Sandia National Laboratories

Securing the future of Nuclear Energy

MELCOR

MELCOR/ORIGEN Integration

2024 European MELCOR Users' Group Meeting

April 15th-18th, 2024

SAND2024-03576PE

Overview

Effort underway to integrate ORIGEN and MELCOR

- ORIGEN functionally replaces MELCOR Decay Heat package (DCH)
- Facilitated with ORNL-developed Melcor ORigen TidY (MORTY) interface
- An alternate DCH “physics” in the language of modernized MELCOR architecture
- Modernized development practices

Review

- ORIGEN
- Conventional DCH in MELCOR
- Integration: assumptions, requirements, implementation, and development

Progress Report (since MCAP ’23 and AMUG ‘23)

- MORTY interface
- Modernized development
- HPR and fixed fuel with a single COR ORIGEN region
- MSRE and fluid fuel with one (and more) CVH ORIGEN regions

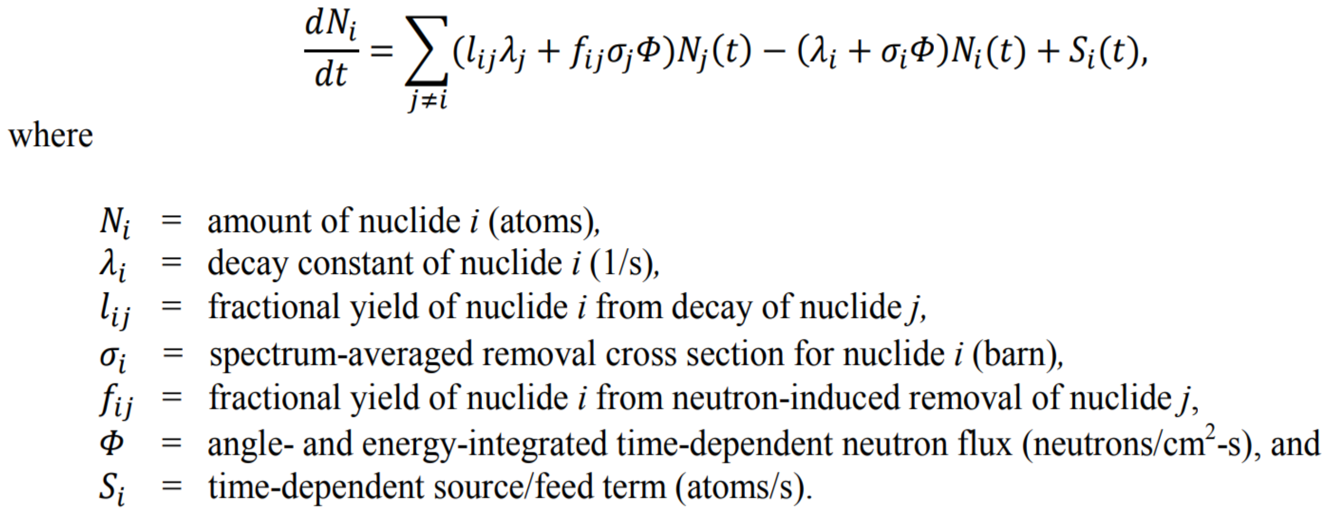
Summary

ORIGEN

ORIGEN does isotopic depletion analysis and enables computation of time-dependent concentrations, activities, and radiation source terms accounting for transmutation, fission, and decay

Arrange isotopic equations into a system with a solution that – spatially – applies "at a point" or that could be viewed as an "average over a volume"

Isotopic equations can account for "continuous feed/removal processes" couched as decay constants and/or elements of a source vector



$$\frac{dN_i}{dt} = \sum_{j \neq i} (l_{ij}\lambda_j + f_{ij}\sigma_j\Phi)N_j(t) - (\lambda_i + \sigma_i\Phi)N_i(t) + S_i(t),$$

where

N_i = amount of nuclide i (atoms),
λ_i = decay constant of nuclide i (1/s),
l_{ij} = fractional yield of nuclide i from decay of nuclide j,
σ_i = spectrum-averaged removal cross section for nuclide i (barn),
f_{ij} = fractional yield of nuclide i from neutron-induced removal of nuclide j,
Φ = angle- and energy-integrated time-dependent neutron flux (neutrons/cm^2-s), and
S_i = time-dependent source/feed term (atoms/s).

