SCALE/MELCOR Non-LWR Source Term Demonstration Project – Fluoride-Salt-Cooled High-Temperature Reactor (FHR)

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U.S.NRC Sandia



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Outline



NRC strategy for non-LWR source term analysis

Project scope

Overview of Fluoride-salt-cooled High-temperature Reactor (FHR)

FHR reactor fission product inventory/decay heat methods & results

MELCOR molten salt models

FHR plant model and source term analysis

Summary

Background slides

- SCALE
- MELCOR

Integrated Action Plan (IAP) for Advanced Reactors





IAP Strategy 2 Volumes



5

NRC strategy for non-LWR analysis (Volume 3)

Evaluation Model and Suite of Codes



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Role of NRC severe accident codes



Dose Criteria Reference Values (10 CFR 50/52)

- 1) An individual located at any point on the boundary of the exclusion area for any 2-hour period following the onset of postulated fission product release, would not receive a radiation dose in excess of 0.25 Sv (25 rem) total effective dose equivalent (TEDE)
- An individual located at any point on the outer boundary of the low population zone, who is exposed to the radioactive cloud resulting from the postulated fission product release (during the entire period of its passage), would not receive a radiation dose in excess of 0.25 Sv (25 rem) TEDE
- 3) Adequate radiation protection is provided to permit access to and occupancy of the control room under accident conditions without personnel receiving radiation exposures in excess of 0.05 Sv (5 rem) TEDE
- Dose criterion not in regulation but found in NUREG-0737/NUREG-0696. GDCs are applicable to light-water reactors. Non-LWRs will have principal design criteria (PDCs) which may have a similar requirement.

Project Scope





Project objectives

Understand severe accident behavior

• Provide insights for regulatory guidance

Facilitate dialogue on staff's approach for source term Demonstrate use of SCALE and MELCOR

- Identify accident characteristics and uncertainties affecting source term
- Develop publicly available input models for representative designs



Project scope

Full-plant models for three representative non-LWRs (FY21)

- Heat pipe reactor INL Design A
- Pebble-bed gas-cooled reactor PBMR-400
- Pebble-bed molten-salt-cooled UCB Mark 1

FY22

- Molten-salt-fueled reactor MSRE
- Sodium-cooled fast reactor To be determined



Project approach

- 1. Build MELCOR full-plant input model
 - Use SCALE to provide decay heat and core radionuclide inventory
- 2. Scenario selection
- 3. Perform simulations for the selected scenario and debug
 - Base case
 - Sensitivity cases

Advanced Reactor Designs





Fluoride-Salt-Cooled High-Temperature Reactor (FHR)





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Molten-salt reactors (1/3)



Aircraft Nuclear Propulsion Program (ANP) – 1946-1961

- Long-term strategic bomber operation using nuclear power
- ORNL developed the nuclear concept with the Aircraft Reactor Experiment (ARE)
 - Originally sodium cooled, but shifted to molten salt
 - 2.5 MW molten salt-cooled reactor operated for 96-MW-hours in November 1954
- Three Heat Transfer Reactor Experiments at Idaho National Laboratory to demonstrate the jet engine propulsion
- Aircraft Shield Test (AFT) B-36 with an operating reactor flew 47 times over West Texas and New Mexico to study shielding (i.e., the reactor was operating but not part of the propulsion system)
- Terminated due to inventing ballistic missile and supersonic aviation



The B-36 Aircraft Shield Test [https://en.wikipedia.org/wiki/Convair_NB-36H#/media/File:NB36H-1.jpg]



Heat Transfer Reactor Experiment #3 [https://en.wikipedia.org/wiki/Aircraft_Nuclear_Propulsion#/med ia/File:HTRE-3.jpg]

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Molten-salt reactors (2/3)

ORNL Molten Salt Reactor (MSR)

- AEC funded the Molten Salt Reactor Experiment (MSRE)
- Operated from 1965 to 1969
- 30 MWt
- Coolant was FLiBe molten salt
- Fuel was dissolved in coolant (molten fuel)





MSRE Graphite Core Structure [https://en.wikipedia.org/wiki/Molten-Salt_Reactor_Experiment]



Molten-salt reactors (3/3)



- Coolant is FLiBe molten salt
- Core is TRISO fuel in a pebble-bed geometry
- Design description
 - "Technical Description of the "Mark 1" Pebble-Bed Fluoride-Salt-Cooled High-Temperature Reactor (PB-FHR) Power Plant," [UCBTH-14-002]
 - "Pebble Bed Reactors Design Optimization Methods and their Application to the Pebble Bed Fluoride Salt Cooled High Temperature Reactor (PB-FHR)," University of California, Berkeley, 2013.
- Used for the SCALE/MELCOR demonstration project





UCB Mark 1 (1/4)

Reactor

- + 236 $\mathrm{MW}_{\mathrm{th}}$ / 100 MW_{e}
- Atmospheric pressure
- 600°C core inlet
- 700°C core outlet
- 976 kg/s core flowrate
- FLiBe molten salt coolant

Core

- 470,000 fueled pebbles + 218,000 unfueled pebbles in core and defueling chute
- 180 MWd/kgHM discharge burnup
- 19.9% enrichment
- Online refueling

Secondary system: gas-turbine at 18.6 bar with natural gas co-firing capability







UCB Mark 1 (2/4)

Recirculation loops

- Salt pumps in the hot well with FLiBe free surface
- 2X cross-over legs to coiled tube air heaters (CTAH)
- 2X cold legs with standpipes with free surface
- Drain tank with freeze valve



UCB Mark 1 (3/4)

Containment

- Most reactor and secondary components below-grade
- Compartmentalized building
- Low-free-volume reactor cavity with fire-brick insulation, steel liner, and concrete walls
- Shield building (above grade)



UCB Mark 1 (4/4)

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 thermosyphoncooled 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: Reactor coolant pump trip causes ball in valve to drop

Reactor cavity cooling subsystem (RCCS) surrounds reactor cavity

• Thermal protection of the concrete





UCB Mark 1 DRACS [UCBTH-14-002]

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UCB Mark 1 fuel

TRISO particle

- TRISO is a portmanteau of tristructural isotropic
- Kernel 1.5 g of UCO, 200 μm radius
- Porous carbon buffer layer
- 3 coatings to contain fission products

TRISO pebble

- Contains 4730 TRISO particles
- 30 mm diameter
- 1 mm graphite outer shell
- TRISO particles are distributed in the carbon matrix region between the solid core and outer shell



TRISO in a Fuel Pebble [http://fhr.nuc.berkeley.edu/wp-content/uploads/2014/10/PEBBLE-SCHEMATIC-V2.png]

Fluoride-salt-cooled High-Temperature Reactor Fission Product Inventory/Decay Heat Methods and Results







