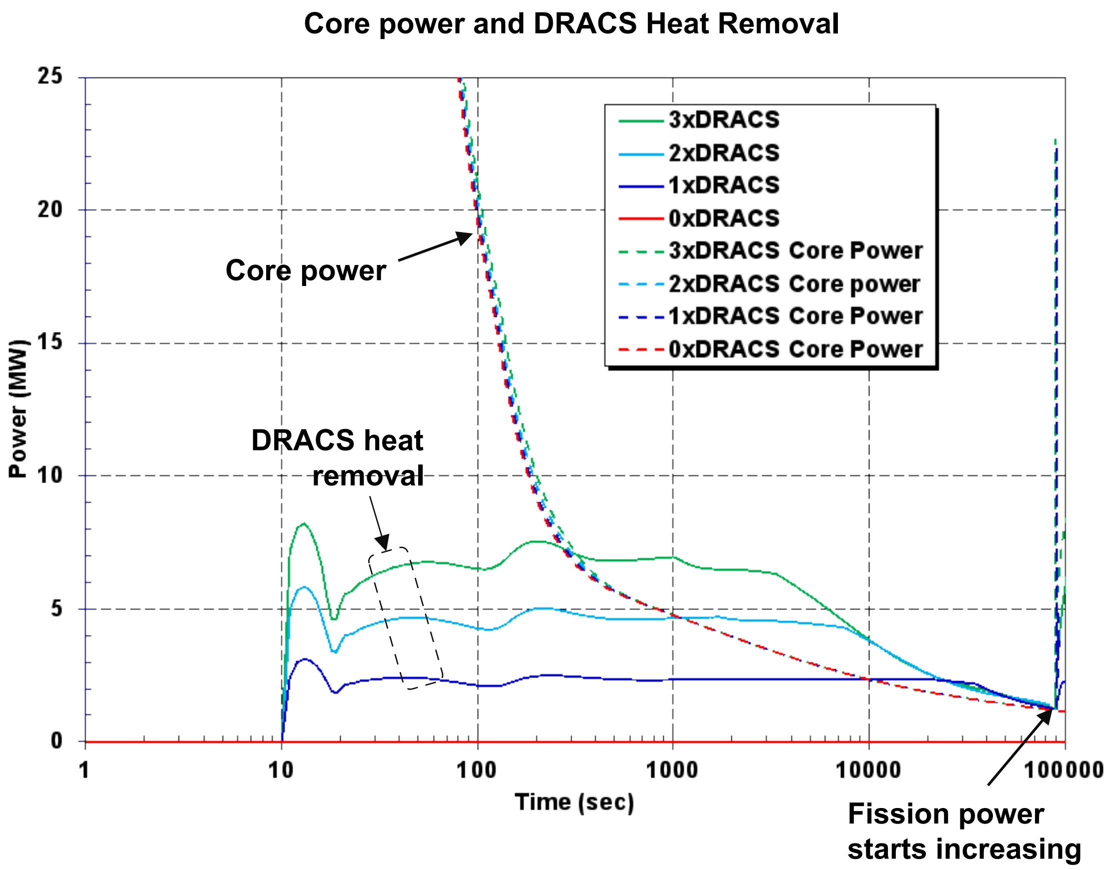
ATWS with variable DRACS (semi-log)

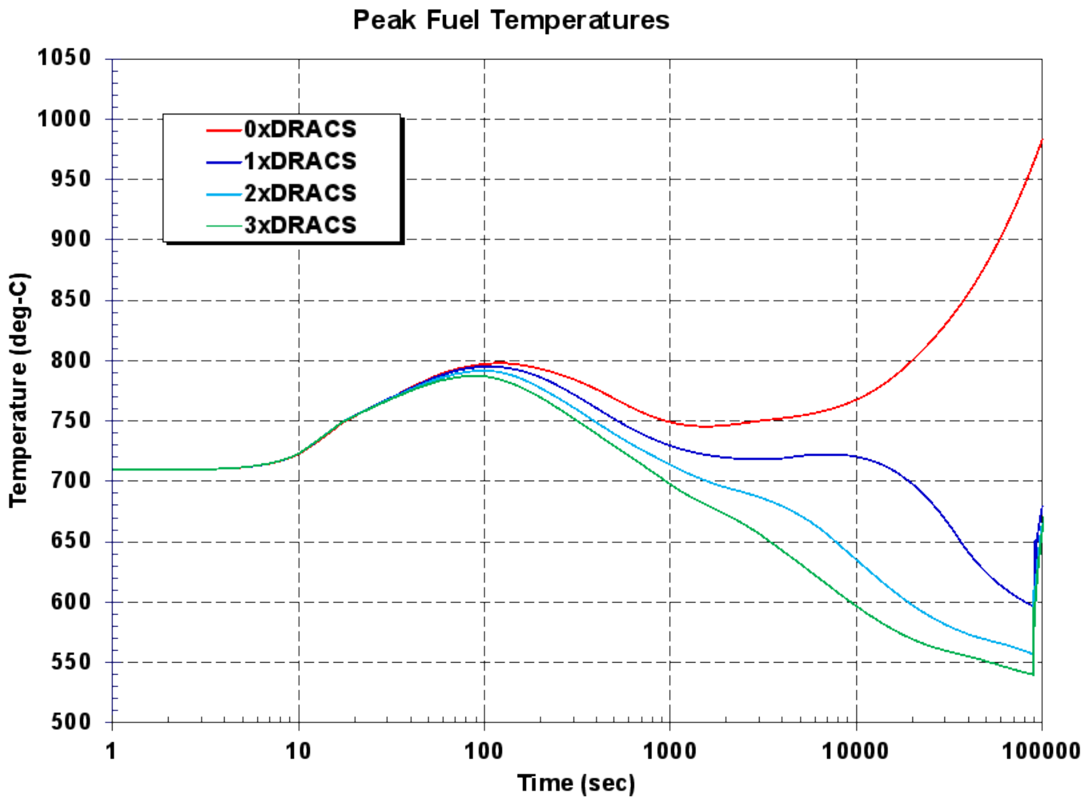
Early power decrease to decay heat level is similar for all cases

- 1xDRACS and 2xDRACS cases exceed decay heat later

Fuel temperatures cool down according to DRACS heat removal rate

- 0xDRACS peak fuel temperature = 990 °C at 10^5 s (T_{sat}~ 1350 °C)





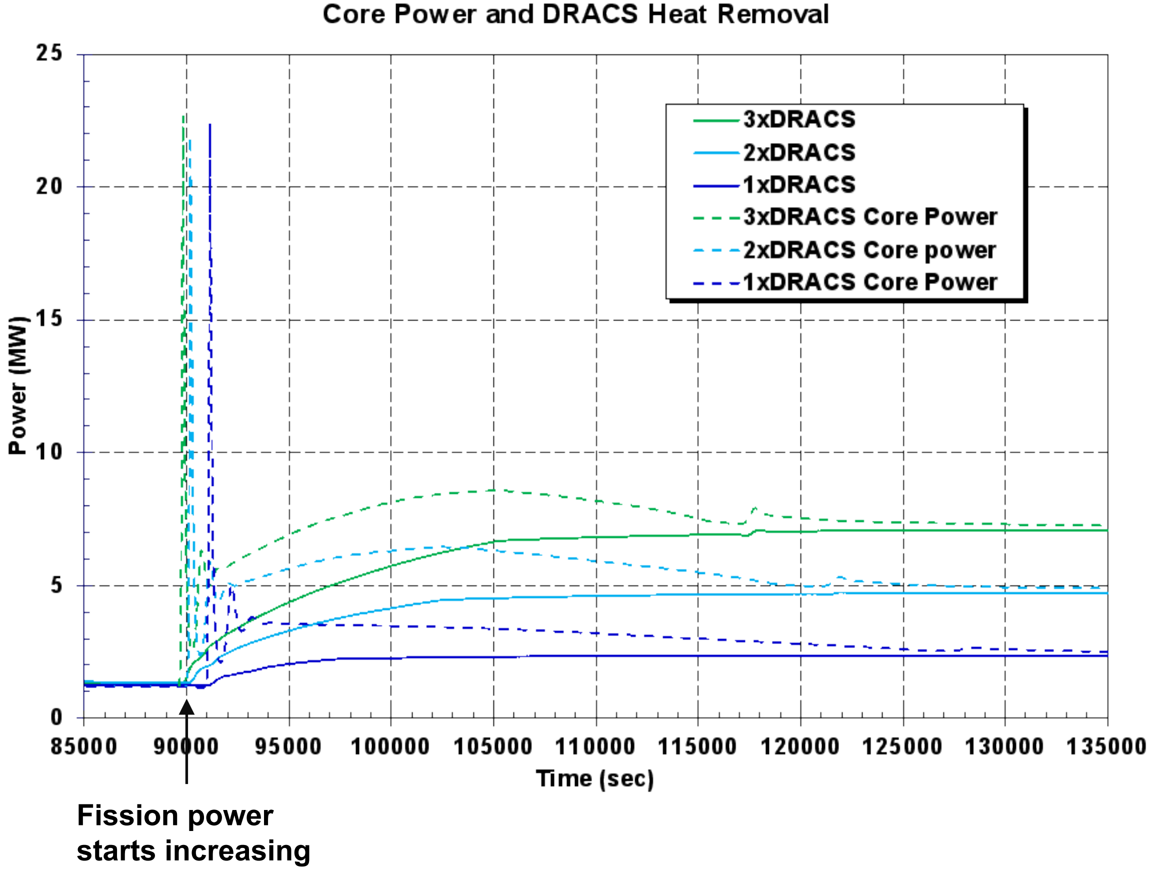
* Xenon transient approximated.