Decay Heat Package

DCH input sets:

- Initial DCH/RN1 class mass inventory via:
  - Element-wise initial mass, and
  - Grouping of elements into classes
- Decay power time tables [time vs W/kg] for each element
- Also any reference core scaling and whole-core power rules (not applicable here)

During a calculation, MELCOR transports radionuclide class mass and loads decay heat in core cells, in CV phases, on HS surfaces, and on filters by reference to DCH

- Radionuclide class mass transfers, the decay power follows the mass
- DCH “decay” does not result in a movement of radionuclide mass between classes
- DCH “decay” cannot alter the fission product chemistry
- Only one DCH decay rule (table) per chemical element in a given DCH/RN1 class which applies to all DCH/RN1 class mass no matter where it resides (COR, CVH, HS, filters)

For certain applications – particularly non-LWR - fission product chemistry and the impact of radioactive decay could be crucial to radionuclide transport/release

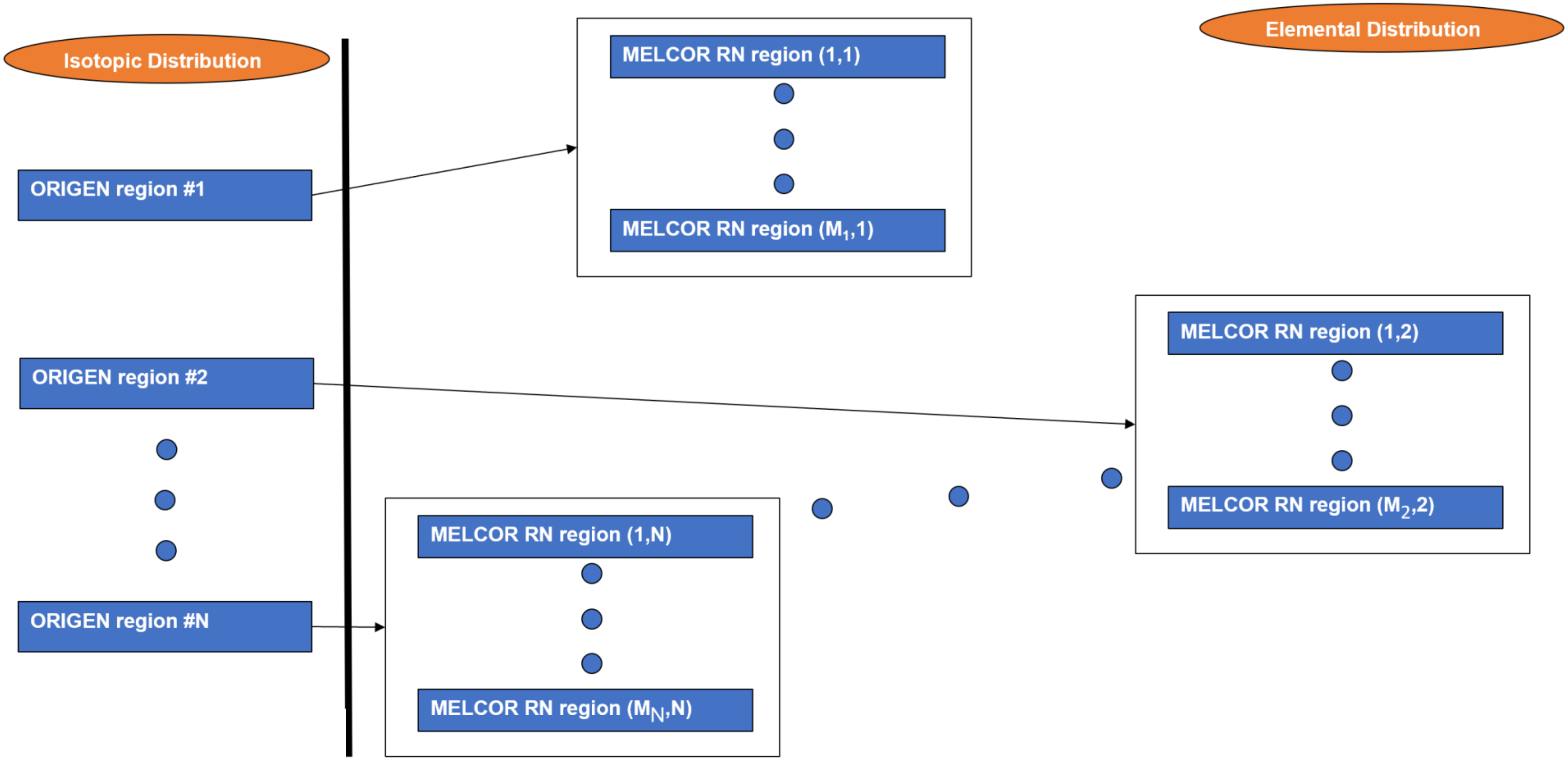
ORIGEN/MELCOR capabilities should be agnostic to reactor type

ORIGEN/MELCOR Integration

Assumptions:

- Pure radioactive decay (no fission product build-in under neutron flux)
- MELCOR and ORIGEN have corresponding spatial domains
  - ORIGEN has “materials” consisting of mass for 2000+ isotopes
  - MELCOR has “ORIGEN regions” consisting of element AND corresponding class mass
- Initialize MELCOR ORIGEN regions and ORIGEN material with ORIGEN JSON file(s)
- Where DCH executes, ORIGEN:
  - Computes isotopics and tallies elements on all materials,
  - Updates elementwise tally on all corresponding ORIGEN regions, and
  - Uses an interface to facilitate the update
- As MELCOR goes on:
  - Class-wise transfer processes move class mass between ORIGEN region spatial domains,
  - Element masses on ORIGEN regions are updated accordingly,
  - Element mass moves between ORIGEN regions are tabulated, and
  - ORIGEN material isotopics are updated accordingly as facilitated by an interface
  - Defer the issue of any MELCOR-side chemistry modeling (individual element moves)
- All DCH MELGEN/MELCOR text outputs, plot variables, CF arguments, etc. are altered to meaningfully reflect the elementwise tracking on ORIGEN regions
- New DCH input structures are created as needed:
  - ORIGEN “activated” as alternate DCH physics model
  - ORIGEN region definition and specification

ORIGEN/MELCOR Integration



Isotopic Distribution

Elemental Distribution

ORIGEN region #1

ORIGEN region #2

ORIGEN region #N

MELCOR RN region (1,1)

MELCOR RN region (M_1,1)

MELCOR RN region (1,2)

MELCOR RN region (M_2,2)

MELCOR RN region (1,N)

MELCOR RN region (M_N,N)

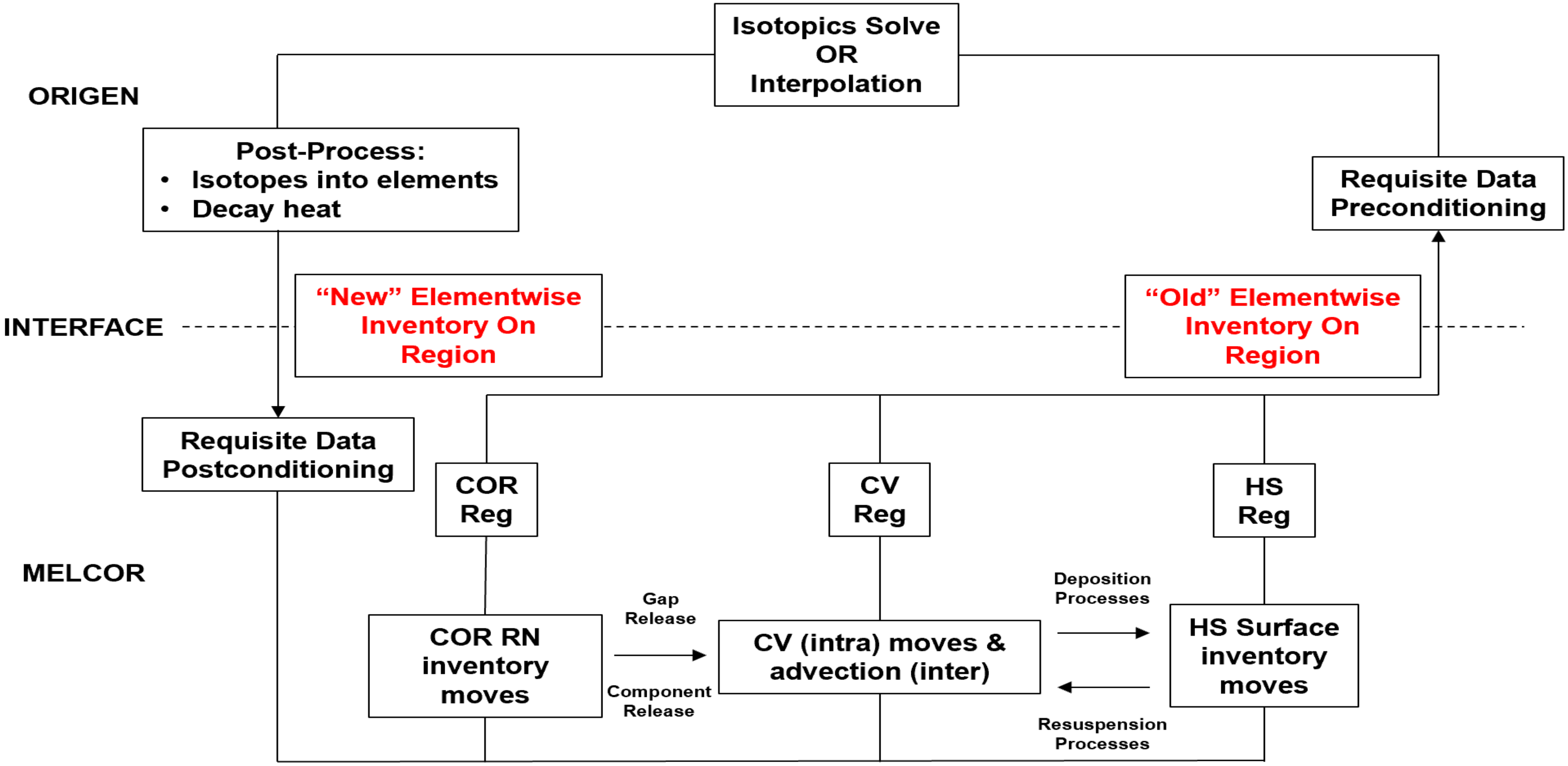
ORIGEN/MELCOR Integration

Ultimate Requirements:

- User can model arbitrarily many ORIGEN regions of any type, where types include:
  - COR regions – consisting of one or more fueled core cells
  - CVH regions – consisting of one or more control volumes (to include all phases)
  - HS regions – consisting of one or more heat structure surfaces
  - FLT regions – consisting of one or more RN2 filters
- Modernized development approach
- Account for future/near-term development and anticipated capabilities
  - GRTR and MELCOR-side element-wise chemistry
  - COR component surfaces as hosts for radionuclide class inventory (e.g. deposition)
- Sufficient user control on ORIGEN execution (not necessarily every time-step)
- MELCOR class-wise radionuclide transport unabridged
- Conservation of mass demonstrated in modified MELGEN/MELCOR text outputs
- New plot variables and CF arguments
- Updated calculations for existing plot variables and CF arguments
- Full MELCOR documentation
  - ORNL developing ORIGEN-side MORTY documentation
  - DCH Users’ Guide for input requirements
  - DCH Reference Manual for modeling/capabilities details
  - Example applications

ORIGEN/MELCOR Integration

Implementation:



```
DCH_ORG BURNFUEL
DCH_ORGCOR 1
          ! REGION NAME    JSON NAME     RESPONSE NAME    MTU SCALAR
          1 'ALLCORCELLS'  'JSON_NAME'   'RESP_NAME'      1.0
```

```
CF_RANGE 'ALLCORCELLS' CELLS 10
CONSTRUCT 1
          1               ALL
```

ORIGEN/MELCOR Integration

Development – An iterative process involving:

- New ORIGEN module/submodule
  - Data and procedure polymorphism
  - Element-wise mass inventory tracking
  - ORIGEN region tracking
- MORTY interface usage/debugging (SNL) and development (ORNL)
- Modernized input parser (DCH primarily)
- Field managers and physics managers (in approximate order of run step execution)
  - DCH – Element/class arrangement, global class inventory tracking, access to ORIGEN
  - COR – Class-wise radionuclide transport processes (e.g. gap release, fuel failure)
  - HS – Class-wise radionuclide transport processes (e.g. deposition, resuspension)
  - RN1/GRTR – Intravolume class-wise radionuclide transport processes (form-wise transfers)
  - CVH/RN2 – Intervolume class-wise radionuclide class advection
  - RN2 – Class-wise radionuclide class deposition on filters
- Testing on demonstration problems
  - HPR – Solid fuel, COR ORIGEN region(s), have a SCALE DCH-only comparison
  - MSRE – Fluid fuel, CVH ORIGEN region(s), have a SCALE DCH-only comparison

Prioritize development by NRC demonstration obligations (e.g. MSRE off-gas first)

Progress Report - MORTY

Melcor ORigen TidY (MORTY) Interface

Functionality not yet fully explored in practice beyond stand-alone unit tests

“ORIGEN implementation”

- Initialize and load ORIGEN material isotopes from JSON(s) during MELGEN execution
- Advance time, get updated decay heat and mass by element by ORIGEN material
- Update ORIGEN material isotopics after MELCOR-side ORIGEN region transfers

Bugs found here and there as development exercises MORTY capabilities

- To be expected…standard development cycle
- Appreciate the timely fixes from ORNL

Future documentation under the SCALE banner by ORNL

Progress Report – Development

In terms of code architecture:

- ORIGEN module/submodule splits data from implementation
  - Region elementwise inventory tracking
  - Implementation of ORIGEN initialization, decay calculations, and material updating
  - Various miscellaneous functions…operations on data encapsulated in ORIGEN module
- Physics manager used extensively to:
  - Instantiate alternate ORIGEN physics where DCH would ordinarily do a table look-up
  - Do additional/alternative initializations (e.g. from JSON not DCH MELGEN input)
  - Do alternative DCH, COR, and RN1 accounting operations and output edit prints
  - Do additional/alternative operations for region-wise class-wise transfer processes

In terms of physical modeling:

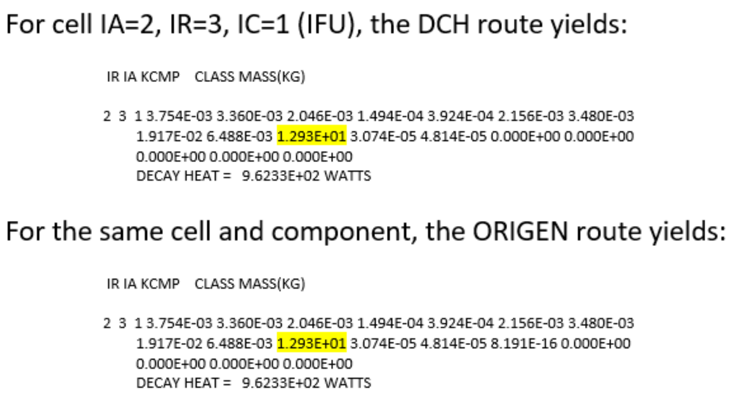
- Online:
  - COR region(s) and core cell (fuel + gap) radionuclide inventory and decay power tracking
  - CVH region(s) and aerosol form only radionuclide inventory and decay power tracking
  - Advection (CVH/RN2) as a means of class-wise ORIGEN region-wise transfer
  - ORIGEN material updates (of isotopics) due to advection and attending element/class move
  - DCH/COR/RN1 accounting for the above
- To-do:
  - Likewise for HS surfaces and filters
  - Address the full spectrum of possible ORIGEN region-wise transfer mechanism (long list)
  - So much more…including demonstrations on non-LWR plant decks

