

ORIGEN Advanced Processing Options

SCALE 6.3.3

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Learning goals



Learn about the advanced features of ORIGIN for blending, feed, and removal



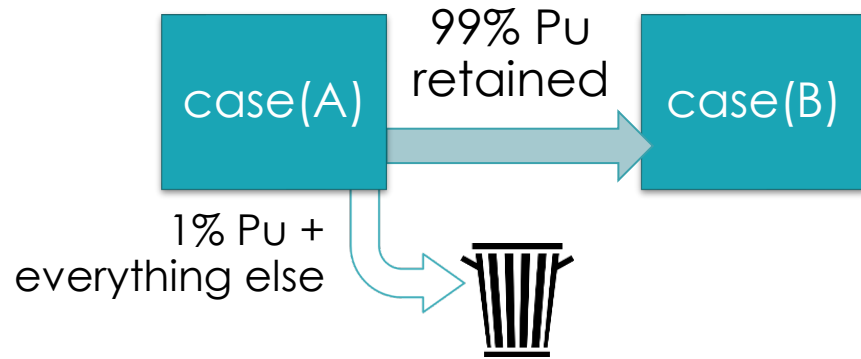
Gain experience using these features for typical applications

Input and Theory

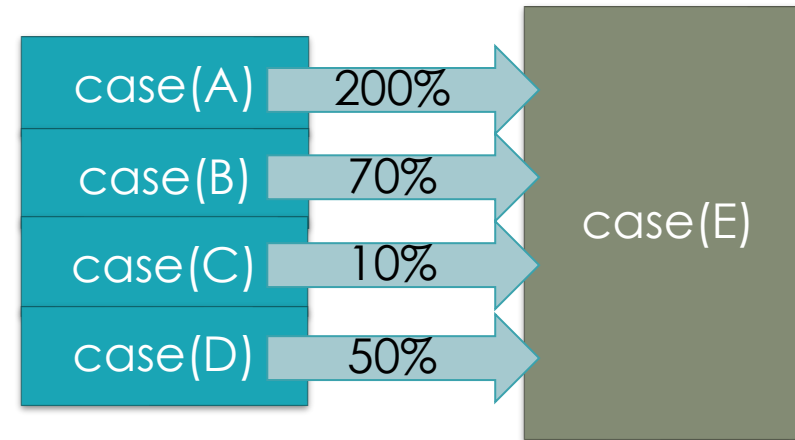


Summary of Advanced Processing Options

Element removal



Stream blending



Continuous removal (elemental)

$$\frac{dN_i}{dt} = \sum_{j=1}^m l_{ij} \lambda_j N_j + \bar{\Phi} \sum_{k=1}^m f_{ik} \sigma_k N_k - (\lambda_i + \bar{\Phi} \sigma_i + r_i) N_i + F_i \quad (i = 1, \dots, m)$$

Continuous feed (isotopic)

Feed and Removal Input



Advanced Operations: removal

```
case{  
    ...  
    processing{  
        %removal rate in 1/s  
        removal{ rate=1e-2 ele=[Xe Ar] }  
        removal{ rate=1e-7 ele=[95 96] }  
    }  
}
```

- continuous removal option, input in the processing block inside a case
- operates on elements, not nuclides
- any number of removals are allowed in a processing block
- define removal by providing
 - removal rate (1/s)
 - list of elements or Z numbers to which the specified removal rate is applied

Advanced Operations: retained

```
case{  
    ...  
    processing{  
        %elementID=atom fraction to retain  
        retained=[ u=1.0 pu=0.5 ]  
    }  
}
```

- retained is input in the processing block inside a case
- operates on elements, not nuclides
- retained specifies the fraction of each element to be retained *at the beginning of case*
- **IMPORTANT:** all elements that are not retained are 0!

Advanced Operations: feed

```
% with feed array
mat{
    % units for iso and feed
    units=GRAMS

    % 1000 kg of natural sodium
    iso=[na=1.0e6]

    % continuous feed of U-235 at 1
    kg/day
    % converted to grams/second
    feed=[u235=0.01157]
}
```

- feed is part of material specification input block
- units are grams per second

Feed and Removal Tutorial Problem



Filtration problem (three cases)

1. Decay 1 g of ^{131}I for 100 days and plot the ^{131}I and $^{131\text{m}}\text{Xe}$ activities
2. Now assume that the generated $^{131\text{m}}\text{Xe}$ is released into a system with a volume of 700 m^3 , and a filtration rate of $5 \text{ m}^3/\text{h}$

$$\text{Noble gas removal rate} = (5 \text{ m}^3/\text{h}) / 700 \text{ m}^3 = 1.98 \times 10^{-6} \text{ s}^{-1}$$

3. Next, in addition to filtration, assume a ^{131}I feed of $1\text{e-}7 \text{ g/s}$

Note difference in results between the three cases

- without filtration or feed
 - with filtration
 - with filtration plus feed
- **Extra Credit:** Estimate the removal rate needed to maintain $^{131\text{m}}\text{Xe}$ system activity $< 100 \text{ Ci}$

