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Nuclide Inventory Sensitivity to a Fine Resolution of Fast-Energy Fission Product Yields

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Evaluating fission product yield energy resolution for accurate nuclide inventory predictions

Nuclear data libraries, including the US ENDF/B library, provide fission product yields (FPY) at few energy points: for example, 0.0253 eV, 500 keV, 2 MeV, 14 MeV

Depletion codes may interpolate FPY to a problem-dependent average energy of fission

Validation of SCALE depletion calculations using these FPY resulted in good agreement between calculation and measurement for spent nuclear fuel inventory of BWRs and PWRs

Questions to answer:

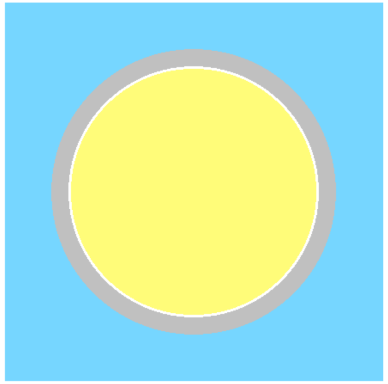
1. Is FPY interpolation between such coarse energy points adequate?
2. Would additional FPY energy points improve code validation results?
3. Do we have enough measured data that can validate FPY data?

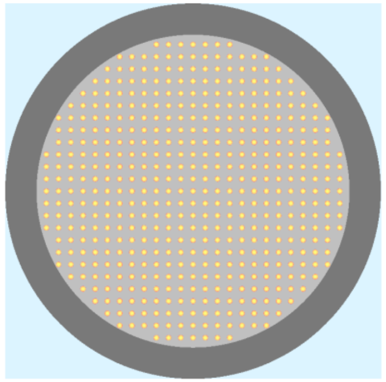
This work:

- Investigate of the relative impact of FPY energy resolution on nuclide inventory predictions
- Deplete small representative reactor models using GEFY FPY data with additional energy points in the fast energy range

Small test models allow investigation of nuclide inventory across various reactor concepts

Model	Fuel	Moderator	Fuel enrichment	Depletion time [years]	Discharge burnup [GWd/tHM]
PWR	UO_2	Water	5.0 wt% U-235	~4.3	59.9
HTGR	UO_2	Graphite	17.0 wt% U-235	~3.3	80.0
MSR	$LiF\text{-}BeF_2\text{-}UF_4$	Graphite	2.29 wt% U-235	4	74.6
SFR	U/TRU-10Zr	-/-	16.5 wt% TRU	~4	94.4
SFR	U-10Zr	-/-	16.5 wt% U-235	~8.9	149.6
MCFR	NaCl-UCl	-/-	12.5 wt% U-235	7	9.7


PWR unit cell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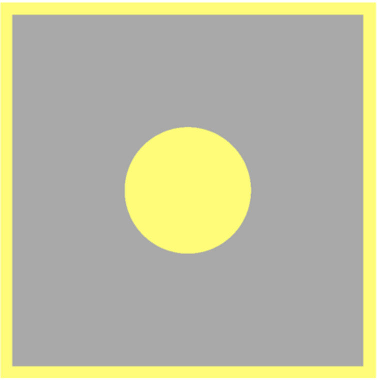
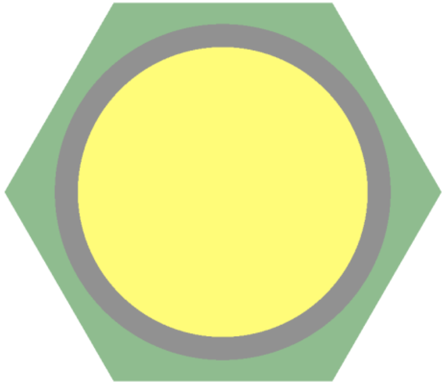
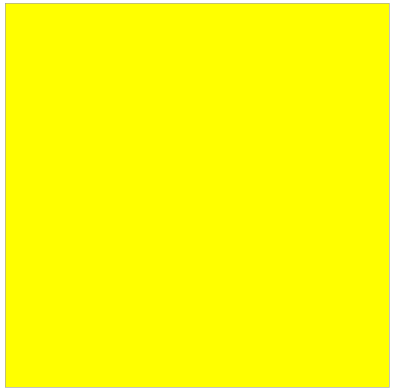

MSR unit cell


SFR unit cell


MCFR unit cell

Each model is a small unit cell that is the smallest, self-contained piece of geometry that represents a repeating portion of the corresponding reactor. Reflective boundary conditions on all sides create an infinite lattice of these unit cells. The neutron spectrum conditions are similar to those of the full reactor so that depletion calculations result in representative nuclide inventory.

Depletion calculations used GEFY FPY libraries with different energy resolution

Fission yield library: GEFY (GEF-based fission-fragment yield library in ENDF format)

Selected actinides: U235, Pu239, Pu241

Energy points in 2 test libraries based on GEFY:

1. FPY for 4 energies to represent the current ENDF/B resolution:
   14 MeV, 2 MeV, 500 keV, 0.0253 eV
2. FPY for all energies available in GEFY:
   0.0253eV, fine resolution between 10 keV and 30 MeV

Available energy points for fission yields in GEFY [eV]

2.53E-02	6.00E+06	1.60E+07
1.00E+05	6.50E+06	1.65E+07
2.00E+05	7.00E+06	1.70E+07
3.00E+05	7.50E+06	1.75E+07
4.00E+05	8.00E+06	1.80E+07
5.00E+05	8.50E+06	1.85E+07
6.00E+05	9.00E+06	1.90E+07
7.00E+05	9.50E+06	1.95E+07
8.00E+05	1.00E+07	2.00E+07
9.00E+05	1.05E+07	2.10E+07
1.00E+06	1.10E+07	2.20E+07
1.50E+06	1.15E+07	2.30E+07
2.00E+06	1.20E+07	2.40E+07
2.50E+06	1.25E+07	2.50E+07
3.00E+06	1.30E+07	2.60E+07
3.50E+06	1.35E+07	2.70E+07
4.00E+06	1.40E+07	2.80E+07
4.50E+06	1.45E+07	2.90E+07
5.00E+06	1.50E+07	3.00E+07
5.50E+06	1.55E+07	

GEFY: https://www.khschmidts-nuclear-web.eu/GEFY.html

Depletion calculations were performed with SCALE and Serpent

Neutron transport code	Neutron transport method	Cross section library
SCALE 7beta/**TRITON: XSDRN+ORIGEN**	1D deterministic	MG (252 groups for thermal systems, 302 groups for fast systems)
SCALE 7beta/**TRITON: Shift+ORIGEN**	3D Monte Carlo	CE
Serpent 2.2.1	3D Monte Carlo	CE

Monte Carlo settings: 50,000 neutrons per generation; 200 active and 100 inactive generations

Cross section and decay data library: ENDF/B-VII.1

Fission yields are interpolated differently between ORIGEN and Serpent

SCALE/ORIGEN:

- For each actinide *j*, an average energy of fission is calculated

$$E_{avg,j} = \frac{\sum_g \bar{E}^g \, \sigma_{f,j}^g \, \phi^g}{\sum_g \sigma_{f,j}^g \, \phi^g}$$

$\bar{E}^g$ average group energy (simple midpoint)
$\sigma_{f,j}^g$ multigroup fission XS of actinide j
ϕ^g flux in energy group g

- The FPY of actinide *j* resulting in FP *i* is then calculated by linearly interpolating the FPYs at this average energy

$$\gamma_{ij}(E_{avg}) = \gamma_{ij}(E_1) + \left(\frac{E_{avg} - E_1}{E_2 - E_1}\right) \cdot \left(\gamma_{ij}(E_2) - \gamma_{ij}(E_1)\right)$$

with $E_1 < E_{avg} < E_2$, and E_1 and E_2 the respective adjacent energy points

- Then the production rate $R_{f,i}$ of FP *i* is:

$$R_{f,i} = \sum_j \gamma_{ij}(E_{avg,j}) \, \sigma_{f,j} \, \phi \, N_j$$

N_j nuclide density of actinide *j*

ORIGEN considers the FPY of 2 adjacent energy points to E_{avg} per fissioning actinide

Serpent:

- The production rate of FP *i* is the sum of partial rates corresponding to the available FPY energies E_k

$$R_{f,i} = \sum_j \sum_k \gamma_{ij}(E_k) \cdot R_{f,j}^k$$

- Partial fission rates: When the fission event occurs at neutron energy E, the corresponding fission rate contribution is distributed between the two adjacent E_k, thereby incrementing the associated partial fission rates according to linear interpolation weights:

$$R_{f,j}^1 \mathrel{+}= \frac{E_2 - E}{E_2 - E_1} R_{f,j}(E) \qquad R_{f,j}^2 \mathrel{+}= \frac{E - E_1}{E_2 - E_1} R_{f,j}(E)$$

Serpent considers energy-dependent FPY using partial fission rates across the whole energy range

