LWR Activation Analysis with Polaris and TRITON

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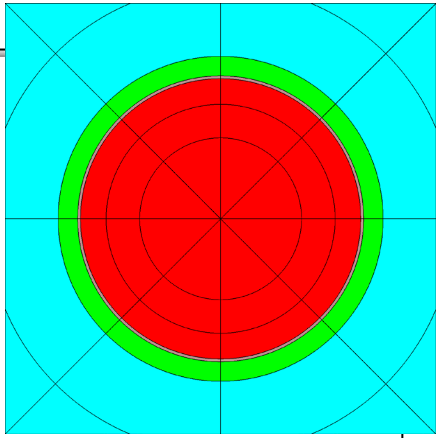
Consider simple coolant activation model in Polaris

- 3.1% enr UO2 fuel
- Zirc4 cladding
- WEC 17x17 geometry
- 600 ppm boron
- 40 MW/MTU
- Coolant and Fuel are depleted from 0 to 10 GWD/MTU
- Output of Interest: H-3 buildup in coolant



```
=polaris

  lib "broad_lwr"
  geom wec_pin : ASSM 1 1.26
  sys PWR

  comp c_uox3 : UOX 3.1
  mat FUEL.1 : c_uox3 10.157

  pin 1 : 0.4096 0.418 0.475 : FUEL.1 GAP CLAD

  mesh FUEL   : nr=2 ns=-4
  shield ALL=P

  state ALL : temp=600 FUEL : temp=900 COOL : boron=600 dens=0.6
  power 40
  bu 0.1 1 2 4 6 8 10
  deplete ALL=no FUEL=yes COOL=yes
  opt DEPL ArchiveF33='ALL'

end
```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Text Output

- F71 Archive Summary:
- Go to positions 9-16 in F71 file in Fulcrum

```
-----------------------------------------------------------------------------
 Depletion Archive F71 Summary for History: BASE_HISTORY
-----------------------------------------------------------------------------

|-----|-----|--------------------|-----------|-----------|
|Index| Pos |          Edit Name |  Time (d) | Time (sec)|
|-----|-----|--------------------|-----------|-----------|
|   1 |   1 |         CLAD.1.p1  | 0.000e+00 | 0.000e+00 |
|   1 |   2 |         CLAD.1.p1  | 2.500e+00 | 2.160e+05 |
|   1 |   3 |         CLAD.1.p1  | 2.500e+01 | 2.160e+06 |
|   1 |   4 |         CLAD.1.p1  | 5.000e+01 | 4.320e+06 |
|   1 |   5 |         CLAD.1.p1  | 1.000e+02 | 8.640e+06 |
|   1 |   6 |         CLAD.1.p1  | 1.500e+02 | 1.296e+07 |
|   1 |   7 |         CLAD.1.p1  | 2.000e+02 | 1.728e+07 |
|   1 |   8 |         CLAD.1.p1  | 2.500e+02 | 2.160e+07 |
|-----|-----|--------------------|-----------|-----------|
|   2 |   9 |         COOL.1.p1  | 0.000e+00 | 0.000e+00 |
|   2 |  10 |         COOL.1.p1  | 2.500e+00 | 2.160e+05 |
|   2 |  11 |         COOL.1.p1  | 2.500e+01 | 2.160e+06 |
|   2 |  12 |         COOL.1.p1  | 5.000e+01 | 4.320e+06 |
|   2 |  13 |         COOL.1.p1  | 1.000e+02 | 8.640e+06 |
|   2 |  14 |         COOL.1.p1  | 1.500e+02 | 1.296e+07 |
|   2 |  15 |         COOL.1.p1  | 2.000e+02 | 1.728e+07 |
|   2 |  16 |         COOL.1.p1  | 2.500e+02 | 2.160e+07 |
|-----|-----|--------------------|-----------|-----------|
|   3 |  17 |         FUEL.1.p1  | 0.000e+00 | 0.000e+00 |
|   3 |  18 |         FUEL.1.p1  | 2.500e+00 | 2.160e+05 |
|   3 |  19 |         FUEL.1.p1  | 2.500e+01 | 2.160e+06 |
|   3 |  20 |         FUEL.1.p1  | 5.000e+01 | 4.320e+06 |
|   3 |  21 |         FUEL.1.p1  | 1.000e+02 | 8.640e+06 |
|   3 |  22 |         FUEL.1.p1  | 1.500e+02 | 1.296e+07 |
|   3 |  23 |         FUEL.1.p1  | 2.000e+02 | 1.728e+07 |
|   3 |  24 |         FUEL.1.p1  | 2.500e+02 | 2.160e+07 |
|-----|-----|--------------------|-----------|-----------|
|   4 |  25 |          GAP.1.p1  | 0.000e+00 | 0.000e+00 |
|   4 |  26 |          GAP.1.p1  | 2.500e+00 | 2.160e+05 |
|   4 |  27 |          GAP.1.p1  | 2.500e+01 | 2.160e+06 |
|   4 |  28 |          GAP.1.p1  | 5.000e+01 | 4.320e+06 |
|   4 |  29 |          GAP.1.p1  | 1.000e+02 | 8.640e+06 |
|   4 |  30 |          GAP.1.p1  | 1.500e+02 | 1.296e+07 |
|   4 |  31 |          GAP.1.p1  | 2.000e+02 | 1.728e+07 |
|   4 |  32 |          GAP.1.p1  | 2.500e+02 | 2.160e+07 |
|-----|-----|--------------------|-----------|-----------|
```