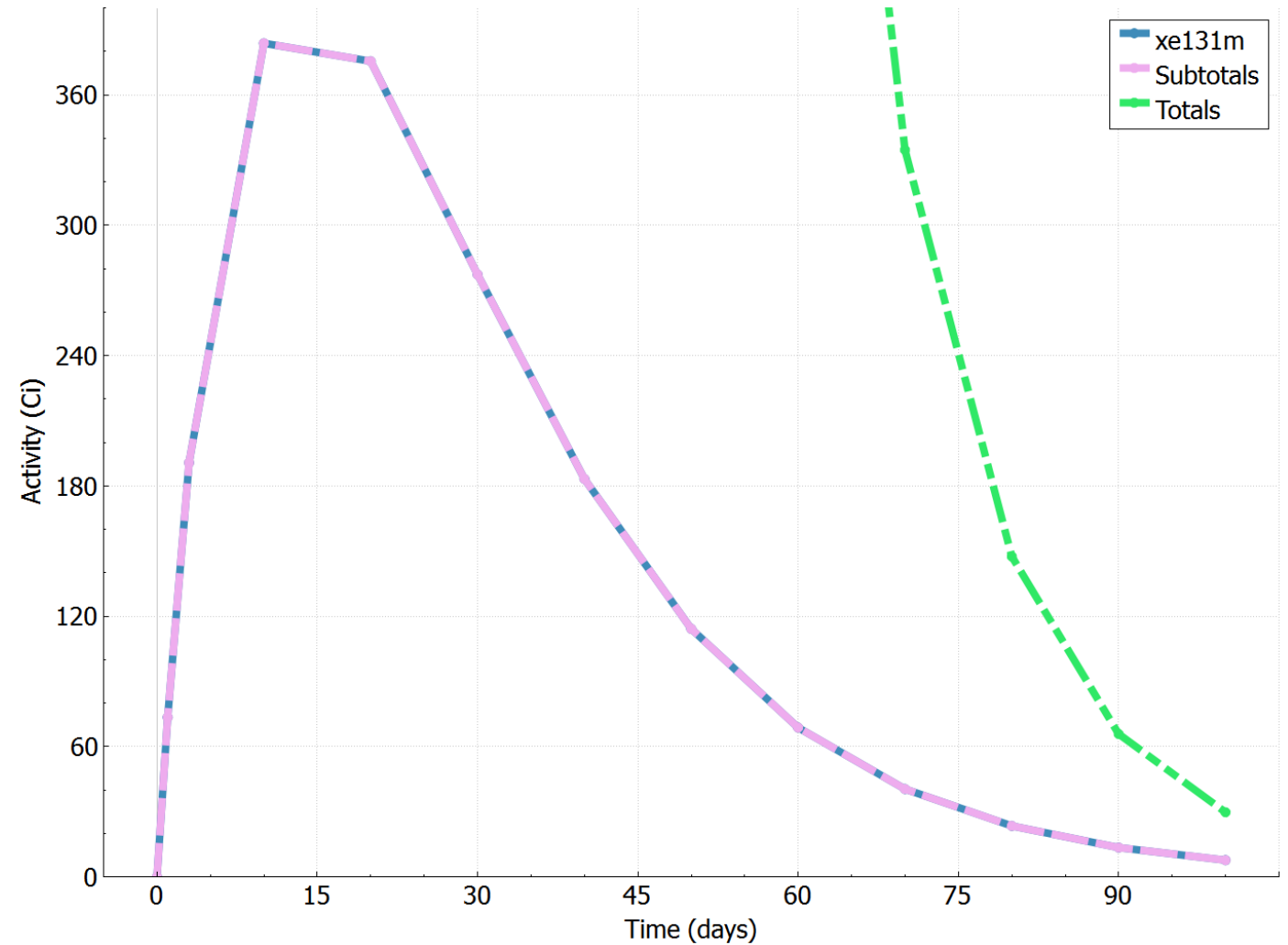
Feed and Removal

Tutorial Solution



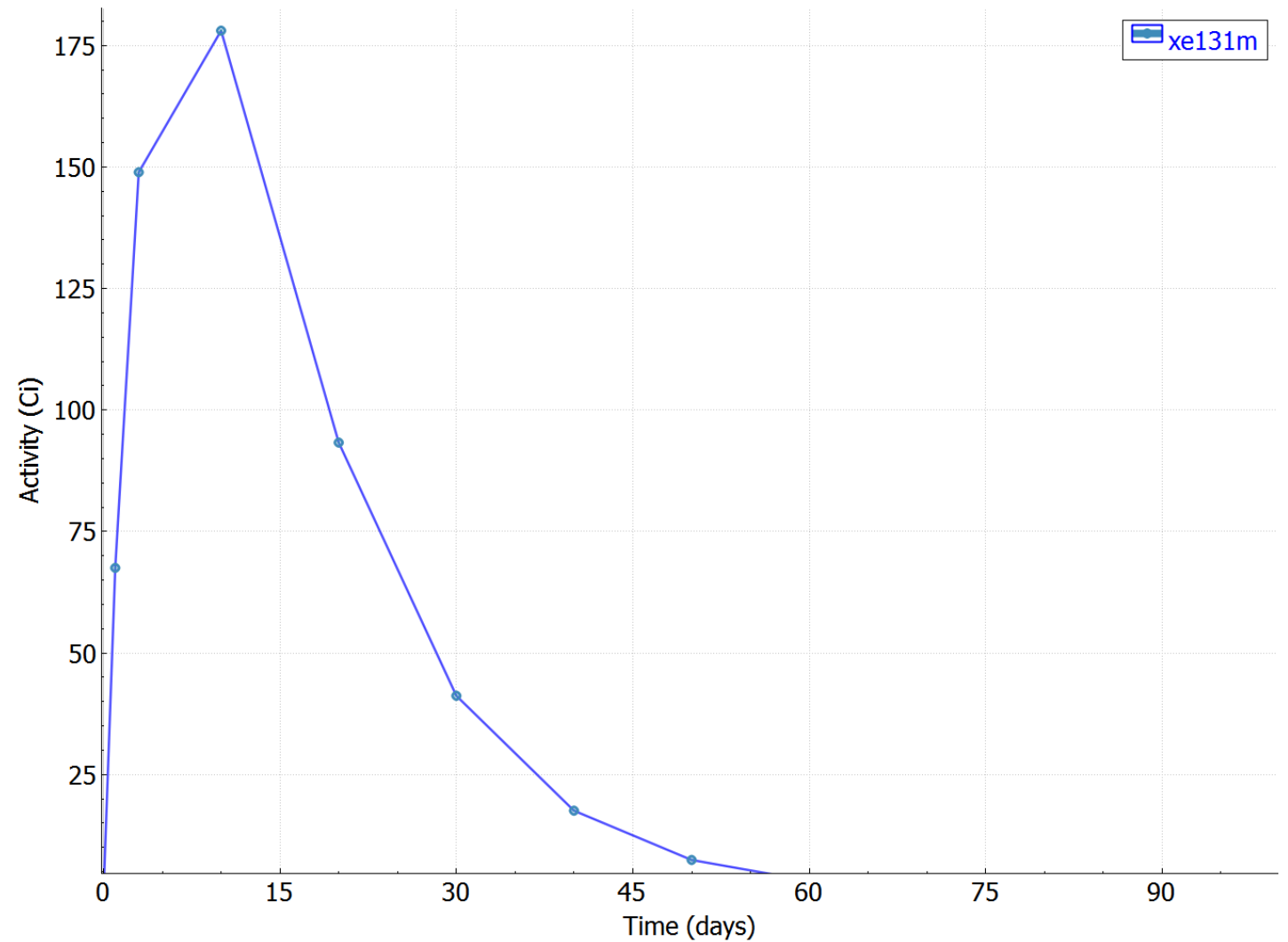
Results: without filtration or feed

```
=origen
case{
  lib{ file="end7dec" }
  mat{
    iso=[ i131(LT)=1.0 ]
    units=GRAMS
  }
  time=[ 1 3 10 20 30 40 50 60 70 80 90 100 ]
  save{
    file="without_filtration.f71"
    steps=all
  }
}
end
```