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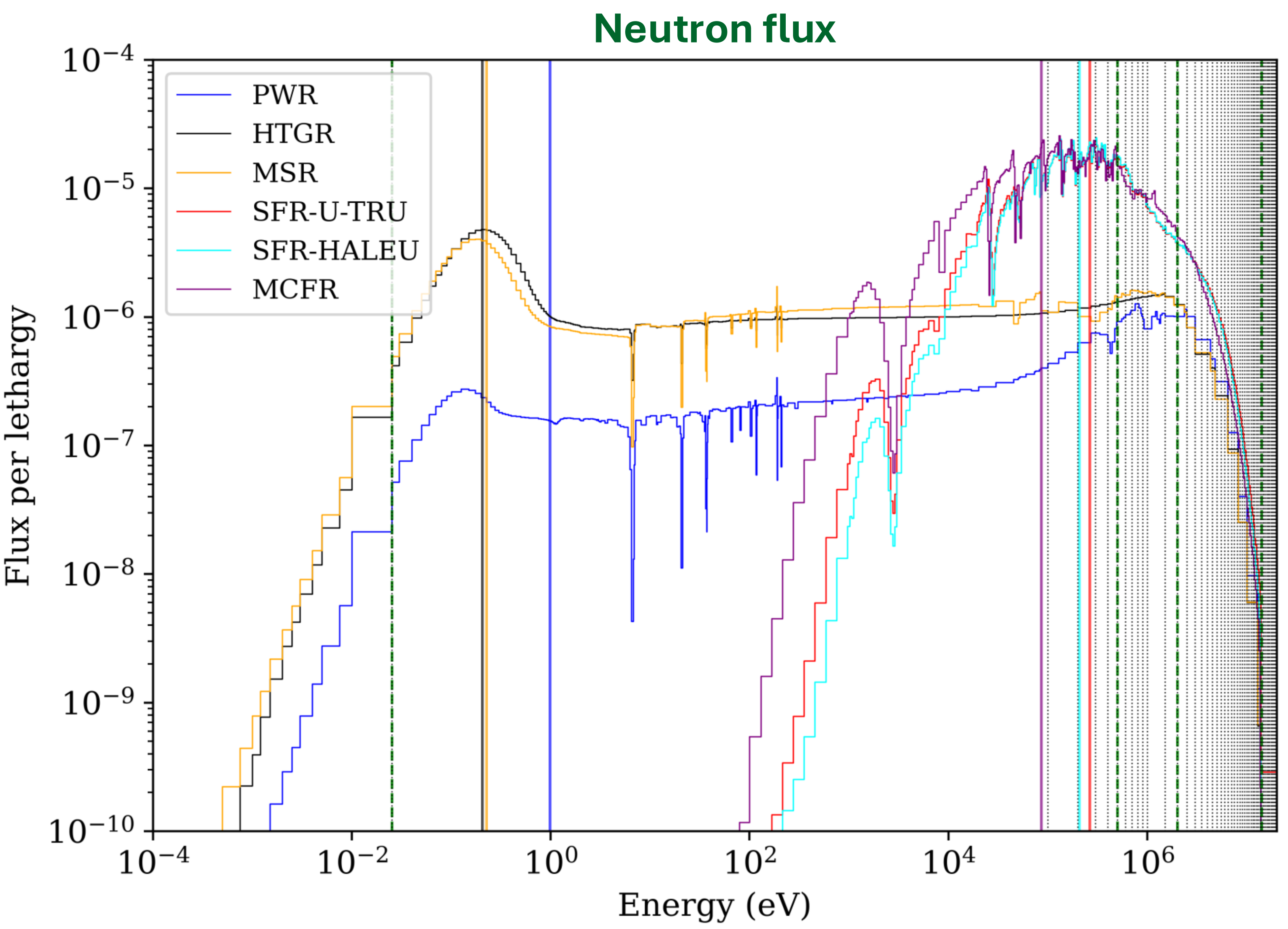
Additional FPY energy points are located in the fast energy range

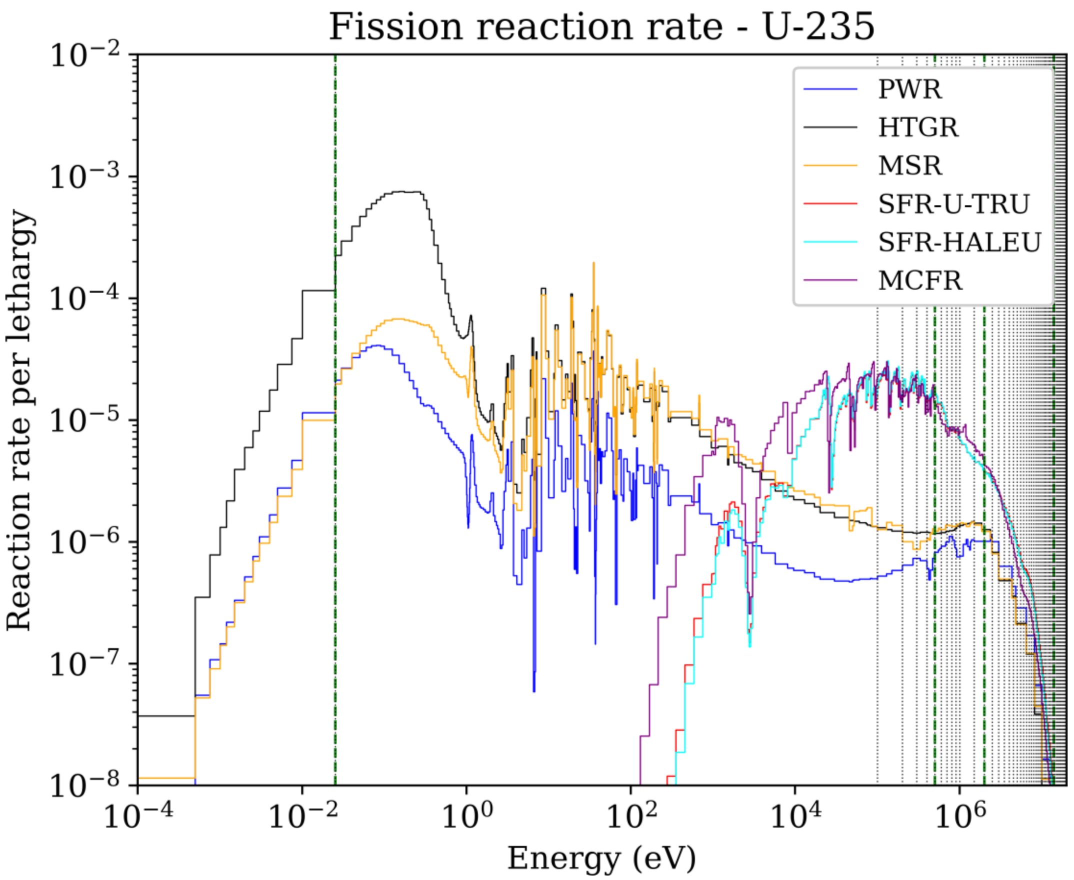
Vertical lines:
Solid color: Energy of average lethargy of fission (EALF)
Dashed green: 4 FPY energies
Dotted gray: all GEFY energies

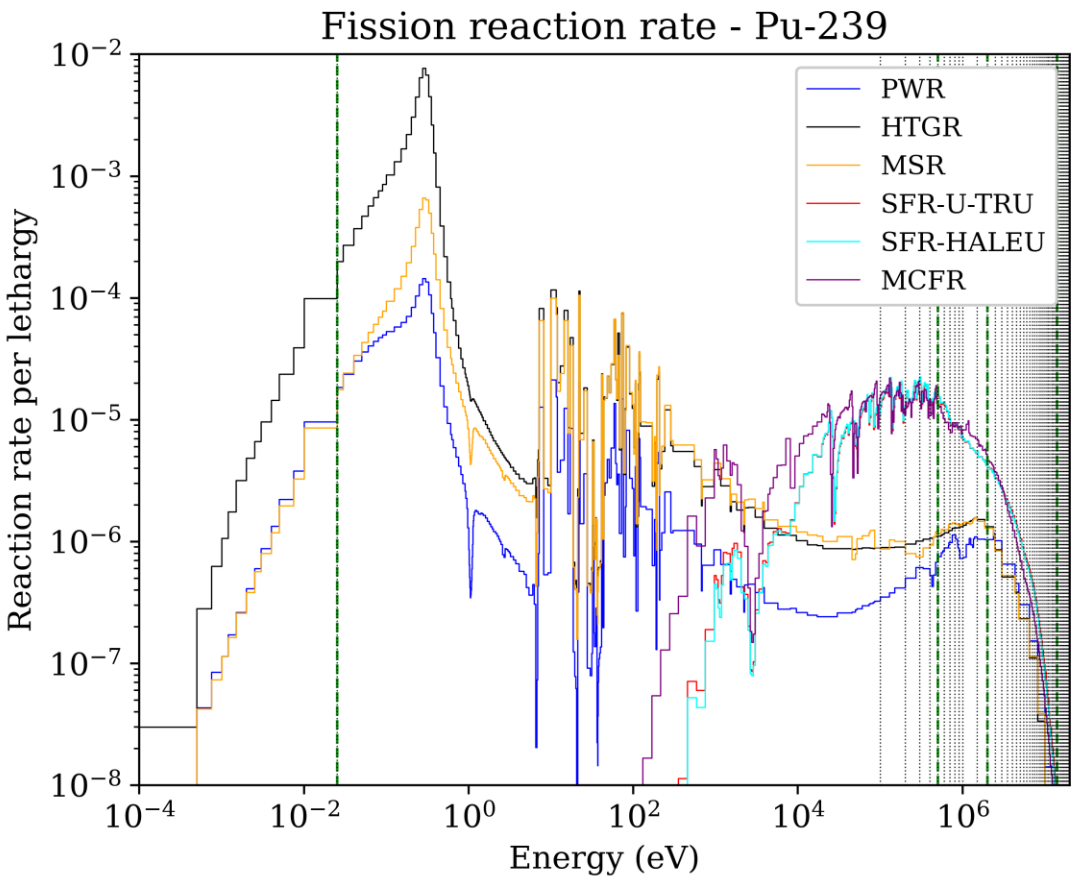
Observation:
Thermal region: only 1 relevant energy point
Fast region: additional relevant energy points that are closer to the EALF than the traditional 500 keV and 2 MeV

