OAK RIDGE National Laboratory

Creating ORIGEN Libraries with Library Builder

SCALE 6.3.1



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U.S. DEPARTMENT OF ENERGY

Learning goals



Summarize the relevant ways in which SCALE treats nuclear data for multigroup cross section processing and why it matters (i.e., resonance self-shielding)



Demonstrate how to use the new Library Builder (build_lib) block with a user-supplied set of flux weighting factors to collapse **multigroup cross sections** down to a **one-group reaction library** for use with ORIGEN

Outline

- Multi-group nuclear data processing basics
- Introduction to ORIGEN Library Builder Input
- Tutorial: Creating ORIGEN activation libraries
- Workshop: Activation libraries and calculations with ORIGEN

Capabilities of ORIGEN Library Builder

Library Builder creates ORIGEN libraries (f33) from fundamental data sources, performing two major functions

1) Converting fundamental decay data into a decay-only f33
2) Updating/adding reaction transition coefficients on an existing f33

Decay and reaction pieces are stored separately in f33 → later in ORIGEN, flux magnitude folded in

Reaction coefficients

Decay coefficients

$$\frac{d\vec{N}}{dt} = \left(\boldsymbol{A}_{\sigma,n}\phi_n + \boldsymbol{A}_{\gamma}\right)\vec{N}(t) + \vec{S}_n$$

$$a_{ij} = \begin{cases} f_{ij}\sigma_j\Phi + l_{ij}\lambda_j & i \neq j \\ -\sigma_i\Phi - \lambda_i & \text{otherwise} \end{cases}$$

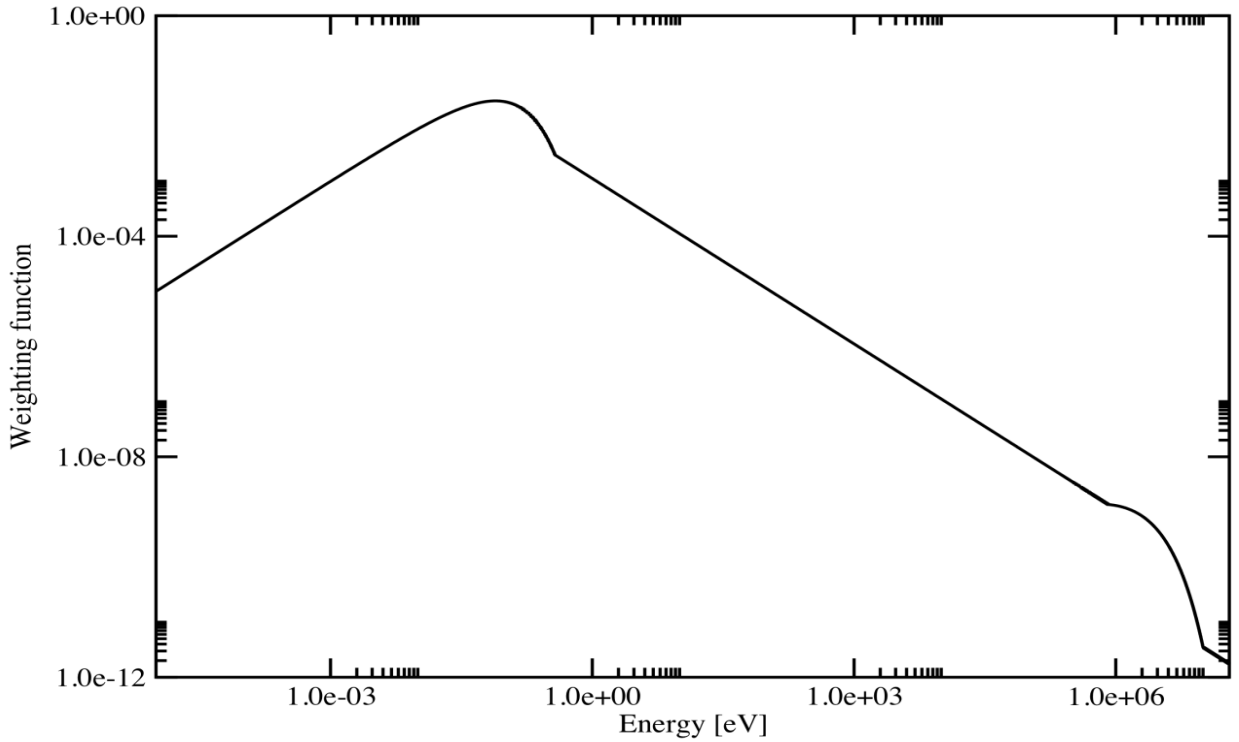
Over time step $t_{n-1} \leq t \leq t_n$

Nuclear data requirements

- Decay and branching data
- Neutron cross sections (transmutation)
- Fission product yields
- Radiation emission data (neutron and gamma)
- Energy release (decay heat)

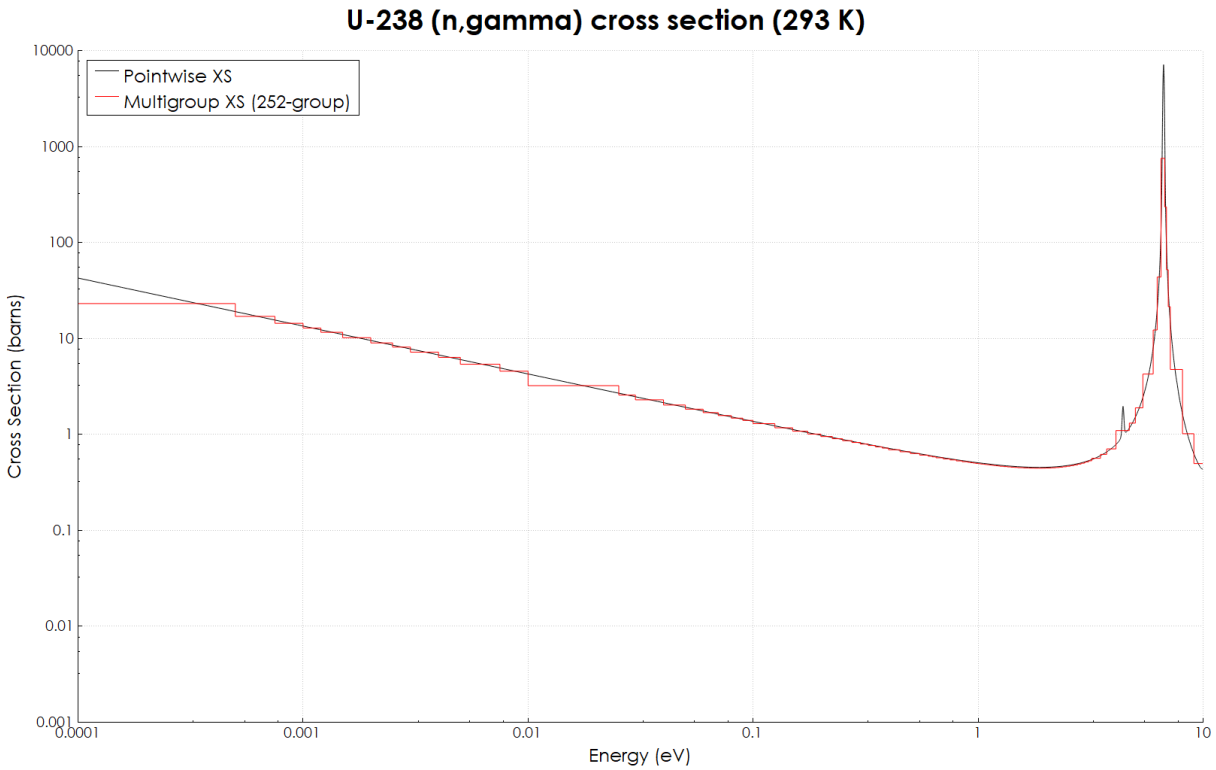
Neutron flux weighting spectrum applied to JEFF-3.1/A