ATWS with variable DRACS – (Linear scale)

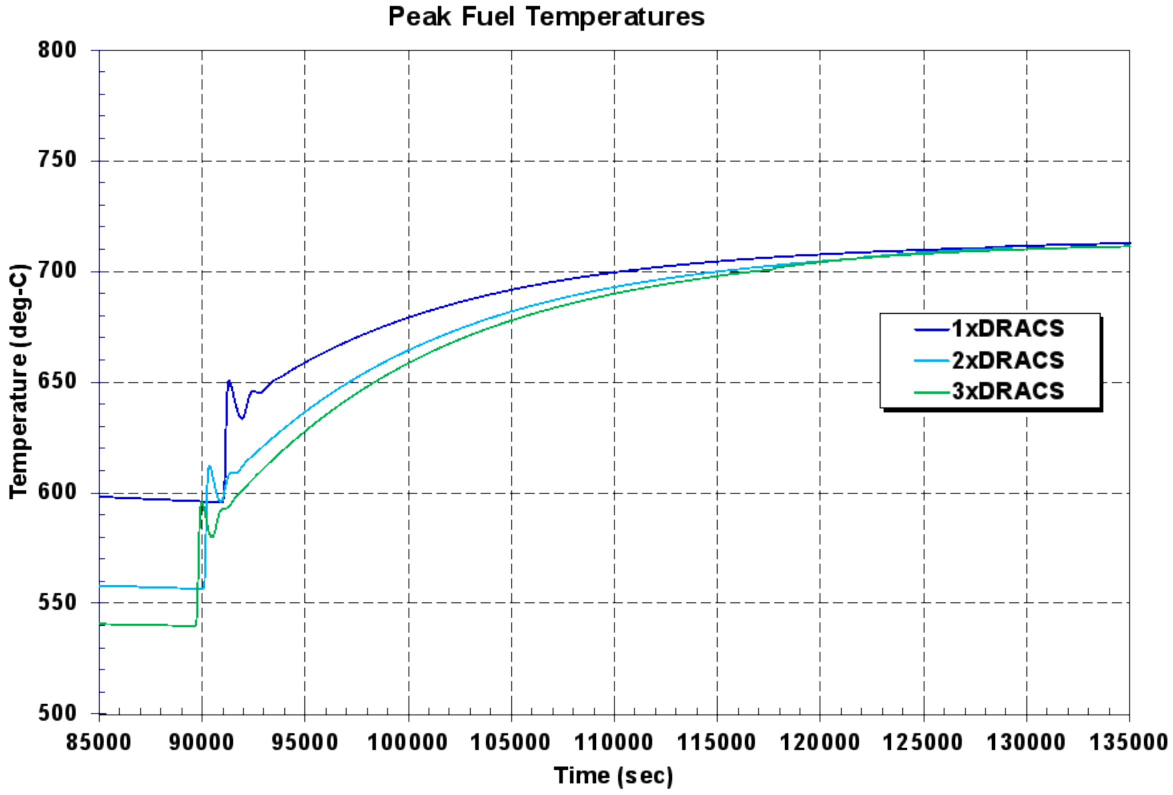
ELCOR

When the total reactivity exceeds zero, the core power increases

- Increased power heats the fuel and reduces the positive fuel reactivity
- Core power eventually converges on the DRACS heat removal rate



The long-term fuel temperatures increase to offset changes in the xenon feedback



* Xenon transient approximated.

Station Blackout

Loss-of-onsite power with SCRAM

- Salt pumps shut off
- Reactor scrams
- Secondary heat removal ends
- Variable DRACS operating (percentage of 1xDRACS)

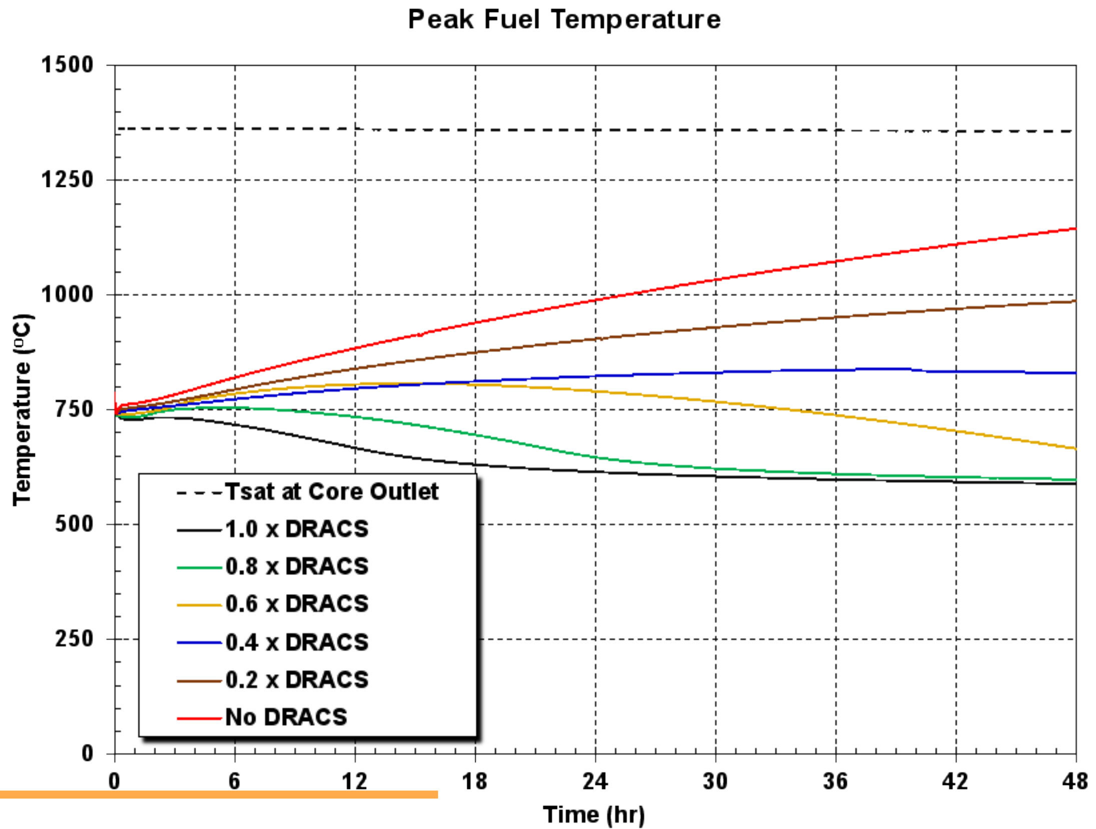
Unmitigated sensitivity case

- No DRACS and extended calculation to 7 days

SBO results (1/3)

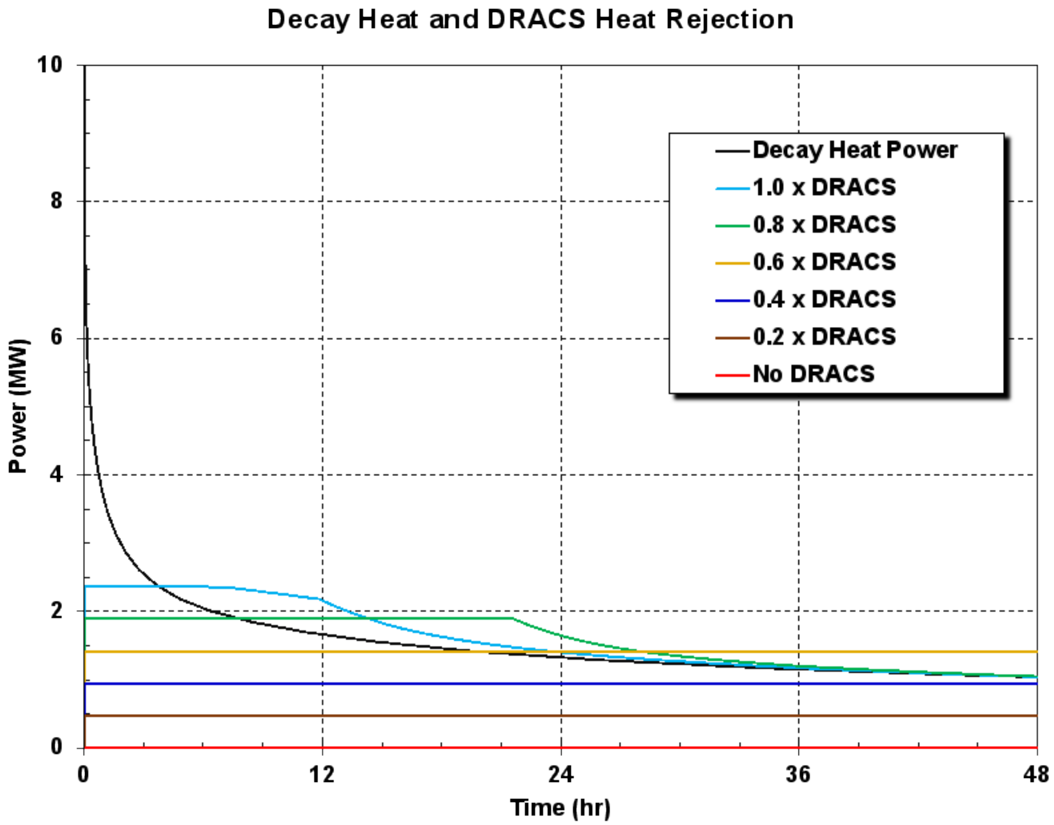
DRACS cases illustrate degraded response