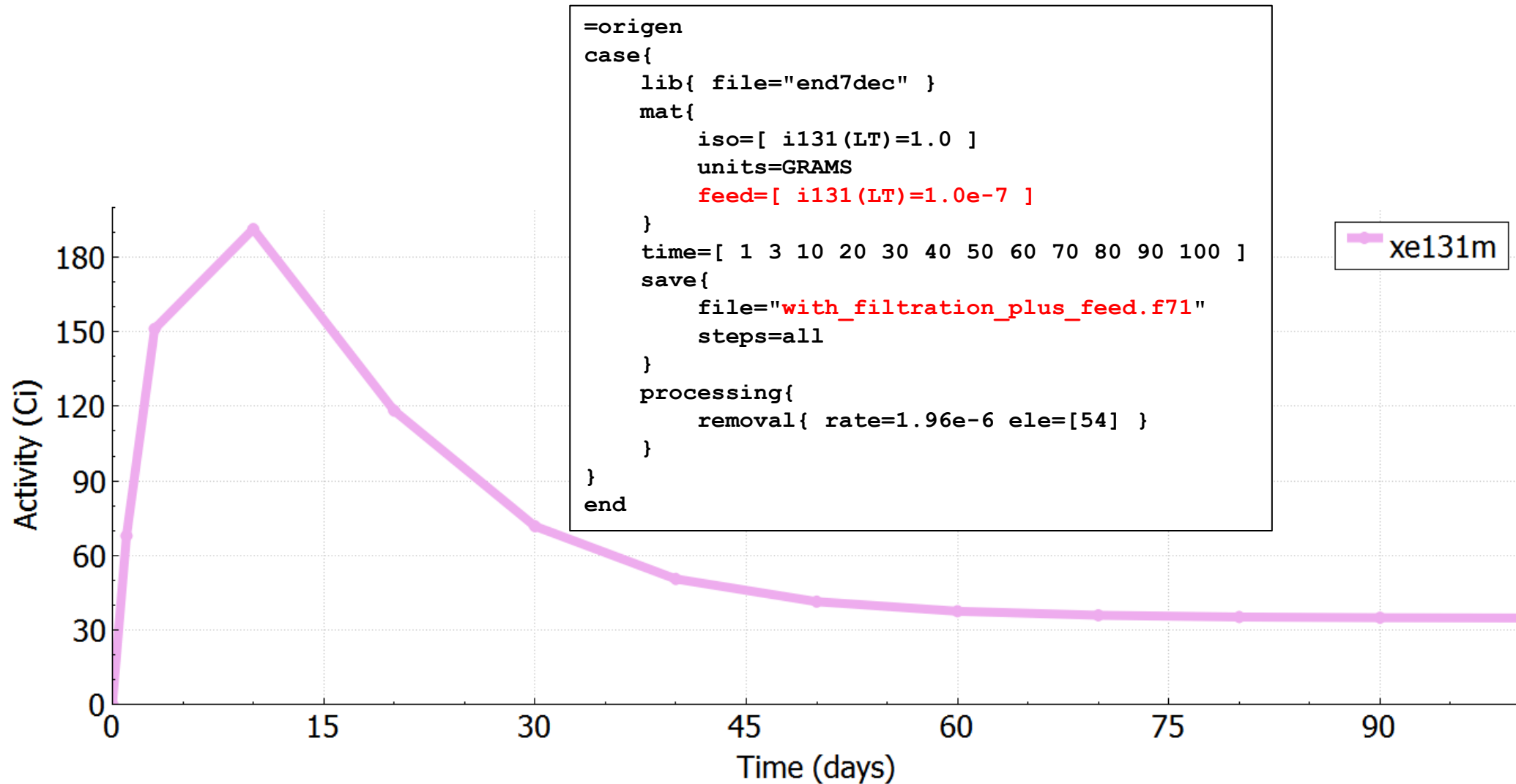


Results: with filtration

```
=origen
case{
  lib{ file="end7dec" }
  mat{
    iso=[ i131(LT)=1.0 ]
    units=GRAMS
  }
  time=[ 1 3 10 20 30 40 50 60 70 80 90 100 ]
}
save{
  file="with_filtration.f71"
  steps=all
}
processing{
  removal{ rate=1.96e-6 ele=[Xe] }
}
end
```



Results: with filtration plus feed



Blending Material Streams

Input



Advanced Operations: **blend**

```
% with blend array
% (only one allowed in an input)
case(A) { ... }
case(B) { ... }
case(C) {
    ...
    mat{
        % case ID(step index)=multiplier
        blend=[ A=0.1 B(2)=0.9 ]
    }
}
```

IMPORTANT: only one blend case is allowed per input (=origen ...end)!

- blends allows fractions of results from specific steps of previous cases to be loaded into a blend
- **case ID(step)=multiplier**
- identifier ID is the case name, or if name not provided the index of the case (default is last case)
- multiplier is the atom fraction of the material composition to be included in the blend
- B(2)=0.9 indicates that 90% of the case(B) isotopics should be taken at the end of step 2 in case B

Blending Material Streams

Tutorial Problem



Blending to simulate a spent fuel pool decay heat power

- Simulate the decay heat power for a spent fuel pool containing three groups of assemblies
 1. 90 assemblies freshly discharged (cooled for 7d after irradiation ends, before being inserted in the pool)
 2. 100 assemblies at 2-yr cooling
 3. 100 assemblies at 4-yr cooling
- Determine the decay heat for the spent fuel pool at 100 days after the discharge from reactor of the group of 90 freshly discharged assemblies
- Assume the same assembly characteristics and irradiation history for all assemblies
 - Westinghouse 15x15 (**w15x15**) assembly, 3.8 wt % ^{235}U enrichment
 - Assembly burnup 40 GWd/MTU, specific power 40MW/MTU
 - For simplicity, assume each assembly has 1 MTU
- Deplete 1 assembly and decay for 4 years months
- “Blend” inventories from the three different cooling times and decay the blend composition to 100 days

Blending Material Streams

Tutorial Solution



Simple irradiation / decay case input

```
=arp
'library type
w15x15
'wt%
3.8
'number of cycles
1
'number of days per cycle
1000
'cycle-average specific power (MW/MTU)
40.0
'number cross section sets generated per
cycle
1
'moderator density (g/cc)
0.723
'interpolated output ORIGEN library
w15.f33
end
...
```

```
...
=origen
case(irrad){
  lib{ file="w15.f33" pos=1 }
  mat{
    units=GRAMS
    iso=[u235=38000 u238=962000]
  }
  time=[ 8I 100 1000 ] %default time in days
  power=[ 10R 40 ] %power in MW
}
case(decay){
  time{
    units=YEARS
    start=0 %reset for input simplicity
    t=[0.019165 0.1 0.3 0.5 1 2 3 4] %points 7d to 4y
  }
  save{ file="discharge.f71" steps=all }
  % f71 has 9 positions, 1st for the end of irradiation
  % the next 8 corresponding to the 8 decay steps
}
end
```

Add blend case

```
=origen
...
t=[0.019165 0.1 0.3 0.5 1 2 3 4] %points 7d to 4y
                                %(positions 1 through 8 in the decay case)
...
case(blend) {
  mat{
    blend=[
      decay(1)=90 % 90 freshly discharged (7d cooled)
      decay(6)=100 % 100 with 2yr cooling
      decay(8)=110 % 110 with 4yr cooling
    ]
  }
  % want 100 days after discharge of the 90 freshly
% discharged assembly; note they are already 7d cooled
  time{
    start=7
    t=[20L 7.1 100]
  }
  % save blended inventory file
  save{ file="blended_sfp.f71" steps=all }
}
end
```