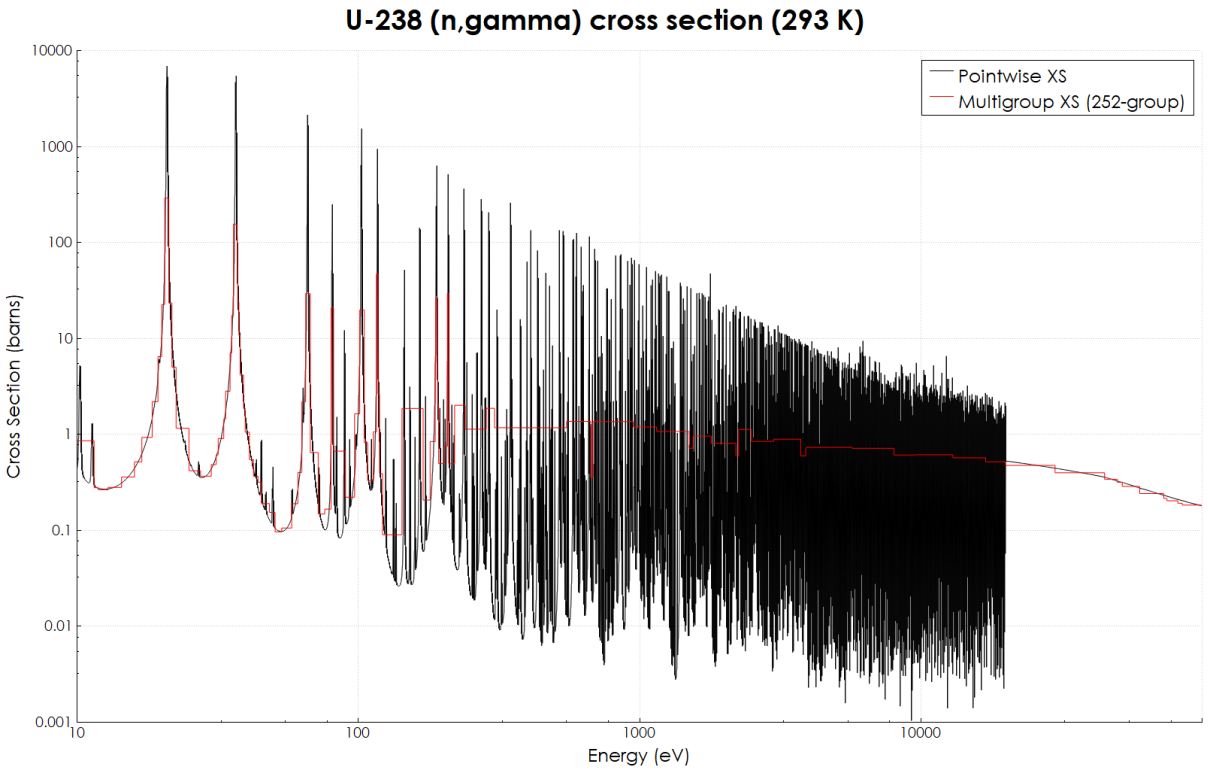
- Infinite dilution (no energy self-shielding)
- **Thermal Maxwellian + 1/E + Fission spectrum + 1/E** used to create various multigroup libraries (238, 252, 56, etc.)



