OAK RIDGE National Laboratory

Non-LWR inventory generation approaches & lessons learned



ORNL is managed by UT-Battelle, LLC for the US Department of Energy

U.S. DEPARTMENT OF ENERGY

Goals of this presentation

- Provide an overview of non-LWR inventory generation approaches with SCALE for
  - Pebble-bed high-temperature gas-cooled reactors (HTGRs) and fluoride salt-cooled high-temperature reactors (FHRs)
  - Fast-spectrum heat pipe reactors (HPRs) and sodium-cooled fast reactors (SFRs)
  - Molten salt reactors (MSRs)
- Provide SCALE input–specific tips & tricks and common pitfalls
  - 3D modeling with CSAS (KENO-V.a, KENO-VI, Shift)
  - TRITON depletion
  - ORIGEN depletion/decay
  - ORIGAMI

OAK RIDGE National Laboratory

Non-LWR inventory generation approaches with SCALE



ORNL is managed by UT-Battelle, LLC for the US Department of Energy

U.S. DEPARTMENT OF ENERGY

General approach

1. Develop understanding of reactor neutronics and reactor physics behavior
   - Location-dependent neutron flux
   - Neutron flux spectrum at different locations
   - Fuel type: liquid vs. solid fuel, fresh fuel vs. reprocessed fuel, LEU vs. HALEU fuel
   - Operating states: continuous operation at equilibrium state, depletion within equilibrium cycle, simple depletion (once-through fuel)
   - Impact of reactor-specific peculiarity: continuous feed of fuel/fuel components, removal of fuel/fuel components/fission products, tritium generation, …

General approach (cont.)

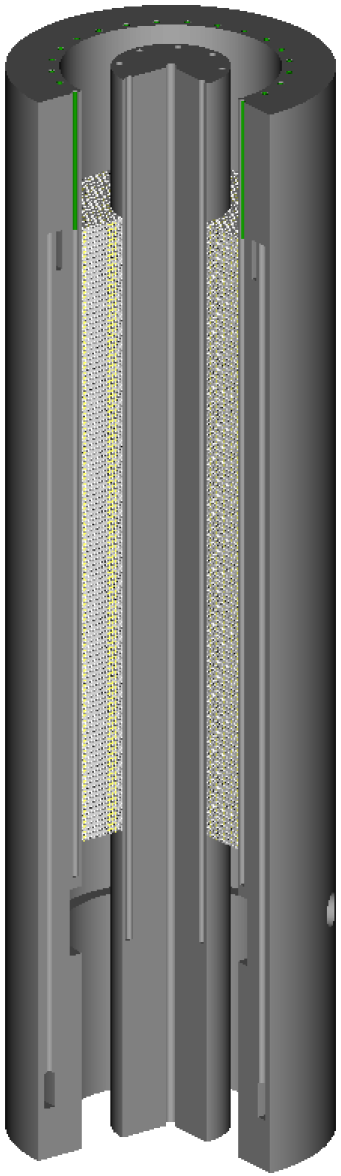
2. ORIGEN reactor library generation
   - Identification of an appropriate surrogate model for detailed depletion calculation with TRITON
   - Choice of parametrization based on sensitivity studies and spectral conditions
   - Potential consideration of multiple fuel types/compositions (e.g., U/TRU fuel, fresh HALEU fuel)

General approach (cont.)

3. Rapid inventory generation with ORIGEN and ORIGAMI
   - Ensure that prepared ORIGEN reactor libraries cover parameter space of interest
   - Rapid inventory generation permits additional sensitivity studies on inventory (e.g., pebble inventory based on various histories)
   - Rapid inventory generation permits prediction of spent fuel compositions (range of burnups, Pu mass, etc.)

Pebble-bed HTGRs and FHRs

- CSAS or TRITON:
  - Use MG calculations with SCALE's MG-doublehet approach to benefit from extremely reduced computation time
  - For CE models:
    - With SCALE 7 beta 4 and later: use the "random" block
    - Develop explicit tristructural isotropic (TRISO) model, avoiding TRISO clipping, and subdividing fuel zone into multiple regions (sub-mesh)
- ORIGEN library generation:
  - Slice model is an adequate surrogate model for ORIGEN library generation with TRITON
  - Sensitivities to fuel and reflector temperature suggest parametrization according to these
  - Strong radial spectral differences require parametrization according to radial zones
  - Different equilibrium compositions and impact of axial effects on spectrum (irregular geometries, leakage, …) in axial levels require parametrization according to axial zones
- Rapid pebble inventory:
  - ORIGAMI of SCALE 7 beta 4 and later provides a new capability for rapid inventory generation of pebble-bed systems