FHR analysis with SCALE

- Objective
 - Provide input for MELCOR accident simulation
 - Radionuclide inventory
 - Decay heat profile
 - Reactivity feedback coefficients
 - Reactivity from xenon transient
- Approach
 - Apply SCALE to generate fuel composition for an equilibrium core
 - Equilibrium core operated for several years so the average burnups are no longer changing
 - Evaluate neutronic characteristics



SCALE model of the UCB Mark 1 core

Workflow





• SCALE capabilities used:

- <u>Codes</u>:
 - ORIGEN for depletion
 - KENO-VI 3D Monte Carlo neutron transport
- <u>Data</u>: ENDF/B-VII.1 nuclear data library*

- <u>Sequences</u>:
 - CSAS for criticality/reactivity
 - TRITON for reactor physics & depletion

* A NUREG about *Nuclear Data Assessment for Advanced Reactors* summarizing the outcome of a recently concluded NRC-sponsored project is going to be published soon. 2

Neutronics overview (1/2)



Relevant characteristics and differences to High Temperature Gas-cooled Reactors:

- Fuel:
 - UCO fuel in TRISO particles in fuel pebbles
 - TRISO particles located in shell instead of sphere
- Coolant: FLiBe salt instead of helium
- Moderator: graphite





Neutronics overview (2/2)



• Challenges for modeling:

- Tritium production in FLiBe
- TRISO particles with very high packing fraction in shell
- Fuel pebble inlet and outlet geometry
- Fuel and unfueled/graphite pebbles in different zones of the core
- Validation
 - SCALE validation with HTGR experiments partially applicable*



UCB Mark 1 Model Description

Description	Value
Reactor power	236 MWth
UCO fuel density	10.5 g/cc
Uranium enrichment	19.9 wt.%
Fuel kernel radius	0.2 mm
Particle coating layer materials (starting from kernel)	Buffer/PyC/SiC/PyC
Fuel particle coating layer thickness	0.100/0.035/0.035/0.035 mm
Number of particles in pebble	4,730
Particle packing fraction in fuel pebble	40%
Radius of fuel pebble	1.5 cm
Inner/outer radius of fuel zone	1.25/1.40 cm
Number of fuel pebbles	470,000
Number of unfueled/graphite pebbles	218,000
Pebble packing fraction	60%
Core Inner reflector radius	35 cm
Outer fuel pebble region radius	105 cm
Outer graphite pebble region radius	125 cm
Volume of active fuel region	10.4 m ³
Average pebble thermal power	500 W
Average pebble discharge burnup	180 GWd/MTIHM
Average pebble full-power lifetime	1.40 years





SCALE model developed based on:

[1] A. T. Cisneros, "Pebble Bed Reactors Design Optimization Methods and their Application to the Pebble Bed Fluoride Salt Cooled High Temperature Reactor (PB-FHR)," University of California, Berkeley, 2013.
[2] C. Andreades et al., "Technical Description of the "Mark 1" Pebble-Bed Fluoride-Salt-Cooled High-Temperature Reactor (PB-FHR) Power Plant," Berkeley, CA, UCBTH-14-002, 2014.

Analysis areas

- 1. Verification of multigroup physics
- 2. Generation of equilibrium core
- 3. Power profile and neutron spectrum
- 4. Temperature feedback
- 5. Decay heat
- 6. 1-group cross sections
- 7. Tritium production
- 8. Xenon reactivity





SCALE model of the UCB Mark 1 core

1. Verification of multigroup physics for UCB Mark 1

 Comparison of multigroup (MG) calculation with continuous energy (CE) calculations for a pebble depletion problem

• Why not always run CE?

- Significant modeling time: random distributions or particle arrays without permitting particle clipping
- Significant computation time: many cells/surfaces (consider thousands of particles) and use of CE data

SCALE's MG approach for double-heterogeneous systems:

- Two self-shielding calculations: (1) particle in graphite matrix,
 (2) pebble in lattice of pebbles
- Generation of problem-dependent cross sections for the fuel region through user-friendly input block
- The MG calculation is 5 times faster than the CE lattice calculation, and 24 times faster than the CE calculation with a random particle distribution





SCALE model a UCB Mark 1 pebble in a cube surrounded by FLiBe

Calculation:

- TRITON/KENO-VI CE and MG
- Depletion calculation to reach discharge burnup of 180 GWd/tHM
- Comparison between calculations: k-eff, nuclide densities, runtime



1. CE model: Random particle distribution

- 2. CE model: particle lattice (no clipping)
- 3. CE model: particle lattice (clipping)



1. Single pebble models







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4. MG model

Note:

- CE-random results are ٠ average of 10 realizations
- All models contain the ٠ same amount of fuel

1. Single pebble initial criticality



Model		C	ZP	HFP		
		k _{eff}	Δρ [pcm]	k _{eff}	Δρ [pcm]	
CE, random	no clipping	1.52539	(ref)	1.44765	(ref)	
CE, lattice	no clipping	1.52449	-39	1.44738	-13	
CE, lattice	clipping	1.51939	-259	1.44092	-323	
MG		1.51986	-239	1.44426	-162	

- **CZP**: all materials 300K
- **HFP**: Fuel 1003K, TRISO layers 973K, graphite center 983K, outer graphite shell 957K, coolant 923K
- All statistical errors of the Monte Carlo calculations < 20 pcm

Result: MG k_{eff} calculations show good agreement with reference CE result independent of the temperature

1. Single pebble k_{eff} over the course of depletion



Calculation details:

- TRITON-KENO depletion of the HFP case
- 540.54 days at 333 MW/MTIHM

Result: MG bias remains below 260 pcm over depletion

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1. Single pebble nuclide density comparison over depletion CAK RIDGE

Comparison of MG against CE random:



Result: MG bias remains below 3% for relevant nuclide densities over depletion

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1. MG performance summary for UCB Mark 1



- We confirmed the performance of SCALE's MG capability for double-heterogeneous systems in terms of k_{eff} and nuclide densities in a UCB Mark 1 single pebble depletion calculation
- SCALE's MG capability permits the calculation of accurate results in a much-reduced runtime (factor of 24 when compared to reference CE calculations)

2. Generation of equilibrium full core





Goal: Determine fuel composition of pebbles in a full core corresponding to an equilibrium state

Boundary conditions:

- Pebble final discharge burnup: 180 GWd/tHM
- Average number of passes per pebble: 8
- Average power: 333 MW/tHM
- Rods fully withdrawn

Full core model discretization:

- 10 axial zones of equal volume
- 3 radial zones with 1/8th, 6/8th, 1/8th fractional volumes

Assumptions:

- All pebbles within a zone contain the same fuel composition
- Fuel composition within a zone represents average of individual pebbles of different passes/burnups in this zone