Model	EALF (eV)	
PWR	0.98 eV	Thermal systems
HTGR	0.21 eV	
MSR	0.23 eV	
SFR U/TRU	262 keV	Fast systems
SFR HALEU	206 keV	
MCFR	86 keV	



Additional FPY energy points are located in the fast energy range (cont.)





Vertical lines:
Solid color: EALF
Dashed green: 4 FPY energies
Dotted gray: all GEFY energies

Observation:
Additional FPY energies in the fast energy range impact all considered systems, but seem most relevant for fast systems

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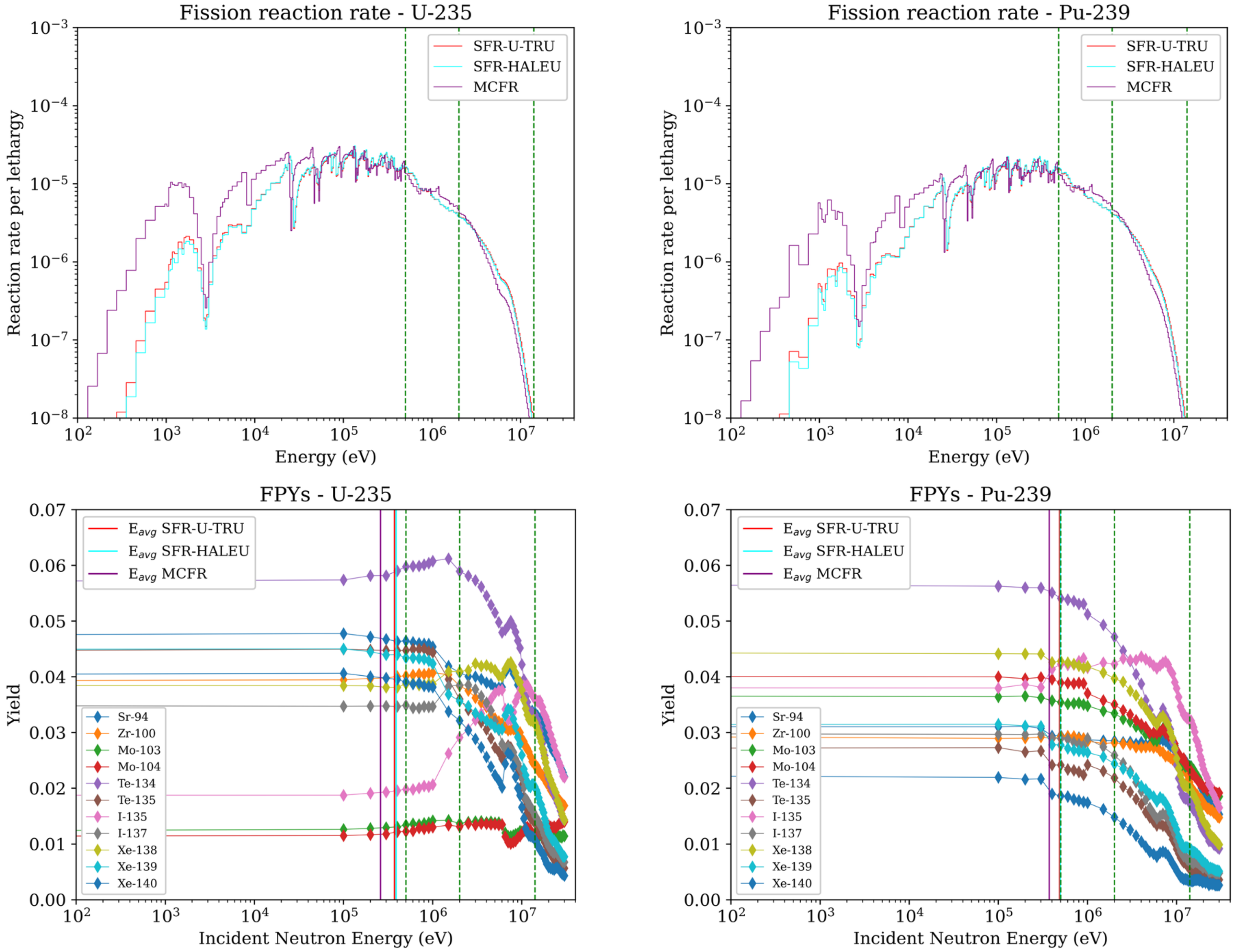
Variation in GEFY FPY at high energies are most relevant for fast systems

Vertical lines:
Dashed green: 4 FPY energies
Solid lines: Average energy of fission E_{avg}

Observation:
FPYs adjacent to E_{avg} does in most cases vary only slightly.



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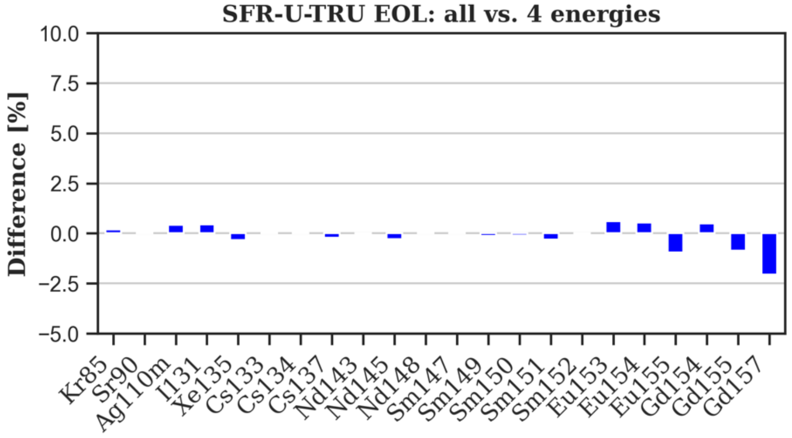
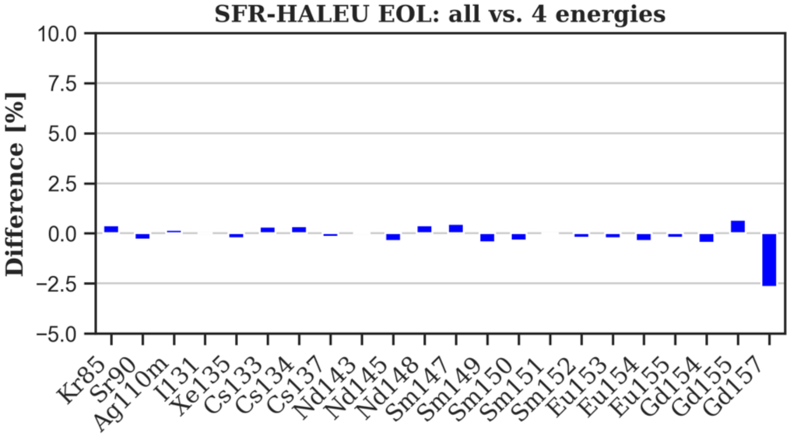
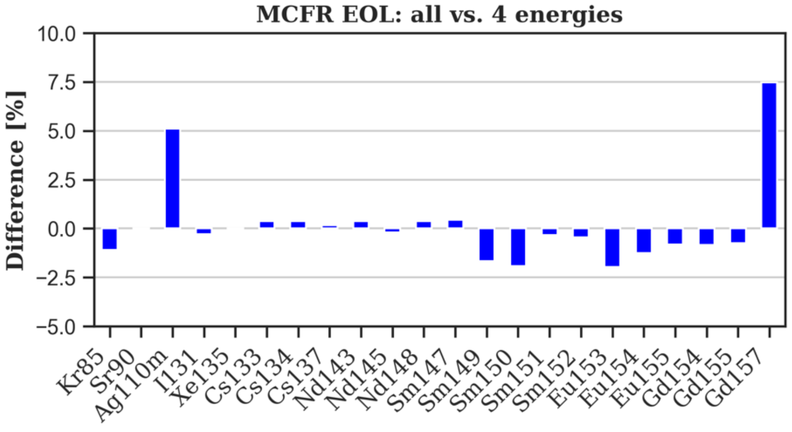
The use of GEFY data with all energies has visible impact on nuclide inventory at EOL for fast systems

