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Description of Transmutation Library for Fuel Cycle System Analyses

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August 2010

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SUMMARY

This report documents the Transmutation Library that is used in Fuel Cycle System Analyses. This version replaces the 2008 version.[Piet2008] The Transmutation Library has the following objectives:

- Assemble past and future transmutation cases for system analyses.
- For each case, assemble descriptive information such as where the case was documented, the purpose of the calculation, the codes used, source of feed material, transmutation parameters, and the name of files that contain raw or source data.
- Group chemical elements so that masses in separation and waste processes as calculated in dynamic simulations or spreadsheets reflect current thinking of those processes. For example, the CsSr waste form option actually includes all alkali metals (Group 1) and alkaline earth metals (Group 2).
- Provide mass fractions at input (charge) and output (discharge) for each case.
- Eliminate the need for either "fission product other" or "actinide other" while conserving mass. Assessments of waste and separation cannot use "fission product other" or "actinide other" as their chemical behavior is undefined.
- Catalog other isotope-specific information in one place, e.g., heat and dose conversion factors for individual isotopes.
- Describe the correlations for how input and output compositions change as a function of UOX burnup (for LWR UOX fuel) or fast reactor (FR) transuranic (TRU) conversion ratio (CR) for either FR-metal or FR-oxide.

This document therefore includes the following sections:

- Explanation of the data set information, i.e., the data that describes each case. In no case are all of the data presented in the Library included in previous documents. In assembling the Library, we returned to raw data files to extract the case and isotopic data, into the specified format.
- Explanation of which isotopes and elements are tracked. For example, the transition metals are tracked via the following: two Zr isotopes, Zr-other, Tc99, Tc-other, two Mo-Ru-Rh-Pd isotopes, Mo-Ru-Rh-Pd-other, four other specific TM isotopes, and TM-other. Mo-Ru-Rh-Pd are separated because their content constrains the loading of waste in glass, so we have to know the mass of those elements independent of others.
- Rules for collapsing long lists of isotopes (~1000) to the 81 items in the library. For each tracked isotope, we define which short-lived isotopes' mass (at t=0) is included with the mass of the tracked isotope at t=0, which short-lived radioactive progeny must be accounted for when the tracked isotope decays, and to which of the other 80 items the mass of the tracked isotope goes when it decays.
- Explanation of where raw data files can be found on the fuel cycle data portal.
- Explanation of generic cross section sets
- Explanation of isotope-specific parameters such as heat and dose conversion factors
- Explanation of the LWR UOX burnup and FR TRU CR correlations.

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4N	Actinide decay chain with mass numbers divisible by 4, including Th232 (1.4e10 years) as longest-lived and ending at Pb208
4N+1	Actinide decay chain with mass numbers 1 greater than a number divisible by 4, including Np237 as longest-lived (2.1e6 years) and ending at Bi209
4N+2	Actinide decay chain with mass numbers 2 greater than a number divisible by 4, including U238 as longest-lived (4.5e9 years) and ending at Pb206
4N+3	Actinide decay chain with mass numbers 3 greater than a number divisible by 4, including U235 as longest-lived (7.0e8 years) and ending at Pb207
ACR	Advanced CANDU (or Canadian) reactor
ANL	Argonne National Laboratory
BNL	Brookhaven National Laboratory
BU	Burnup (MWth-day/kg-iHM or equivalently GWth-day/tonne-iHM)
BWR	Boiling water reactor
CANDU	Canada deuterium uranium (reactor)
COEX	Co-extraction of U and Pu
CORAIL	*Combustible recyclage a ilot* French fuel cycle variant of MOX
CR	Transuranic conversion ratio (similar but not identical to breeding ratio)
CY	Calendar year (365.25 days)
DU	Depleted uranium
Echem	Electrochemical separation process (a.k.a. pyroprocessing)
EFPD	Effective full power days
EFPY	Effective full power years = capacity factor times calendar years
EU	Enriched uranium
FP	Fission product
FR	Fast reactor or fast reactor fuel
FR-ox	Oxide fast reactor fuel
FR-mtl	Metal fast reactor fuel
FR-NpPu	Fast reactor fuel with Np, Pu, and no other transuranic elements
FR-NpPuAm	Fast reactor fuel with Np, Pu, Am, and no other transuranic elements
FR-Pu	Fast reactor fuel and no other transuranic elements
FR-TRU	Fast reactor fuel with all the transuranic elements
GWe	Gigawatt-electric (one billion watts of electricity)
GWth	Gigawatt-thermal (one billion watts of heat)
HTGR	High temperature gas reactor
HWR	Heavy water reactor
iHM	Initial heavy metal
IMF	Inert matrix fuel (uranium free)
IMF-NpPu	Inert matrix fuel with Np, Pu, and no other transuranic elements
IMF-NpPuAm	Inert matrix fuel with Np, Pu, Am, and no other transuranic elements
IMF-Pu	Inert matrix fuel and no other transuranic elements
IMF-TRU	Inert matrix fuel with all the transuranic elements
INL	Idaho National Laboratory or its predecessor laboratories INEL (Idaho National Engineering Laboratory) or INEEL (Idaho National Engineering and Environmental Laboratory)
Ln	Lanthanide elements
LWR	Light water reactor

