Target Activation and Analysis GUI (TAAG) Introduction and Test Problem

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Outline

Introduction and background

Test Problem: Mo-99 Production in OPAL
- Problem description
- Activation setup
- Operating history
- Results

Conclusions

TAAG Background

- Grew from need for simplified interface to perform activation calculations using ORIGEN
- Activation simulations have always been available in ORIGEN, but access to the feature has been somewhat more difficult
  - Available in the legacy ORIGEN-ARP GUI (SCALE 6.0 and earlier)
  - Available using the text input format
    - FIDO input in SCALE 6.1 and earlier: *very* difficult to use—recommended only for super users
    - ORIGEN modern input in SCALE 6.2 and beyond: easier to use, but still requires knowledge of the text-based input
- Activation libraries are the same as typical ORIGEN libraries, but setup in the `arpdata.txt` file is different
- Activation calculations have a significant number of degrees of freedom
  - Typical ORIGEN fuel depletion simulations use a known fuel material in a particular reactor
  - Interpolation performed for enrichment, moderator density, burnup, and Pu vector for MOX
  - For activation, any target can be put in an irradiation location in a reactor, meaning spectrum and material may be unknown

Depletion/Activation Equation

$$\text{Rate of change in nuclide concentration} = \text{Production rate of nuclide} - \text{Loss rate of nuclide}$$

$$\overbrace{\frac{\mathrm{d}N_i}{\mathrm{d}t}}^{\text{Rate of change in nuclide concentration}} = \overbrace{\sum_j l_{ij}\lambda_j N_j}^{\text{Decay into nuclide by other nuclides}} + \overbrace{\phi \sum_j f_{ij}\sigma_j N_j}^{\text{Production of nuclide from irradiation}} - \overbrace{(\lambda_i + \phi\sigma_i + r_i)N_i}^{\text{Loss of nuclide through decay, irradiation, etc}}$$

N_i : amount of nuclide i

λ_i : decay constant of nuclide i (s^{-1})

l_{ij} : branching ratio for decay from nuclide j to nuclide i

ϕ : angle- and energy-integrated neutron flux ($\mathrm{n}/\mathsf{cm}^2\mathsf{s}$)

σ_i : spectrum-averaged removal cross section for nuclide i (b)

f_{ij} : fractional yield of nuclide i from neutron-induced removal of nuclide j

r_i : linear removal rate of nuclide (s^{-1})

Depletion/Activation Equation for TAAG

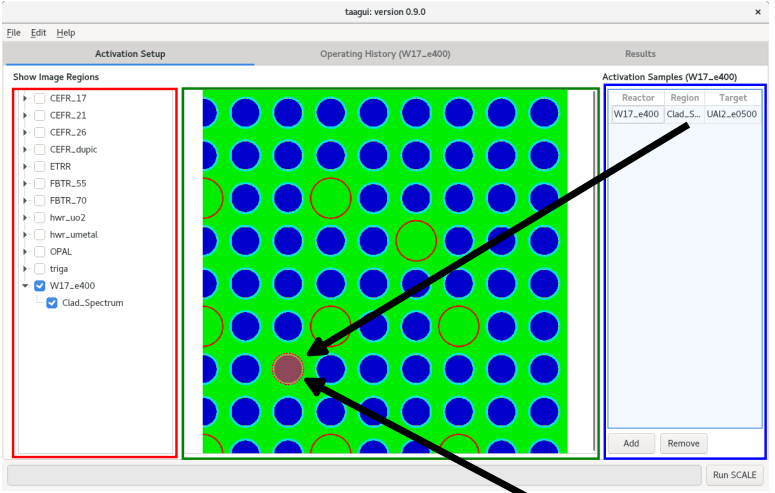
- User input
  - Initial target composition $N_i(t_0)$: can vary for many different types of targets
  - Irradiation time Δt
  - Neutron flux ϕ: derived from reactor power
- Material data
  - Neutron cross-sections σ_i and reaction yields f_{ij} for activation simulations
    1. Group XS $\sigma_{g,i}$ generated for generic material (air, cladding, etc.)
    2. Flux spectrum ϕ_g in that region used to collapse location-dependent XS data

$$\sigma_i = \frac{\sum_g \phi_g \sigma_{g,i}}{\sum_g \phi_g}$$

  - Decay constants λ_i and branching ratios l_{ij}

$$\frac{\mathrm{d}N_i}{\mathrm{d}t} = \sum_j l_{ij}\lambda_j N_j + \phi \sum_j f_{ij}\sigma_j N_j - (\lambda_i + \phi\sigma_i + r_i)N_i$$