Progress Report – HPR Demo

DCH-only vs ORIGEN JSON, cycle 0, decay power

		DCH		ORIGEN	
Class Number	Class Name	Class Specific Power	Class Power	Class Specific Power	Class Power
1	XE	2.27736E+04	3.01334E+04	2.27736E+04	3.01333E+04
2	CS	4.54254E+04	5.37956E+04	4.54254E+04	5.37956E+04
3	BA	5.34472E+04	3.85400E+04	5.34472E+04	3.85400E+04
4	I	6.90674E+05	3.63647E+04	6.90674E+05	3.63647E+04
5	TE	1.11599E+05	1.54345E+04	1.11599E+05	1.54344E+04
6	RU	2.56859E+03	1.95167E+03	2.56859E+03	1.95167E+03
7	MO	3.61492E+04	4.43293E+04	3.61492E+04	4.43293E+04
8	CE	3.85053E+03	2.60087E+04	3.85053E+03	2.60088E+04
9	LA	3.05700E+04	6.99030E+04	3.05700E+04	6.99030E+04
10	UO2	1.252713E+00	5.70672E+03	1.25271E+00	5.70670E+03
11	CD	1.14154E+06	1.23664E+04	1.14154E+06	1.23664E+04
12	AG	2.71994E+05	4.61502E+03	2.71994E+05	4.61502E+03
13	BO2	0	0	1.45216E+04	4.19175E-09
14	H2O	0	0	0	0
15	CON	0	0	0	0
16	CSI	3.60597E+05	0	0	0
17	CSM	4.29653E+04	0	0	0
TOTAL			3.39149E+05		3.39149E+05

DCH-only vs ORIGEN JSON, cycle 0, RN1 class masses in core cells



For cell IA=2, IR=3, IC=1 (IFU), the DCH route yields:

```
 IR IA KCMP    CLASS MASS(KG)

2  3  1 3.754E-03 3.360E-03 2.046E-03 1.494E-04 3.924E-04 2.156E-03 3.480E-03
        1.917E-02 6.488E-03 1.293E+01 3.074E-05 4.814E-05 0.000E+00 0.000E+00
        0.000E+00 0.000E+00 0.000E+00
        DECAY HEAT =   9.6233E+02 WATTS
```

Computed as classes from element mass on DCH_EL using RN1_FPN

For the same cell and component, the ORIGEN route yields:

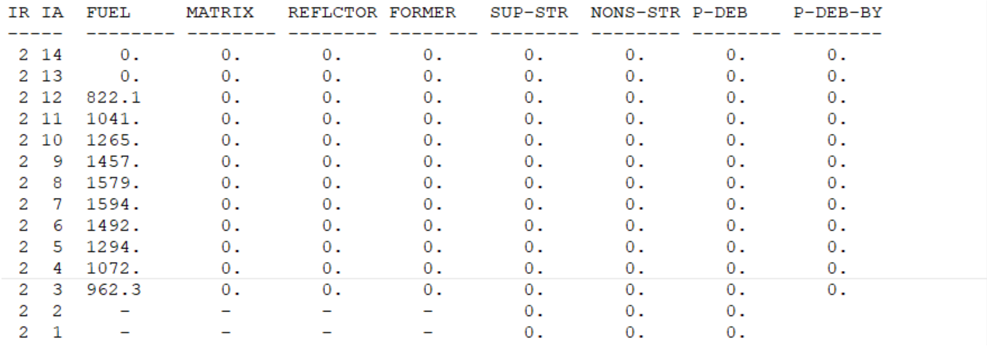
```
 IR IA KCMP    CLASS MASS(KG)

2  3  1 3.754E-03 3.360E-03 2.046E-03 1.494E-04 3.924E-04 2.156E-03 3.480E-03
        1.917E-02 6.488E-03 1.293E+01 3.074E-05 4.814E-05 8.191E-16 0.000E+00
        0.000E+00 0.000E+00 0.000E+00
        DECAY HEAT =   9.6233E+02 WATTS
```