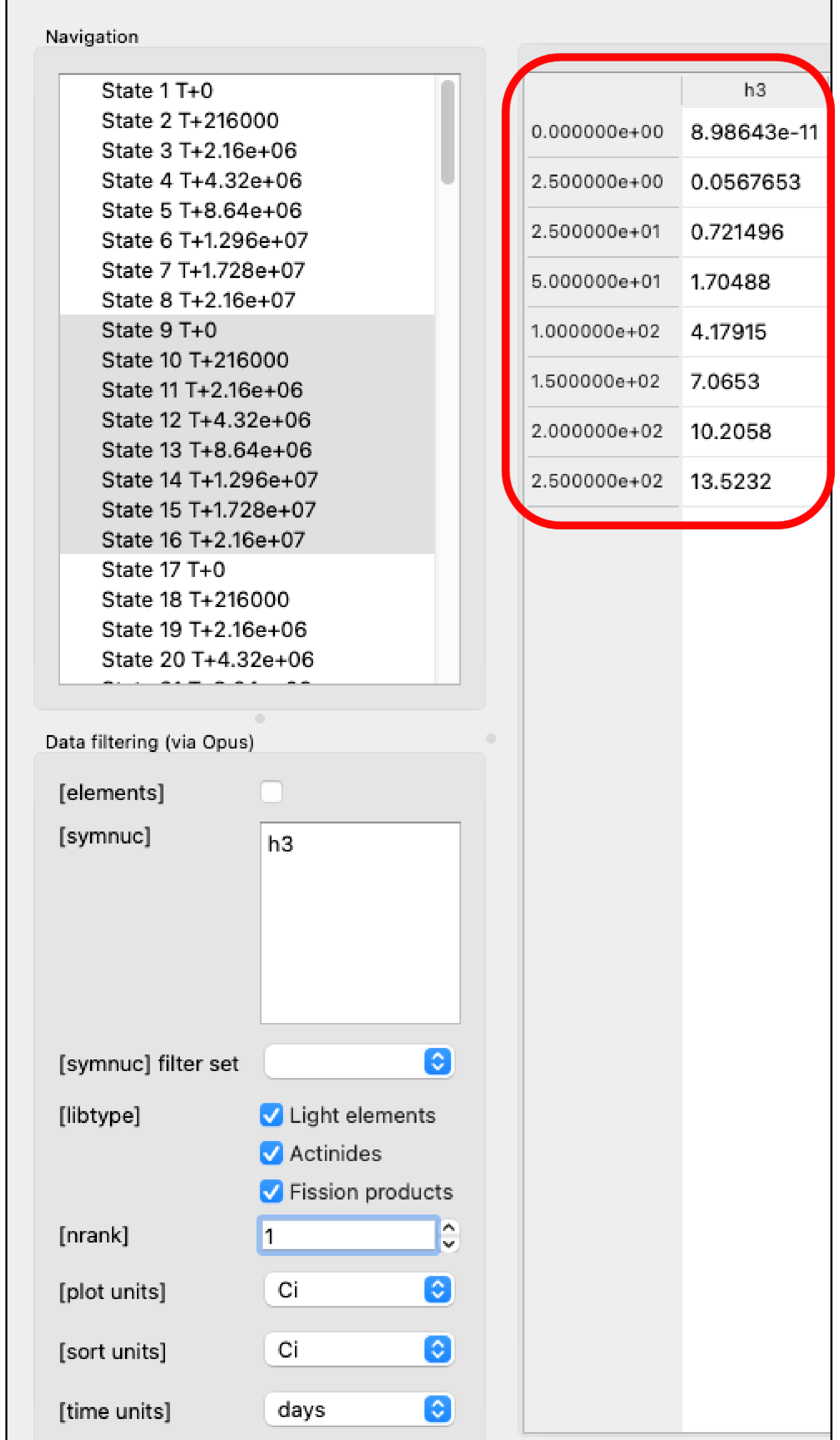
Fulcrum Output

- F71 Archive Summary:
- Go to positions 9-16 in F71 file in Fulcrum
- H-3 activity is13.5 Ci @ 250 days (or 10 GWD/MTU)

Concern

- Calculation above used 56-group LWR library
- If 252-group library is used:
- H-3 activity is 3.6 Ci @ 250 days (or 10 GWD/MTU)
- Similar results for equivalent TRITON model

Why is 252G library calc produce ~4x less tritium in coolant than equivalent 56G calc?