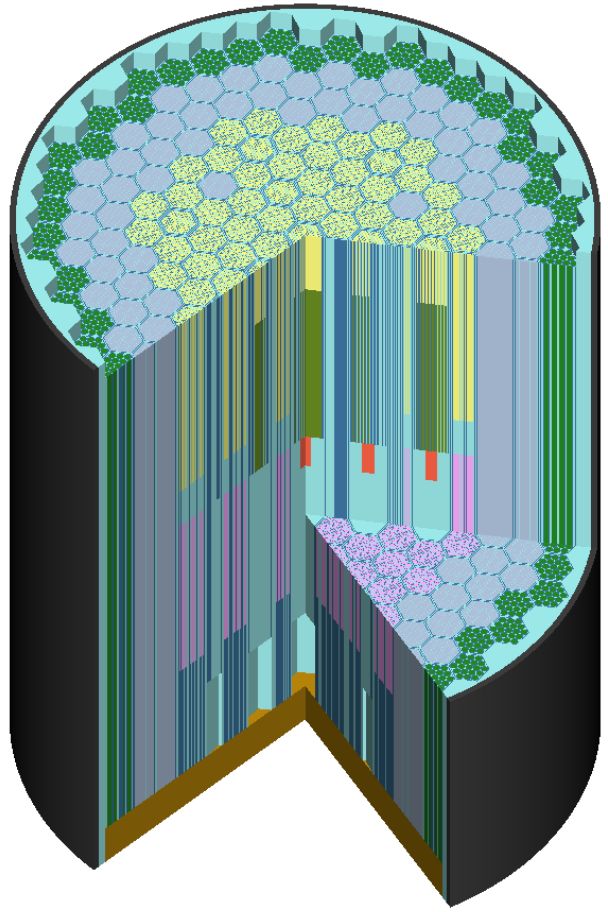


SCALE PBMR-400 model*

*Ref.: S. E. Skutnik and W. A. Wieselquist (2021). Assessment of ORIGEN Reactor Library Development for Pebble-Bed Reactors Based on the PBMR-400 Benchmark, ORNL/TM-2020/1886. https://doi.org/10.2172/1807271

Fast spectrum SFRs and HPRs

- CSAS or TRITON:
  - Use CE ENDF 7.1 in 6.3 and later (with the p-table fix)
- ORIGEN library generation:
  - For large cores, a slice model shows representative spectral conditions compared to the full core and can be used for ORIGEN library generation
  - Smaller cores require full-core models to properly consider axial leakage
  - Parametrization according to fuel type required: U/TRU fractions, fresh HALEU fuel, different U-235 enrichments, etc.

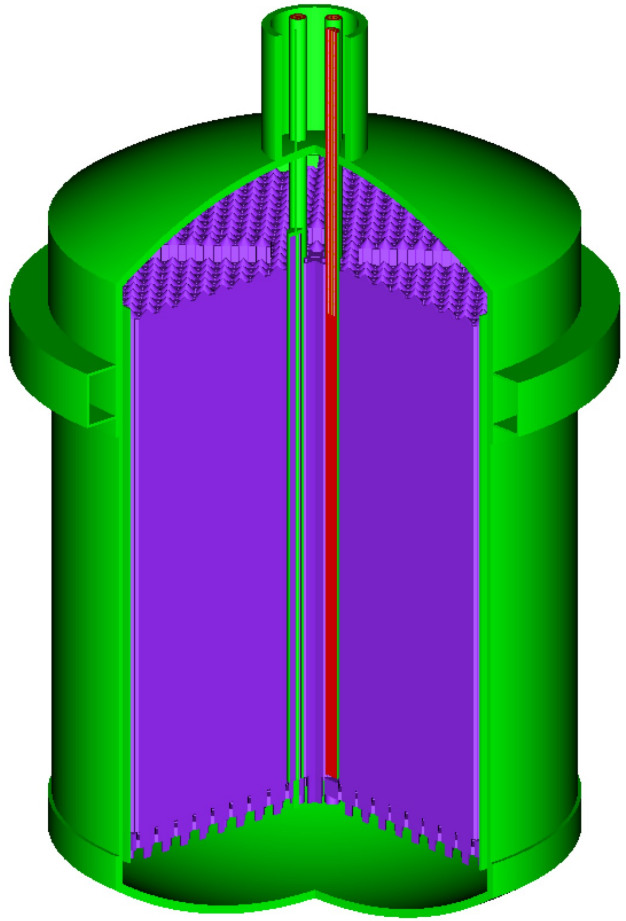


SCALE ABTR model*

*Ref.: A. Shaw, et al. (2023). SCALE Modeling of the Advanced Burner Test Reactor, ORNL/TM-2022/2758. https://doi.org/10.2172/1991734