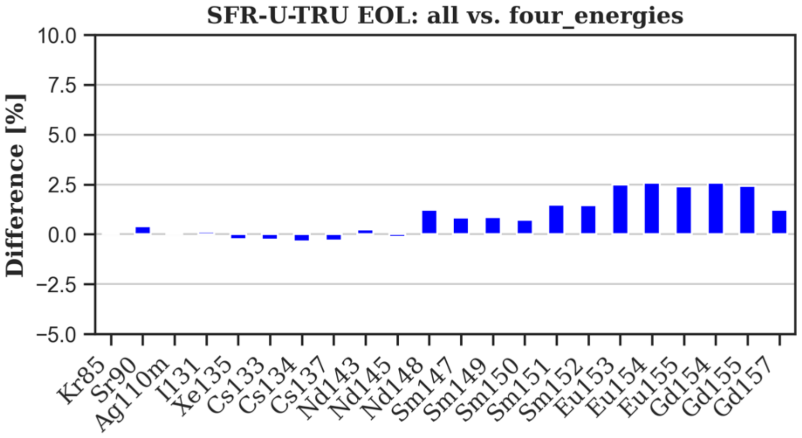
SCALE

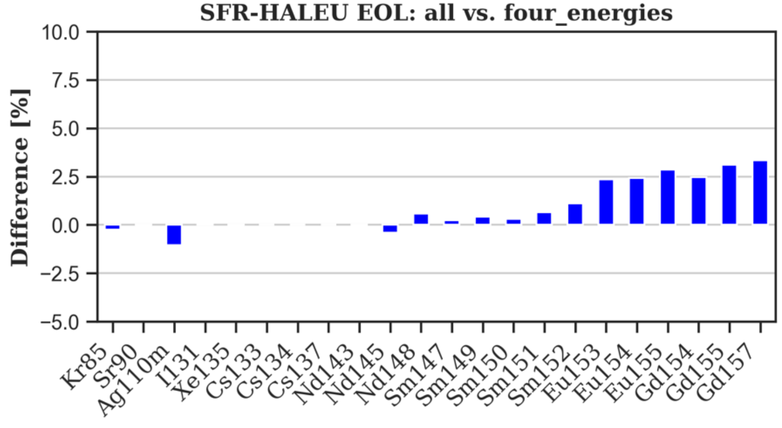


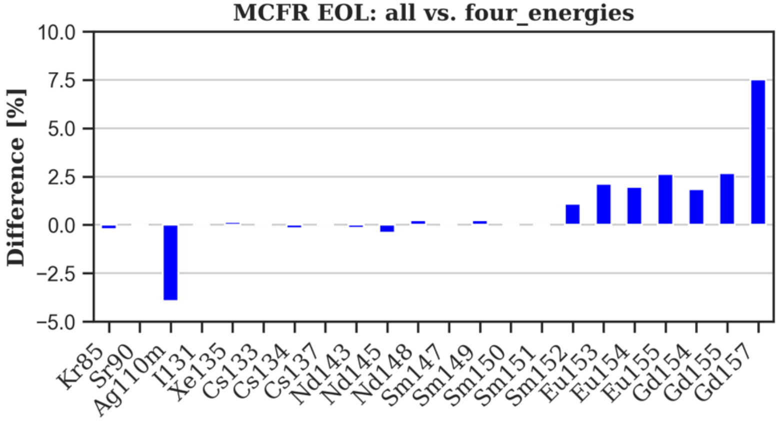




Serpent







SCALE and Serpent show different trends due to different approaches of using the available FPY.
The impact of using FPY at all energies vs. the traditional 4 energy points is clearly visible, with up to ~8% for some fission products.

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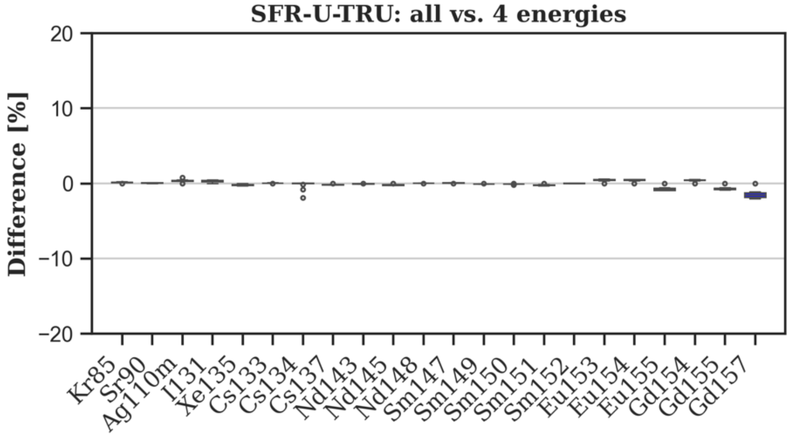
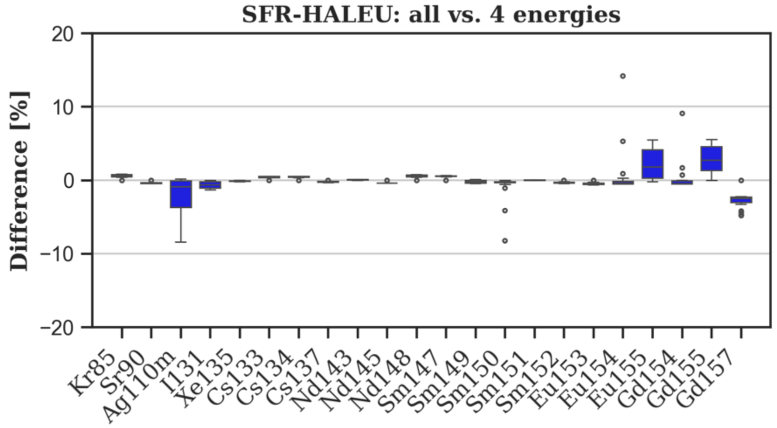
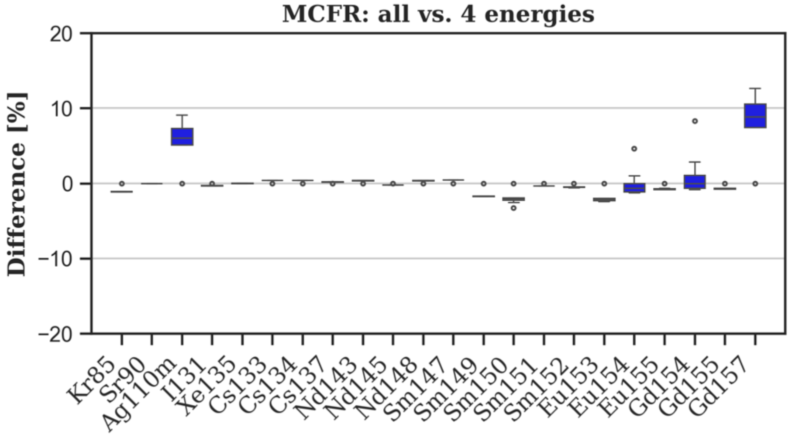
The use of GEFY data with all energies has visible impact on nuclide inventory across the entire irradiation history for fast systems