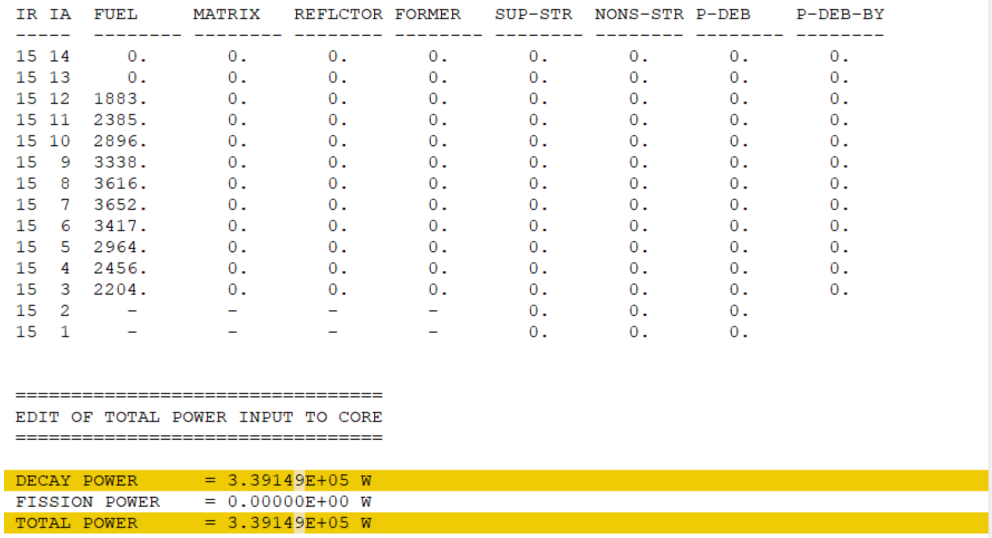
Computed as sums over elements in classes according to DCH_CL, with element mass from JSON using RN1_FPN

Progress Report – HPR Demo

DCH-only vs ORIGEN JSON, cycle 0, component-wise cell decay power



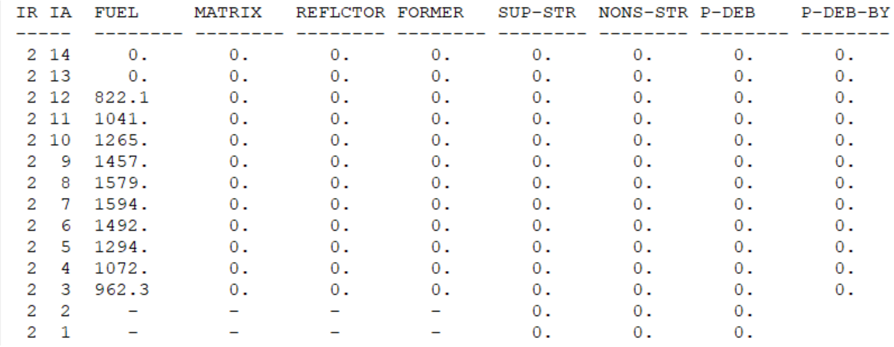
```
IR IA  FUEL     MATRIX   REFLCTOR FORMER   SUP-STR  NONS-STR P-DEB    P-DEB-BY
-----  -------- -------- -------- -------- -------- -------- -------- --------
 2 14      0.       0.       0.       0.       0.       0.       0.       0.
 2 13      0.       0.       0.       0.       0.       0.       0.       0.
 2 12  822.1      0.       0.       0.       0.       0.       0.       0.
 2 11  1041.      0.       0.       0.       0.       0.       0.       0.
 2 10  1265.      0.       0.       0.       0.       0.       0.       0.
 2  9  1457.      0.       0.       0.       0.       0.       0.       0.
 2  8  1579.      0.       0.       0.       0.       0.       0.       0.
 2  7  1594.      0.       0.       0.       0.       0.       0.       0.
 2  6  1492.      0.       0.       0.       0.       0.       0.       0.
 2  5  1294.      0.       0.       0.       0.       0.       0.       0.
 2  4  1072.      0.       0.       0.       0.       0.       0.       0.
 2  3  962.3      0.       0.       0.       0.       0.       0.       0.
 2  2      -        -        -        -       0.       0.       0.
 2  1      -        -        -        -       0.       0.       0.
```



```
IR IA  FUEL     MATRIX   REFLCTOR FORMER   SUP-STR  NONS-STR P-DEB    P-DEB-BY
-----  -------- -------- -------- -------- -------- -------- -------- --------
15 14      0.       0.       0.       0.       0.       0.       0.       0.
15 13      0.       0.       0.       0.       0.       0.       0.       0.
15 12  1883.      0.       0.       0.       0.       0.       0.       0.
15 11  2385.      0.       0.       0.       0.       0.       0.       0.
15 10  2896.      0.       0.       0.       0.       0.       0.       0.
15  9  3338.      0.       0.       0.       0.       0.       0.       0.
15  8  3616.      0.       0.       0.       0.       0.       0.       0.
15  7  3652.      0.       0.       0.       0.       0.       0.       0.
15  6  3417.      0.       0.       0.       0.       0.       0.       0.
15  5  2964.      0.       0.       0.       0.       0.       0.       0.
15  4  2456.      0.       0.       0.       0.       0.       0.       0.
15  3  2204.      0.       0.       0.       0.       0.       0.       0.
15  2      -        -        -        -       0.       0.       0.
15  1      -        -        -        -       0.       0.       0.

=================================
EDIT OF TOTAL POWER INPUT TO CORE
=================================

DECAY POWER        = 3.39149E+05 W
FISSION POWER      = 0.00000E+00 W
TOTAL POWER        = 3.39149E+05 W
```



```
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-----  -------- -------- -------- -------- -------- -------- -------- --------
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 2 13      0.       0.       0.       0.       0.       0.       0.       0.
 2 12  822.1      0.       0.       0.       0.       0.       0.       0.
 2 11  1041.      0.       0.       0.       0.       0.       0.       0.
 2 10  1265.      0.       0.       0.       0.       0.       0.       0.
 2  9  1457.      0.       0.       0.       0.       0.       0.       0.
 2  8  1579.      0.       0.       0.       0.       0.       0.       0.
 2  7  1594.      0.       0.       0.       0.       0.       0.       0.
 2  6  1492.      0.       0.       0.       0.       0.       0.       0.
 2  5  1294.      0.       0.       0.       0.       0.       0.       0.
 2  4  1072.      0.       0.       0.       0.       0.       0.       0.
 2  3  962.3      0.       0.       0.       0.       0.       0.       0.
 2  2      -        -        -        -       0.       0.       0.
 2  1      -        -        -        -       0.       0.       0.
```