CE/Multigroup comparison

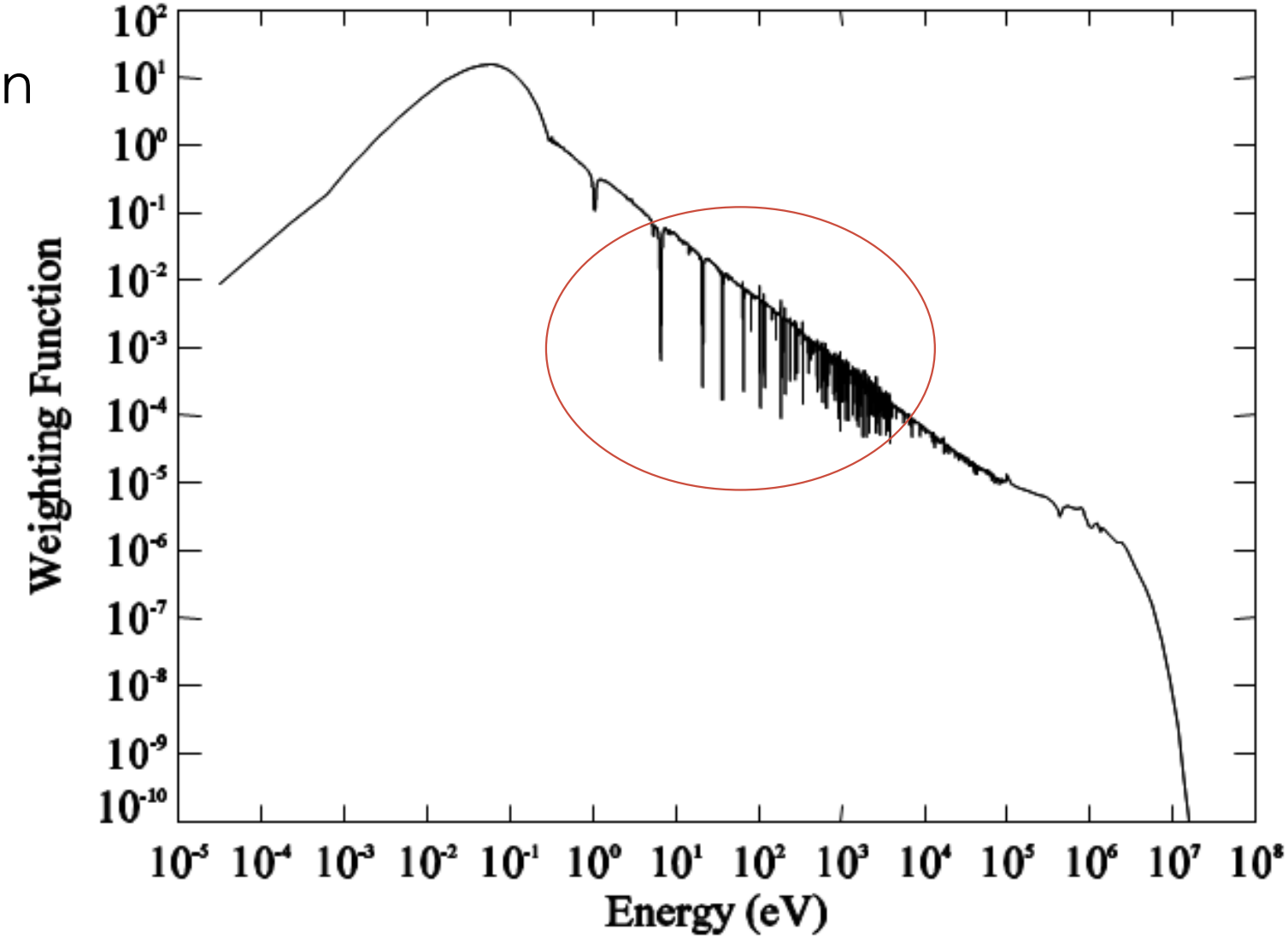
^{238}U (n,γ) neutron cross section



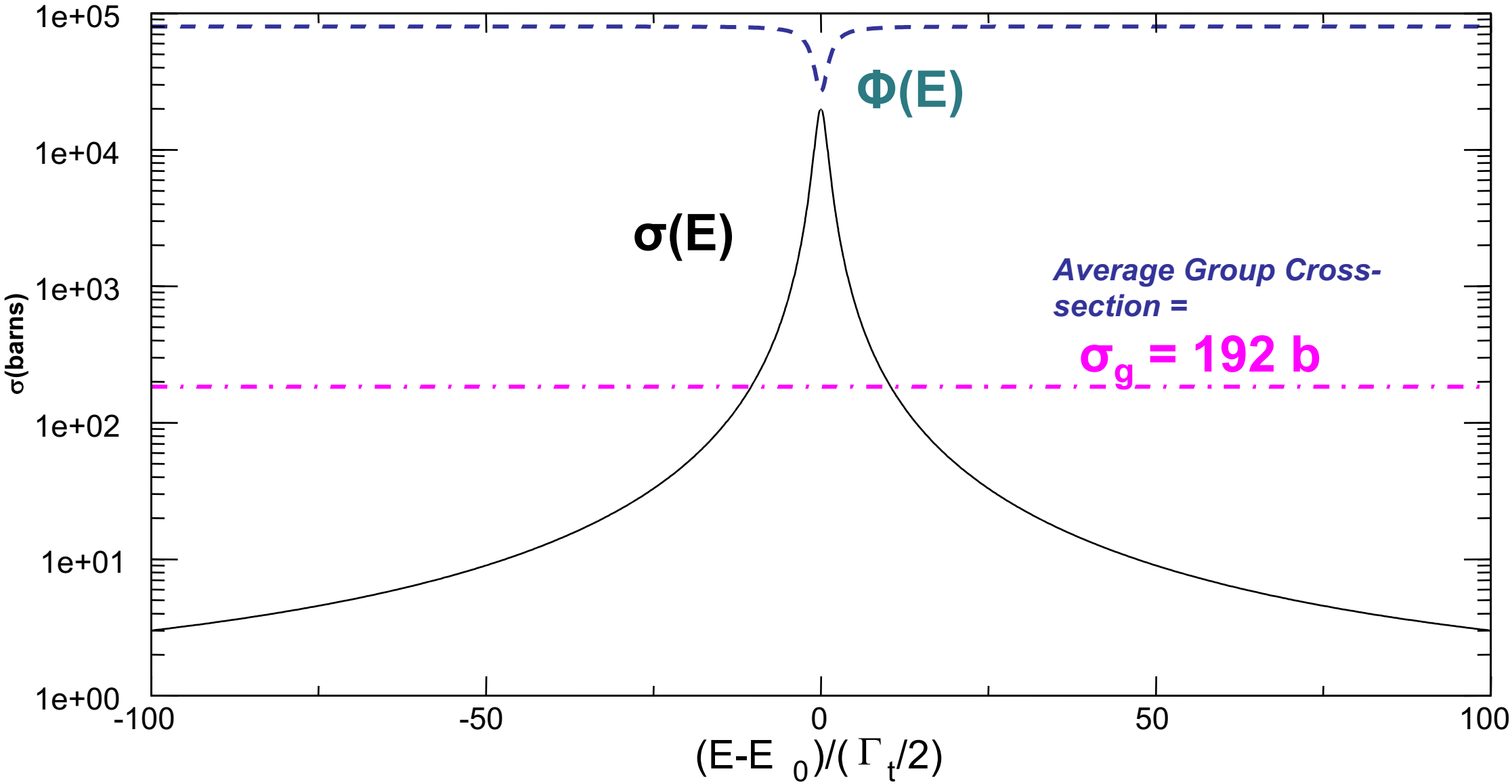


Actual LWR fuel neutron spectrum

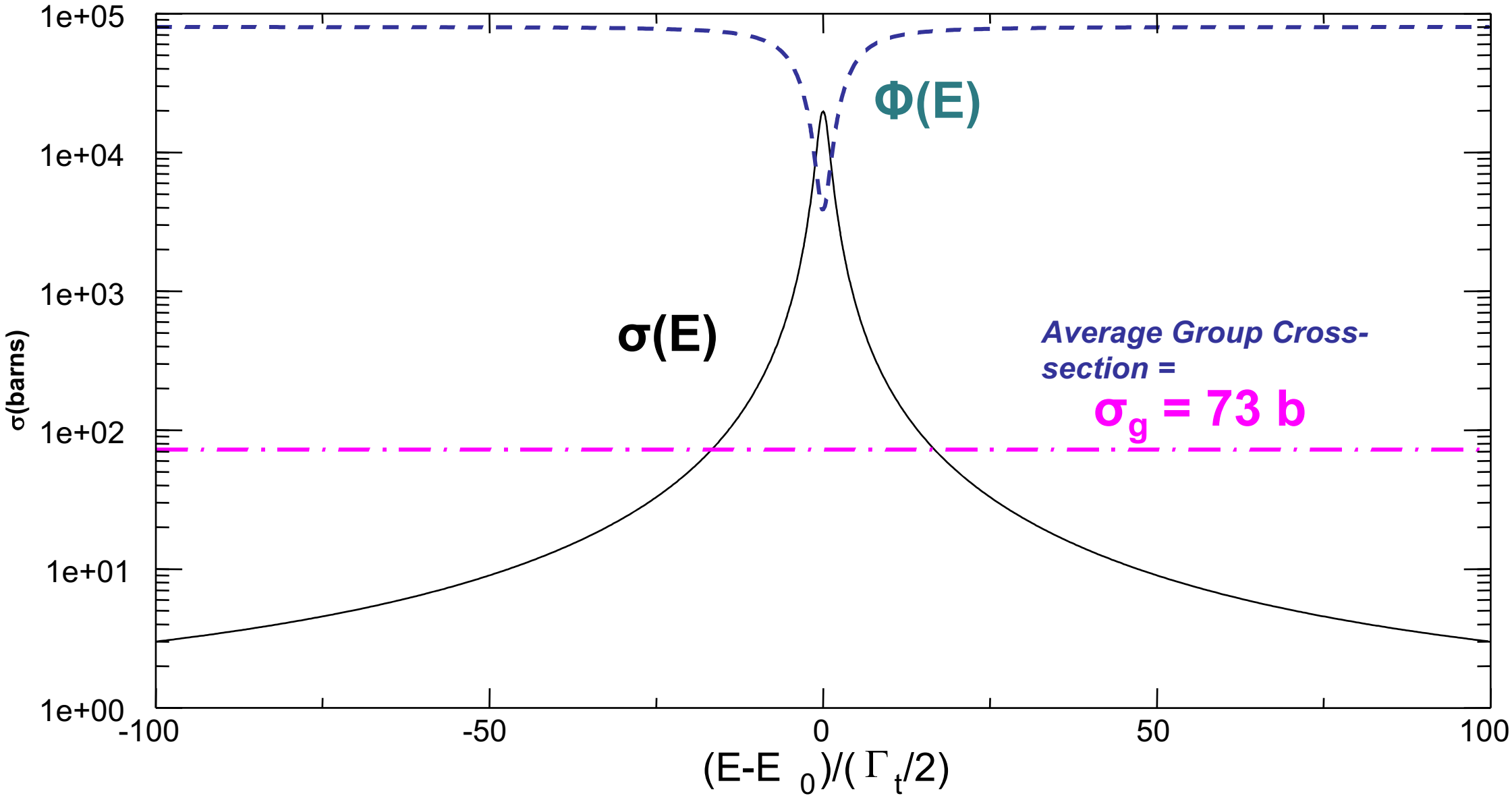
Absorption in the neutron resonances results in **reduction** in the flux at the resonance energy



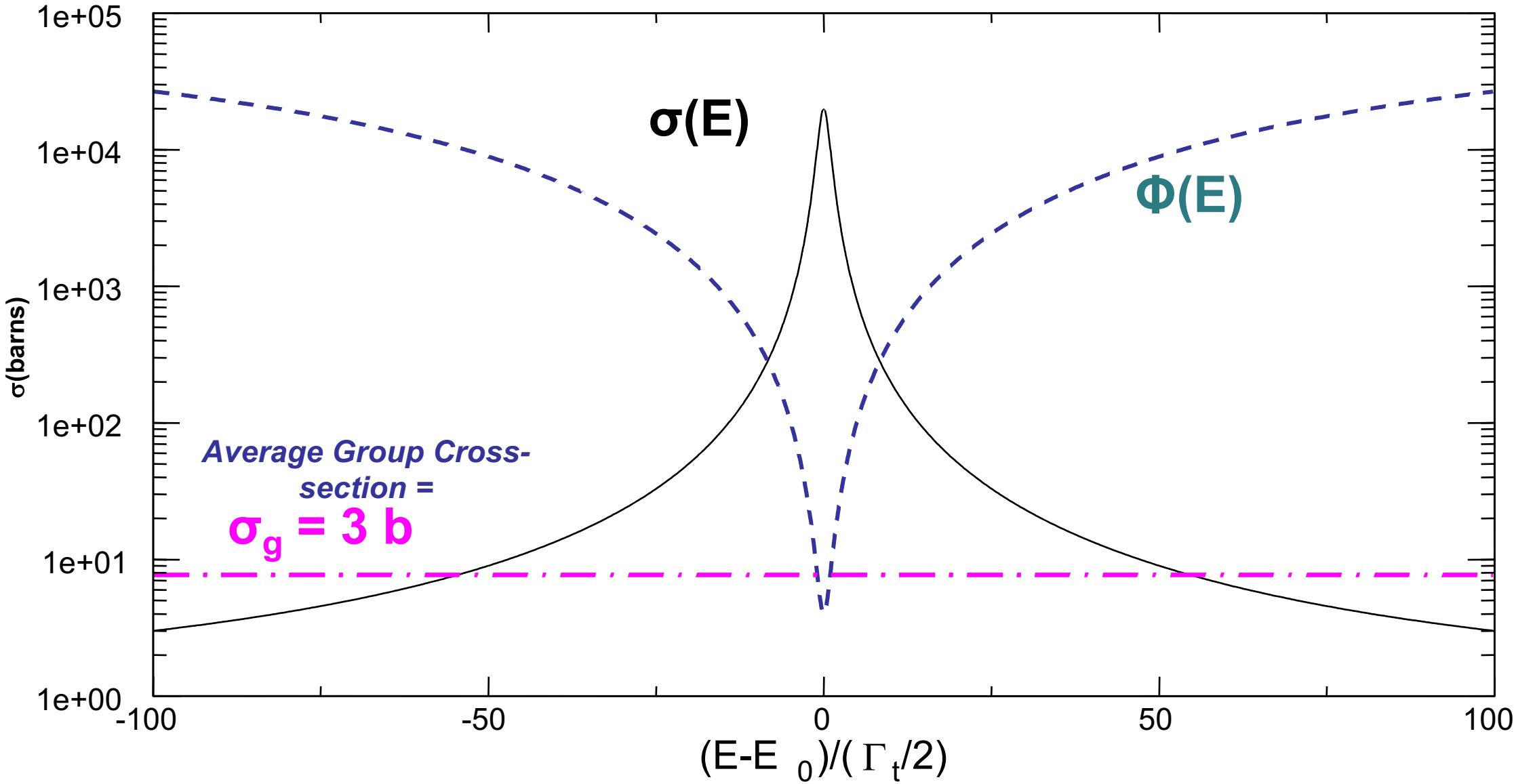
Groupwise cross-section: Infinitely dilute absorber