MSRs

- CSAS or TRITON:
  - MG approaches are usually sufficient but require some effort to determine an appropriate self-shielding unit cell because of irregular lattices
  - TRITON's FLOW block provides the capability for continuous feed (e.g., refueling) and fractional removal (e.g., fission product removal)
- ORIGEN:
  - Permits location-dependent inventory prediction
  - ORIGEN permits removal of nuclides
- Location dependence of inventory was not found relevant for MSR loops with short loop transit times (e.g., 25 seconds for MSRE)
  - TRITON calculation of system-average (i.e., core+loop) inventory found adequate



SCALE MSRE model*

*Ref.: F. Bostelmann, et al. (2022). Modeling of the Molten Salt Reactor Experiment with SCALE. Nuclear Technology, 208(4), 603–624. https://doi.org/10.1080/00295450.2021.1943122

All non-LWRs

- CSAS and TRITON's definitions and tallies block can be used to analyze:
  - spatial distribution of neutron flux and the fission density (good proxy for power) over a full core, and
  - neutron flux spectrum at any location in the core
- Depletion calculations require material/region volumes to be specified or calculated:
  - Fulcrum provides a convenient ray tracer that works for most geometries
  - KENO provides a Monte Carlo and a trapezoidal integration method
  - Shift provides a parallelized ray tracer that rapidly calculates volumes
- The development and use of a JSON-formatted inventory interface file simplify a streamlined analysis approach and data exchange with others
- The OBIWAN command-line utility offers a fast way to interrogate F71 and F33 files

OAK RIDGE National Laboratory

SCALE input tips & tricks and common pitfalls



ORNL is managed by UT-Battelle, LLC for the US Department of Energy

U.S. DEPARTMENT OF ENERGY

OAK RIDGE National Laboratory

Cross section libraries, materials, and cross section processing



Which cross section library should I use?

- Depends on:
  - Spectral conditions of the model (thermal vs. fast)
  - Desired solution accuracy
  - Available simulation time
- For thermal systems and with limited applicability for other spectral conditions:
  - If time allows, use the 252-group ENDF/B-VII.1 (v7-252) library
  - If a quick answer is needed, use the 56-group ENDF/B-VII.1(v7-56) library (but be careful since this library was specifically optimized for LWRs)
- For fast spectrum calculations:
  - Try out the 302-group SFR library or 1596-group library
  - Compare neutron transport calculation results (k_{eff}, neutron flux) with CE before proceeding with depletion calculation
- For anything else:
  - Use a CE library
- Always compare MG calculations with CE to assess the bias due to cross section processing and choice of the multigroup cross section library

Which cross section processing options should I use?

- The most accurate solution is obtained using CENTRM and a fine-group cross section library
- **Latticecell**: sufficient for most unit cells
  - Assumes that the fuel pin lies in an infinite lattice of other fuel pins
- **Multiregion**: to be used if unit cell needs to be divided into multiple rings or in more complex scenarios
  - Example: Complex geometry such as in MSRs not easily modeled using Latticecell
  - Note: Default boundary condition for multiregion is white – double check!
- **Doublehet**: to be used for double-heterogeneous systems with fuel particles dispersed in a pebble, compact, or slab
- If approximation of infinite lattice of fuel pins is insufficient, then modify the Dancoff factor for that fuel pin so that $|k_{MG} - k_{CE}| < 300$ pcm
- If a unit cell geometry is widely different from repeated fuel lattices, try to create a multiregion with representative radii, use Dancoff factors, and perform thorough comparisons to CE calculations.
  - Example: Many MSR systems have irregular repeating geometries

What are common input errors?