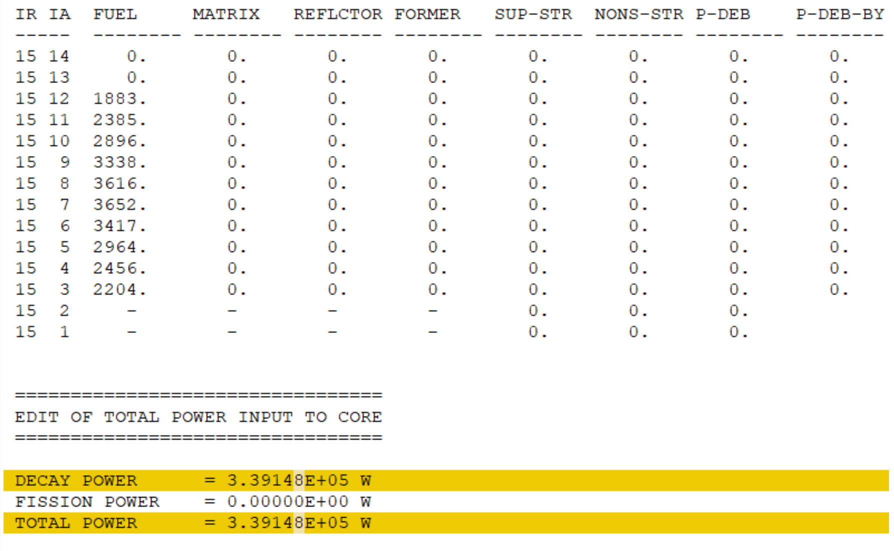

```
IR IA  FUEL     MATRIX   REFLCTOR FORMER   SUP-STR  NONS-STR P-DEB    P-DEB-BY
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15 13      0.       0.       0.       0.       0.       0.       0.       0.
15 12  1883.      0.       0.       0.       0.       0.       0.       0.
15 11  2385.      0.       0.       0.       0.       0.       0.       0.
15 10  2896.      0.       0.       0.       0.       0.       0.       0.
15  9  3338.      0.       0.       0.       0.       0.       0.       0.
15  8  3616.      0.       0.       0.       0.       0.       0.       0.
15  7  3652.      0.       0.       0.       0.       0.       0.       0.
15  6  3417.      0.       0.       0.       0.       0.       0.       0.
15  5  2964.      0.       0.       0.       0.       0.       0.       0.
15  4  2456.      0.       0.       0.       0.       0.       0.       0.
15  3  2204.      0.       0.       0.       0.       0.       0.       0.
15  2      -        -        -        -       0.       0.       0.
15  1      -        -        -        -       0.       0.       0.

=================================
EDIT OF TOTAL POWER INPUT TO CORE
=================================

DECAY POWER        = 3.39148E+05 W
FISSION POWER      = 0.00000E+00 W
TOTAL POWER        = 3.39148E+05 W
```
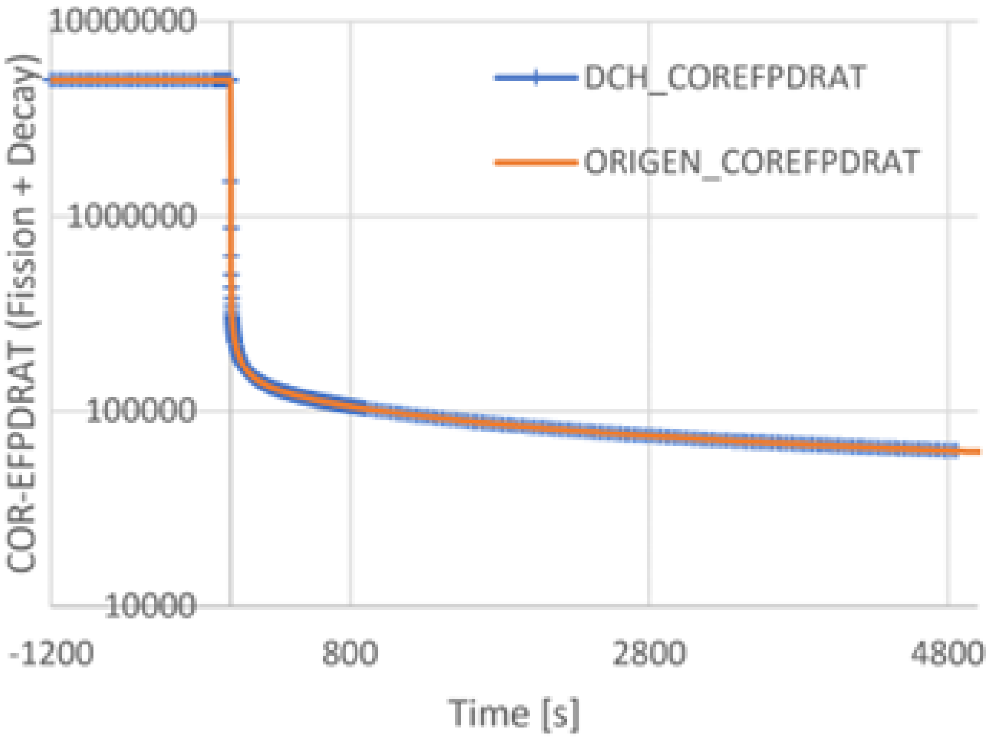