- Results for fraction of 1xDRACS
- ≥40% of one DRACS stops the temperature rise within 48 hr



DRACS power follows heat removal requirements

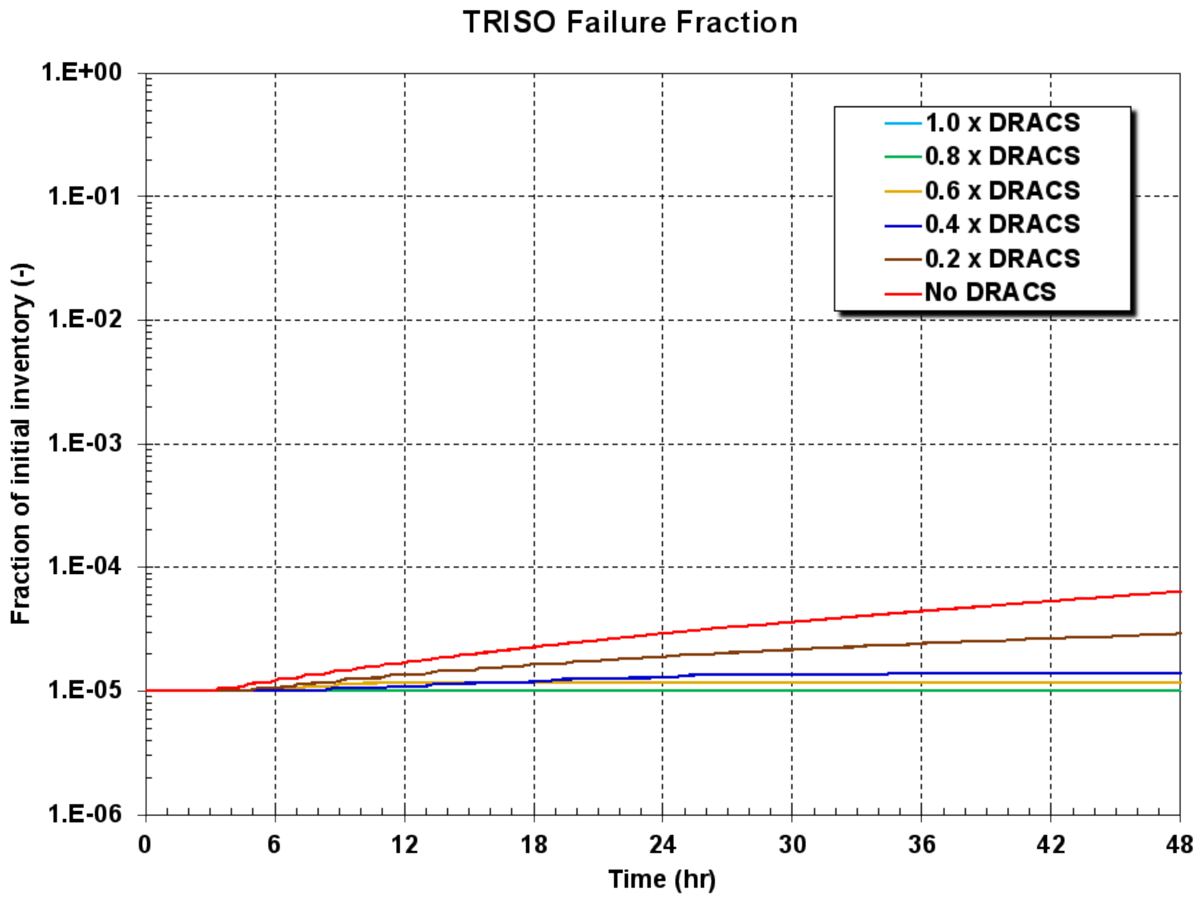
- 1xDRACS exceeds decay heat within 3 hr



SBO results (2/3)

The TRISO failure fraction remains low ($1x10^{-5}$) in the SBO with one DRACS operating *