Groupwise cross-section: Moderately dilute absorber



Groupwise cross-section: Undiluted (pure) absorber



Effective/one-group cross sections

reaction rate

$$R = N \int_0^\infty \sigma(E)\Phi(\mathrm{E})dE$$

number density *N*

$$\approx N \sum_g \sigma^g \Phi^g$$

multigroup approximation

$$= \frac{N\Phi \sum_g \sigma^g w^g}{\sum_g w^g}$$

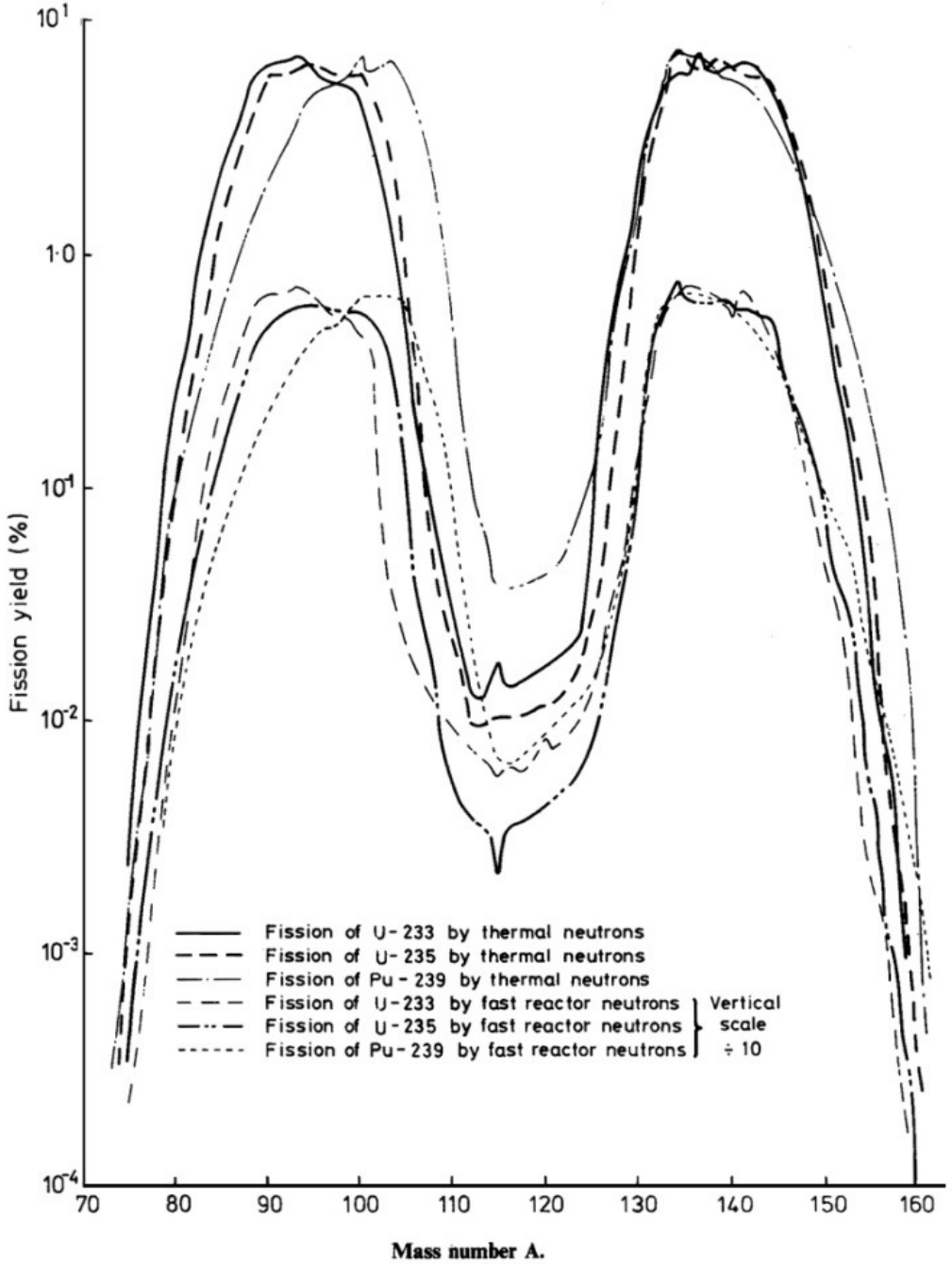
multigroup weighting function w^g

flux magnitude Φ (n/cm^2-s)

$$= N\Phi\sigma$$

Energy of neutrons causing fission

Energy dependence of fission product distribution on the energy of incident neutrons is calculated by ORIGEN for each actinide



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Introduction to ORIGEN library builder input



Introduction to the ORIGEN Library Builder

- ORIGEN's new Library Builder replaces COUPLE and uses the same SON-based syntax as ORIGEN
- Using Library Builder, users can:
  - Specify sources of decay and neutron reaction data, neutron-induced fission yields, and spontaneous fission yield data
  - Collapse multigroup cross sections to the one-group form usable by ORIGEN via either:
    - A user-defined flux weighting spectra
    - A flux defined in an AMPX library (i.e., resonance self-shielded flux)
  - Define and adjust reaction cross sections, decay constants, and branching ratios

The ORIGEN library builder block: `build_lib`

- The top-level `build_lib` block for the ORIGEN library builder has three main components:
  - `nuclide`: Define the nuclide set to be used on the library
  - `decay`: Define the problem-independent **decay data** to be used with the library
  - `neutron`: Define the neutron-induced **reaction** data to be used, including:
    - Collapsing spectrum weight
    - Reaction data
    - Fission product yields

Library Builder: Basic input structure (**nuclide**)

```
build_lib("my_lib.f33") {
  nuclide{ type=NAMED_SET list="complete_v6.2" }




}
```

Builds a new F33 library called "my_lib.f33"

Creates a decay library using the full SCALE 6.2 nuclide set

Library Builder: Basic input structure (**decay**)

```
build_lib("my_lib.f33") {
  nuclide{ type=NAMED_SET list="complete_v6.2" }
  decay{ type=ENDF_DECAY
         resource="${DATA}/origen_data/origen.rev03.decay.data"
  }
}
```

Decay data can come from an existing ORIGEN library (**type=ORIGEN_LIBRARY**) or from an ENDF decay resource (**type=ENDF_DECAY**)

Manually specify the location of the ORIGEN decay data (OPTIONAL)

Library Builder: Basic input structure (**decay**)

```
build_lib("my_lib.f33") {
  nuclide{ type=NAMED_SET list="complete_v6.2" }
  decay{ type=ENDF_DECAY
         resource="${DATA}/origen_data/origen.rev03.decay.data"
         coeff_update[
           u238 "5" 1e-12 % alpha decay (MT=5) in 1/s
           u238 "5(0)" 0.9000 % alpha decay (5) yield to residual in ground (0)
           u238 "5(1)" 0.1000 % alpha decay (5) yield to residual in 1st meta (1)
         ]
  }
}
```

Decay constants (1/s) and branching fractions of decay states can also be manually overridden by reaction channel ID in the **coeff_update** block

Format: **parent** "channel(yield) value"

"Yield" is the metastable state identifier of the daughter (0 = ground, 1 = metastable)

Library Builder decay channel IDs

Channel	Decay
1	Gamma
2	Beta-
3	Beta+
4	Isomeric transition
5	Alpha
6	Neutron
7	Spontaneous fission
8	Proton
9	Unknown

Note that decays can consist of multiple, chained modes;

e.g., $2\beta^- + n$ would have id “226”

Library Builder: Basic input structure (**neutron**)

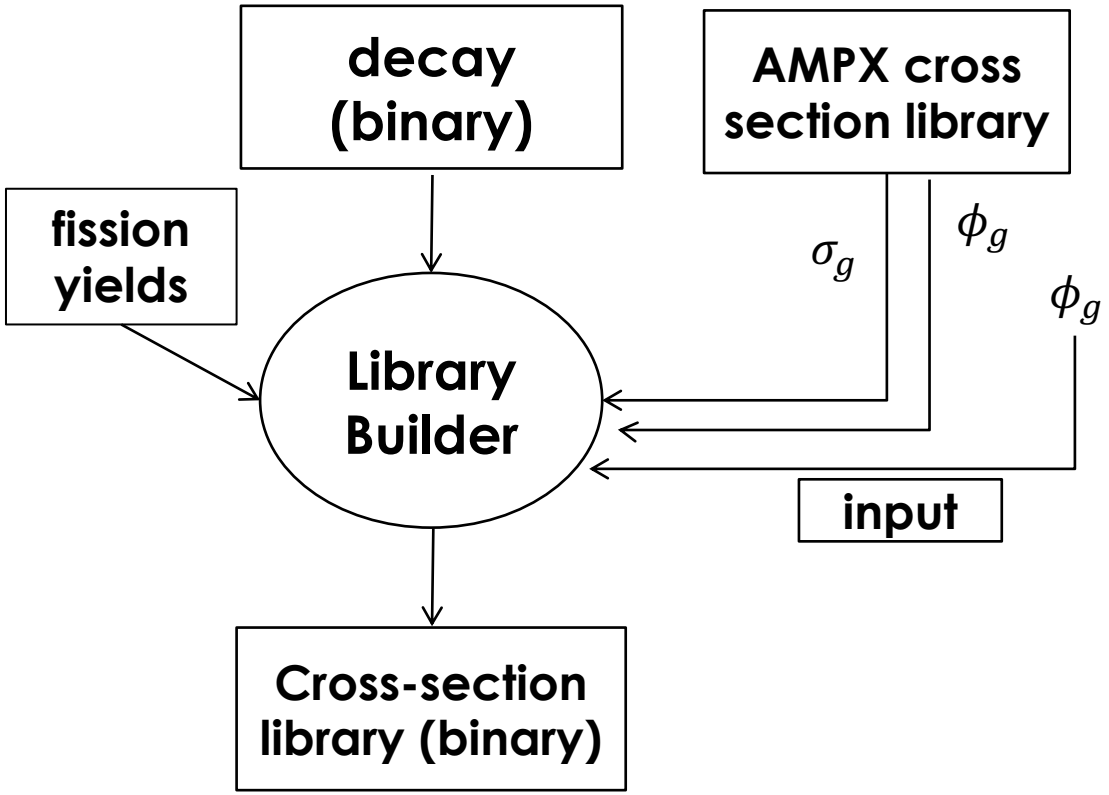
```
build_lib("my_lib.f33") {
  nuclide{ type=NAMED_SET list="complete_v6.2" }
  decay{ type=ENDF_DECAY
         resource="${DATA}/origen_data/origen.rev03.decay.data"
  }
  neutron(1){
   type=ENDF_ENERGY_DEPENDENT
   reaction_resource="${DATA}/origen.rev01.jeff56g"
   fp_yield_resource="${DATA}/origen_data/origen.rev05.yield.data"
  }



}
```

User can specify ENDF-formatted data resources for neutron-induced reactions and energy-dependent fission product yields

Library Builder: Weighting flux (**spectrum** block)



- Library Builder collapses **multigroup** cross sections to **one group** for ORIGEN to calculate reaction rates
- A flux weighting spectrum must therefore be specified, either input directly or via resonance self-shielded flux from an AMPX-formatted library
- Finished ORIGEN library contains decay data, fission yields (optional), and one group XS (optional).