2. Generation of isotopics for an equilibrium state





Fuel pebble burnup (GWd/MTIHM) in each axial zone depending on the pass through the core assuming constant axial/radial power:

	pass through the core							
axial zone		2	3	4	5	6	7	8
10	21.4	43.9	66.4	88.9	111.4	133.9	156.4	178.9
9	19.1	41.6	64.1	86.6	109.1	131.6	154.1	176.6
8	16.9	39.4	61.9	84.4	106.9	129.4	151.9	174.4
7	14.6	37.1	59.6	82.1	104.6	127.1	149.6	172.1
6	12.4	34.9	57.4	79.9	102.4	124.9	147.4	169.9
5	10.1	32.6	55.1	77.6	100.1	122.6	145.1	167.6
4	7.9	30.4	52.9	75.4	97.9	120.4	142.9	165.4
3	5.6	28.1	50.6	73.1	95.6	118.1	140.6	163.1
2	3.4	25.9	48.4	70.9	93.4	115.9	138.4	160.9
1	1.1	23.6	46.1	68.6	91.1	113.6	136.1	158.6

Mix fuel compositions of these burnups to get average composition of axial zone 3

2. Approach to generate equilibrium inventory



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2. Slice depletion model

Pebbles containing averaged equilibrium core fuel composition (not changing during depletion)





Why a slice and not a single pebble:

- Representative moderator/fuel ratio
- Representative neighboring conditions (spectral effects)

Depletion model:

- Slice through center of the core
- Depletion of surrogate pebbles surrounded by coreaverage fuel composition
- Axially reflected, radially vacuum boundary conditions



(always starting with fresh fuel, depleted during depletion)



2. K_{eff} and nuclide density convergence

Outer iteration 1 using constant core power



- Outer iteration 1: convergence of k_{eff} and nuclide densities achieved after 8 inner iterations
- Outer iteration 2 using 3D power map showed similar convergence behavior



3. Full core power profile



3. Example fuel cell flux spectrum comparison





- UCB Mark 1 and PBMR show a larger thermal peak compared to LWR
- UCB Mark 1 shows smaller fast flux due to scattering with the salt



Elastic scattering cross section

3. Energy-dependent flux profile







3. 3D full core flux visualizations









Total flux at the axial center of the core

3.45e-05 - 3.59e-05 3.30e-05 - 3.45e-05 3.16e-05 - 3.30e-05 3.02e-05 - 3.16e-05 2.87e-05 - 3.02e-05 2.73e-05 - 2.87e-05 2.58e-05 - 2.73e-05 2.44e-05 - 2.58e-05 2.30e-05 - 2.44e-05 2.15e-05 - 2.30e-05 2.01e-05 - 2.15e-05 1.87e-05 - 2.01e-05 1.72e-05 - 1.87e-05 1.58e-05 - 1.72e-05 1.44e-05 - 1.58e-05 1.29e-05 - 1.44e-05 1.15e-05 - 1.29e-05 1.01e-05 - 1.15e-05 8.62e-06 - 1.01e-05 7.18e-06 - 8.62e-06 5.74e-06 - 7.18e-06 4.31e-06 - 5.74e-06 2.87e-06 - 4.31e-06 1.44e-06 - 2.87e-06

2.81e-14 - 1.44e-06

Fast flux, E > 0.625 eV

Thermal flux, E < 0.625 eV

3. Radial flux distribution at axial core center (axial zone 5)



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3. Axial flux distribution in the fuel region







4. Reactivity coefficients

- Isothermal temperature coefficient calculation:
 - k_{eff} calculations with material temperatures varying over a range of several hundred K
 - Assuming constant temperature within material
 - Fitting of reactivity ρ to determine coefficient
- β_{eff} and coolant void coefficient

Valu

Quantity

Coolant void

β_{eff}

Nominal temperatures:

- Fuel: 1003 K
- Salt coolant: 923 K
- Graphite moderator*: 973/983 K
- Inner graphite reflector: 873 K
- Outer graphite reflector: 973 K

*All carbonaceous materials in fuel pebbles

	Component	Temperature Reactivity Coefficient at nominal temperature [pcm/K]	
ie [pcm]	Salt coolant	-0.48	Einear fit
541 ± 20	Fuel	-3.90	
5094 <u>+</u> 21	Graphite moderator	-1.10	Slope from
	Inner graphite reflector	+1.21	polynomial fit
	Outer graphite reflector	+0.61	



 2σ statistical error bars are displayed

4. Isothermal temperature coefficients



- 1. Linear fit for salt temperature coefficient
- Polynomial fit or tabulated values for fuel, 2. moderator, and graphite temperature coefficients

	a	b	С	d
Fuel	4.57E-02	-7.08E-05	1.59E-08	
Moderator	-2.02E-03	-2.48E-05	3.88E-08	-2.16E-11
Inner graphite	-2.18E-02	2.07E-05	-7.55E-09	
Outer graphite	-3.10E-02	3.49E-05	-1.31E-08	

 $\rho = a + bT + cT^2 + dT^3$

1000

1200

1400



46

5. Generation of decay heat file for MELCOR



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5. Generation of decay heat file for MELCOR



Relative contribution of top fission products

Relative contribution of top actinides



5. Decay heat comparisons





- UCB Mark 1: equilibrium core
- PWR: approximate end of cycle core (mixture of assemblies at burnup of 20, 40, 60 GWd/tHM)

6. Towards rapid inventory calculations with ORIGAMI

Purpose of 1-group cross section analysis: understand the spectral variations and their impact on 1-group cross sections which influence all inventory calculations



 Only small variation of 1group removal cross section over depletion

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• Small changes visible mainly in Pu-240

6. Axial variation of 1-group removal cross section



51

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6. Radial variation of 1-group removal cross section Actional Laboratory





Radial variation:

Significant radial variation for various nuclides

IRC

7. Tritium production

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Tritium overview

- FHR uses FLiBe coolant
 - Lithium is enriched to >99.5%
 Li-7 because Li-6 is a neutron poison
- Li-6 and Li-7 react with neutrons to produce tritium
 - ${}^{6}\text{Li} + n \rightarrow {}^{4}\text{He} + {}^{3}\text{H}$
 - $^{7}\text{Li} + n \rightarrow {}^{4}\text{He} + {}^{3}\text{H} + n'$
- Tritium is a potential radiological dose hazard

- Mass of FLiBe defined in the ORIGEN model is the total FLiBe mass in the entire system
 - To irradiate just the FLiBe in the core at a given time, we scale the flux in our ORIGEN model based on what volume fraction of FLiBe is in the core
- ORIGEN flux is equal to $\phi \times \left(\frac{V_{core}}{V_{total}}\right)$
- Determine the flux spectrum and 1-group cross sections in FLiBe in this core
- Irradiate FLiBe using explicit flux magnitude scaled based on the fraction of system FLiBe in the core at any given time