- Higher TRISO failures were calculated as the DRACS degrades

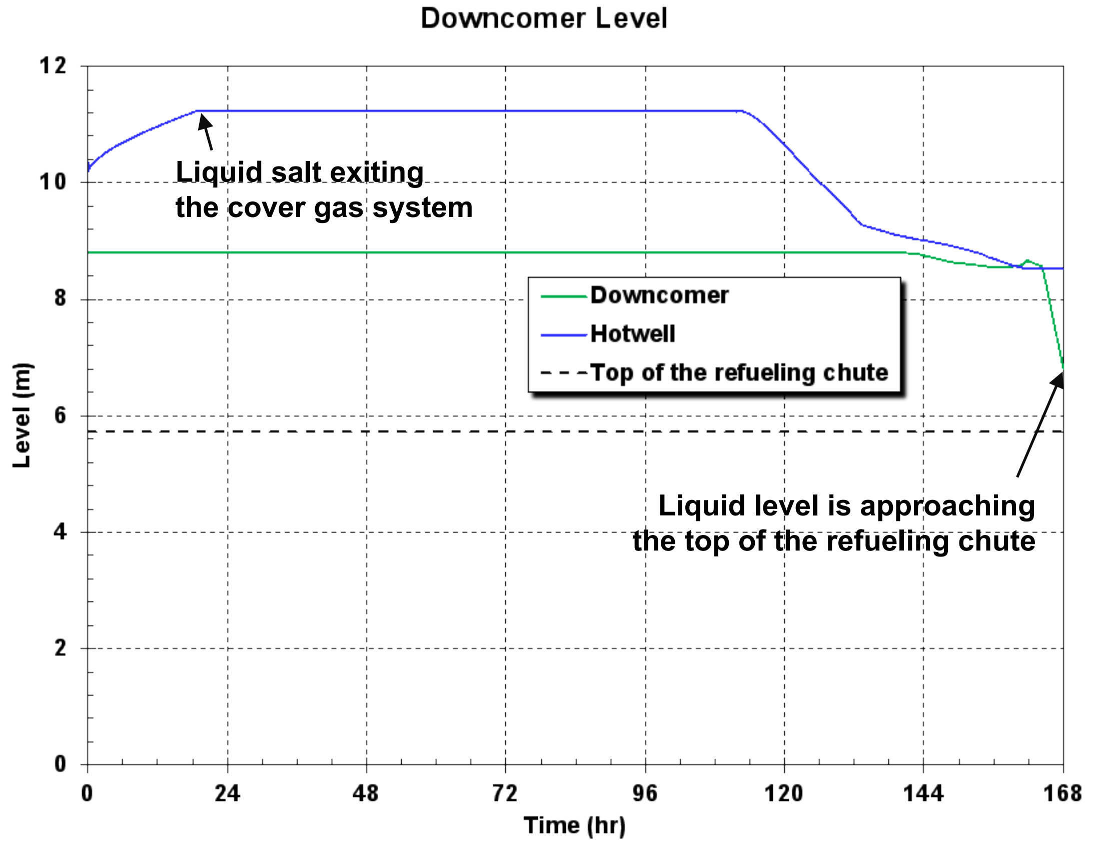


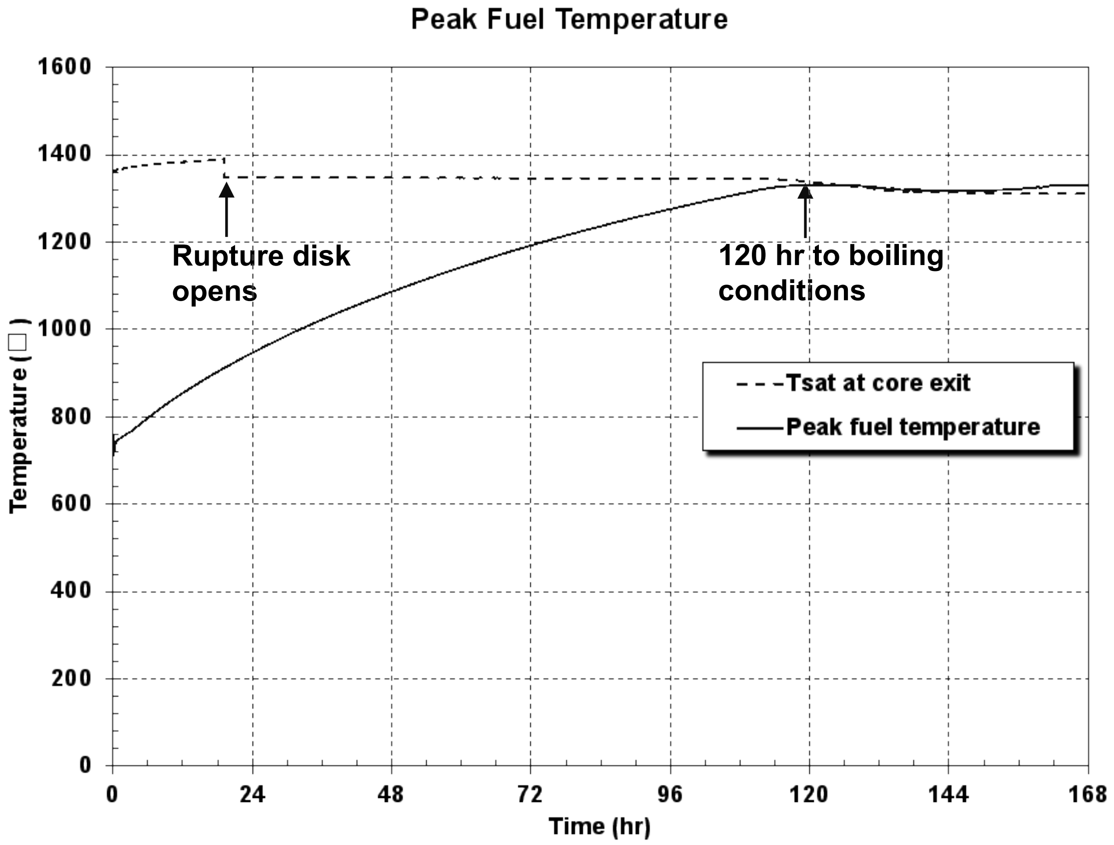
* UCO TRISO thermal failure characteristics were not available, so UO_2 TRISO diffusivity and UO_2 failure data were used. Both are changeable through user input with design-specific data.

SBO results (3/3)

The SBO with no DRACS was extended to 7 days

- No fuel uncovery
- Peak fuel temperature approximately at Tsat (~1350 °C)





LOCA

Loss-of-onsite power with LOCA

- Variable size leaks of the 3” pipe of the drain tank line
- Salt pumps shut off
- Reactor scrams
- Secondary heat removal ends
- 1 or no trains of DRACS operating
- With or without a cover gas connection path between the hotwell and the standpipes

Unmitigated sensitivity case

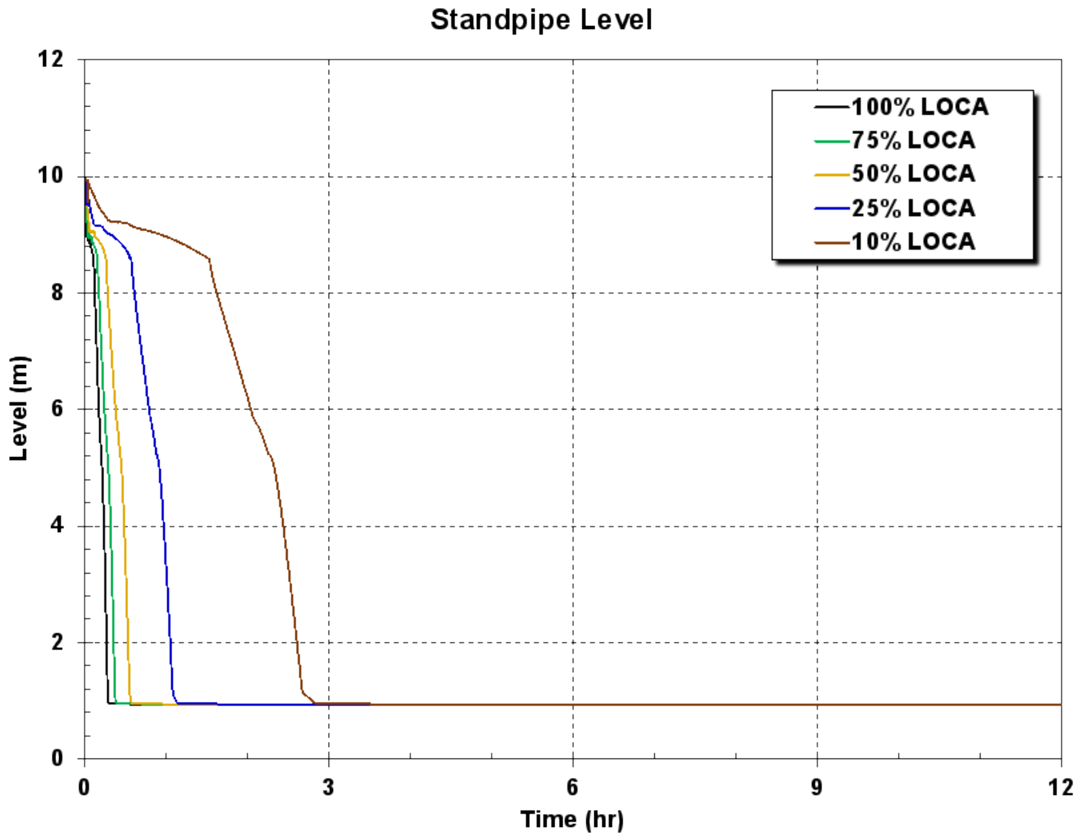
- No DRACS case extended to include fuel uncovery

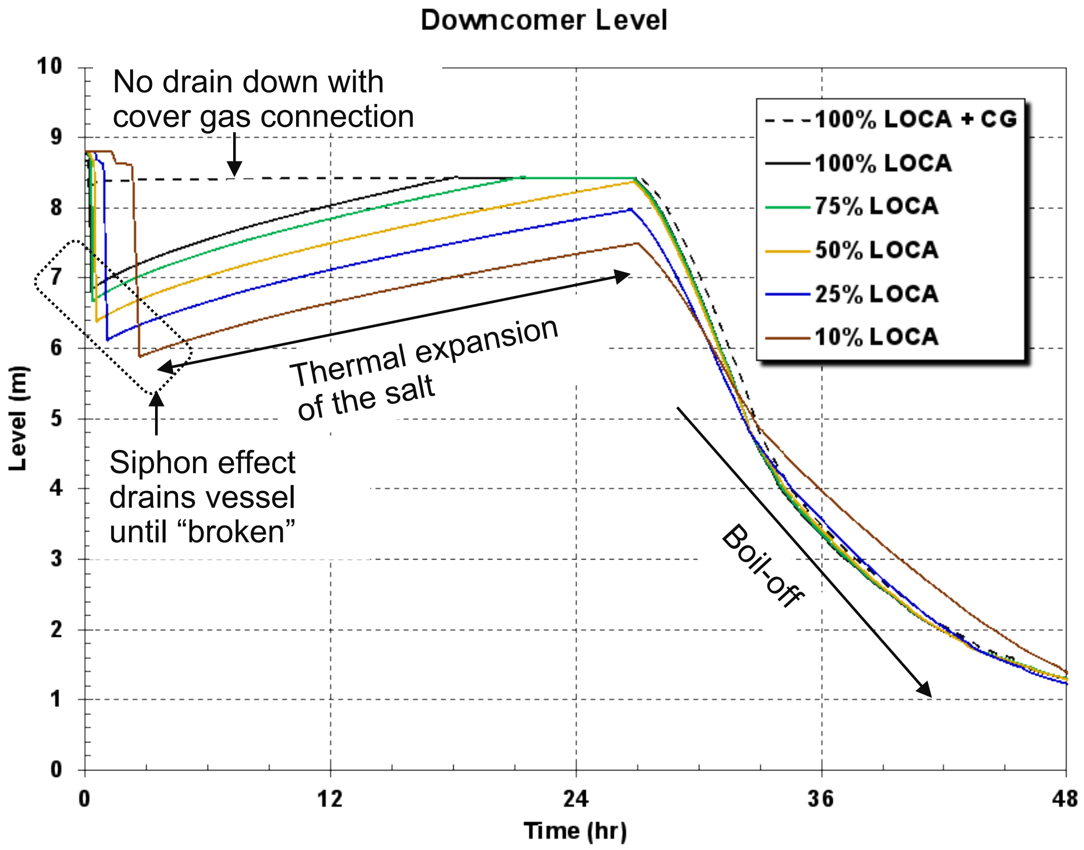
LOCA results (1/6)

10% to 100% LOCA size did not significantly impact vessel boiloff timing

Cover gas connection (+ CG) between hotwell and standpipe prevents siphon

- Stops initial drain down of vessel fluid
- No significant impact on vessel boiloff timing





LOCA results (2/6)