Library Builder: Weighting flux (**spectrum** block)

User-defined neutron spectrum (type=MULTIGROUP)

```
spectrum{
   type=MULTIGROUP
   flux=[56R1.0]
}
```

Use a uniform flux weighting across 56 energy groups

Neutron flux from an AMPX library (type=AMPX_LIBRARY)

```
spectrum{
   type=AMPX_LIBRARY
   file="sysin.microWorkLib_0.f44"
   mixture=1
}
```

Read fluxes from **mixture 1** of the working library "**sysin.microWorkLib_0.f44**" in **${TMPDIR}**

Library Builder:
Importing self-shielded XS from an AMPX library

```
xs_update {
   type=AMPX_LIBRARY
   file="sysin.microWorkLib_0.f44"
   mixture=1
}
```

Reads self-shielded XS from **mixture 1** of the working library "**sysin.microWorkLib_0.f44**" in **${TMPDIR}**

Used **in addition** to getting MG fluxes from an AMPX library!

Library Builder: Putting it all together

```
build_lib("my_lib.f33") {
  nuclide{ type=NAMED_SET list="complete_v6.2" }
  decay{ type=ENDF_DECAY
         resource="${DATA}/origen_data/origen.rev03.decay.data"
  }
  neutron(1){
   type=ENDF_ENERGY_DEPENDENT
   reaction_resource="${DATA}/origen.rev01.jeff56g"
   fp_yield_resource="${DATA}/origen_data/origen.rev05.yield.data"
   spectrum{
     type=MULTIGROUP
     flux=[56R1.0]
   }
 }
}
```

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Activation calculations in ORIGEN



Irradiation and activation calculations in ORIGEN

- With a library with the appropriate neutron reaction data, we can now perform irradiation and activation calculations using ORIGEN
- Depleting materials by **flux:**

`flux=[` Φ_1 Φ_2 … Φ_N `]` Stepwise interval flux in units of **n/cm^2·sec**

- Depleting materials by **power**:

`power=[` P_1 P_2 … P_N `]` Stepwise interval power in units of **MW** (absolute units!)

Conversion of power to flux

- Internally, ORIGEN converts all user-specified powers into a corresponding flux by summing the **recoverable energy** (Q) from each reaction type
  - Fission ($Q_{fission}$)
  - Non-fission capture ($Q_{capture}$)
- Note that ORIGEN always works in **absolute** units (i.e., MW), so making sure that the total power (or flux) corresponds to the correct mass basis is important

Irradiation example with a user-built activation library

```
=origen
build_lib("my_lib.f33") {
  nuclide{ type=NAMED_SET list="complete_v6.2" }
  decay{ type=ENDF_DECAY resource="decay.data" }
  neutron(1){  ... }
 }
}
Case(irrad){
  mat{ iso=[92235=500.0 92238=9500] units=GRAMS } % 10 kgU, 5% enriched
  flux=[9R5.0E14 0.0 ] % 9 time intervals at 5E14 n/cm^2-sec and one decay
  time{ t=[ 8I 10.0 100.0 ] } % 8 linear intervals between 10.0 and 100.0 days
                              % => 11 time points (including 0)
                              % => 10 time intervals
}
```

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Tutorial: Creating ORIGEN activation libraries



Goals



Gain experience using Library Builder to create ORIGEN libraries



See the impact of self-shielding for fuel depletion calculations

UO_2 pin cell exercise

- Evaluate the Pu-239 content for a 3.3% ^{235}U PWR fuel pin, power 30 MW/MTU, 1100 d irradiation at 10 years' cooling time
- Create the library in two ways:
  1. Use ORIGEN's library builder and the 252-group flux spectrum provided → ORIGEN uses JEFF-3.1/A **infinitely dilute cross sections** (**pwr_inf.f33**)
  2. Use Library Builder with the same flux but **AMPX library** from SCALE **self-shielding** module CSAS-MG (**pwr_ss.f33**)

ORIGEN library builder (infinitely dilute XS) starter

```
=origen
build_lib("pwr_inf.f33") {
  nuclide{ type=NAMED_SET list="complete_v6.2" }
  decay{ type=ENDF_DECAY
         resource="${DATA}/origen_data/origen.rev03.decay.data"
  }
  neutron(1){
   type=ENDF_ENERGY_DEPENDENT
   reaction_resource="${DATA}/origen.rev01.jeff56g"
   fp_yield_resource="${DATA}/origen_data/origen.rev05.yield.data"
   spectrum{
     type=MULTIGROUP
     flux=[ ... ]
   }
 }
}
case(irradiation){
  ...
}
case(decay) {
 ...
}
end
```

Use the flux provided in "flux.txt" (copy and paste into the flux array)

Irradiate 3.3 wt. % U-235 @ for 1100 days @ 30 MW/MTU

Cool for 10 years' decay time & save

CSAS-MG + Library Builder (pwr_ss.f33) 2/2

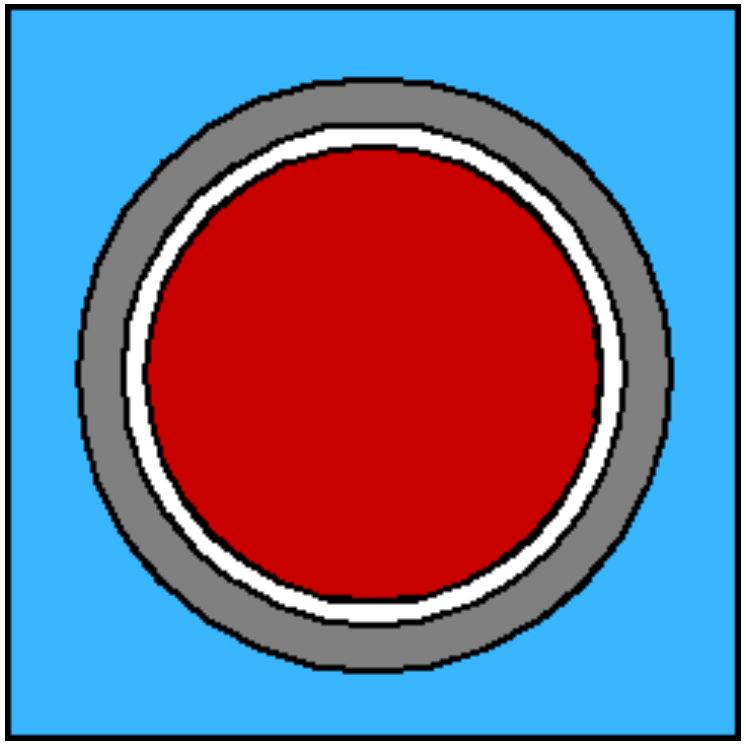
CSAS input

```
=csas-mg
centrm problem pwr:JAEA Next Gen PWR Benchmark: UO2 pincell, COLD
v7-252
read comp
u-235 1 0 1.5122e-3 300 end
u-238 1 0 2.1477e-2 300 end
o     1 0 4.5945e-2 300 end
zr    2 0 4.3107e-2 300 end
h     3 0 4.4148e-2 300 end
o     3 0 2.2074e-2 300 end
end comp
read celldata
latticecell squarepitch pitch=1.265 3 fueld=0.8240 1 cladd=0.9520 2 end
end celldata
end
```

CSAS-MG + Library Builder (pwr_ss.f33) 1/2

Pin cell definition

- Temperature 300K
- compositions atoms/(barn-cm)
  - Fuel (UO2)
    - u-235 1.5122e-3
    - u-238 2.1477e-2
    - o 4.5945e-2
  - Cladding (Zr)
    - zr 4.3107e-2
  - Coolant (water)
    - h 4.4148e-2
    - o 2.2074e-2
- Fuel square pitch (cm) =1.265
- Fuel pellet diameter (cm) = 0.8240
- Clad outer diameter (cm) = 0.9520



UO_2 pin cell Results

- ORIGEN libraries generated and copied back
  - **pwr_inf.f33** – infinitely dilute xs
  - **pwr_ss.f33** – self-shielded xs
- Run provided **origen_pwr.inp**
  - Copies in **pwr_inf.f33** and **pwr_ss.f33** and runs depletion case
  - Search for "pu-239" in decay case and extract final value

origen_pwr.inp

```
=origen
case(irrad){
    lib{ file="pwr_inf" }
    mat{
        iso=[u235=3.3e4 u238=96.7e4]
        units=GRAMS
    }
    time=[9I 100 1100]
    power=[11R 30]
}
case(decay){
    title="Infinitely Dilute XS"
    time{
        units=YEARS
        start=0
        t=[10L 0.01 10]
    }
}
end
=origen
case(irrad){
    lib{ file="pwr_ss" }
    mat{
        iso=[u235=3.3e4 u238=96.7e4]
        units=GRAMS
    }
    time=[9I 100 1100]
    power=[11R 30]
}
case(decay){
    title="Self-Shielded XS"
    time{
        units=YEARS
        start=0
        t=[10L 0.01 10]
    }
}
end
```

UO_2 pin cell conclusions

Self-shielding (mainly ^{238}U) has a huge effect on the neutron absorption rate and thus on the production of Pu in reactor fuel.