- If we used more steps in the decay, we would need to make sure they corresponded to the intended times
- Use **start=7** to reset the time for the decay of the blend case to 7d, because 1st group of assembly is already cooled for 7 days.
- Save f71 for blend case decay
- Open f71 in Fulcrum to get decay heat

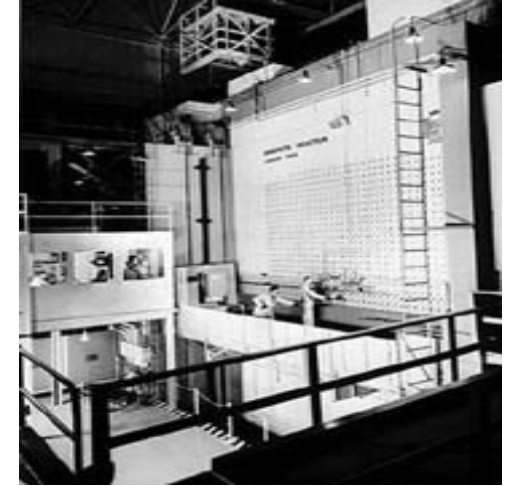
Workshop Problems



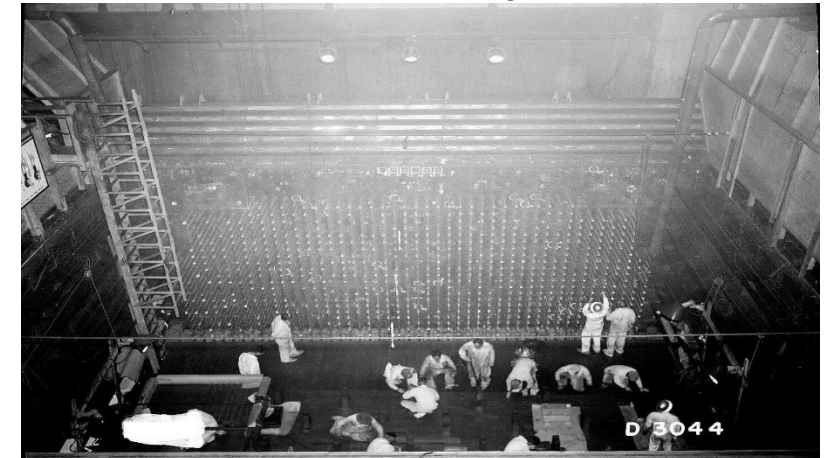
Problem 1: Graphite-moderated reactor

- **Estimate the U and Pu isotopic compositions** evolving in natural U fuel irradiated in a graphite-moderated lattice similar to the configurations of the Oak Ridge Graphite Reactor or the Hanford B Reactor
- Compare calculated data with measurement data for a Hanford B sample
- Need an ORIGEN library representing graphite reactor spectrum—we will use TRITON to generate one.