MOX	Mixed oxide fuel							
MOX-NpPu	Mixed oxide fuel with Np, Pu, and no other transuranic elements							
MOX-NpPuAm	Mixed oxide fuel with Np, Pu, Am, and no other transuranic elements							
MOX-Pu	Mixed oxide fuel with Pu and no other transuranic elements							
MOX-TRU	Mixed oxide fuel with all the transuranic elements							
MT	Montana, it is not used as metric ton or million tons							
MWe	Megawatt-electric (one million watts of electricity)							
MWth	Megawatt-thermal (one million watts of heat)							
NA	Not applicable							
NGNP	Next Generation Nuclear Plant (a type of VHTR/HTGR)							
NU	Natural uranium							
ORNL	Oak Ridge National Laboratory							
P	Recycle pass (not to be confused with batch)							
P0 or p=0	Unrecycled material, i.e., uranium-based fuel							
P1 or p=1	Startup recycle pass, reactor in equilibrium with feed material from separated uranium-based fuel, i.e., first use of recycled material							
Pn or p=n	Nth recycle pass, reactor in equilibrium with feed material that has been through reactors n-1 times							
ppm	parts per million							
PHWR	Pressurized heavy water reactor							
PWR	Pressurized water reactor							
PUREX	Plutonium-Uranium Extraction separation process							
RU	Recovered uranium							
SFR	Sodium fast reactor							
t	Time							
TBD	To be determined							
ThOX	Thorium oxide							
TM	Transition metal							
Tonne	1000 kg, metric ton							
TRU	Transuranic elements							
UCO	Uranium oxycarbide fuel							
UOX or UO_2	Uranium oxide fuel							
UOX-nn	Uranium oxide fuel with nn MWth-day/kg-iHM burnup							
UREX	Uranium Extraction separation process							
UREX+1	UREX producing …	U	Tc	CsSr	TRU (with or without Ln)			Other fission products
UREX+2	UREX producing …	U	Tc	CsSr	NpPu	AmCm+Ln		Other fission products
UREX+3	UREX producing …	U	Tc	CsSr	NpPu	AmCm		Other fission products
UREX+4	UREX producing …	U	Tc	CsSr	NpPu	Am	Cm	Other fission products
VHTR	Very high temperature reactor							
VISION	Verifiable Fuel Cycle Simulation dynamic fuel cycle model							
W	Watt							
Xsec	cross section							
Yr	Year (generally “year” is calendar year when the differentiation between calendar year and effective full power years is obvious)							

SYSTEM ANALYSIS

DESCRIPTION OF TRANSMUTATION LIBRARY FOR FUEL CYCLE SYSTEM ANALYSES

1. INTRODUCTION

This report documents the format of the Transmutation Library for Fuel Cycle System Analyses. This report is intended to be used by the following types of people:

- Reactor physicists who perform transmutation calculations.
- Experts who translate raw transmutation calculations into the format used in the Library, namely provide data on the calculations themselves, and collapse the huge amount of raw data (of order 1000 isotopes) into a defined set of 81 isotopes and chemical elements.
- System analyses who use transmutation calculations, especially for studies with the Fuel-cycle Integration & Tradeoff (FIT) or system dynamic calculations with the Verifiable Fuel Cycle Simulation (VISION) model.