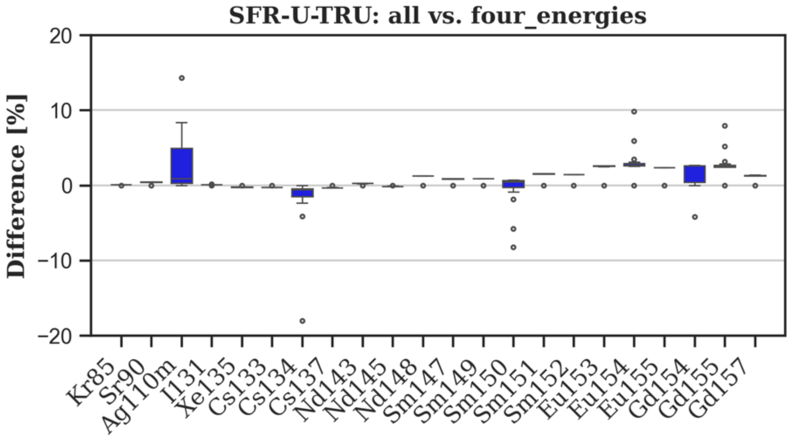
SCALE

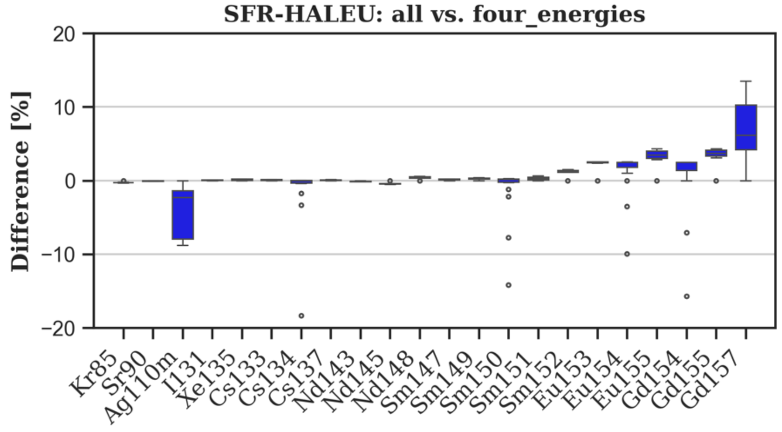


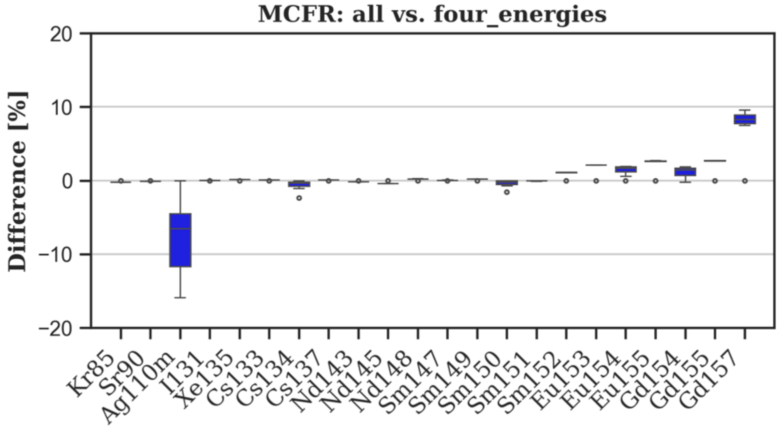




Serpent







The impact of using FPY at all energies vs. the traditional 4 energy points can be higher over the course of depletion compared to EOL

The boxes represent the interquartile range (IQR), from the 25th percentile to the 75th percentile; the horizontal line presents the median (50th percentile); the error bars go to the most extreme data points within 1.5×IQR; and the dots are outliers.

Summary and Conclusions

Use of additional FPY data points in fast energy range in GEFY impacts prediction of fission product inventory:

- Several % difference at EOL for fast spectrum systems; negligible impact for thermal spectrum systems
- Varying magnitude of differences at specific times during depletion compared to EOL
- Varying magnitude of differences between SCALE and Serpent due to different FPY interpolation schemes
- Visible impact despite only few additional energy points in relevant energy range

We need:

- Additional FPY energy points in thermal and intermediate range
- FPY interpolation based on appropriate weighting with fission reaction rate
- Analysis of the impact with respect to validation data
    - Destructive radiochemical assay data for 76 BWR fuel samples and 129 PWR fuel samples is used in SCALE's nuclide inventory validation

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References

GEFY:

- https://www.khschmidts-nuclear-web.eu/GEFY.html

PWR:

- Model: Westinghouse 17x17 model of the ORIGEN reactor library generation files in SCALE 6.3
- W. A. Wieselquist, R. A. Lefebvre, Eds. (2024), SCALE 6.3.2 User Manual, ORNL/TM-2024/3386

HTGR:

- Model: HTR-10 fuel pebble
- R. Elzohery, F. Bostelmann, G. Ilas, "Nuclear Data Impact Assessment for the HTR-10 Pebble-Bed Reactor Using SCALE," Nuclear Science and Engineering (submitted)
- F. Bostelmann, C. Celik, M. L. Williams, R. J. Ellis, G. Ilas, W. A. Wieselquist (2020), "SCALE capabilities for high temperature gas-cooled reactor analysis," Annals of Nuclear Energy, 147. DOI: 10.1016/j.anucene.2020.107673.

MSR:

- Model: Unit cell of a modified version of the Molten Salt Breeder Reactor
- D. Hartanto, G. Redulescu, F. Bostelmann, W. Wieselquist (2025), SCALE Analyses of Scenarios in the Molten Salt Reactor Fuel Cycle, ORNL/TM-2024/3659

SFR:

- Model: Advanced Burner Test Reactor pin cell
- D. Hartanto, G. Radulescu, F. Bostelmann, R. Elzohery, W. Wieselquist (2024), SCALE Demonstration for Sodium-cooled Fast Reactor Fuel Cycle Analysis, ORNL/TM-2023/3214
- A. Shaw, F. Bostelmann, D. Hartanto, E. Walker, and W. A. Wieselquist (2023), SCALE Modeling of the Sodium Cooled Fast-Spectrum Advanced Burner Test Reactor, ORNL/TM-2022/2758

MCFR:

- Model: Molten Chloride Fast Reactor fuel
- G. Ilas, F. Bostelmann, R. Elzohery, "Nuclear Data Impact on Key Metrics for a Representative Molten Chloride Fast Reactor Model," PHYSOR2025, Turin, Italy, April 19-23, 2025 (submitted)
- M. Wargon, J. Latkowski, T. Cisneros (2023), Representative Neutronics Models of MCFR Reactors, DOI: 10.13140/RG.2.2.15127.55208

SCALE:

- W. A. Wieselquist, R. A. Lefebvre, Eds. (2024), SCALE 6.3.2 User Manual, ORNL/TM-2024/3386

Serpent:

- J. Leppänen, V. Valtavirta, A. Rintala, R. Tuominen (2025), "Status of Serpent Monte Carlo code in 2024," EPJ Nuclear Sci. Technol., 11(3). DOI: 10.1051/epjn/2024031

Backup

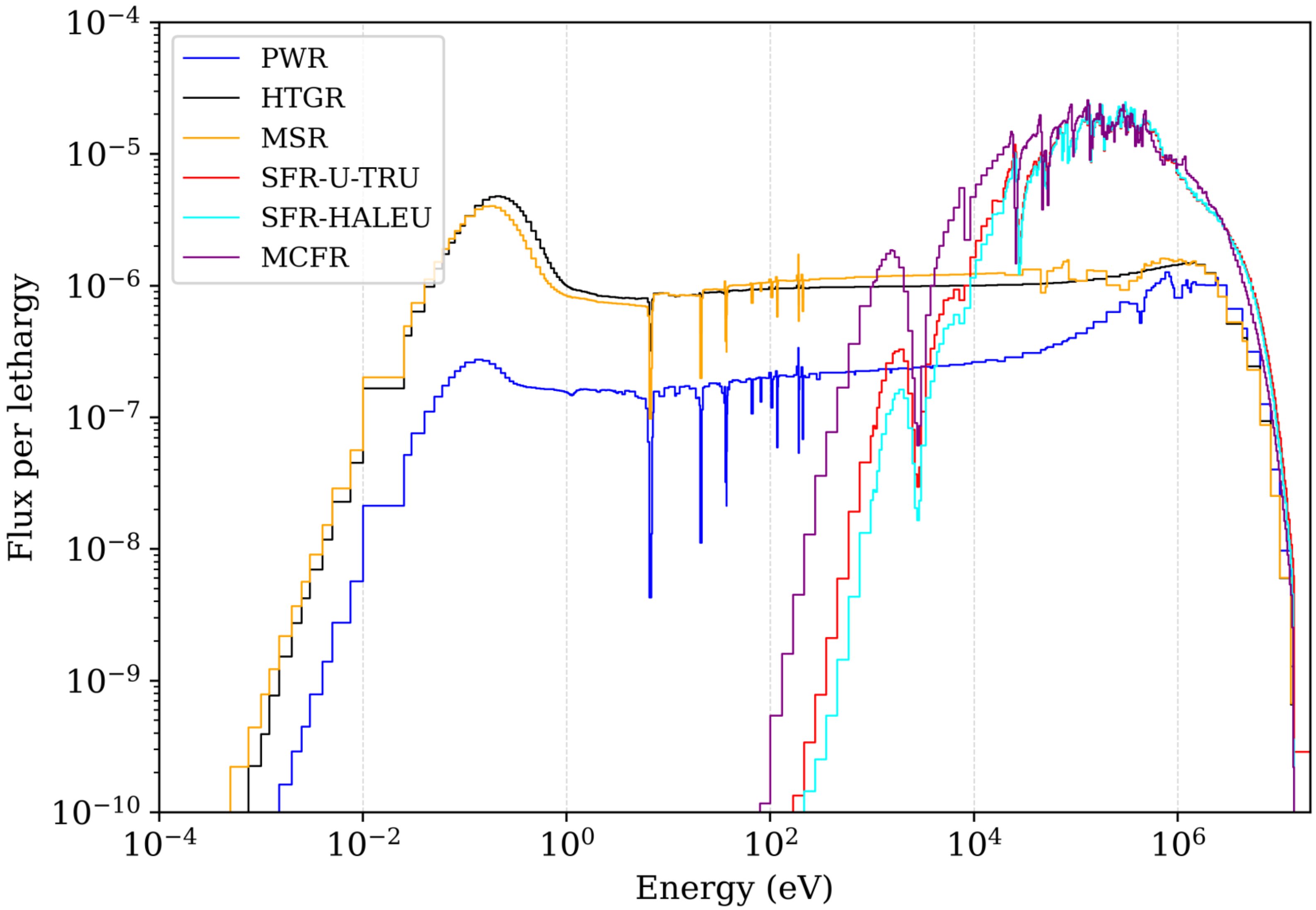
Reactor models covering thermal and fast neutron spectral conditions