Progress Report – HPR Demo

DCH-only vs ORIGEN JSON, Total Fission and Decay Power

- Time trace shows excellent agreement b/t SCALE-supplied W/kg tables and ORIGEN
- Point kinetics transient with scram and negative reactivity insertion at time zero



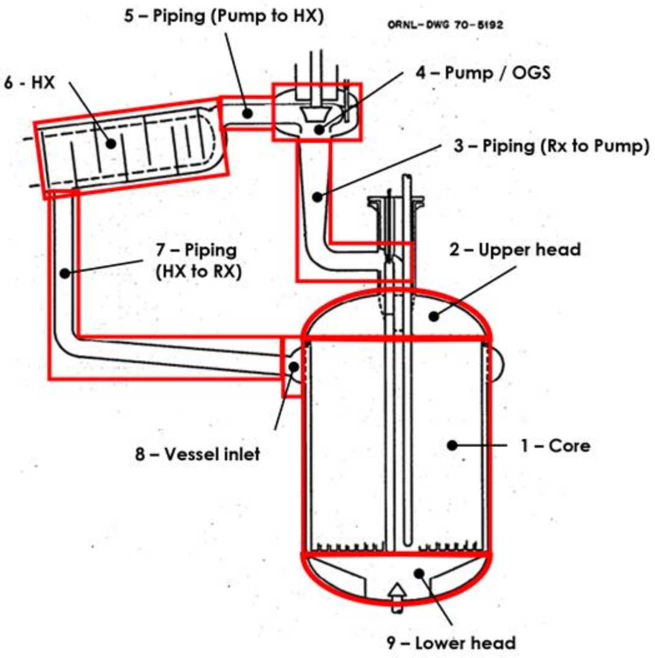
Progress Report – MSRE Demo

MSRE from NRC public demonstration workshop, but

- Add CVH ORIGEN regions (each a CF range of CVs) tracking to multiple JSON files
- Assume initial radionuclide mass is distributed in the primary loop…
  - Uniformly by volume across all CVs belonging to a region correlating to a JSON, and
  - As aerosol in the pool
- Work through:
  - CVH form-wise (e.g. aerosol) element/class-wise inventory accounting
  - CVH form-wise (e.g. aerosol) decay power addition to host phase (e.g. pool)
  - CV-to-CV class-wise advection of form-wise (e.g. aerosol) mass
  - MELCOR-to-ORIGEN updates of region/material elements

From there, work towards:

- HS surfaces and HS ORIGEN regions,
- Filters and FLT ORIGEN regions,
- More region-wise transfer processes and accounting,
- A scenario that releases to an off-gas system,
- Scenarios that demonstrate fluid fuel point kinetics…
  - Alongside ORIGEN/MELCOR,
  - With possible feedback terms informed by ORIGEN ?
  - With delayed neutron precursors informed by ORIGEN ?



Summary

Reviewed ORIGEN and conventional DCH functions in MELCOR

Discussed MELCOR/ORIGEN integration:

- Assumptions,
- Requirements,
- Implementation, and
- Development

Gave updates on:

- MORTY interface,
- MELCOR development,
- HPR demonstration, and
- MSRE demonstration (in progress)

More to come at CSARP/MCAP in June