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Data Mining with obiwan

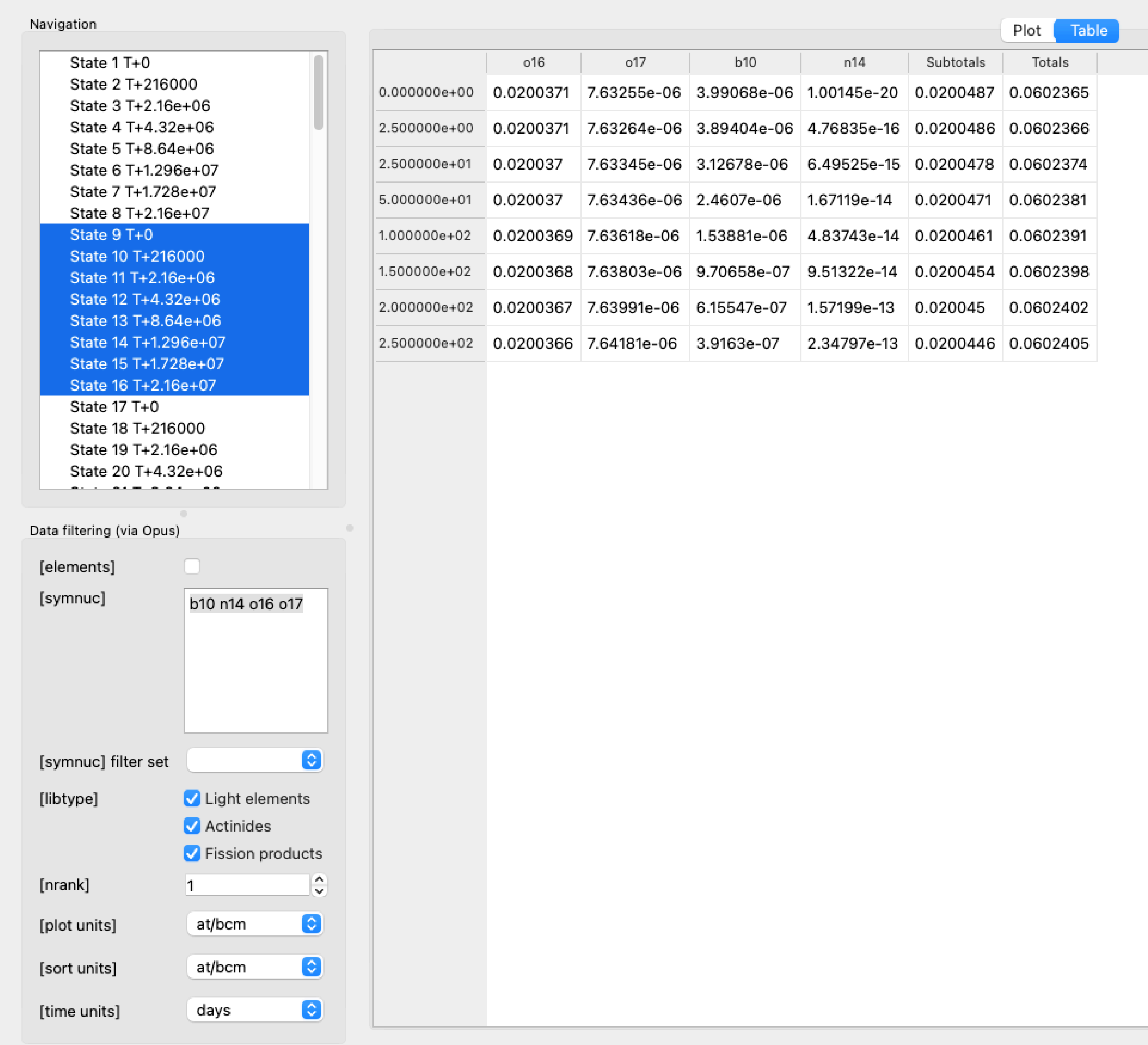
- Use obiwan to get micro XS
- Command : obiwan view -format=coefft <file.f33> | grep '10001003<‘
- Columns: bu= 0.0, 0.1, 1, 2, 4, 6, 8, 10

```
[m8j ~/Downloads/trit]$ /Users/Shared/build/master_rel/INSTALL/bin/obiwan view -format=coefft pol56.COOL.1.f33 | grep '10001003<'
 10001003<--[102]--10001002  3.9814e-05  3.9140e-05  3.8358e-05  3.7626e-05  3.6434e-05  3.5498e-05  3.4746e-05  3.4128e-05
 10001003<--[103]--10002003  3.8805e+02  3.8102e+02  3.7270e+02  3.6488e+02  3.5220e+02  3.4225e+02  3.3427e+02  3.2773e+02
 10001003<--[105]--10003006  6.8783e+01  6.7543e+01  6.6074e+01  6.4695e+01  6.2457e+01  6.0702e+01  5.9294e+01  5.8139e+01
  10001003<--[22]--10003007  6.3795e-03  6.3895e-03  6.4549e-03  6.5208e-03  6.6259e-03  6.7079e-03  6.7748e-03  6.8311e-03
  10001003<--[33]--10004009  2.8772e-05  2.8874e-05  2.9287e-05  2.9699e-05  3.0375e-05  3.0922e-05  3.1383e-05  3.1782e-05
  10001003<--[33]--10004010  1.4563e-06  1.4615e-06  1.4824e-06  1.5032e-06  1.5374e-06  1.5651e-06  1.5884e-06  1.6086e-06
 10001003<--[105]--10005010  1.7316e-02  1.7279e-02  1.7358e-02  1.7442e-02  1.7563e-02  1.7643e-02  1.7700e-02  1.7741e-02