1.1 Purpose

This report documents the format of the Transmutation Library to be used in future Fuel Cycle System Analyses. The Transmutation Library and hence its format described here has the following objectives:

- Assemble past and future transmutation data sets for system analyses.
- For each case, assemble descriptive information.
- Group chemical elements so that masses in separation and waste processes reflect current thinking of how those processes would work.
- Provide mass fraction recipes at input (charge) and output (discharge) for each case.
- Eliminate the need for either “fission product other” or “actinide other” while conserving total mass as it is impossible to assess the waste and environmental consequences of a undefined mass of material.
- Catalog other isotope-specific information in one place, e.g., heat and dose conversion factors for individual isotopes.
- Describe the correlations for how input and output compositions change as a function of UOX burnup (for LWR UOX fuel) or fast reactor (FR) transuranic (TRU) conversion ratio (CR) for either FR-metal or FR-oxide.

1.2 Scope

The document includes the following sections:

- Explanation of the data set information. Note that in no case is all of the data presented in the Library included in any of the previous documents. In assembling the Library, we have gone back to raw data files to extract the case data and isotopic data, and process into the specified format.
- Explanation of which isotopes and elements are tracked.

- Rules for collapsing long lists of isotopes to the 81 items in the library. For each tracked isotope, we define which short-lived isotopes' mass (at t=0) is to be added to the mass of the tracked isotope at t=0, which short-lived radioactive progeny must be accounted for when the tracked isotope decays, and to which of the other 80 items the mass of the tracked isotope is assigned when it decays.
- A check whether the set of isotopes is adequate for our purposes.
- Preliminary information on ways to adjust recipes when simulation conditions warrant, e.g., if burnup or cooling time before separation is 20% higher than assumed in a previous calculation.
- Explanation of where raw data files can be found on the fuel cycle data portal.
- Explanation of generic cross section sets
- Explanation of isotope-specific parameters such as heat and dose conversion factors
- Explanation of the LWR UOX burnup and FR TRU CR correlations.

Table 1-1 summarizes the classes of transmutation cases included in the Library. The classes span all four fuel cycle strategies. Except for once-through cases, a single simulation will require use of several recipes. For example, a 2-tier UOX-MOX-FR case will require a UOX recipe, a MOX recipe, and one or more FR recipes. A case involving two recycles in MOX before insertion into a fast reactor would require two MOX recipes, recycle pass 1 and recycle pass 2. The fast reactor would generally include the startup recycle pass and equilibrium recycle pass. Note that "recycle pass" and "equilibrium" refers to the status of the *system*, not a *reactor core*. (At present, all cases in the Library involve an equilibrium core condition, as opposed to the startup core or the last batches before reactor retirement.) A "startup recycle pass" recipe means the core is at equilibrium with the initial feed material, for example, TRU from separated UOX. An "equilibrium recycle pass" means the core is at equilibrium with equilibrium system feed material; for fast reactors with TRU conversion ratio less than one, this would be a mix of TRU from separated UOX plus TRU from separated FR fuel.

Table 1-1. Classes of Transmutation Cases

Class	Illustrative source of feed material	Illustrative reactors	Corresponding Strategy
Once through	Enriched U	PWR	Once through
MOX	Separated UOX fuel	PWR	Single or multiple recycling in thermal reactors
IMF	Separated UOX fuel	PWR	
UOX-FR (1-tier)	Separated UOX & FR fuels	FR	Multiple recycling using thermal and fast reactors
UOX-MOX-FR (2-tier)	Separated UOX, MOX, & FR fuels	FR	
UOX-IMF-FR (2-tier)	Separated UOX, IMF, & FR fuels	FR	
UOX-breeder	Separated FR fuel	FR	Multiple recycling using fast reactors

In dynamic simulations of fuel cycles, the isotopic composition of material that is available in a given time step "never" exactly matches the fixed static calculation one obtains from a transmutation analysis calculation. For example, the average age of separated material available to make fuel might be 11.5 years whereas the closest calculation might be for 10. Therefore, for several years, we have been building a set of tools that would allow adjustments in models such as VISION. There are three types of tools:

- Higher density of cases so that the deviation between available material composition and a case is minimized; assembly of the Library gives us a better assessment of "case" density.

- Correlations of input/output recipes for UOX as a function of burnup and for FR fuel as a function of FR TRU conversion ratio.[Yacout2008]
- 1-group cross section perturbation approach for adjusting recipes.[Bays2009, Yee2008]

1.3 Methodology

One of the motivations for the Library is to improve the ability of transmutation calculations to support fuel cycle waste management assessments. It is therefore no longer adequate to track a few individual isotopes and lump everything else into "fission product other".

Instead, the Library is carefully structured to preserve mass in fuel cycle simulations and to differentiate mass based on the range of separation and waste management options being studied. The following paragraphs explain the approach.