TAAG Activation Setup Panel



Selected reactor
Highlighted regions

Reactor image

Region with
activation target

TAAG Operating History Panel

taagui: version 0.9.0

File Edit Help

Activation Setup | Operating History (W17_e400) | Results

Operating History

Full Power = 40 MW/MTIHM, Cycle Length = 365 days

User Inputs

Cycle	Step	Time Interval (days)	Time Total (days)	EFPD Interval (days)	EFPD Cycle (days)	EFPD Total (days)	Power (MW/MTIHM)	Percent Full Power (%)
1	1	2	2	1	1	1	20	50
1	2	10	12	7.5	8.5	8.5	30	75
1	3	20	32	20	28.5	28.5	40	100
1	4	40	72	40	68.5	68.5	40	100
1	5	90	162	90	158.5	158.5	40	100
1	6	90	252	90	248.5	248.5	40	100
1	7	90	342	85.5	334	334	38	95
1	8	30	372	27	361	361	36	90

Δt

ΔEFPD = $\Delta t \times$ [% Full Power]

Power

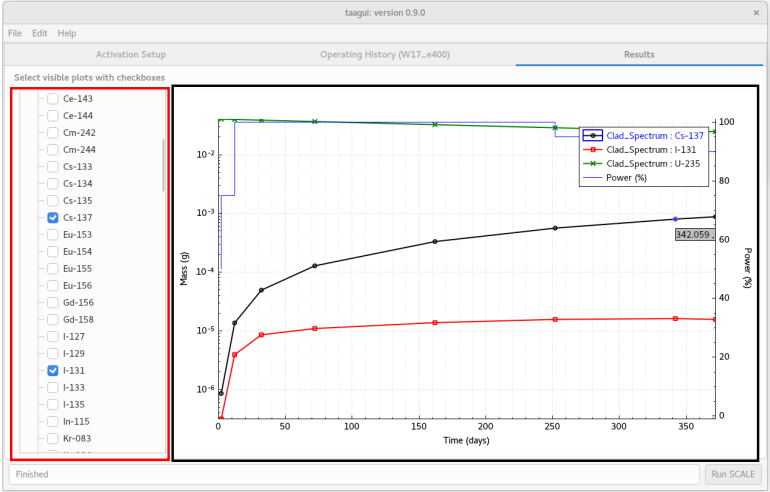
Cumulative EFPD

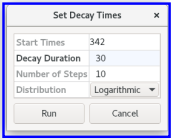
Flux ϕ

Copy Insert Delete Import Save

Run SCALE

TAAG Results Panel





Pure decay calculation of nuclide from selected time

Target nuclides

Plot of target nuclide masses [g] and reactor power [%] vs time

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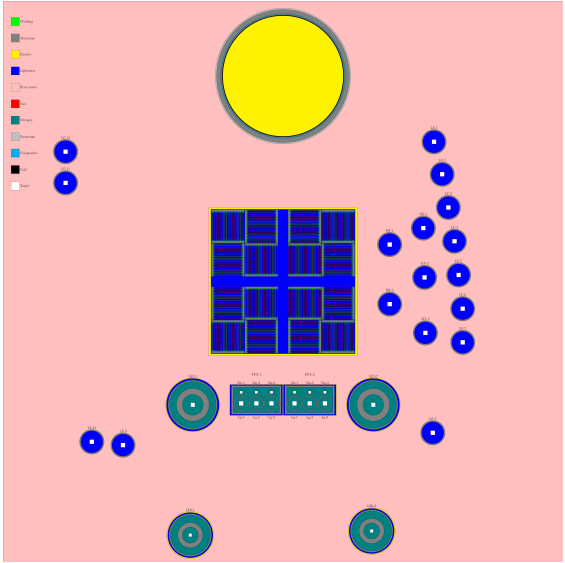
Open Pool Australian Light Water (OPAL) Reactor

- 20 $\mathrm{MW_{th}}$ open pool type light water research reactor
- Australian Nuclear Science and Technology Organisation (ANSTO) in Sydney, AU
- Officially opened April 2007 replacing High Flux Australian Reactor (HIFAR)
- Multi-purpose facility: neutron beams, radiopharmaceuticals, irradiation of materials
- Heavy water ($\mathrm{D_2O}$) neutron reflector
- LEU (19.8% $^{235}\mathrm{U}$) $\mathrm{U_3Si_2}$ fuel on Al plates
- Maximum neutron irradiation flux: $\phi_{\mathrm{th}} \lesssim 3 \times 10^{14}\ \mathrm{n/cm^2/s}$
- 30-35 day cycles with 5-day shutdown for refueling or reshuffling