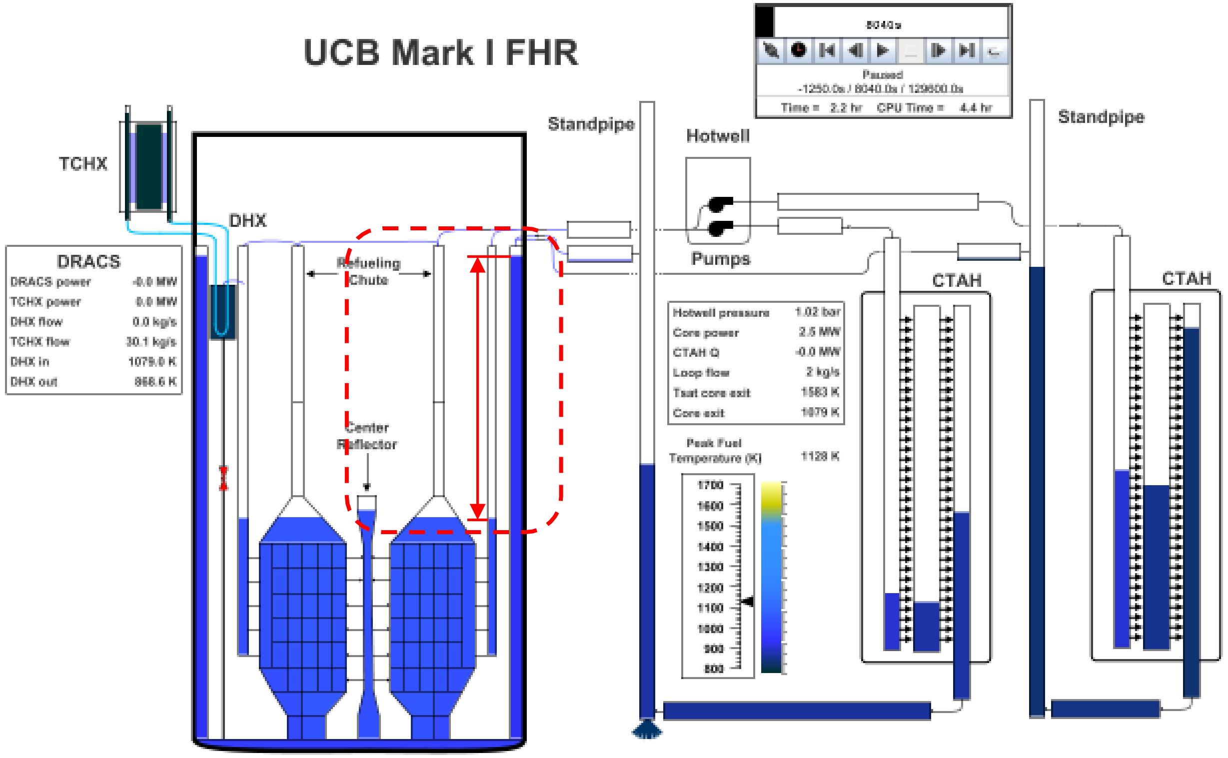
IIIELCOR

Liquid drain down initially creates siphon and then low pressure region

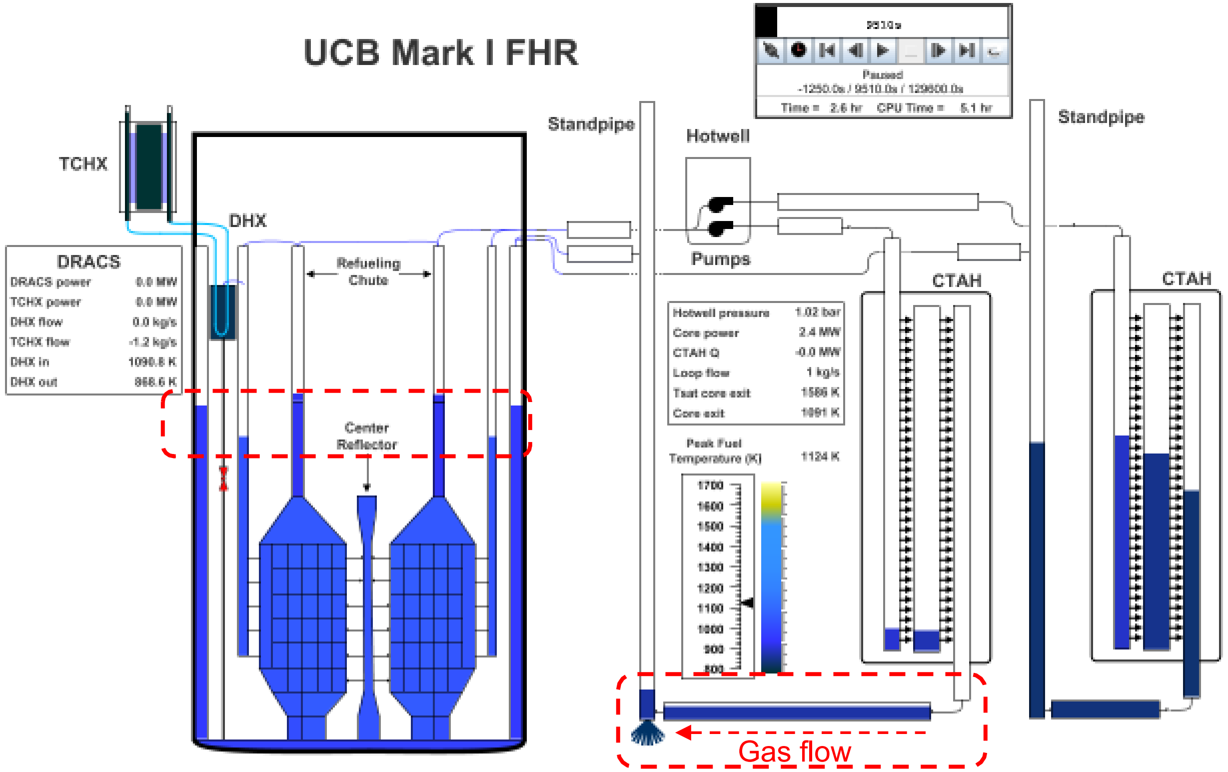
- Causes a level difference between the core and downcomer

Core and downcomer levels equilibrate once there is gas flow around the loop

- Standpipe connections to the cover gas system are closed



10% LOCA at maximum point in the “siphon”