7. Equilibrium tritium production rate

- SCALE-predicted equilibrium value is 0.021 mol/day
 - Equilibrium value from Cisneros was 0.023 mol/day
- Equilibrium is a balance between Li-6 production and destruction
 - ${}^{9}\text{Be} + n \rightarrow {}^{4}\text{He} + {}^{6}\text{Li} + e^{-} + \overline{\nu_{e}}$
 - ${}^{6}\text{Li} + n \rightarrow {}^{4}\text{He} + {}^{3}\text{H}$
- The calculated behavior is consistent with established trends in the literature





55

7. Sensitivity analysis on tritium production

- We ran 5,000 combinations of initial Li-7 enrichment and flux using SAMPLER to determine their impact on equilibrium tritium production
- Variations in initial tritium production rate are quite large and depend on flux and initial Li-7 enrichment
 - Li-6 is a neutron poison, so FHR systems seek to enrich coolant in Li-7
 - Natural Li is 7.59% Li-6

Property	Minimum Value	Maximum Value
Flux (n/cm ² -s)	3.528x10 ¹⁴	4.312x10 ¹⁴
Initial Li-7 Enrichment (w/o)	99.95	100.0





7. Sensitivity analysis on tritium production

Initial Li-7 enrichment has no effect on *equilibrium tritium* production rate, while flux has a significant impact



No correlation for initial Li-7 enrichment

Strong correlation for neutron flux

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8. Transient xenon reactivity

- Steady-state Xe-135 reactivity worth is -6.48\$
- Using equilibrium I-135 and Xe-135 concentrations from UCB Mark 1 model, we can calculate time-dependent concentrations analytically
- When flux goes to zero, Xe-135 inventory is dictated only by decay of I-135 and Xe-135
- Peak Xe-135 reactivity is -18.6\$ and occurs at 9.49 hours
- Xe-135 reactivity drops below steadystate value after 34.67 hours



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Neutronics Summary

Demonstrated SCALE's capabilities for FHR modeling

- SCALE's multigroup physics was confirmed adequate through FHR fuel pebble analysis: k_{eff} bias smaller than 260 pcm, while achieving 24 times faster runtime
- Fuel compositions for an equilibrium core were developed using an iterating scheme
- Power profiles and decay heat were determined for equilibrium core
- Temperature feedback: linear behavior found for salt, nonlinear trend for fuel and for materials containing graphite
- Strong radial variation for 1-group cross section was observed, while axial variation was limited to inlet/outlet regions
- Tritium production rate in coolant salt was estimated
- Preliminary results for time-dependent Xe-135 concentration



MELCOR Molten Salt Models



MELCOR Molten Salt Reactor Modeling

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





Core components

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



- 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

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TRISO particle

0.045

0.025 Fuel Compact Radius [m]

Radionuclide Diffusion Release Model



Intact TRISO Particles

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

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



		-		-	-	-	
Padionuclida	UO	UCO	DyC	Porous	SiC	Matrix	TRISO
Radionucilde	002	000	1 yC	Carbon	SIC	Graphite	Overall
Ag	Some	g	Some		Extensive	Some	Extensive
Cs	Some	gate	Some	р	Extensive	Some	Some
Ι	Some	stig	Some	onr	Some	Not found	Not found
Kr	Some	лvе	Some	ot f	Not found	Some	Some
Sr	Some	ot i	Some	ž	Extensive	Some	Some
Xe	Some	Ž	Some		Some	Some	Not found

Diffusivity Data Availability

Data used in the demo calculation [IAEA TECDOC-0978]

	FP Species							
	Kr		Cs		Sr		Ag	
D (m ² /s) Q D (m ² /s) Q		Q	D (m ² /s)	Q	D (m2/s)	Q		
Layer		(J/mole)		(J/mole)		(J/mole)		(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

lodine assumed to behave like Kr

Radionuclide Release Models

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- 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

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

Steam oxidation

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

Air oxidation

Reactions

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

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

Reactions

1. $C + O_2 \rightarrow CO_2(g)$

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

 $R_{OX} = 1.7804 \, x 10^4 \, \exp\left(-\frac{20129}{T}\right) \left(\frac{P}{0.21228 \, x 10^5}\right)^{0.5}$

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

4. $C + CO_2(g) \rightarrow 2CO(g)$



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

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

Energy Transport between Discrete Core Volumes



Effective conductivity prescription for pebble bed (bed conductance)

• Zehner-Schlunder-Bauer, without radiation heat transfer

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

where:

- $\varepsilon = \mathrm{Bed}\ \mathrm{porosity}\ [-]$
- $k_f =$ Fluid (FLiBe) conductivity [W/m/K]
- $k_c =$ Effective bed conductivity [W/m/K], used with zero radiative conductivity
- $k_s = \text{Solid conductivity [W/m/K]}$
- 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

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

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



Interface Between Thermal Hydraulics and Reactor Core Structures



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

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

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

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	C₃	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

Standard treatment

$$\frac{dP}{dt} = \left(\frac{\rho - \beta}{\Lambda}\right)P + \sum_{i=1}^{6} \lambda_i Y_i + S_0$$
$$\frac{dY_i}{dt} = \left(\frac{\beta_i}{\Lambda}\right)P - \lambda_i C_i, \quad for \ i = 1 \dots 6$$

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)



Derived from standard PRKEs and solved similarly

$$\begin{split} \frac{dP(t)}{dt} &= \left(\frac{\rho(t) - \bar{\beta}(t)}{\Lambda}\right) P(t) + \sum_{i=1}^{6} \lambda_i C_i^C(t) + S_0 \\ \frac{dC_i^C(t)}{dt} &= \left(\frac{\beta_i}{\Lambda}\right) P(t) - \left(\lambda_i + 2/\tau_c\right) C_i^C(t) + \left(\frac{V_L}{V_c}\right) \left(\lambda_i + 2/\tau_L\right) C_i^L(t), \qquad i = 1 \dots 6 \\ \frac{dC_i^L(t)}{dt} &= \left(\frac{V_c}{\tau_c V_L}\right) C_i^C(t) - \left(\lambda_i + 1/\tau_L\right) C_i^L(t), \qquad i = 1 \dots 6 \\ \bar{\beta}(t) &= \beta - \beta(t)_{lost} = \beta - \left(\frac{\Lambda}{P(t)}\right) \sum_{i=1}^{6} \lambda_i C_i^L(t) \end{split}$$

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

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



Fluoride-salt-cooled High-Temperature Reactor Plant Model and Source Term Analysis





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 overpressurized

Secondary-side air cools primaryside 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)



Equilibrium inventory and decay heat from SCALE

Radial and axial power profiles from SCALE

Reactivity feedbacks from SCALE

Cell-to-cell radial and axial heat transfer in the pebble bed and to adjacent reflector structures