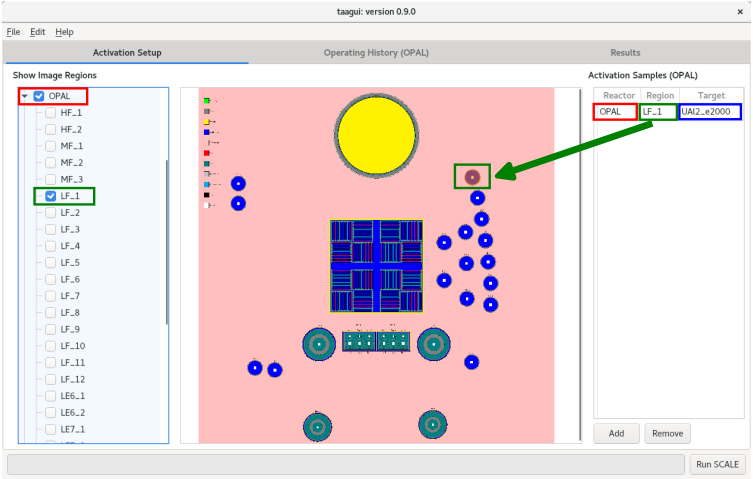
OPAL Mo-99 Production

- Target
  - Manufactured by CERCA[1] or CNEA[2]
  - LEU (19.75% $^{235}\mathrm{U}$) UAl_x, $x \in \{2, 3, 4\}$
  - Assume 49 g total mass UAl_x but can range 25-50 g
- Irradiation
  - Bulk production
  - Low-flux ($\phi_{\mathrm{th}} \lesssim 10^{14}\,\mathrm{n/cm^2/s}$)
  - Assume 6 days but can range 3-13 days
- Mo-99 production: 2150 to 3500 6-day Ci/week
  - A 6-day Ci is the measurement of the remaining radioactivity of Mo-99 six days after it leaves the processor's facility (from end of processing)
  - Assuming 24 hours of processing following irradiation
    - We will decay for 7 days after irradiation to compare to the 6-day Ci output
    - We will also irradiate for 6 days to have weekly production

[1] CERCA is a fuel production subsidiary of Areva.

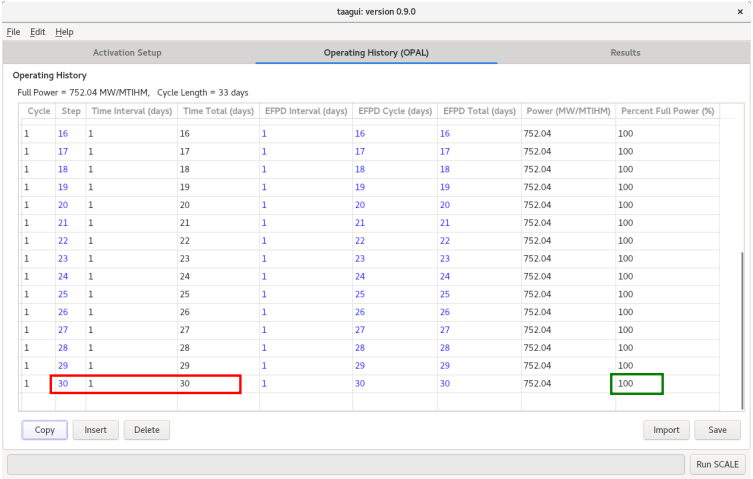
[2] CNEA is the Argentine National Atomic Energy Commission for nuclear energy R&D.