EALF: Energy of average lethargy of fission

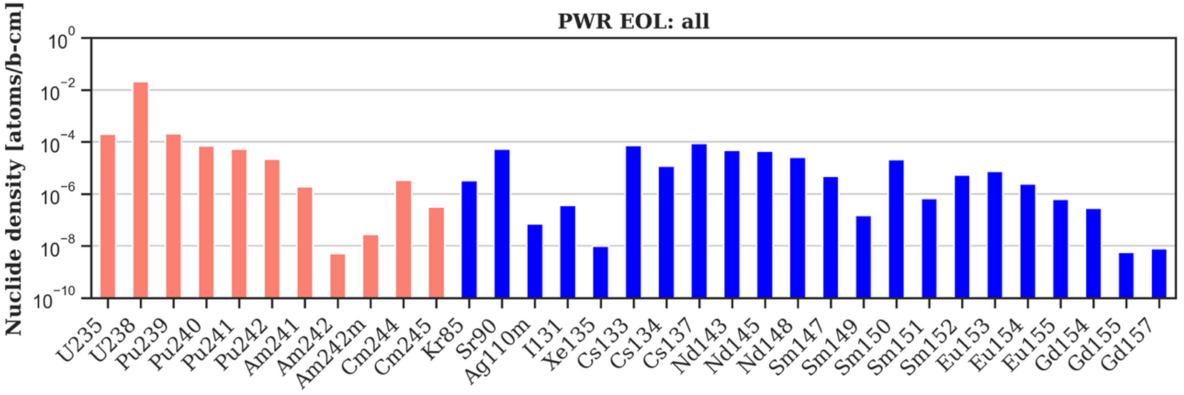
Model	EALF (eV)
PWR	0.98 eV
HTGR	0.21 eV
MSR	0.23 eV
SFR U/TRU	262 keV
SFR HALEU	206 keV
MCFR	86 keV

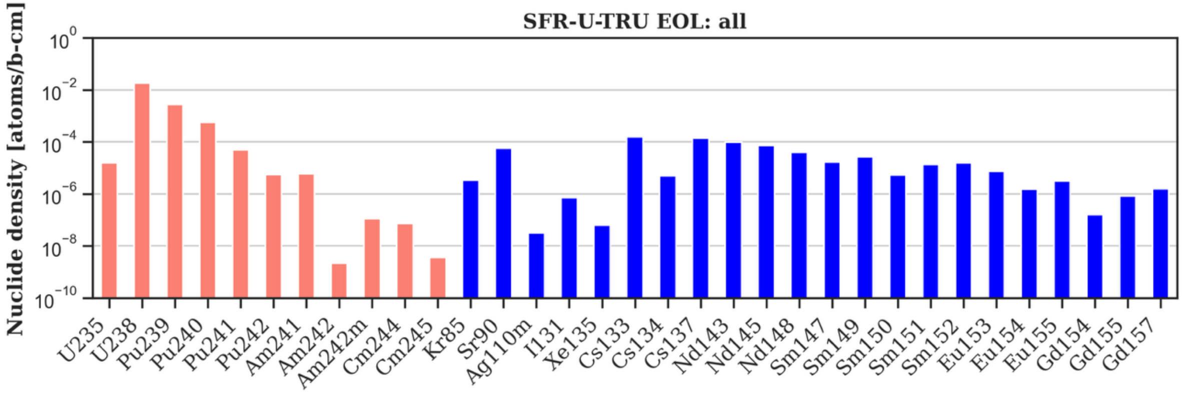
Thermal systems (PWR, HTGR, MSR)

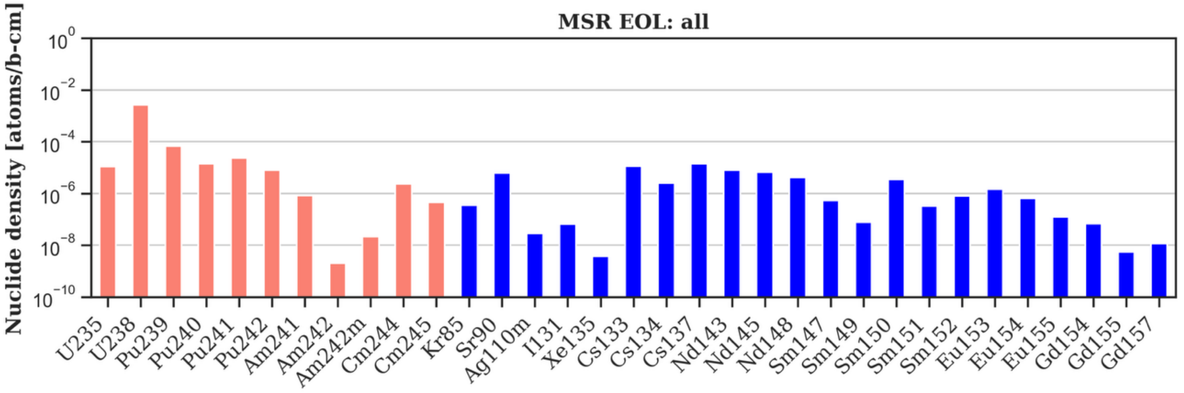
Fast systems (SFR U/TRU, SFR HALEU, MCFR)