Oak Ridge Graphite Reactor 1943



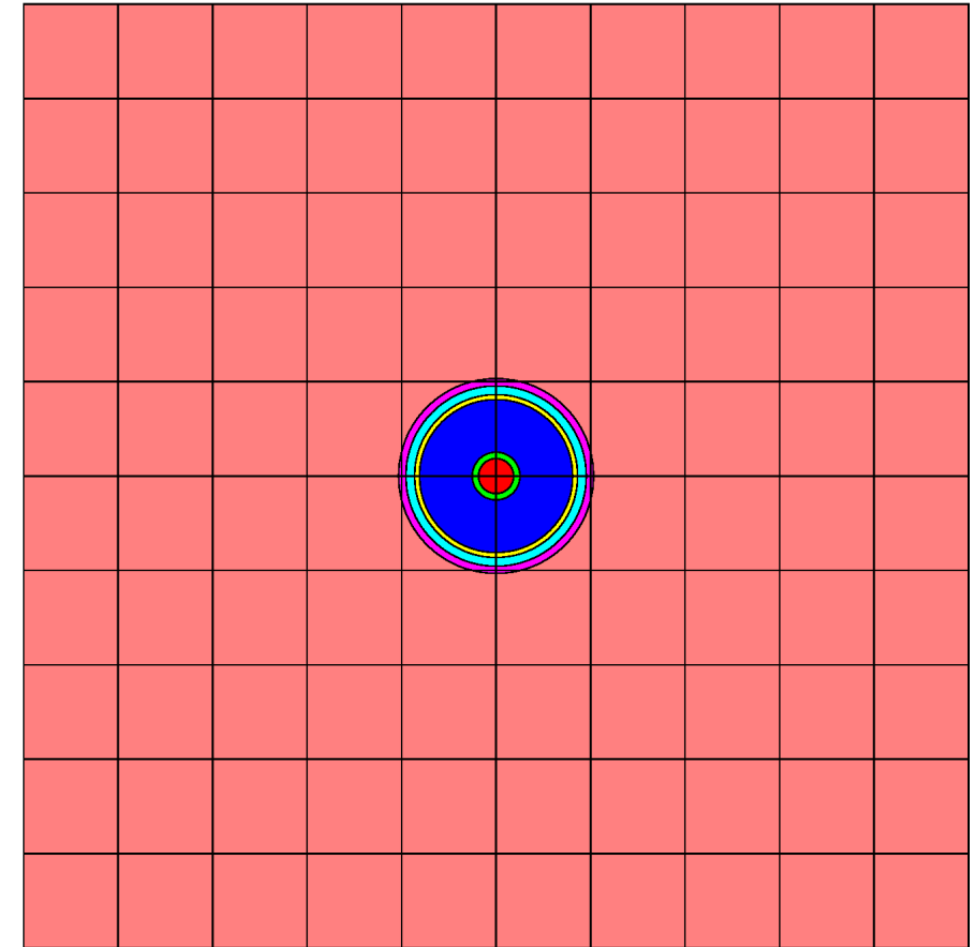
Hanford B Reactor 1944



Problem 1: ORIGIN reactor library generation

- Run the provided TRITON input* for a unit cell to obtain the ORIGIN library
- Create a folder **my_arlibs** and create a new my_arpdata.txt file with the following information:
 - Name: “**graphite_pile**”
 - Library file name: “**graphcell.lib**”
 - Number of enrichment points: 1
 - Number of burnup points: 11
 - Burnup values (MWd/MTU)
0. 150. 450. 750. 1050. 1350. 1650. 1950. 2250. 2550.
2850.
- Copy **my_arlibs** and **my_arpdata.txt** file into \$TMPDIR via a shell command before the SCALE input:

```
=shell
ln -s ${INPDIR}/my_arlibs ${TMPDIR}/arlibs
ln -s ${INPDIR}/my_arpdata.txt ${TMPDIR}/arpdata.txt
end
```



*The provided TRITON input uses a cylindrical lattice cell for computational speed-up

Problem 1: Initial conditions and operating history data

- Based on data sample #4 in ORNL/TM-2014/53

G. Ilas, I. C. Gauld, R. M. Westfall, and M. Pigni, "Evaluation of Hanford B Reactor Experiments (PTA-069 and PTA-084) for Code and Data Benchmarking", ORNL/TM-2014/53, Oak Ridge National Laboratory (March 2014); temperature updated for graphite here

- Uranium isotopic composition (in wt% relative to total U)

U-234 0.0050%

U-235 0.7116%

U-236 0.0006%

U-238 99.2828%

- Specific power 17.56 MW/MTU
- Total irradiation time 30 days
- Decay time after discharge 60 days

Problem 1: Graphite-moderated reactor lattice

Sample measurement data

$^{234}\text{U}/\text{U}$		$^{235}\text{U}/\text{U}$		$^{236}\text{U}/\text{U}$		$^{238}\text{U}/\text{U}$	
content (wt%)	error (wt%)	content (wt%)	error (wt%)	content (wt%)	error (wt%)	content (wt%)	error (wt%)
0.0051	0.0004	0.6600	0.0300	0.0084	0.0010	99.3270	0.0030
$^{238}\text{Pu}/\text{Pu}$		$^{239}\text{Pu}/\text{Pu}$		$^{240}\text{Pu}/\text{Pu}$		$^{241}\text{Pu}/\text{Pu}$	
content (wt%)	error (wt%)	content (wt%)	error (wt%)	content (wt%)	error (wt%)	content (wt%)	error (wt%)
0.0043	0.0004	95.8300	0.0400	4.0000	0.0400	0.1730	0.0090

Problem 2: Fukushima Daiichi 3

Example of using ORIGEN for scoping analysis

- BWR plant
- **Assumptions:**
 - Assume release of 1% of the core inventory into containment water mass of 10,000 MT ($10,000 \text{ m}^3 \rightarrow 1\text{e}4 \text{ m}^3 \rightarrow 1\text{e}10 \text{ cm}^3$)
 - Assume release into water 6 days after shutdown
 - Release I, Cs, Ba, Ce, Mo
- Calculate specific activities in water 14 days after shutdown
- Estimate release fractions based on activities results



Problem 2: Fukushima Measured Water Activities

location	Puddle in underground floor of turbine building of Unit 3
Name of nuclide	Concentration of sample(Bq/cm ³)
Cobalt60	Approximately 7.0×10^2
Technetium99m	Approximately 2.5×10^3
Iodine131	Approximately 1.2×10^6
Cesium134	Approximately 1.8×10^5
Cesium136	Approximately 2.3×10^4
Cesium137	Approximately 1.8×10^5
Barium140	Approximately 5.2×10^4
Lanthanum140	Approximately 9.4×10^3
Cerium144	Approximately 2.2×10^5
total	Approximately 3.9×10^6

<http://www.tepco.co.jp/en/press/corp-com/release/11032503-e.html>

Problem 2: Procedure

- Use ORIGAMI to generate spent fuel inventory (**fukushima.inp**)
 - GE 8x8-2 assembly
 - Core-average burnup: 25 GWd/MTU, Average power 25 MW/MTU
 - Moderator density: 0.45 g/cm³
 - Enrichment: 3.8 wt% ²³⁵U
 - Core inventory: 94 MTU
 - Shutdown cooling: 0 days
 - Run ORIGAMI, examine **fukushima.f71**
- Use ORIGEN to decay post-shutdown (**containment.inp**)
 - Create a decay case for 6 days, loading final isotopics from **fukushima.f71**
 - Create a second decay case for when release is assumed to occur
 - Retain 1% of I, Cs, Ba, Ce, Mo
 - Decay 8 more days (14 days after shutdown)