- Unshielded (infinite dilution) ^{239}Pu = 13 kg per metric ton U
- Shielded ^{239}Pu = 7.3 kg per metric ton U
- 44% lower Pu content!

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Workshop: Activation libraries and calculations with ORIGEN



Problem 1: Silene experiments

- CEA Valduc experimental facility, France
- Critical pulse 93% ^{235}U uranyl nitrate solution
- Threshold activation foil measurements





Problem 1: Silene – measurements

- Aluminum holders have three foil cavities containing Fe, Ni, and Mg foils with > 99% elemental purity
  - Nickel, 1 mm thick, 2.807 g
  - Iron, 3 mm thick, 7.292 g
  - Magnesium, 2 mm thick, 1.089 g
- Activation from fast (*n,p*) reactions were measured
- Measured activities per unit mass and relative uncertainties (2 sigma)
  - $^{54}Fe(n,p)^{54}Mn$, ^{54}Mn activity 0.1961 Bq/g ± 4.1%
  - $^{58}Ni(n,p)^{58}Co$, ^{58}Co activity 12.99 Bq/g ± 3.2%
  - $^{24}Mg(n,p)^{24}Na$, ^{24}Na activity 59.10 Bq/g ± 4.1%

Problem 1: Silene – problem description

Goals

- Calculate the specific activity (Bq/g) for each foil
- Observe time-dependence post-irradiation
- Compare to experiment plus uncertainty

Assumptions

- Neutron energy spectrum provided
- Natural isotopic abundance for foil elements
- Total fluence of 1.6351×10^{11} n/cm^2

Problem 1: Silene – procedure

- Begin with **silene.starter.inp**
- Copy/paste in **flux.txt** to finish the Library Builder setup
- Create an ORIGEN activation input with three cases, one for each sample
  - Note that starter has outline and follow-on OPUS post-processing
  - Make "iron" case work first
  - Then copy/paste/modify for the "nickel" and "magnesium" cases
  - Uncomment the OPUS inputs for "nickel" and "magnesium"
- *Alternatively, you could open each .f71 in Fulcrum and use OPUS F71 Viewer*

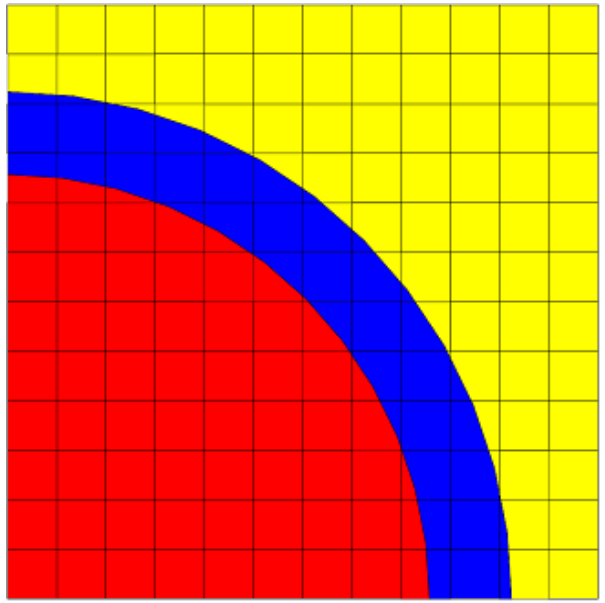
Problem 2: Sodium fast reactor (SFR) library

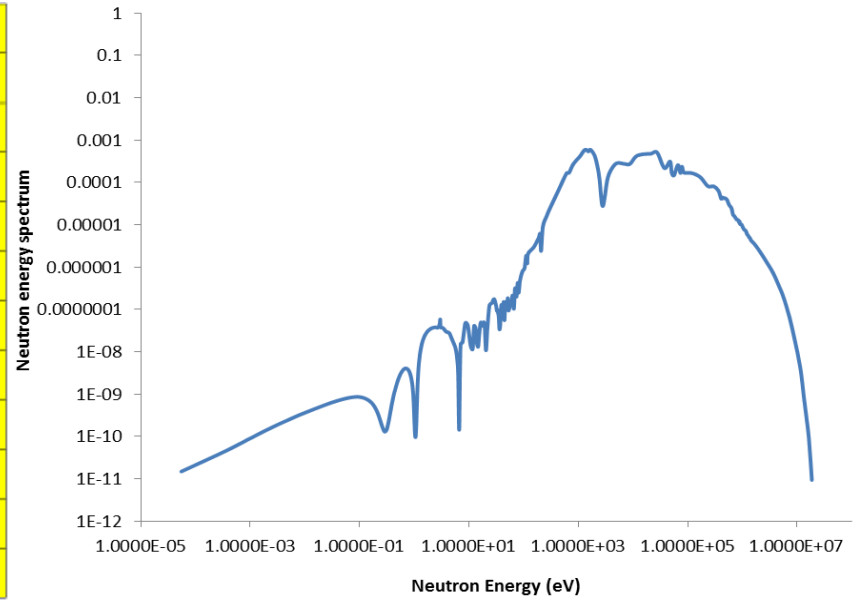
Goal: Assess effect of self-shielding on Pu-239 mass in a fast system

Advanced Burner Test Reactor

Specifications:

- Compositions atoms/(barn · cm)
  - Fuel (U-Pu-Zr-Mo)
  - Gap (Na bond)
  - Cladding (Fe-Mo alloy)
  - Coolant (sodium)
- Fuel hex pitch (cm) = 0.908
- Fuel pellet diameter (cm) = 0.603
- Clad outer diameter (cm) = 0.800
- Clad inner diameter (cm) = 0.696





Problem 2: SFR – procedure

- Process identical to tutorial with PWR library
- Create ORIGEN libraries by copy/paste flux.txt into
  - **lib_builder_sfr_inf.starter.inp –** infinitely dilute version (sfr_inf.f33)
  - **lib_builder_sfr_ss.starter.inp –** self-shielded version (sfr_ss.f33)
- Run **origen_sfr.inp and** extract Pu-239 content at end of irradiation when using the two different libraries
- Compare the variation with irradiation time of the Pu-239 mass as a function of the library used
- Compare the variation with irradiation time of the Pu-239 consumption as a function of the library used

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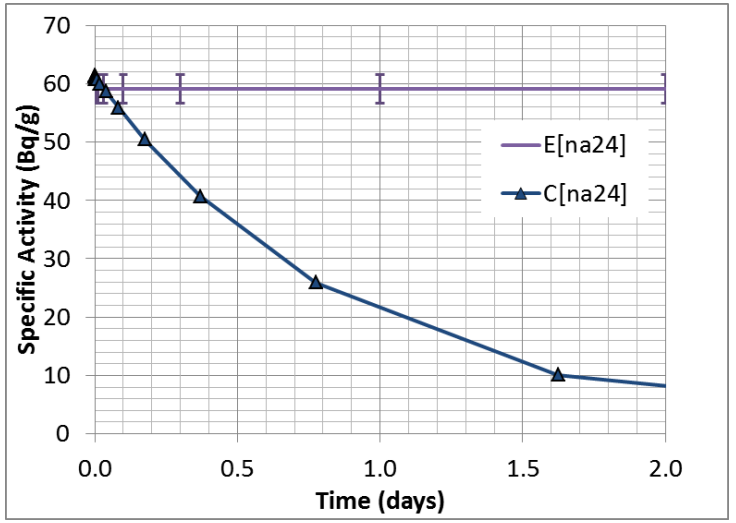
Solutions

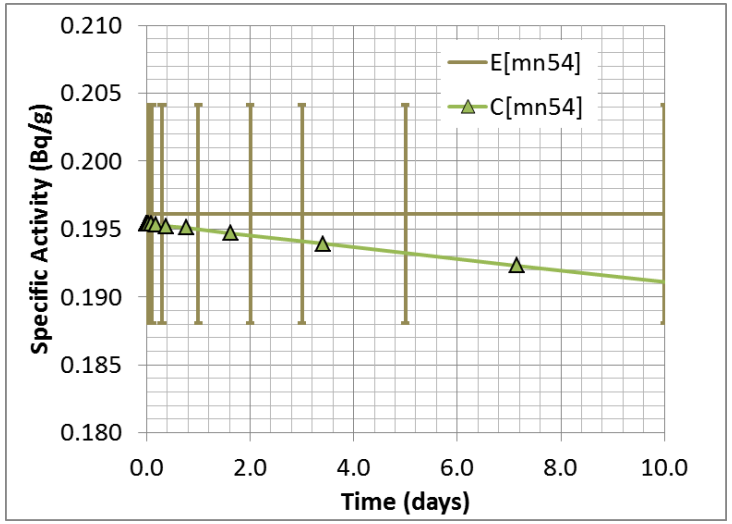


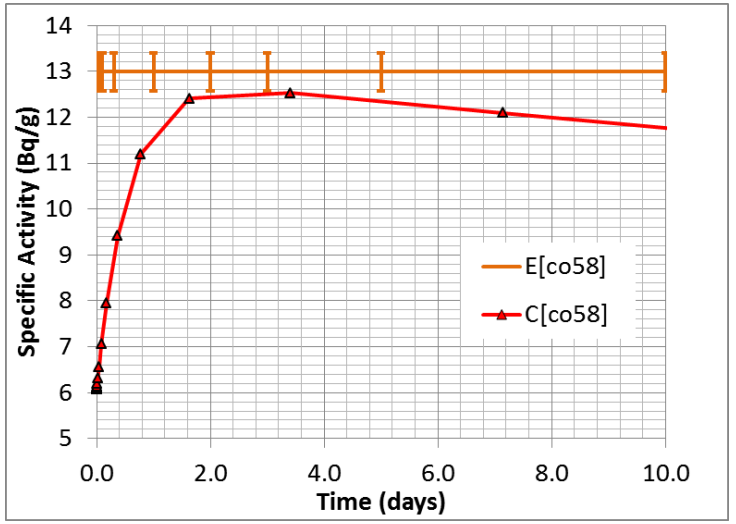
Silene results

Reaction	Measured (Bq/g)	Uncertainty 2-sigma (%)	Calculated (Bq/g)	Error C/E-1 (%)
$^{54}Fe(n,p)^{54}Mn$	0.1961	4.1	0.1953	-0.4
$^{58}Ni(n,p)^{58}Co$	12.99	3.2	12.53*	-3.5
$^{24}Mg(n,p)^{24}Na$	59.10	4.1	61.31	3.7