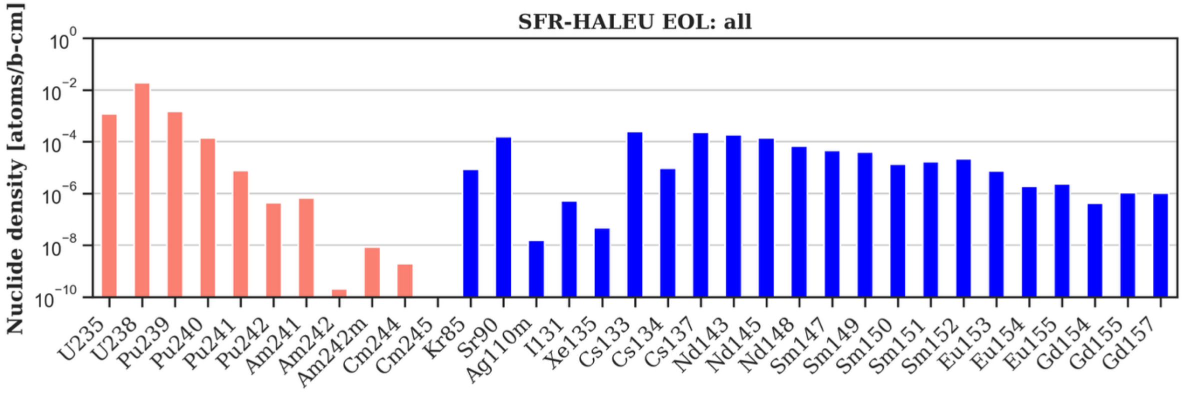


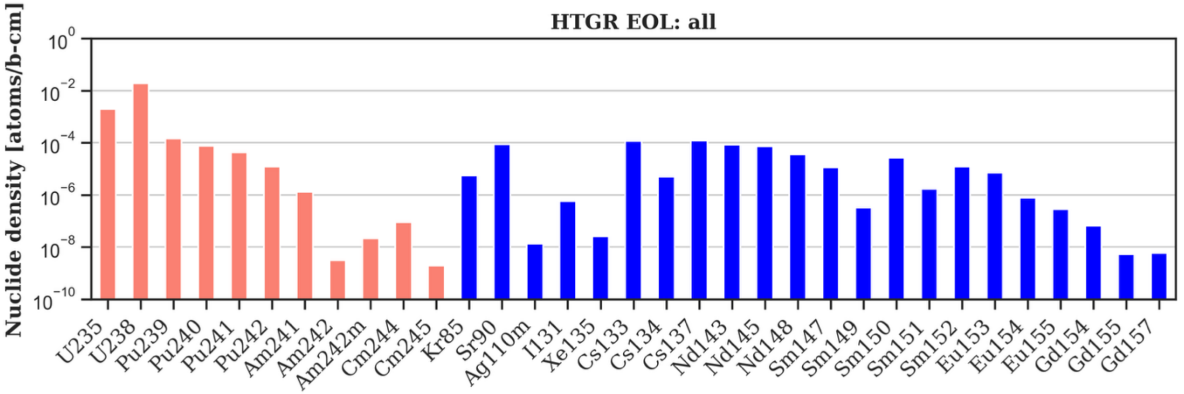
EOL nuclide densities

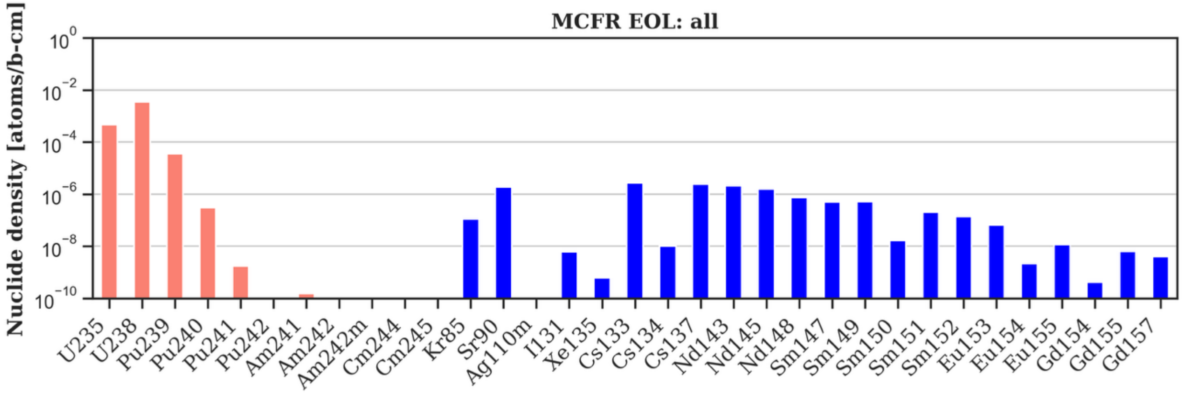






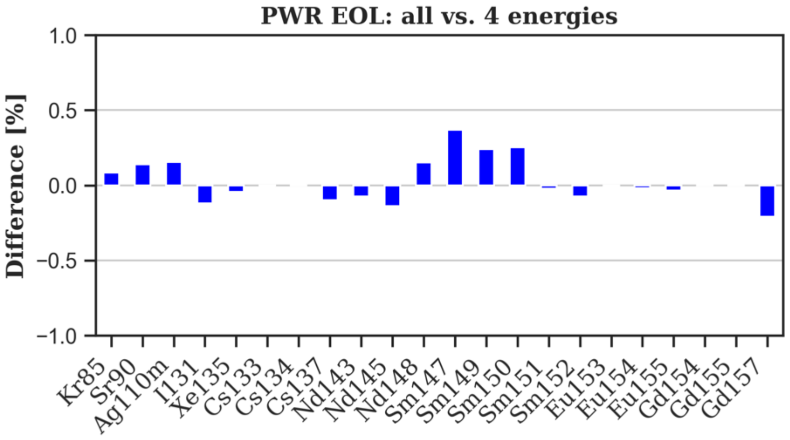


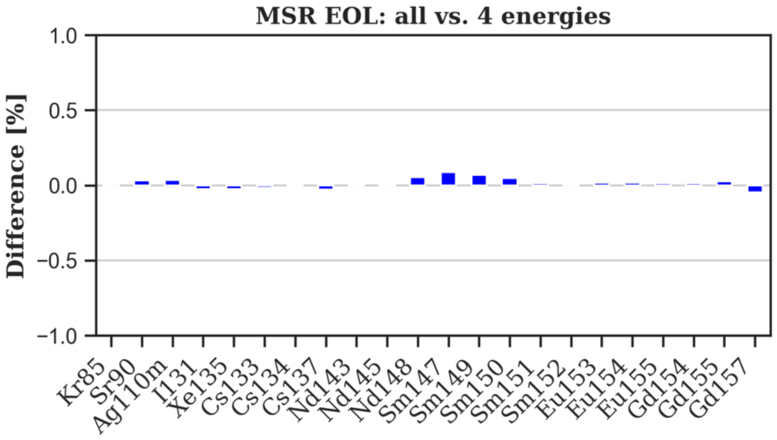


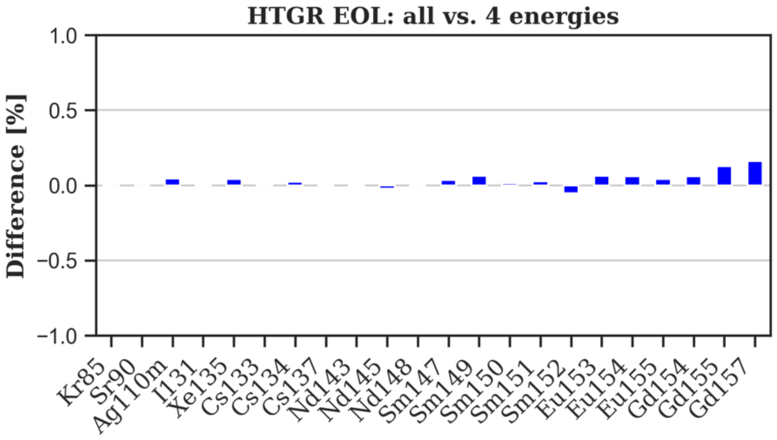


The use of GEFY data with all energies has negligible impact on nuclide inventory at EOL for thermal spectrum systems

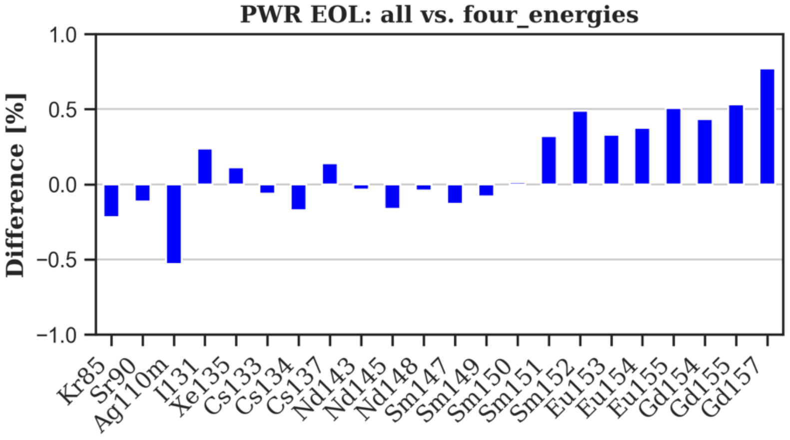
SCALE

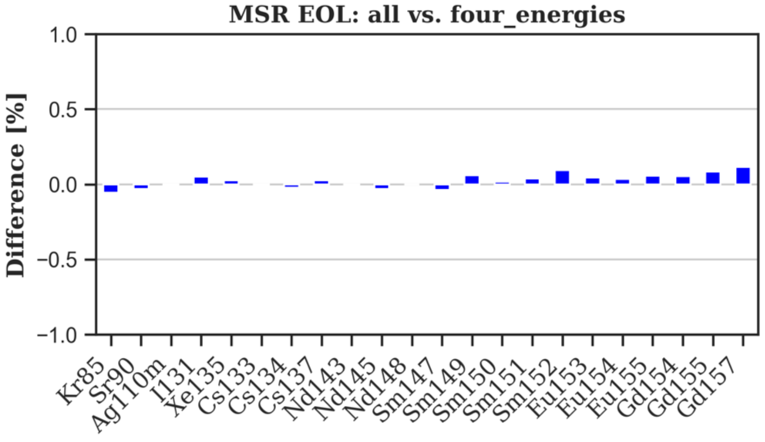


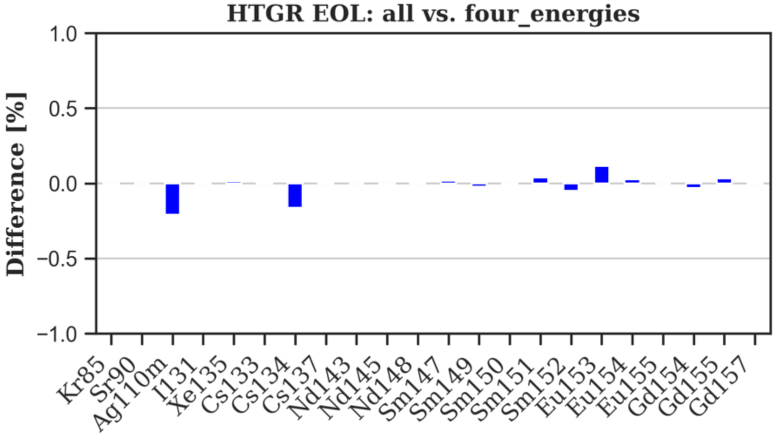




Serpent







SCALE and Serpent show different trends due to different FPY interpolation
The impact of using FPY at all energies vs. the traditional 4 energy points is negligible (<1% for all systems) because the FPY are finely resolved only in the fast energy range.