Workshop Solutions



Problem 1: Graphite-moderated Reactor Inventory

	Calculated		Measured		C/M
	g/MTU	wt% Pu	wt% Pu	2 sigma (%)	
Pu-238	1.735E-02	0.0036	0.0043	18.6	0.837
Pu-239	4.482E+02	95.002	95.8300	0.1	0.991
Pu-240	2.247E+01	4.7629	4.0000	2.0	1.191
Pu-241	1.072E+00	0.2272	0.1730	10.4	1.313
Pu-242	1.967E-02	0.0042	NA		
	g/MTU	wt% U	wt% U	2 sigma (%)	
U-234	4.909E+01	0.0049	0.0051	15.7	0.961
U-235	6.549E+03	0.6556	0.6600	0.9	0.993
U-236	9.701E+01	0.0097	0.0084	23.8	1.155
U-238	9.923E+05	99.3298	99.3270	0.0	1.000

Problem 2: Fukushima Daiichi 3

Nuclide	Z	Measured			Calculated		Ratio C/M	Estimated Release Fraction (%)
		Bq/cm ³	Ci/cm ³	Ci/m ³	Ci	Ci/m ³		
Co-60	27	700	1.89E-08	0.02				
Tc-99m	43	2.50E+03	6.76E-08	0.07	3.38E+04	3.38	50.05	0.02
I-131	53	1.20E+06	3.24E-05	32.43	1.96E+05	19.64	0.61	1.65
Cs-134	55	1.80E+05	4.86E-06	4.86	7.04E+04	7.04	1.45	0.69
Cs-136	55	2.30E+04	6.22E-07	0.62	1.08E+04	1.08	1.74	0.57
Cs-137	55	1.80E+05	4.86E-06	4.86	7.53E+04	7.53	1.55	0.65
Ba-140	56	5.20E+04	1.41E-06	1.41	5.30E+05	53.05	37.60	0.03
La-140	57	9.40E+03	2.54E-07	0.25	5.76E+05	57.62	226.74	<0.01
Ce-144	58	2.20E+06	5.95E-05	59.46	8.28E+05	82.83	1.39	0.72

Workshop Problem

Modeling the MSRE Flow Loop in ORIGIN



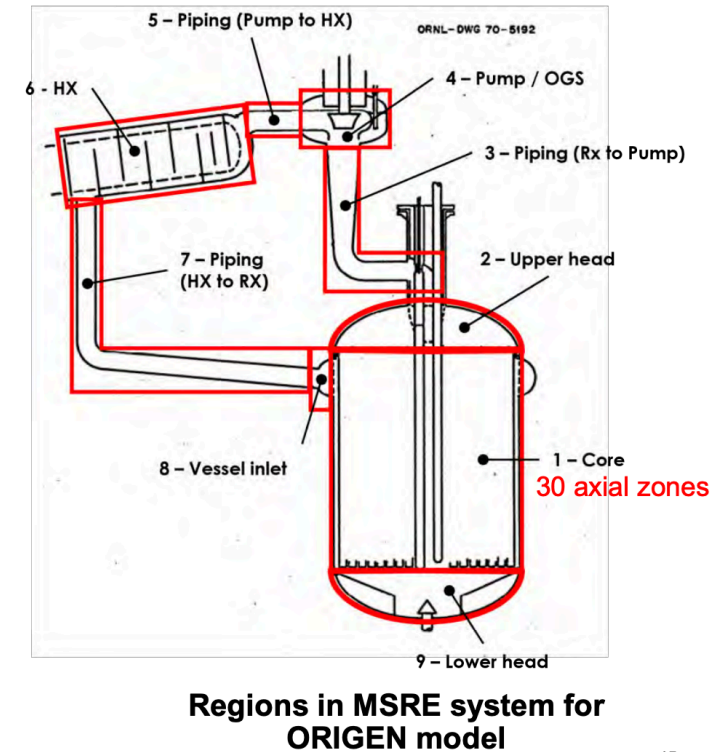
Two approaches Molten-salt fueled systems

- Power production time-scales (months)
 - Consider the loop+core as the main generator of nuclides and consider other “compartments” based on where nuclides will be removed/added to loop
 - Heat Exchanger
 - Off-gas
- Loop transit time-scales (seconds)
 - Consider following a “slug” of fuel as it moves through the system to estimate the “location-dependent” inventory

Location dependent inventory – model development

Developed ORIGEN model to predict nuclide inventory **in each region** of the loop at ~375 days