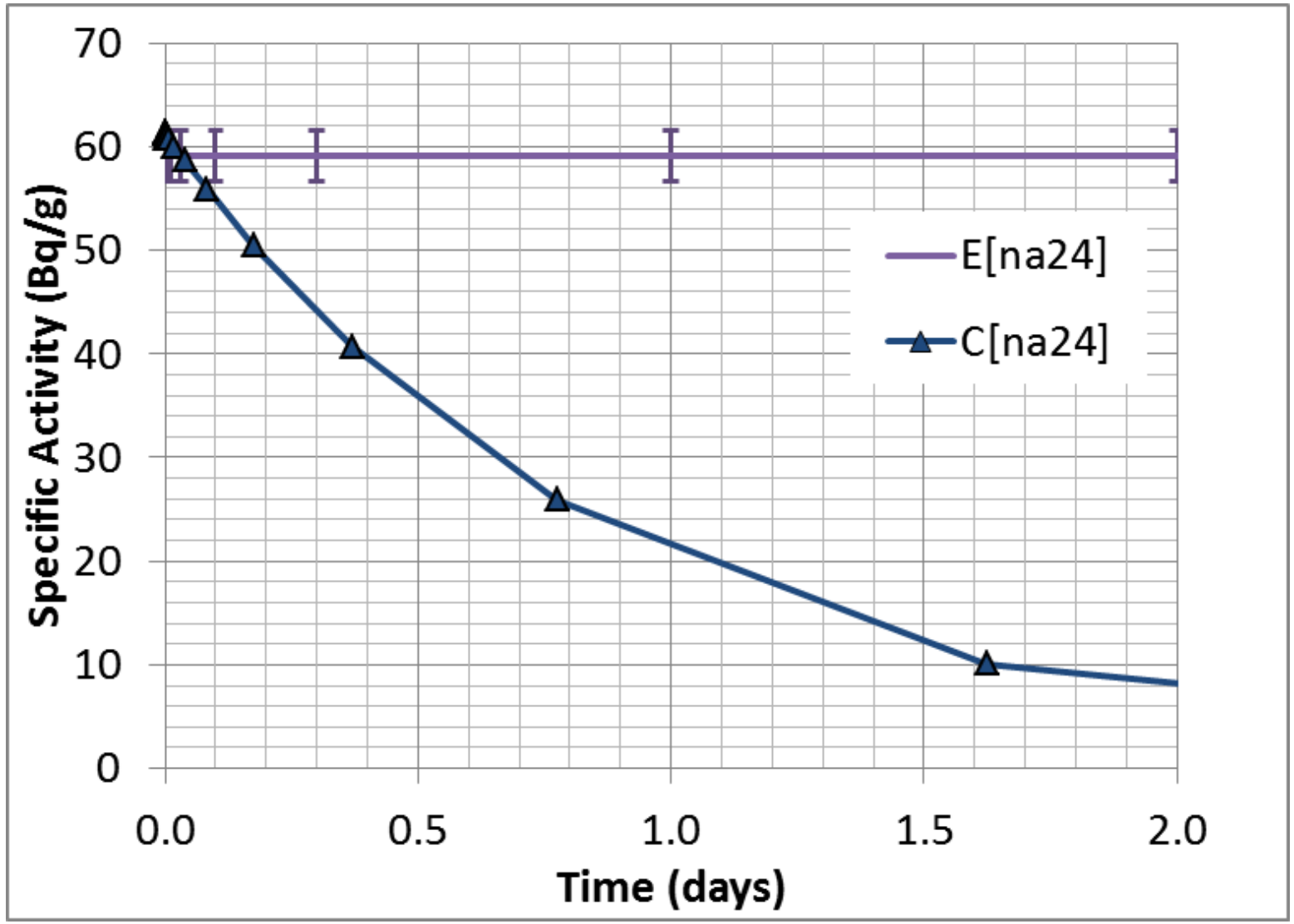
*Estimated maximum activity



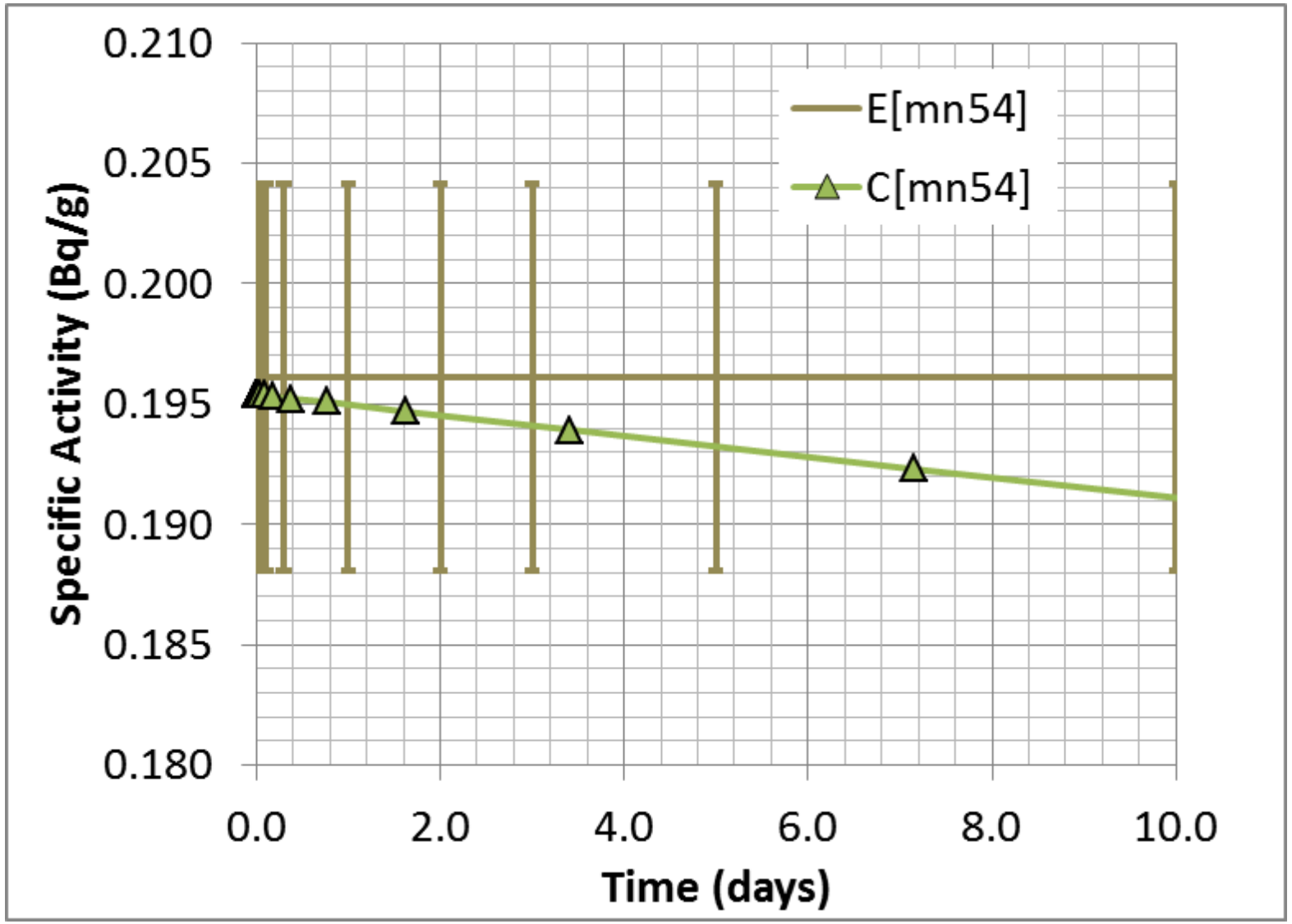




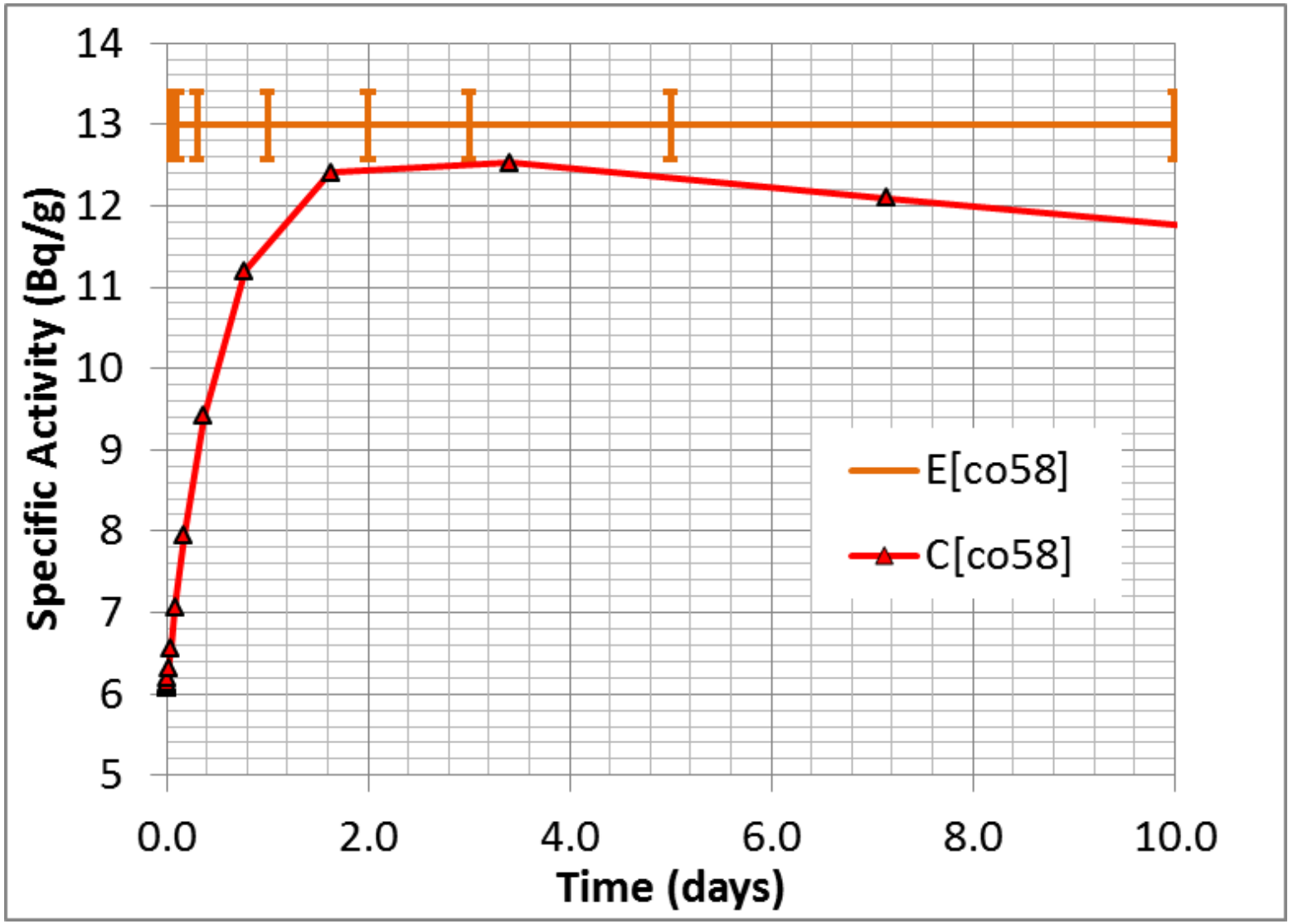
Silene results: Na-24 ($T_{1/2}$= 15 h)



Silene results: Mn-54 ($T_{1/2}$= 312.2 d)

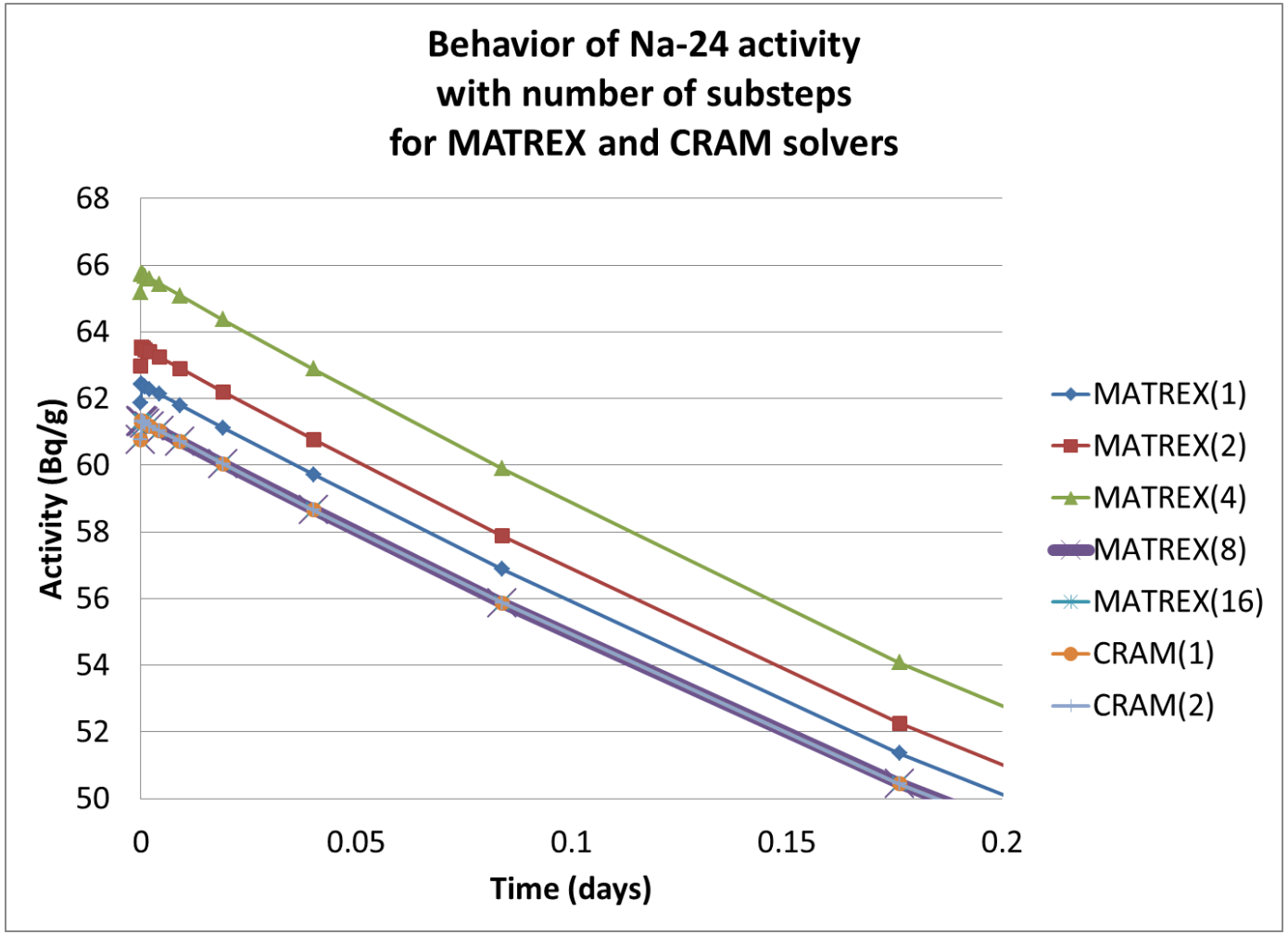


Silene results: Co-58 ($T_{1/2}$= 70.86 d)



Silene results: Solver comparison on Na-24

- Activation for 1 second still needs multiple time steps for MATREX solver
  - Always use 4 or more steps is conventional rule of thumb
  - Turns out using 8 substeps is required to converge
- **`solver{ … opt{ substeps=N } }`** is a painless way to check convergence w.r.t. time discretization (N=1,2,4,8,…)
- CRAM solver is converged with a single substep



SFR results

- Self-shielding is less important in fast systems than in thermal systems
- 7% more plutonium consumed when using self-shielded cross sections vs infinite dilute
- Examining ORIGEN output for cross section data relevant to Pu-239
  - Inf. Dilute (in barns):

```
92238 to 922390  2.30913E-01   mt= 102