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SCALE/ORIGEN average energy of fission

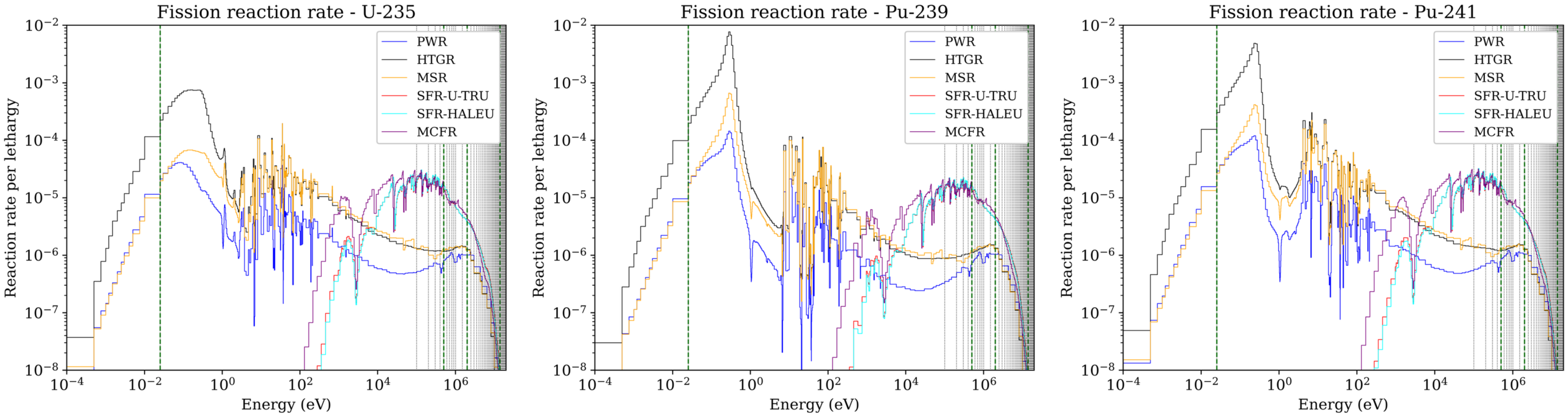
Model	EALF at BOL	EALF at EOL	Actinide	E_{avg} [keV] at BOL	E_{avg} [keV] at BOL
PWR	0.98 eV	1.73 eV	U-235	28.9	35.1
			Pu-239	16.0	23.0
			Pu-241	13.9	18.3
MSR	0.23 eV	0.96 eV	U-235	2.9	14.4
			Pu-239	1.2	7.9
			Pu-241	1.2	7.2
SFR U/TRU	262 keV	252 keV	U-235	371.2	348.6
			Pu-239	484.3	458.9
			Pu-241	367.7	345.9
SFR HALEU	206 keV	215 keV	U-235	387.8	342.3
			Pu-239	495.8	449.3
			Pu-241	383.4	339.8
MCFR	86 keV	87 keV	U-235	259.4	257.7
			Pu-239	370.6	369.0
			Pu-241	261.9	260.3

Available energy points for fission yields in GEFY

2.53E-02	6.00E+06	1.60E+07
1.00E+05	6.50E+06	1.65E+07
2.00E+05	7.00E+06	1.70E+07
3.00E+05	7.50E+06	1.75E+07
4.00E+05	8.00E+06	1.80E+07
5.00E+05	8.50E+06	1.85E+07
6.00E+05	9.00E+06	1.90E+07
7.00E+05	9.50E+06	1.95E+07
8.00E+05	1.00E+07	2.00E+07
9.00E+05	1.05E+07	2.10E+07
1.00E+06	1.10E+07	2.20E+07
1.50E+06	1.15E+07	2.30E+07
2.00E+06	1.20E+07	2.40E+07
2.50E+06	1.25E+07	2.50E+07
3.00E+06	1.30E+07	2.60E+07
3.50E+06	1.35E+07	2.70E+07
4.00E+06	1.40E+07	2.80E+07
4.50E+06	1.45E+07	2.90E+07
5.00E+06	1.50E+07	3.00E+07
5.50E+06	1.55E+07	

Difference in E_{avg} between calculations "all" vs. 4 FPY energies is <0.01%

EOL fission reaction rates



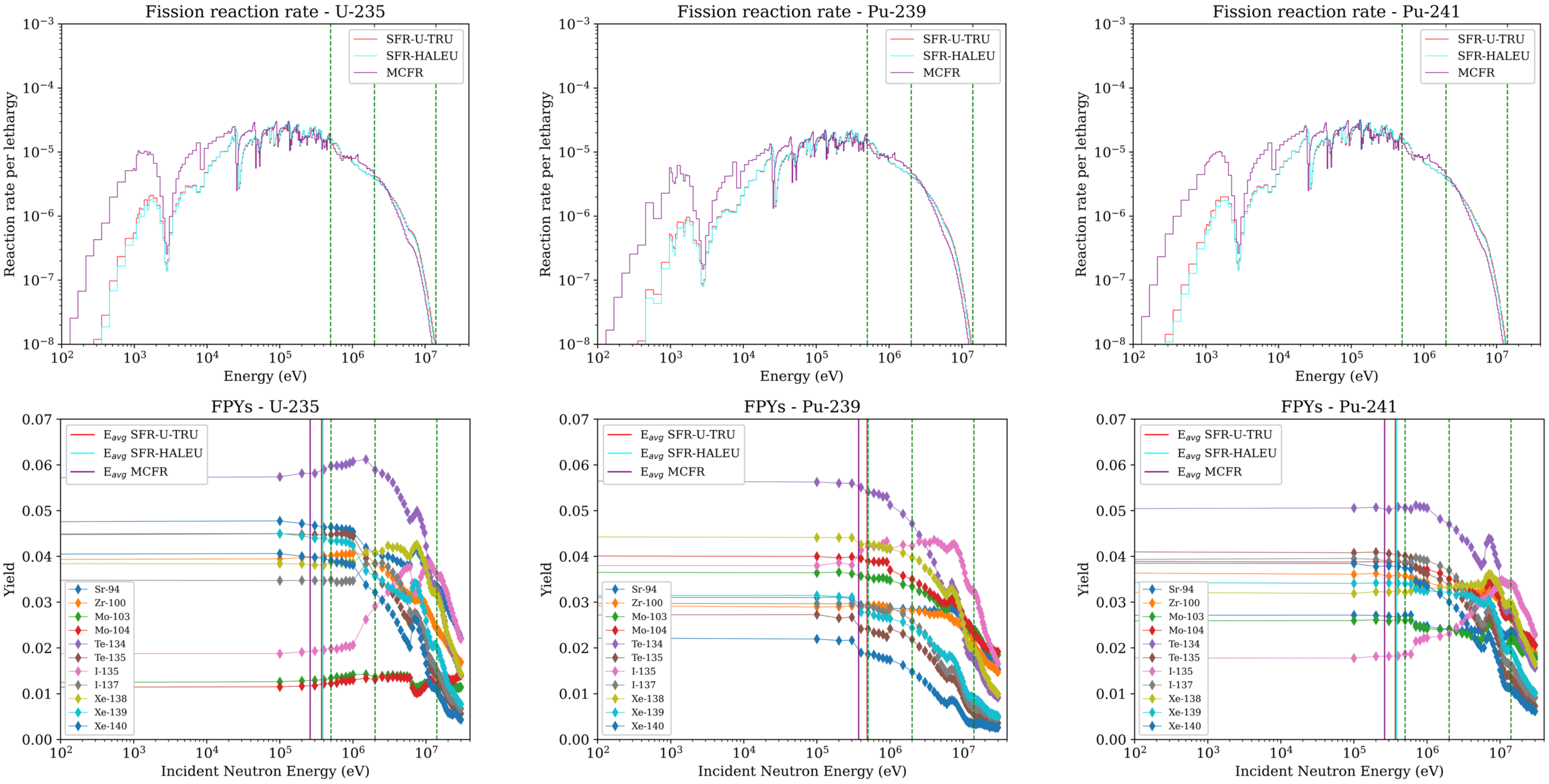
Vertical lines:

Dashed green: 4 FPY energies

Dotted gray: all GEFY energies

GEFY FPY

Vertical dashed green lines: 4 FPY energies
FPYs adjacent to E_{avg} does in most cases vary only slightly.



EOL FPY used by SCALE/ORIGEN