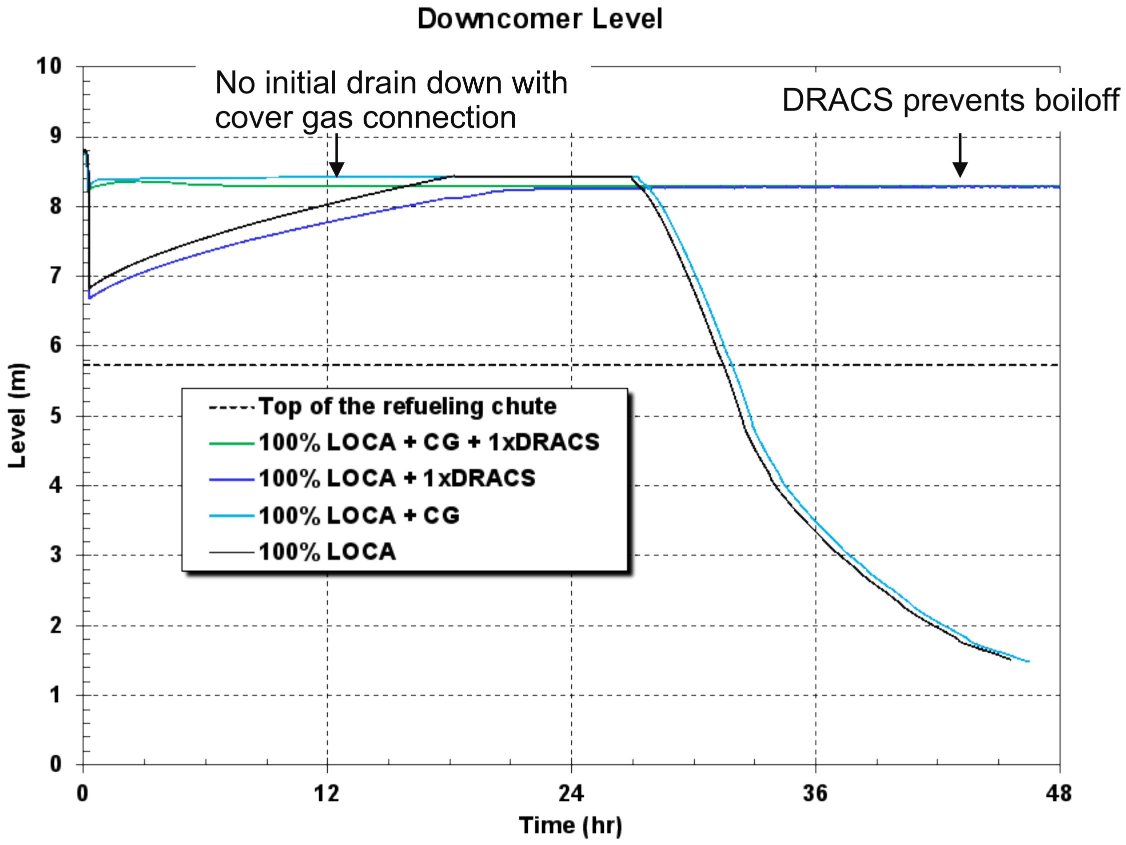
10% LOCA after equilibration

LOCA results **(3/6)**

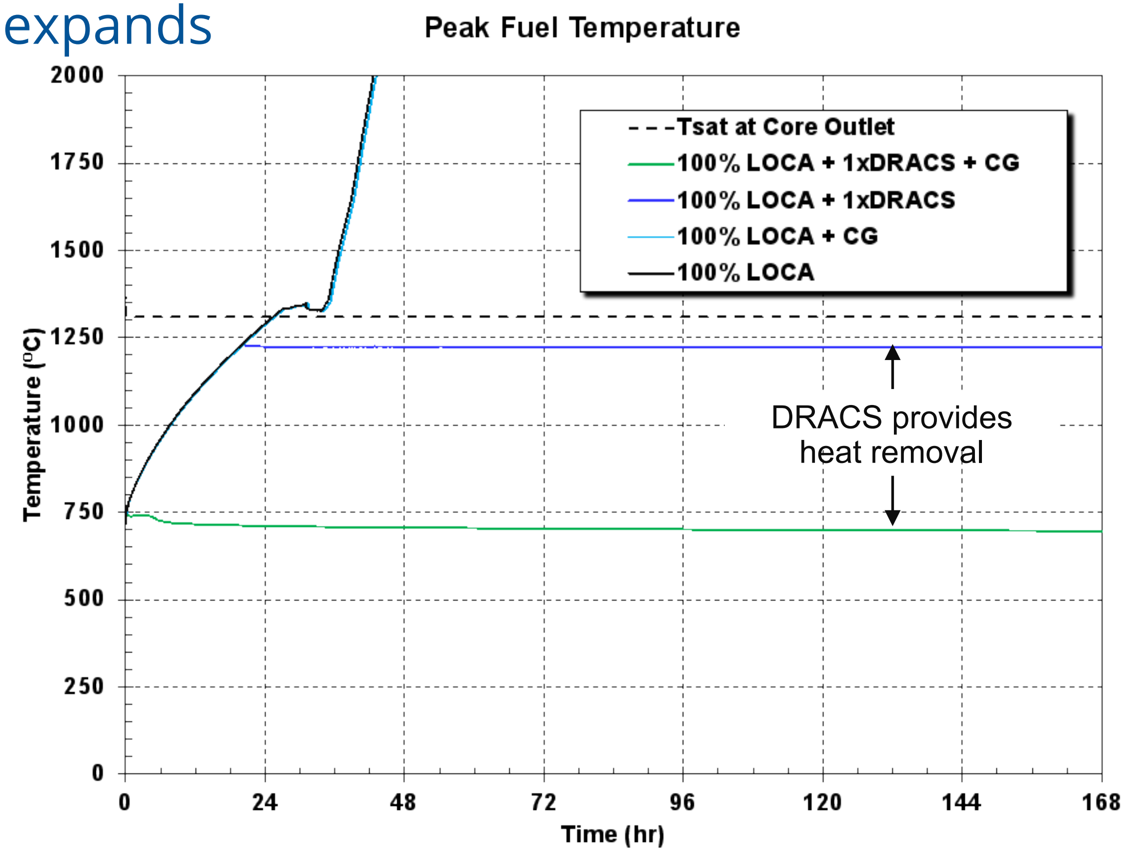
LOCA cases without DRACS proceed to fuel uncovery at ~31 hr

Connection through the cover gas system keeps the DRACS active during the drain down

Without the cover gas connection, the DRACS heat removal is delayed until the salt heats and expands



100% LOCA cases

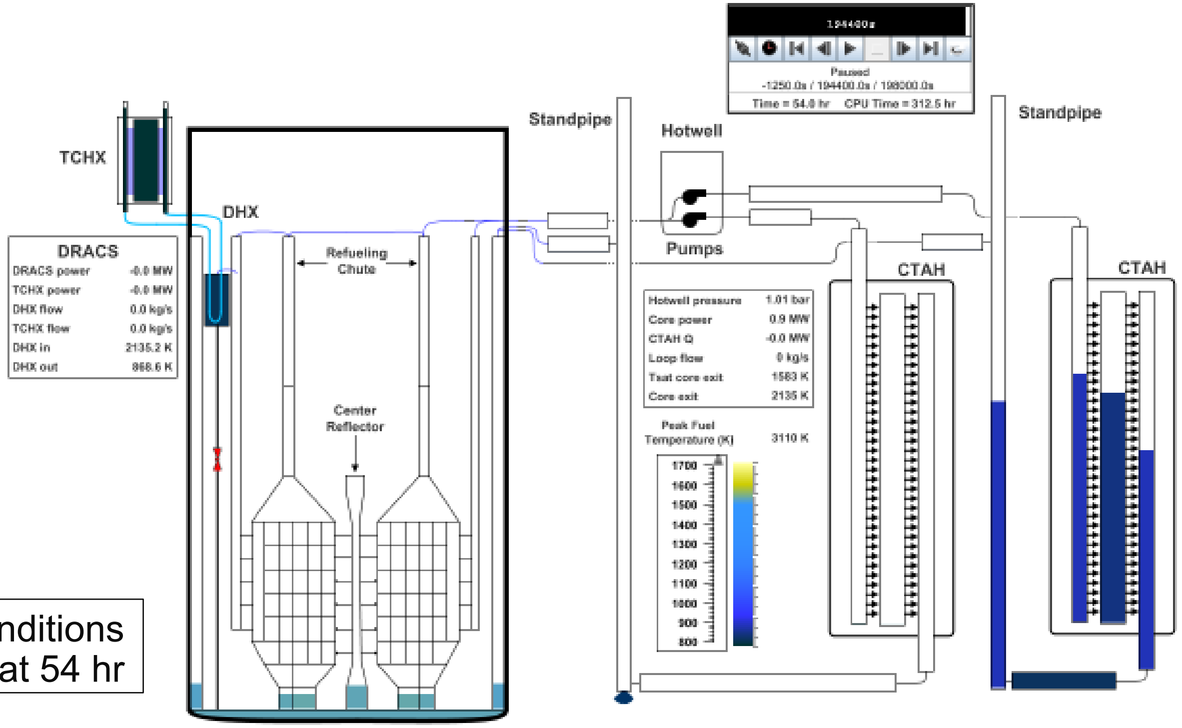


100% LOCA cases

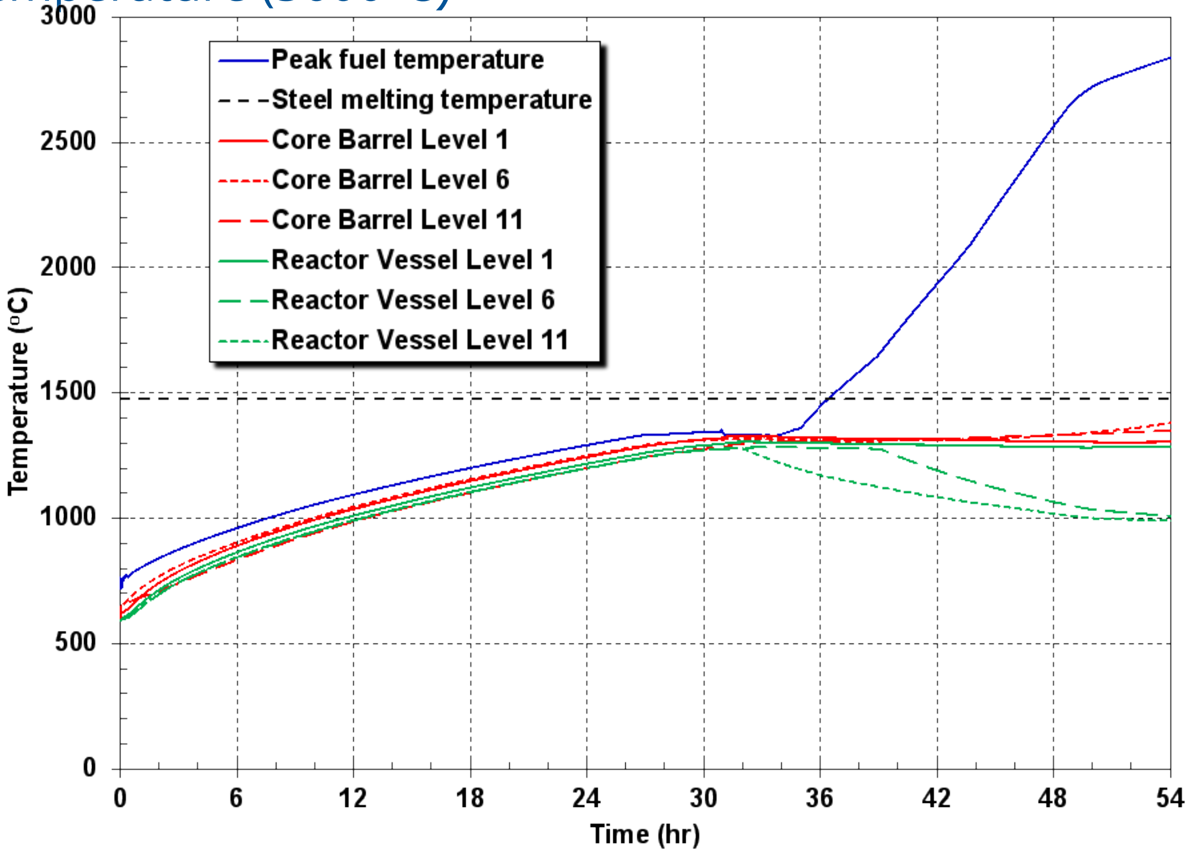
LOCA results (4/6)