 10001003<--[105]--10005011  1.7868e-05  1.7931e-05  1.8188e-05  1.8444e-05  1.8864e-05  1.9203e-05  1.9489e-05  1.9737e-05
```

```
[m8j ~/Downloads/trit]$ /Users/Shared/build/master_rel/INSTALL/bin/obiwan view -format=coefft pol252.COOL.1.f33 | grep '10001003<'
 10001003<--[102]--10001002  4.0181e-05  3.9508e-05  3.8715e-05  3.7973e-05  3.6776e-05  3.5844e-05  3.5101e-05  3.4497e-05
 10001003<--[103]--10002003  3.9190e+02  3.8489e+02  3.7644e+02  3.6853e+02  3.5578e+02  3.4587e+02  3.3799e+02  3.3160e+02
 10001003<--[105]--10003006  6.9467e+01  6.8229e+01  6.6738e+01  6.5342e+01  6.3091e+01  6.1344e+01  5.9953e+01  5.8825e+01
  10001003<--[22]--10003007  6.4912e-03  6.5044e-03  6.5746e-03  6.6450e-03  6.7575e-03  6.8456e-03  6.9177e-03  6.9784e-03
  10001003<--[33]--10004009  8.3262e-07  8.3595e-07  8.6824e-07  9.0113e-07  9.5643e-07  1.0040e-06  1.0469e-06  1.0865e-06
  10001003<--[33]--10004010  7.3576e-13  8.9324e-13  2.2240e-12  4.8230e-12  1.5468e-11  3.3265e-11  5.6673e-11  8.4129e-11
 10001003<--[105]--10005010  1.7375e-02  1.7342e-02  1.7424e-02  1.7511e-02  1.7636e-02  1.7720e-02  1.7779e-02  1.7822e-02
 10001003<--[105]--10005011  5.9215e-07  5.9456e-07  6.1875e-07  6.4336e-07  6.8459e-07  7.1984e-07  7.5149e-07  7.8060e-07
```