94239 capture    3.35290E-01   mt= 102
```

  - Self-shielded (in barn):

```
922380 to 922390  2.14476E-01  mt= 102
942390 capture    3.06939E-01  mt= 102
```

Pu-239 variation with irradiation time

				consumed	consumed
days	inf. dilute (g/MTHM)	self-shielded (kg/MTHM)	diff (kg/MTHM)	inf. dilute (kg)	self-shielded (kg)
0	145.30	145.30	0.00	0.00	0.00
30	144.38	144.33	0.04	0.92	0.97
60	143.63	143.53	0.10	1.67	1.77
90	142.89	142.74	0.15	2.41	2.56
120	142.16	141.95	0.21	3.14	3.35
150	141.43	141.17	0.26	3.87	4.13
180	140.70	140.39	0.31	4.60	4.91
210	139.98	139.62	0.36	5.32	5.68
240	139.27	138.86	0.41	6.03	6.44
270	138.56	138.10	0.46	6.74	7.20
300	137.86	137.35	0.51	7.44	7.95

Conclusions

- ORIGEN's built-in Library Builder is the new way to generate ORIGEN activation and decay libraries in SCALE 6.3
- Library Builder can read in a user-defined flux spectrum (assumes infinitely dilute absorbers) or a resonance self-shielded flux from AMPX
- Neglect of self-shielding for cross-section resonance regions can lead to **overestimation** of multi-group removal cross-sections