- Modified Zehner-Schlunder-Bauer model formulation
- Combined conductive and radiative (when core uncovered) heat transfer depends on the coolant and fuel conductivities, fuel (graphite) emissivity, pebble bed porosity

Pebble bed friction losses – Achenbach pressure drop formulation

•
$$K_{loss} = 2 + 320 \left(\frac{(1-\epsilon)}{Re}\right) + 20 \left(\frac{(1-\epsilon)}{Re}\right)^{0.4}$$

Pebble to fluid heat transfer within a cell

• Forced convection using Wakao correlation, $Nu = 2 + 1.1 Re^{0.66} Pr^{0.33}$



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 UO₂ TRISO pebbles
 - UO₂ 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





Scenarios



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

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 10⁵ s (T_{sat}~ 1350 °C)





ATWS with variable DRACS – (Linear scale)

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





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)

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48

84

DRACS cases illustrate degraded response

- Results for fraction of 1xDRACS
- <u>></u>40% of one DRACS stops the temperature rise within 48 hr

Peak Fuel Temperature

DRACS power follows heat removal requirements

• 1xDRACS exceeds decay heat within 3 hr

Decay Heat and DRACS Heat Rejection





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 UO₂ TRISO diffusivity and UO₂ failure data were used. Both are changeable through user input with design-specific data. ⁸⁵



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)



86



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



Downcomer Level

48

LOCA results (2/6)



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)

No initial drain down with

----- Top of the refueling chute

100% LOCA + 1xDRACS

100% LOCA + CG

-100% LOCA

12

100% LOCA + CG + 1xDRACS

cover gas connection

10

9

8

7

6

5

4

3

2

1

0

Level (m)

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

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

Peak Fuel Temperature





100% LOCA cases

24

Time (hr)

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)





3000

2500

2000 ව

femperature (

1000

500

54

48

TRISO Failure Fraction and Peak Fuel Temperature

LOCA results (5/6)

TRISO failure rate extrapolated from available UO₂ 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



1.E+00

1.E-01

Failure fraction

Peak fuel temperature

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 in²)

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



94

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



Summary





Conclusions

- Demonstrated use of SCALE and MELCOR for FHR safety analysis
- Simulated the entire accident starting with the initiating event
 - system thermal hydraulic response
 - fuel heat-up
 - heat transfer through the reactor to the surroundings
 - radiological release
- Evaluated effectiveness of passive mitigation features

Background Slides



Further SCALE analysis details



Comparison of the FHR with other concepts

	Mk1 PB-FHR	ORNL 2012 AHTR	Westing- house 4-loop PWR	PBMR	S- PRISM
Coolant	flibe	flibe	water	helium	sodium
Core inlet/outlet temperatures (°C)	600-700	650-700	292/326	500/900	355/510
Reactor thermal power (MWt)	236	3400	3411	400	1000
Reactor electrical power (MWe)	100	1530	1092	175	380
Fuel enrichment †	19.90%	9.00%	4.50%	9.60%	8.93%
Fuel discharge burn up (MWt-d/kg)	180	71	48	92	106
Fuel full-power residence time in core (yr)	1.38	1.00	3.15	2.50	7.59
Power conversion efficiency	42.4%	45.0%	32.0%	43.8%	38.0%
Core power density (MWt/m3)	22.7	12.9	105.2	4.8	321.1
Fuel average surface heat flux (MWt/m2)	0.189	0.285	0.637	0.080	1.13
Fuel specific surface area (area/volume) (1/m)	120	45	165	60	285
Reactor vessel diameter (m)	3.5	10.5	6.0	6.2	9.2
Reactor vessel height (m)	12.0	19.1	13.6	24.0	19.6
Reactor vessel specific power (MWe/m3)	0.866	0.925	2.839	0.242	0.292
Start-up fissile inventory (kg-U235/MWe) ††	0.79	0.62	2.02	1.30	6.15
EOC Cs-137 inventory in core (g/MWe) *	30.8	26.1	104.8	53.8	269.5
EOC Cs-137 inventory in core (Ci/MWe) *	2672	2260	9083	4667	23359
Spent fuel dry storage density (MWe-d/m3)	4855	2120	15413	1922	
Natural uranium (MWe-d/kg-NU) **	1.56	1.47	1.46	1.73	121
Separative work (MWe-d/kg-SWU) **	1.98	2.08	2.43	2.42	- 14 - I



[†] For S-PRISM, effective enrichment is the Beginning of Cycle weight fraction of fissile Pu in fuel

†† Assume start-up U-235 enrichment is 60% of equilibrium enrichment; for S-PRISM startup uses fissile Pu

* End of Cycle (EOC) life value (fixed fuel) or equilibrium value (pebble fuel)

** Assumes a uranium tails assay of 0.003.

C. Andreades et al., "Technical Description of the "Mark 1" Pebble-Bed Fluoride-Salt-Cooled High-Temperature Reactor (PB-FHR) Power Plant," Berkeley, CA, UCBTH-14-002, 2014.



1. Single pebble nuclide density over depletion



1. Single pebble nuclide density comparison over depletion Content Laboratory Internal Laboratory

Comparison of MG against CE random:



Result: MG bias remains below 3% for relevant nuclide densities over depletion

1. Single pebble nuclide density comparison of against reference CE random results





CE, lattice, clipped



200

200







1. Single pebble runtime comparison

Monte Carlo calculation settings:

- 25,000 neutrons per cycle in 500 active and 100 inactive generations
- 1 node with 32 processors

Model		Runtime [min]
CE, random	no clipping	~79 (per realization)
CE, lattice	no clipping	15.28
CE, lattice	clipping	15.78
MG		3.25



SCALE model a UCB Mark 1 pebble in a cube surrounded by FLiBe



2. Generation of isotopics for an equilibrium state

Zone-wise power

profile

zone-wise fuel composition

Outer iteration 1:

- Flat axial power profile
- Consider only axial zones
- No radial zones or radial power distribution
- Outer iteration 2:
 - Use axial and radial power profile from outer iteration 1
 - Consider axial and radial zones
 - Additional assumption: homogenization of compositions of all radial zones after each pass \rightarrow initial composition for next pass





2. Convergence of results during iterations

i	t _{final} (days)	bu _{final} (^{GWd} / _{tHM})	$\frac{bu_{final}}{180 \ GWd/tHM} - 1$	k _{eff}	$k_i - k_{i-1}$ (pcm)	$N_D^{235}\mathrm{U}_{(atoms/_{b-cm})}$	$\frac{N_{D_i}}{N_{D_{i-1}}} - 1$	$N_D {}^{239}{ m Pu}$ (atoms/b-cm)	$\frac{N_{D_i}}{N_{D_{i-1}}} - 1$
0	540.54	144.56	-19.69%	1.32689	_	2.454E-03	_	2.063E-04	_
1	673.08	194.90	8.28%	1.03112	-29577	2.257E-03	-8.00%	2.147E-04	4.10%
2	621.63	187.44	4.13%	1.00464	-2648	2.273E-03	0.71%	2.104E-04	-2.02%
3	596.95	182.68	1.49%	1.00680	216	2.294E-03	0.91%	2.098E-04	-0.27%
4	588.21	180.39	0.22%	1.00954	274	2.304E-03	0.44%	2.102E-04	0.16%
5	586.94	180.15	0.08%	1.01046	92	2.307E-03	0.14%	2.114E-04	0.59%
6	586.45	180.01	0.00%	1.01120	74	2.314E-03	0.27%	2.123E-04	0.40%
7	586.43	179.84	-0.09%	1.01128	8	2.315E-03	0.04%	2.126E-04	0.18%
8	586.95	179.95	-0.03%	1.01126	-2	2.316E-03	0.06%	2.127E-04	0.05%

Table 4. Slice depletion calculation iterations of outer iteration 1 (constant power).