We terminated the calculation at ~54 hr peak when the fuel kernel melting starts

- Reactor vessel wall and core barrel below the steel melting temperature
- Residual molten salt keeps the bottom level (level 1) at T_{sat}
- Upper vessel wall cools after downcomer salt level drops
- Pebbles and reflectors below graphite sublimation temperature (3600°C)



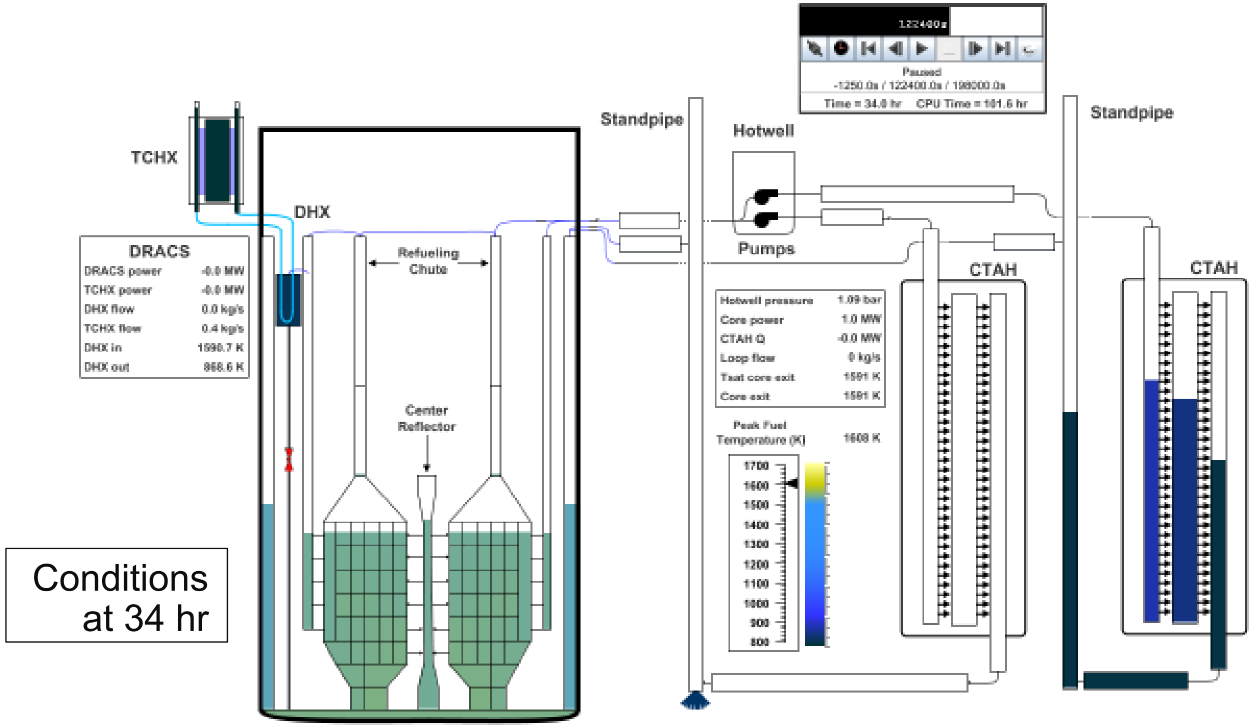
Conditions at 54 hr



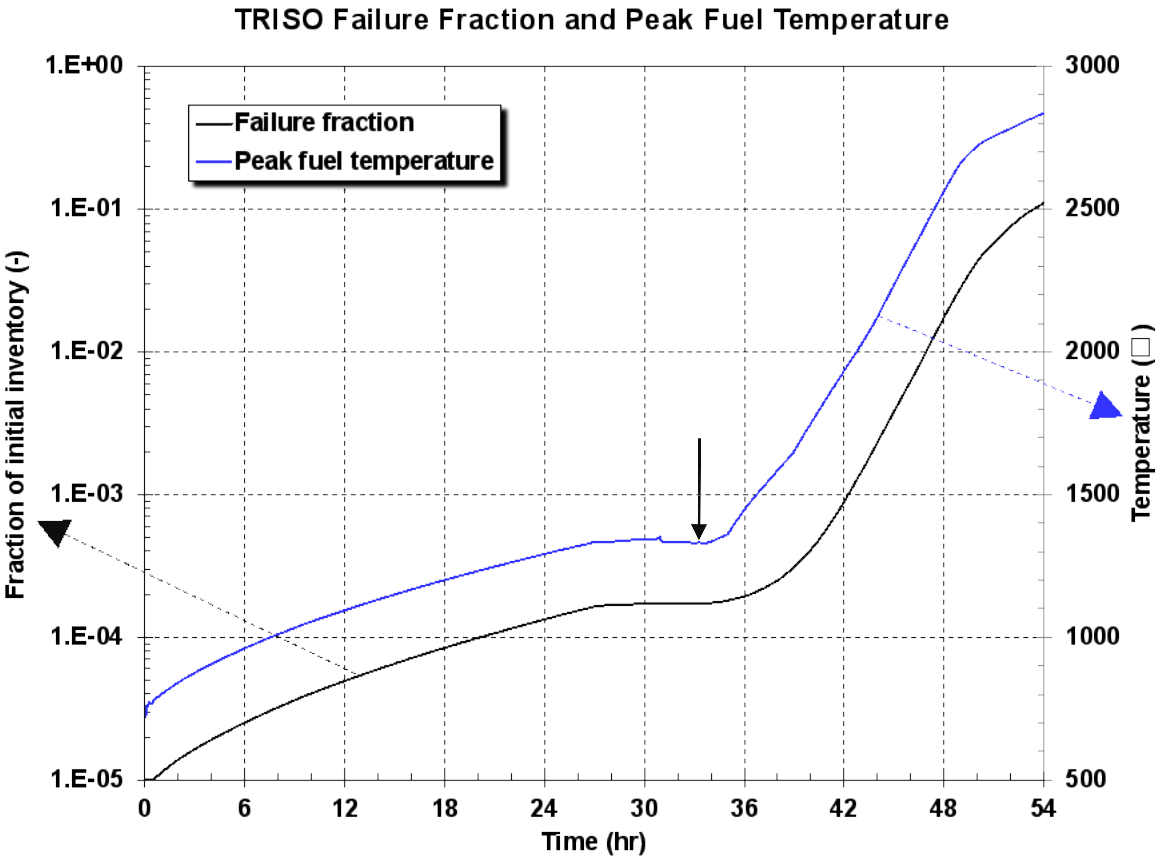
LOCA results (5/6)

TRISO failure rate extrapolated from available UO_2 TRISO data

- Correlation is based on data to 1800°C
- Initial failures set to 10^{-5} (0.001%)
- 0.017% of the TRISOs failed at 34 hr
- 7.5% of the TRISOs failed at 54 hr



Low failure rate when $<T_{sat}$



Note:
** Fuel used thermal-physical properties of UO_2.