Data Mining with Fulcrum

- Use Fulcrum (or obiwan) to get number densities



	o16	o17	b10	n14	Subtotals	Totals
0.000000e+00	0.0200371	7.63255e-06	3.99068e-06	1.00145e-20	0.0200487	0.0602365
2.500000e+00	0.0200371	7.63264e-06	3.89404e-06	4.76835e-16	0.0200486	0.0602366
2.500000e+01	0.020037	7.63345e-06	3.12678e-06	6.49525e-15	0.0200478	0.0602374
5.000000e+01	0.020037	7.63436e-06	2.4607e-06	1.67119e-14	0.0200471	0.0602381
1.000000e+02	0.0200369	7.63618e-06	1.53881e-06	4.83743e-14	0.0200461	0.0602391
1.500000e+02	0.0200368	7.63803e-06	9.70658e-07	9.51322e-14	0.0200454	0.0602398
2.000000e+02	0.0200367	7.63991e-06	6.15547e-07	1.57199e-13	0.020045	0.0602402
2.500000e+02	0.0200366	7.64181e-06	3.9163e-07	2.34797e-13	0.0200446	0.0602405

Results and Analysis

- 8 top contributors to the production of H-3 at 10 GWD/MTU
- The sum macro xs of the production of H-3 is 6x bigger in 56g calculation compared to 252g
- Errors can come from
  - Number density differences
  - Microscopic XS differences
- "Rel Err in Sum" is the contribution of each reaction to the error in the sum macro xs
- Notice that He-3 (n,p) reaction has the most error

H-3 Parent	56g micro	252g micro	56g numden	252g numden	56g macro	252g macro	Rel Err in Sum
Li-7	6.8E-03	7.0E-03	3.6E-06	3.6E-06	2.5E-08	2.5E-08	-2%
B-10	1.8E-02	1.8E-02	3.9E-07	3.9E-07	6.9E-09	6.9E-09	0%
He-3	3.3E+02	3.3E+02	5.2E-10	3.6E-12	1.7E-07	1.2E-09	501%
H-2	3.4E-05	3.4E-05	1.3E-05	1.3E-05	4.3E-10	4.4E-10	0%
Li-6	5.8E+01	5.9E+01	7.7E-12	5.4E-12	4.5E-10	3.2E-10	0%
B-11	2.0E-05	7.8E-07	1.6E-05	1.6E-05	3.2E-10	1.3E-11	1%
Be-9	3.2E-05	1.1E-06	1.3E-11	4.3E-12	4.0E-16	4.7E-18	0%
Be-10	1.6E-06	8.4E-11	4.9E-11	4.5E-11	7.9E-17	3.8E-21	0%
				sum	2.0E-07	3.4E-08	6

Results and Analysis

- 4 top contributors to the production of He-3 at 10 GWD/MTU
- The sum macro xs of the production of He-3 is 5465x bigger in 56g calculation compared to 252g
- Errors can come from
  - Number density differences
  - Microscopic XS differences
- "Rel Err in Sum" is the contribution of each reaction to the error in the sum macro xs
- Notice that O-16 (n,He-3) reaction has the most error

He-3 Parent	56g micro	252g micro	56g numden	252g numden	56g macro	252g macro	Rel Err in Sum
O-16	9.2E-06	1.7E-09	2.0E-02	2.0E-02	1.8E-07	3.4E-11	546432%
B-10	6.2E-06	3.2E-10	3.9E-07	3.9E-07	2.4E-12	1.3E-16	7%
O-17	1.3E-08	6.8E-13	7.6E-06	7.6E-06	9.9E-14	5.2E-18	0%
N-14	1.2E-06	6.2E-11	2.3E-13	1.2E-13	2.8E-19	7.4E-24	0%
				sum	1.8E-07	3.4E-11	5465

- O-16 (n,He-3) is a threshold reaction > 14 MeV
- In the 252g structure, the top 3 energy groups are above this threshold
- In the 56g structure, the top energy group lower bound is 6.43 MeV
- This coarse structure in the 56g library leads to over prediction of the ORIGEN transition coefficient (in this case by 5400x)

Best practices

- LWR depletion calculations in SCALE (TRITON or Polaris) can utilize either the 56g library or the 252g library
- The transition coefficients in ORIGEN depend on the flux-volume collapse of cross sections.
- Several of the 54,000 transitions tracked in ORIGEN are threshold reactions, with Q-values above 6 MeV
- Flux-volume collapse of these threshold reactions tend to produce over-estimated transition coefficients for a 56g library calculation
- Non-threshold or fission transitions are not as sensitive to library structure, but are still susceptible to errors if the model spectrum is different than the collapsing spectrum
- **For non-fuel LWR activation studies, best practice is to use the 252g library with SCALE 6.3**