Table 5. Slice depletion calculation iterations using outer iteration 2 (axial/radial power profile).

i	t _{final} (days)	bu _{final} (^{GWd} /tHM)	$\frac{bu_{final}}{180 \ GWd/tHM} - 1$	k _{eff}	$k_i - k_{i-1}$ (pcm)	N_D^{235} U (atoms/b-cm)	$\frac{N_{D_i}}{N_{D_{i-1}}}-1$	N_D^{239} Pu (atoms/b-cm)	$rac{N_{D_i}}{N_{D_{i-1}}}-1$
0	540.54	144.56	-19.69%	1.32689	_	2.454E-03	_	2.0881E-04	_
1	673.08	194.18	7.88%	1.03206	-29483	2.257E-03	-8.20%	2.1643E-04	3.65%
2	623.93	187.83	4.35%	1.00585	-2621	2.273E-03	0.93%	2.1384E-04	-1.20%
3	597.91	182.83	1.57%	1.00772	187	2.294E-03	0.96%	2.1432E-04	0.22%
4	588.67	180.46	0.26%	1.00991	219	2.304E-03	0.61%	2.1516E-04	0.39%
5	587.16	179.74	-0.14%	1.01122	131	2.307E-03	0.06%	2.1491E-04	-0.11%
6	588.01	179.62	-0.21%	1.01218	96	2.314E-03	0.03%	2.1403E-04	-0.41%
7	589.24	180.11	0.06%	1.01256	38	2.315E-03	-0.06%	2.1468E-04	0.31%
8	588.87	179.76	-0.13%	1.01178	-78	2.316E-03	-0.10%	2.1390E-04	-0.36%
9	589.66	180.40	0.22%	1.01168	-10	2.316E-03	0.01%	2.1432E-04	0.20%

Convergence after 8 or 9 iterations:

• k_{eff} converged

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- Nominal discharge
 burnup achieved
- Nuclide densities converged



2. Comparison of final core average fuel compositions

106

Relative difference of core-average fuel composition is
negligible besides very few exceptions in case of small
nuclide densities.

Nuolido	Density	Relative	
Nuchae	Outer iteration 1	Outer iteration 2	difference
xe-135	4.587E-08	4.422E-08	-3.6%
cs-134	1.542E-05	1.509E-05	-2.2%
cs-137	1.570E-04	1.568E-04	-0.1%
nd-148	4.405E-05	4.414E-05	0.2%
sm-149	4.019E-07	4.122E-07	2.6%
sm-151	1.856E-06	1.861E-06	0.3%
gd-154	6.098E-08	6.104E-08	0.1%
gd-155	2.865E-09	3.137E-09	9.5%
eu-153	1.077E-05	1.065E-05	-1.1%
eu-154	1.788E-06	1.759E-06	-1.6%
eu-155	5.965E-07	5.876E-07	-1.5%

Nuolido	Density [Relative	
nuciae	Outer iteration 1	Outer iteration 2	difference
u-235	2.316E-03	2.306E-03	-0.4%
u-238	1.786E-02	1.788E-02	0.1%
pu-239	2.127E-04	2.143E-04	0.7%
pu-240	8.041E-05	8.033E-05	-0.1%
pu-241	6.724E-05	6.662E-05	-0.9%
pu-242	2.980E-05	2.910E-05	-2.3%
am-241	6.746E-07	6.873E-07	1.9%
cm-242	4.772E-07	4.672E-07	-2.1%
cm-244	1.467E-06	1.420E-06	-3.2%



3. Full core power profile





Results:

- Power is peaking in the inner fuel region
- Consideration of axial/radial power profile in the iterations to obtain the equilibrium core compositions has minor effect.

4. Comparison of isothermal temperature coefficients

- Reactivity coefficient calculation:
 - k_{eff} calculations with material temperatures varying over a range of several hundred K
 - Assuming constant temperature within material
 - Fitting of ρ to determine coefficient

Component	Temperature Reactivity Coefficient at HFP [pcm/K]		
	Cisneros [1]	ORNL	
Fuel	-3.8	-3.90	
Salt coolant	-1.8	-0.48	
Graphite moderator	-0.7	-1.10	
Inner graphite reflector	+0.9	+1.21	
Outer graphite reflector	+0.9	+0.61	



[1] A. T. Cisneros, "Pebble Bed Reactors Design Optimization Methods and their Application to the Pebble Bed Fluoride Salt Cooled High Temperature Reactor (PB-FHR)," University of California, Berkeley, 2013.


6. Towards rapid inventory calculations with ORIGAMI

Purpose of 1-group cross section analysis: understand the spectral variations and their impact on 1-group cross sections which influence all inventory calculations



- Only small variation of 1-group removal cross section over depletion
- Small changes visible mainly in Pu-240

*S. Skutnik, W. Wieselquist, ORNL/TM-2020/1886, 2021. <u>https://www.osti.gov/servlets/purl/1807271</u> 109

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6. Comparison between UCB Mark 1 and PBMR-400



- Both cores showed significant radial variation for various nuclides
- Only UCB Mark 1 showed axial variation due to inlet/outlet geometry

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7. Analytical model to calculate tritium production



 A simplified analytical model was developed by Cisneros et al*. using a flux and one-group cross sections to allow estimation of tritium generation rates for an arbitrary initial Li-7 enrichment

$$\dot{T}(t) = \phi \sigma_{Li-7}^{T} N_{Li-7} + \phi \sigma_{Li-6}^{T} \left(N_{Li-6}^{0} e^{-\frac{V_{core}}{V_{Loop}} \phi \sigma_{Li-6}^{abs} t} + \frac{\phi \sigma_{Be-9}^{\alpha} N_{Be-9}}{\phi \sigma_{Li-6}^{abs}} \left(1 - e^{-\frac{V_{core}}{V_{Loop}} \phi \sigma_{Li-6}^{abs} t} \right) \right)$$

- SCALE results using TRITON/ORIGEN: 0.021 mol/day
- Equilibrium value from Cisneros analytical approach: **0.023 mol/day**

*Cisneros, A. T., 2013. Pebble Bed Reactors Design and Optimization Methods and their Application to the Pebble Bed Fluoride Salt Cooled High Temperature Reactor (PB-FHR) (PhD). University of California Berkeley.