- Check that all necessary unit cell parameters are included: all radii, pitches and heights; but remove optional ones that you don't need
- Check that boundary conditions are correct (e.g., **`right_bdy=vacuum`** – most likely incorrect for lattices)
- Do not confuse pitches (pitch) and half pitches (**h**pitch) or radii (fuel**r**) and diameter (fuel**d**)
- For doublehet cells:
  - Be aware that coatings can be specified via radius, diameter, or thickness: coat**r**, coat**d**, coat**t**
  - Specify either the volume fraction of fuel particles (vf) **OR** the number of particles (numpar)
  - You need to define a doublehet mixture ID → don't confuse this ID with the fuel mixture ID from a possible CE model
- Triple check material IDs in unit cell specifications, especially after a copy/paste from an old input
- "more data" and "centrm data" only apply to the unit cell specified immediately above the line

OAK RIDGE National Laboratory

Neutron transport model development tips & tricks



What options should I use for Monte Carlo calculations?

- **NPG**: Ensure that a sufficient number of particles per generation is used
  - ≥ 100,000 for reactor physics models; ≥ 10,000 for crit safety models
- **NSK**: Check convergence to ensure NSK is large enough
  - ≥ 100 for reactor physics models; ≥ 25 for simple crit safety models
- Larger numbers of bodies and larger separations in the geometric model require greater NPG, NSK, and GEN values
- **SIG**: Use SIG parameter to converge k_{eff} result to specific level; for this option, also set GEN to a large number (10,000+)
- **RND**: For spatially dependent output quantities (e.g., power profile), run multiple calculations with different random seeds (parameter RND) and determine average of these runs

What are some common KENO and Shift input errors?

- Incorrect array definition or array placement:
  - Incorrect number of units listed in array fill statement
  - Array placement leads to undefined region in the geometric unit that contains the array
  - Units used in array don't have the same outer boundaries (e.g., not the same axial expansion)
  - Fulcrum can help detect input errors
  - Sometimes it is easier to run a problem with a very small number of neutrons and obtain KENO/Shift's error message instead of the input validation/parser messages
- Overlapping holes
- Undefined space
- Missing "end data" at the end of the input before the final "end" statement

OAK RIDGE National Laboratory

TRITON model development tips & tricks



Tracking of nuclides on the neutron transport side

- Use an adequate addnux level: **parm=(addnux=N) with N=1,2,3,4**.
- Default addnux=2 is adequate for most cases
- Higher addnux values mean increased accuracy, but longer run time
- addnux=4 is desired for best-estimate benchmark models and when calculating a model different from LWRs (it's always good to start with addnux=4 and to then determine whether one can decrease the level)

Alias block

- Aliases make the input file shorter and much easier to read; you can read a descriptive name for a material rather than just a number
- Aliases are especially useful when defining multiple fuel components
  - Example: repeated graphite layers in TRISO particles
- Aliases are especially useful when analyzing power profile via mixture-specific power
- Fulcrum offers an alias expansion, and expanded input is also printed in the output
- Note that CSAS does not permit aliases; only TRITON does

Burndata block

- The specific power density can be given in a few ways
  - The power density can be calculated from the total reactor power, the number of assemblies, and the mass of heavy metal in each assembly
  - It can also be calculated from the linear heat rate, fuel pin dimensions, and fuel density
- In TRITON, the power density must be input in megawatts per metric ton of heavy metal (MW/MTHM)
- If a full-core model is depleted, the total heavy metal mass (printed in TRITON output) and the specific power can be used to confirm the total reactor power

Depletion steps

- The TRITON "nlib" option is used in the burndata block to specify the number of cross section updates per burn period
- The user should specify a first step that is very small (~ 100 hours) to set xenon and samarium equilibrium concentrations
- Remember that "burn=0" can be used for transport-only calculations (since SCALE 6.3)
- Note the calculation of different results for different points in time due to TRITON's predictor-corrector approach:
  - **Nuclide inventory** as calculated by ORIGEN is available **at the end** of each depletion and decay step
  - **Neutron flux, k_{eff},** and other quantities as calculated by the neutron transport solver is available **in the middle** of each depletion step
  - If neutron transport output is needed at the end of a depletion step or at the end of the irradiation history, users can add very small depletion intervals as needed (e.g., "burn=1e-5").

What are some common mistakes or issues?