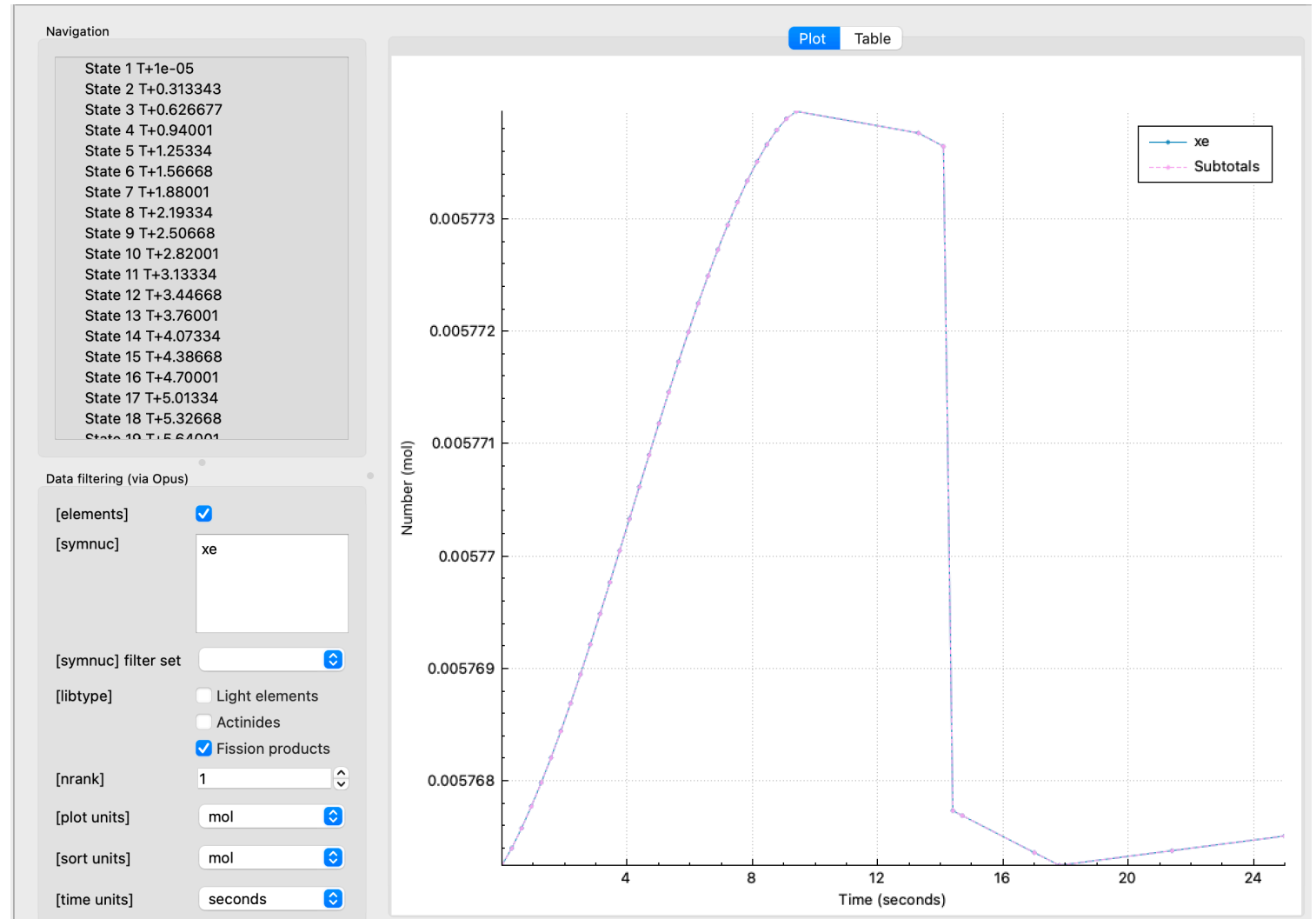
- Divided MSRE system into 9 general regions, with the core region subdivided into 30 axial zones
- Used fuel salt composition from 2D TRITON-MSR calculation at 375 days as the start
- Developed chain of ORIGEN inputs that use residence time and flux of the fuel salt in each region and removes noble gases (Kr, Xe) in off-gas system
- 1 ORIGEN input corresponds to the salt traveling 1 time through the whole loop



Slide from volume 3 MSRE workshop explaining the 9 different regions a “slug” of fuel will travel through.
<https://code.ornl.gov/scale/analysis/non-lwr-models-vol3>

Procedure

- Examine the models for the “location-dependent” inventory calculation.
 - They start from equilibrium conditions and simulate a few loops with ORIGEN to attempt to converge the spatial distribution around the loop
 - The equilibrium solution (TRITON) should have the loop+core average approximately correct, but we want to see how nuclides could change around the loop.
- 10 successive loop inputs are prepared in the starter directory



We want to examine the Xe inventory as a function of loop time (25 seconds for the full loop) and confirm the different effects.

Strategy

- The ORIGEN models are set up correctly, but you must run them in order
- Use F71 viewer in Fulcrum to view particular nuclides or elements
 - Check the “elements” box
 - Reduce the NRANK to 1 or 2
 - Change the y-axis units to moles or grams
 - Change the x-axis units to seconds
 - Right-click the legend “Total” and “remove selected” so it doesn’t affect the axis scale so much
 - You could also click on the Table tab and copy/paste the data into Excel

Answer the following based on the Xe plot

1. Why does Xe increase over the first 9 seconds?
2. Why does it increase slower near the beginning and end of the first interval?
3. Why is there a sharp drop at ~14 seconds?
4. Why is there a slow increase after that?
5. **Extra:** does Kr show the same or different effect?