Activation Setup



1. Select the OPAL reactor
2. Irradiate in a bulk-production irradiation LF (low-flux) region
   There are 12 such identical regions: will re-scale results by 12
3. Use 1 g `UAl2_e2000` target material (20% $^{235}\mathrm{U}\ \mathrm{UAl_2}$) similar to CERCA or CNEA LEU targets
   Will re-scale results by actual target mass (49 g)

Operating History

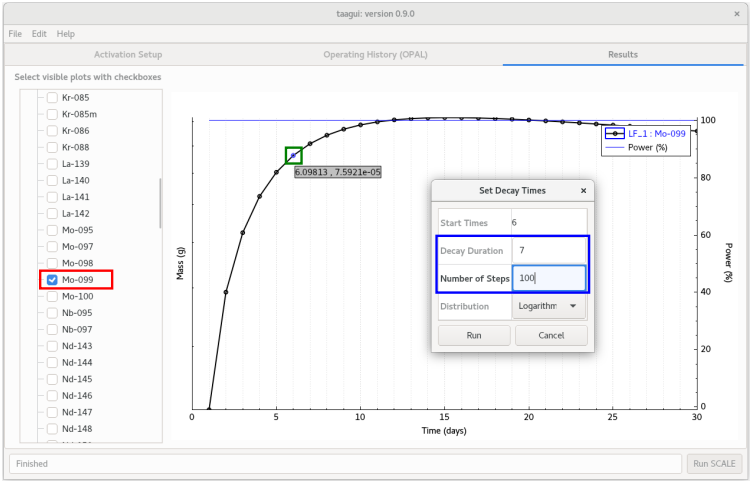


Cycle	Step	Time Interval (days)	Time Total (days)	EFPD Interval (days)	EFPD Cycle (days)	EFPD Total (days)	Power (MW/MTIHM)	Percent Full Power (%)
1	16	1	16	1	16	16	752.04	100
1	17	1	17	1	17	17	752.04	100
1	18	1	18	1	18	18	752.04	100
1	19	1	19	1	19	19	752.04	100
1	20	1	20	1	20	20	752.04	100
1	21	1	21	1	21	21	752.04	100
1	22	1	22	1	22	22	752.04	100
1	23	1	23	1	23	23	752.04	100
1	24	1	24	1	24	24	752.04	100
1	25	1	25	1	25	25	752.04	100
1	26	1	26	1	26	26	752.04	100
1	27	1	27	1	27	27	752.04	100
1	28	1	28	1	28	28	752.04	100
1	29	1	29	1	29	29	752.04	100
1	30	1	30	1	30	30	752.04	100

We only need the first 6 days of irradiation, but we can observe the peak (i.e., saturation) Mo-99 production behavior over 30 days

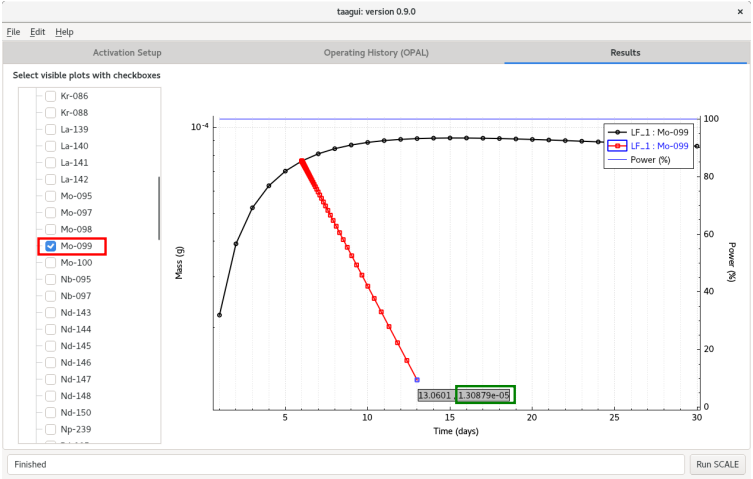
1. Add 30 steps with interval $\Delta t = 1\,\mathrm{d}$
2. Irradiate at full power during each time step

Results: Activation



1. Select the Mo-99 activation data
2. Select the 6-day data point
3. Decay for 7 days with 100 steps

Results: Decay



1. Select the Mo-99 decay data
2. Observe the 7-day decayed value (includes 24 hours of processing): 1.31×10^{-5} g

Results: 6-day Ci Mo-99 Conversion

- Convert 6-day mass units to 6-day activity:
  - 1.31×10^{-5} g/week/1 g $\mathrm{target/region} = 6.28$ Ci/week/1 g $\mathrm{target/region}$
- Re-scale by actual target mass (49 g) and number of LF target regions (12):
  - 3700 6-day Ci/week
- Close to the estimated 2150 to 3500 6-day Ci/week
- May be overestimate potentially due to processing losses
- Exact value may vary depending on irradiation times, processing times, and target composition and masses

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- TAAG is a simple interface for performing activation calculations using ORIGEN
- There are several reactors and targets available with the ability to add more
- Can control the reactor irradiation time and power history
- Can simply perform post-irradiation decay calculations

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