MELCOR for Accident **Progression and Source** Term Analysis





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MELCOR Development for Regulatory Applications



What Is It?

MELCOR is an engineering-level code that simulates the response of the reactor core, primary coolant system, containment, and surrounding buildings to a severe accident.

Who Uses It?

MELCOR is used by domestic universities and national laboratories, and international organizations in around 30 countries. It is distributed as part of NRC's Cooperative Severe Accident Research Program (CSARP).

How Is It Used?

MELCOR is used to support severe accident and source term activities at NRC, including the development of regulatory source terms for LWRs, analysis of success criteria for probabilistic risk assessment models, site risk studies, and forensic analysis of the Fukushima accident.

How Has It Been Assessed?

MELCOR has been validated against numerous international standard problems, benchmarks, separate effects (e.g., VERCORS) and integral experiments (e.g., Phebus FPT), and reactor accidents (e.g., TMI-2, Fukushima).

U.S.NRC

Sandia National Laboratories

Source Term Development Process

104 / T(K)













SCALE/MELCOR/MACCS



Neutronics Oriticality Shielding Radionuclide inventory Burnup credit Decay heat

Y Integrated Severe

- Hydrodynamics for range
- of working fluids
- Accident response of
- plant structures, systems
- and components
- Fission product transport

Radiological Consequences

- 1AC
 - Near- and far-field atmospheric transport and deposition
 - Assessment of health and economic impacts

Nuclear Reactor System Applications

Non-Reactor Applications

Fusion

Neutron beam injectors

• Li loop LOFA transient

ITER cryostat modeling

• He-cooled pebble test

analysis

blanket (H³)

Spent Fuel

- Risk studies
 - Multi-unit accidents
 - Dry storage
 - Spent fuel
 - transport/package applications

Facility Safety

- Leak path factor calculations
- DOE safety toolbox codes
- DOE nuclear facilities (Pantex, Hanford, Los Alamos, Savannah River Site)

Safety/Risk Assessment

- Technology-neutral
- o Experimental
- o Naval
- Advanced LWRs
- Advanced Non-LWRs
- Accident forensics (Fukushima, TMI)
- Probabilistic risk assessment

Regulatory

- License amendments
- Risk-informed regulation
- Design certification (e.g., NuScale)
- Vulnerability studies
- Emergency preparedness
- Emergency Planning Zone Analysis

Design/Operational Support

- Design analysis scoping calculations
- Training simulators

MELCOR Attributes Foundations of MELCOR Development



Phenomena modeled

Reactor coolant thermal hydraulics

ssion product removal processes

Release of fission products to environment

down and fission product release

Engineered safety systems - sprays, fan coolers, etc.

Accident initiation

oss of core coolant

actor vessel failure

odine chemistry and more

Fully integrated, engineering-level code

- Thermal-hydraulic response of reactor coolant system, reactor cavity, rector enclosures, and auxiliary buildings
- · Core heat-up, degradation and relocation
- Core-concrete interaction
- Flammable gas production, transport and combustion
- Fission product release and transport behavior

Level of physics modeling consistent with

- State-of-knowledge
- Necessity to capture global plant response
- Reduced-order and correlation-based modeling often most valuable to link plant physical conditions to evolution of severe accident and fission product release/transport

Traditional application

- Models constructed by user from basic components (control volumes, flow paths and heat structures)
- Demonstrated adaptability to new reactor designs HPR, HTGR, SMR, MSR, ATR, Naval Reactors, VVER, SFP,...





CONTAINMENT SPRAYS

AND

HYDROGEN

PRODUCT

AEROSOLS



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MELCOR Pedigree

Validated physical models

- International Standard Problems, benchmarks, experiments, and reactor accidents
- Beyond design basis validation will always be limited by model uncertainty that arises when extrapolated to reactor-scale

Cooperative Severe Accident Research Program (CSARP) is an NRC-sponsored international, collaborative community supporting the validation of MELCOR



International Collaboration Cooperative Severe Accident Research Program (CSARP) – June/U.S.A MELCOR Code Assessment Program (MCAP) – June/U.S.A European MELCOR User Group (EMUG) Meeting – Spring/Europe European MELCOR User Group (EMUG) Meeting – Fall/Asia



International LWR fleet relies on safety assessments performed with the MELCOR code



Common Phenomenology





MELCOR Modeling Approach



Modeling is mechanistic consistent with level of knowledge of phenomena supported by experiments

Parametric models enable uncertainties to be characterized

- Majority of modeling parameters can be varied
- Properties of materials, correlation coefficients, numerical controls/tolerances, etc.

Code models are general and flexible

- Relatively easy to model novel designs
- All-purpose thermal hydraulic and aerosol transport code





MELCOR State-of-the-Art



		MELCOR	Code Developm	ent		Ve	ersion	Date
odels Conve	ecting Molten Pool ♦	Point Kinetics ♦	Turbulent Deposition		Eutectics Vector CFs	တ္တ 2.2	2.18180	December 202
Curved Lower	Head Stefan Model	Smart Resta	H2 Production Mechanis	tic Fan Cooler A Homologou	s Pump nsion	BSB 2.2	2.14959	October 201
· · · · · · · · · · · · · · · · · · ·				♦ Aac	liation Enclosure		2.11932	November 201
hasis		MELCOR 2.X Robustnes	ss & User Flexibility	Code Performance Impro	ovements	2.2	2.9541	February 20 ⁻
(Conversion from F77 to F95	HTGR Mo	dels	Na Fire Models	Non-LWR Models	epc 2.	1.6342	October 20 [°]
Molter	n Pool / Lower Head	odels		SMR Models	a successive sectors and	Ŭ 2.	1.4803	September 20 ⁻
al Release	MELCO	R 2.0 (beta)	M2.1.3649		· MELCOR 2.2	.cia 2.	1.3649	November 20
OR 1.8.5	MELCOR 1.8.6	\$	M2.1.1576 M2.1.4803	♦ IVI2.1.6342	MILLOUR 2.2	iiii 2.	1.3096	August 20
1 1	· · · · ·	I I I I	1 I I I	· · · · ·	Year	× 2.	1.YT	August 20
00 2001 2002	2 2003 2004 2005	2006 2007 2008	2009 2010 2011 2012 2	013 2014 2015 2016	2017 2018 2019 2020	\geq 2.0	0 (beta)	Sent 20
Blanket 440 water cooled me servery neutrons and Divertor 5 This removes impuri 440 water cooled me 5 This removes impuri 440 water cooled me 5 This removes impuri 5 This rem	dules, each odules, each sel from high ites (exhaust) in vessel r vessel rutron Beam Injectors DVA) Loop LOFA transient alysis ER Cryostat modeling	Spent fuel pool risk studies Multi-unit accidents (la area destruction) Dry Storage	rge Non-Nuclear Facilities Leak Path Factor Calculation (LPF) Release of hazardous materials from facilities, buildings, confined space	 Accelerated steady state initialization Two-sided reflector (RF) component Modified Fuel components (PMR/PBR) Point kinetics Fission product diffusion, transport and release TRISO fuel failure 	Sodium Equation of Sodium Thermo-m properties Containment Mode Sodium pool fire m Sodium spray fire n Atmospheric chem Sodium-concrete in	of State echanical ling odel nodel istry model iteraction	Molten Salt Reactors Properties for LiF-BeF2 have been added Equation of State Thermal- mechanical properties	
 Hell 	lium Lithium lium Cooled Pebble	Here is a submitted in the second sec	 DOE Safety Toolbox code DOE nuclear facility users Pantex 	Person Carton Buller Layer Person Inner Pyrodolic and		Noybonum Darlsings Man Partemanys	sic	