- Incorrect volumes lead to incorrect mixture powers
  - Calculate and explicitly define all possible volumes
  - Use volume block with tight settings for automatic volume calculations
- Specific case: Incorrect volumes are applied in units used in arrays; volumes applied in a unit refer to the total volume of that unit in a model
  - Example: Volumes of a pin cell unit correspond to the single pin cell volumes multiplied by the number of times that pin cell is used in an array
- Typos in shell blocks lead to injection files not being found or files not being copied back from TMPDIR
- Common error when converting input from CSAS to TRITON: missing "read model" and "end model" block, missing "end data"
- Remember the data on ORIGEN concentration (F71) files are normalized to 1 MTIHM
  - Example: All fuel of a model is depleted – total (case=0) heavy metal mass on F71 is 1 MTIHM
  - Example: Depletion of only a few out of many fuel pebbles causes the total (case=0) heavy metal mass on the F71 file to be lower than 1 MTIHM because not all fuel mixtures end up on the file

OAK RIDGE National Laboratory

ORIGEN and ORIGAMI development tips & tricks



Which tool is right for me?

ORIGEN + ARP

- Depletion of one or a few regions
- Complex irradiation histories and/or advanced processing
- Any fuel type (incl. MOX, CANDU, etc.)



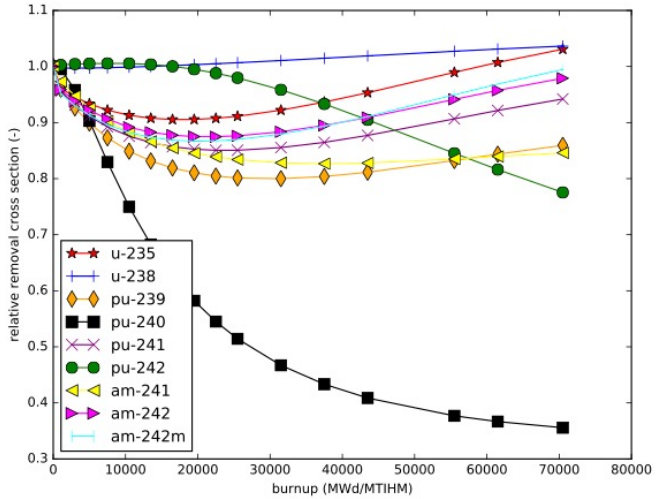
ORIGAMI

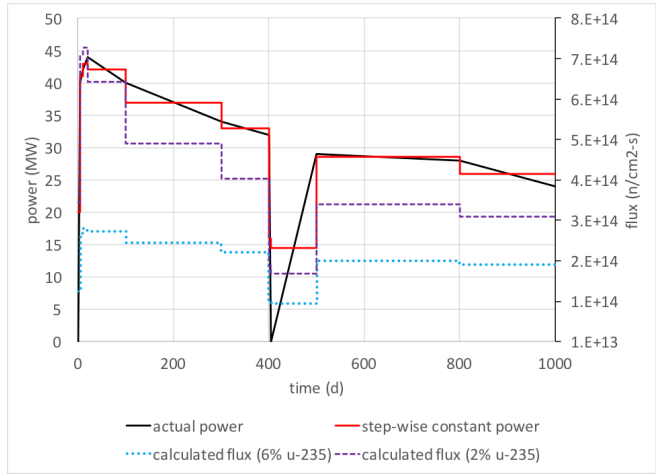
- Depletion of many regions / compositions (several depletion problems)
- Relatively simple (TRITON-like) irradiation histories
- Follow-on analysis using tools such as CSAS, MAVRIC, and MCNP
- UOX only (presently)



Tips for more accurate depletion calculations

- Cross section sensitivity to burnup can be highest at lower burnups
  - Avoid large timesteps for depletion
  - Use more sub-steps or sub-cycles
  - At least **one** library interpolation per cycle
- Avoid large swings in flux
  - Verify consistency between power and mass basis
  - Use smaller time intervals for large power changes





Balancing performance & accuracy in ORIGAMI depletion

- ORIGAMI allows one to control the number of library interpolations per cycle using nlib
  - default: nlib=4
  - Users should typically test a second higher nlib to ensure that the interpolated cross section grid is sufficient
- For higher burnups or later cycles, fewer interpolations are needed to obtain accurate results
  - relatively slower change in effective one-group cross sections with burnup
  - reducing the number of libraries for these cycles will yield some speedup with minimal loss of accuracy

Best practices for decay calculations

- Use sufficiently granular timesteps to capture phenomena of interest
  - MATREX solver (default): Follow *the rule of 3s* where $\Delta t_i \leq 3\Delta t_{i-1}$
  - CRAM: no specific rule, but logarithmically spaced steps recommended
- Split up very long decay intervals across multiple cases
  - E.g.: tracking (alpha,n) sources over very long decay times