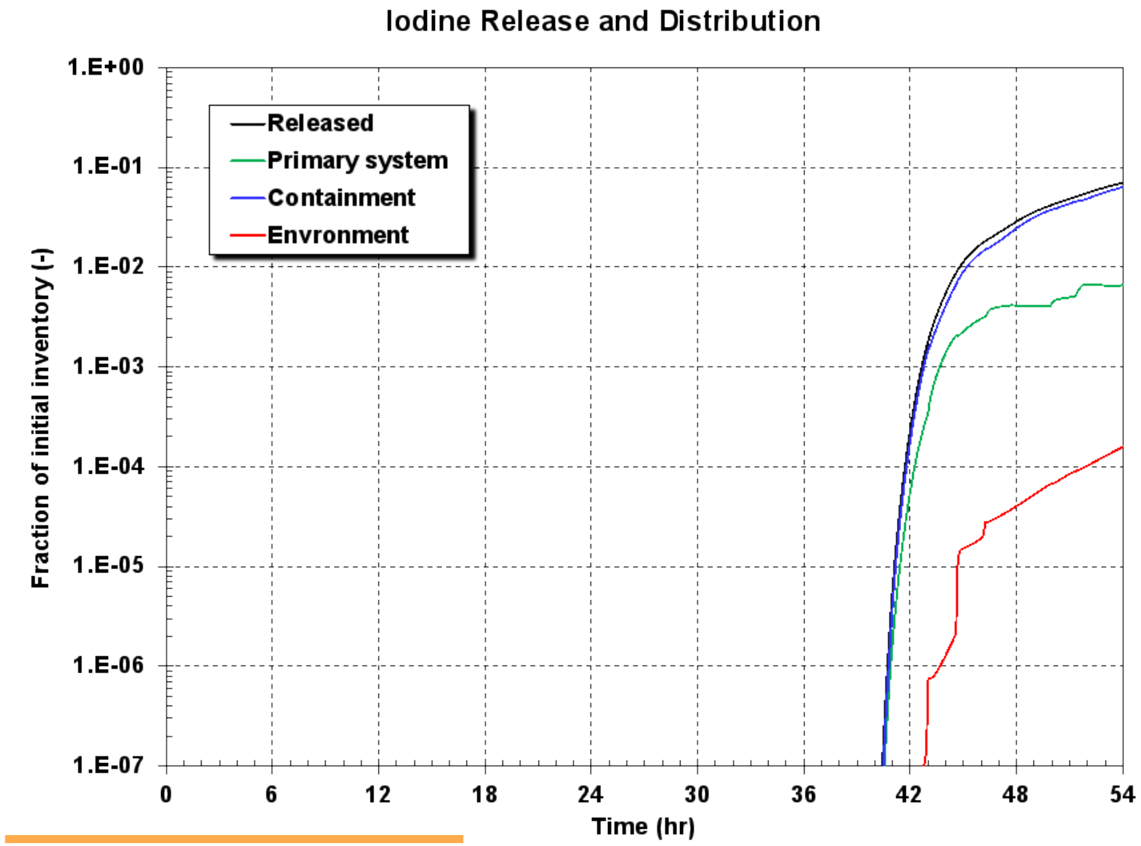
LOCA results **(6/6)**

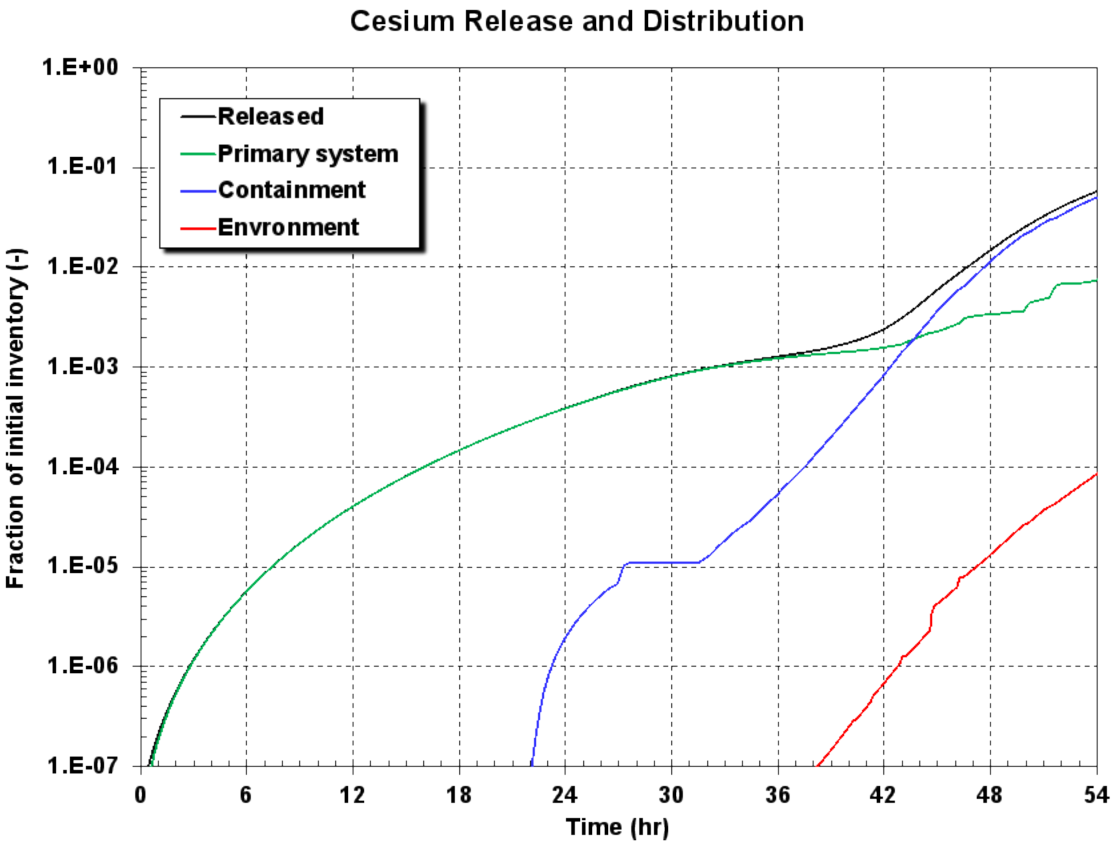
Most of the fission product release from fuel is retained in the containment

- Assumed hole size equivalent to 100% volume per day at 0.25 psig (8.7 in^2)

The radionuclide distribution is affected by the timing of the release from the TRISO

- Cesium release from the pebbles to the liquid molten salt starts earlier at lower fuel temperatures
- Most aerosols leaving the primary system settle in the containment





Cesium vaporization from the molten salt

ELCOR

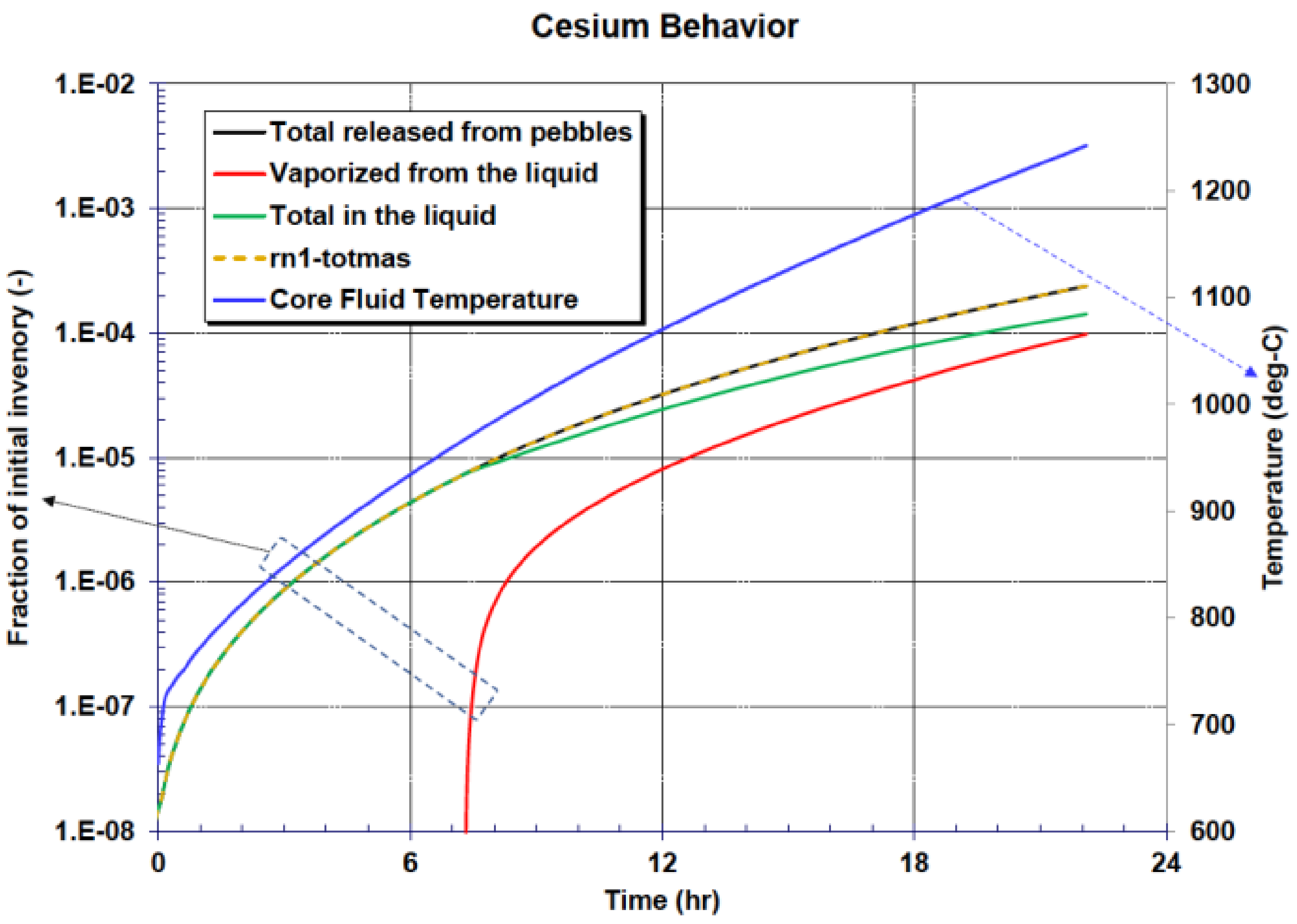
Molten salt chemistry and radionuclide release model calculates cesium and cesium fluoride release to the gas spaces

- Results use OECD/NEA JRC database for Thermochimica *
- Includes vapor phase data for CsF

LOCA sequence

- No accelerated steady state
- No core uncovery through 24 hr
  - Cesium releases are from pebbles → liquid → gas

Model shows Cs/CsF vaporization to gas spaces at higher temperatures



* With modifications by Ontario Tech.