MELCOR Software Quality Assurance – Best Practices

MELCOR SQA Standards SNL Corporate procedure IM100.3.5 CMMI-4+ NRC NUREG/BR-0167

MELCOR Wiki

- Archiving information
- Sharing resources (policies, conventions, information, progress) among the development team.

Code Configuration Management (CM)

- 'Subversion'
- TortoiseSVN
- VisualSVN integrates with Visual Studio (IDE)

Reviews

- Code Reviews: Code Collaborator
- Internal SQA reviews

Continuous builds & testing

- DEF application used to launch multiple jobs and collect results
- Regression test report
- More thorough testing for code release
- Target bug fixes and new models for testing

Emphasis is on Automation Affordable solutions Consistent solutions

Bug tracking and reporting

• Bugzilla online

Code Validation

- Assessment calculations
- Code cross walks for complex phenomena where data does not exist.

Documentation

- Available on 'Subversion' repository with links from wiki
- Latest PDF with bookmarks automatically generated from word documents under Subversion control
- Links on MELCOR wiki

Project Management

- Jira for tracking progress/issues
- Can be viewable externally by stakeholders

Sharing of information with users

- External web page
- MELCOR workshops
- MELCOR User Groups (EMUG & AMUG)







	BUR	CAV	CF	COR	CVH	DCH	FCL	FDI	FL	HS	NCO	PAR	RN	SPR
Case		Ť		Ť	Ŭ	_					· · ·			
M-8-1 NoMix			х		х				х	х	х			
M-8-1 SYM			х		х				х	х	х			
Lace7			х		х	х			х	х	х		х	
Lace8			х		х	х			х	х	х		х	
Vanam-M3			х		х				х	х	х		х	
Molten Salt			х	х	х				х	х	х			
PHEBUS-B9			х	х	х				х	х	х			
FPT1			Х	Х	х	х			Х	х	х		х	
LOFT			х	х	х	х			х	х	х			
Test lnew	х	х	х	х	х	х	х	х	х	х	х	х	х	х
SURRY	х	х	х	х	х	х	х	х	х	х	х		х	х
(LBLOCA)														
Zion (SBO)		х	х	х	х	х	х	х	х	х	х	х	х	х
PeachBottom	х	х	х	х	х	х			х	х	х		х	х
(SBO)														
Grand Gulf (SBO)	х	Х	х	х	х	х		х	х	х	х		х	

Table 1-1: Physics Package Coverage

MELCOR Verification & Validation Basis





Volume 1: Primer & User Guide Volume 2: Reference Manual Volume 3: MELCOR Assessment Problems [SAND2015-6693 R]

Analytical Problems

Saturated Liquid Depressurization Adiabatic Expansion of Hydrogen Transient Heat Flow in a Semi-Infinite Heat Slab Cooling of Heat Structures in a Fluid Radial Heat Conduction in Annular Structures Establishment of Flow



non

5

Specific





Sample Validation Cases

IAEA CRP-6 Benchmark Fractional Release										
Case	1a	1b	2a	2b	3a	3b				
US/INL	0.467	1.0	0.026	0.996	1.32E-4	0.208				
US/GA	0.453	0.97	0.006	0.968	7.33E-3	1.00				
US/SNL	0.465	1.0	0.026	0.995	1.00E-4	0.208				
US/NRC	0.463	1.0	0.026	0.989	1.25E-4	0.207				
France	0.472	1.0	0.028	0.995	6.59E-5	0.207				
Korea	0.473	1.0	0.029	0.995	4.72E-4	0.210				
Germany	0.456	1.0	0.026	0.991	1.15E-3	0.218				

TRISO Diffusion Release

LACE LA1 and LA3 tests experimentally examined the transport and retention of aerosols through pipes with high speed flow





Resuspension

STORM (Simplified Test of Resuspension Mechanism) test facility



(1a): Bare kernel (1200 °C for 200 hours)
(1b): Bare kernel (1600 °C for 200 hours)
(2a): kernel+buffer+iPyC (1200 °C for 200 hours)
(2b): kernel+buffer+iPyC (1600 °C for 200 hours)
(3a): Intact (1600 °C for 200 hours)
(3b): Intact (1800 °C for 200 hours)

A sensitivity study to examine fission product release from a fuel particle starting with a bare kernel and ending with an irradiated TRISO particle;

Aerosol Physics

- Agglomeration
- Deposition
- Condensation and Evaporation at surfaces

Validation Cases

- •Simple geometry: AHMED, ABCOVE (AB5 & AB6), LACE(LA4),
- •Multi-compartment geometry: VANAM (M3), DEMONA(B3)
- •Deposition: STORM, LACE(LA1, LA3)



ABCOVE AB5





and transport





XOAK RIDGE

 $\begin{array}{l} TP = Transfer Process\\ DCH = Decay Heat\\ COR = Core\\ SPR = Containment Spray\\ BUR = Gas Combustion\\ FDI = Fuel Dispersal Interaction\\ CAV = Cavity (MCCI)\\ ESF = Engineered Safety Features\\ MP = Material Properties\\ \end{array}$

RN = Radionuclide HS = Heat Structure CVH = CV Hydrodynamics EDF = External Data File CF = Control Function MES = Special Messages MEX = Executive CVT = CV Thermodynamics NCG = Non Condensible Gas

Separate Physics

Numerics

&

National Laboratories





Molten Salt Chemistry and Radionuclide Release – * Concerns Integration into MELCOR

MELCOR provides mass of radionuclides released into salt, chemistry, T and P







Cs vapor pressures in MSM calculations