In determining which isotopes and chemical elements to include in the Library, we followed certain procedures.

- Only isotopes with halflife greater than 0.5 year are candidates for being tracked in fuel cycle simulations. A half year is two VISION time steps. Section 3 and Appendix A show that not tracking such short-lived isotopes does not significantly impact mass and radiotoxicity assessments. (Spot checks of gamma and heat indicate the same thing.) Short-lived progeny of other isotopes, however, must be considered. Their heat and decay energy emission must be included when their parent isotopes decay. For example, Y90 decay energy must be included with decay of Sr90.
- For actinide and decay chain isotopes, we started with all isotopes with halflife greater than 0.5 year. Because of the complexity of the decay chains (Appendix B), we only discard five of the candidate isotopes (Np235, Np236, Pu236, Cf248, and Es254) because their yield is so low. The behavior of actinide and decay chain isotopes is so complex that we essentially have to include all isotopes with halflife greater than 0.5 years. In subsequent calculations of radiotoxicity, heat, etc, the decay input of those isotopes less than 0.5 years must be accounted for as being in equilibrium with longer-lived parents.
- For fission products, the complexity of behavior is less and the number of candidate isotopes is greater. For fission products, we started with the set of isotopes previously studied in AFCI system studies and added isotopes (and blocks of "stable" elements) such that the mass and radiotoxicity of each of the candidate waste streams (inert gases, lanthanides, CsSr, transition metal, Tc, halogens) calculated from the reduced set of isotopes and elements in the Library was within a few percent of calculations using all the isotopes for UOX at 51 MWth-day/kg-iHM burnup. See Section 3 and Appendix A.

At present, we only have fast reactor recipes for the startup recycle pass (p=1) and equilibrium recycle pass (p designated as 5). When both startup and equilibrium recipes exist, the Library performs an interpolation between p1 and p5 to provide recipes for p2, p3, and p4. At present, we use a log interpolation for actinide and decay chain isotopes as they vary orders of magnitude and a linear interpolation for fission product isotopes as they vary little.

All recipes are mass fractions that must sum to 1.000.

All recipes only include the fuel and its fission and decay products; these part of the system dominate fuel cycle assessments to date. At present, the current Library does not include data for cladding, matrix materials, and structures in reactors.

To preserve mass, we have to designate where each of the 81 item's mass goes when it decays into one of the other 80 items. For example, Sr90 ultimately decays into Zr90, which must be included as part of Zr-other.

Another example of the importance of getting the mass right is that the high-heat CsSr waste form will actually contain all the Group 1 and 2 elements. There is insignificant mass, heat, gamma, and radiotoxicity from isotopes of Li, Be, Na, M, Ka, Ca so their designation does not matter. The dominant heat, gamma, and radiotoxicity isotopes are Sr90, Cs134, Cs135, and Cs137, so these must be tracked. To get the mass of waste forms correct, however, we must also track the mass of all other Sr isotopes, all other Cs isotopes, Rb, and Ba. These four other items are treated as "stable" in VISION simulations. As Sr90 decays, it reduces the mass of Group 1 and 2 as it moves to Zr-other. All three individual Cs isotopes decay into Ba isotopes, so their decay does not change the mass of Group 1 and 2, but the mass does move from the individual isotopes to Ba.

Figure 1-1 shows how chemical elements are grouped per discussions (summer 2008) between S. Piet and D. Gombert (Integrated Waste Management Strategy), verified by T. Todd (Separations Campaign Director) et al. The most complicated issue is the treatment of the so-called transition metals, which are divided as follows:

- Zr93, Zr95, and Zr-other
- Tc99 and Tc-other
- Ru106, Pd107, and Mo-Ru-Rh-Pd-other
- Se79, Cd113m, Sn126, Sb125, and TM-other

Zirconium is grouped by itself because in systems with Zr alloy cladding or Zr-alloy metal fuel most of the mass of Zr will be from those other sources, not the Zr fission products. So, future assessments will have the Zr isotopes and mass as fission products available for combination with non-fuel sources of Zr. Tc is grouped by itself because the UREX family of separation options extracts Tc as its own waste stream. Mo-Ru-Rh-Pd are grouped together because their content in glass waste form is limited to 3% per D. Gombert, so we must know the mass of those elements independent of others to know the loading of the combined set of transition metals (and other stuff) into glass. TM-other is what remains.

Yttrium is not included with the transition metals because it tends to flow with the lanthanides per D. Gombert and T. Todd et al.

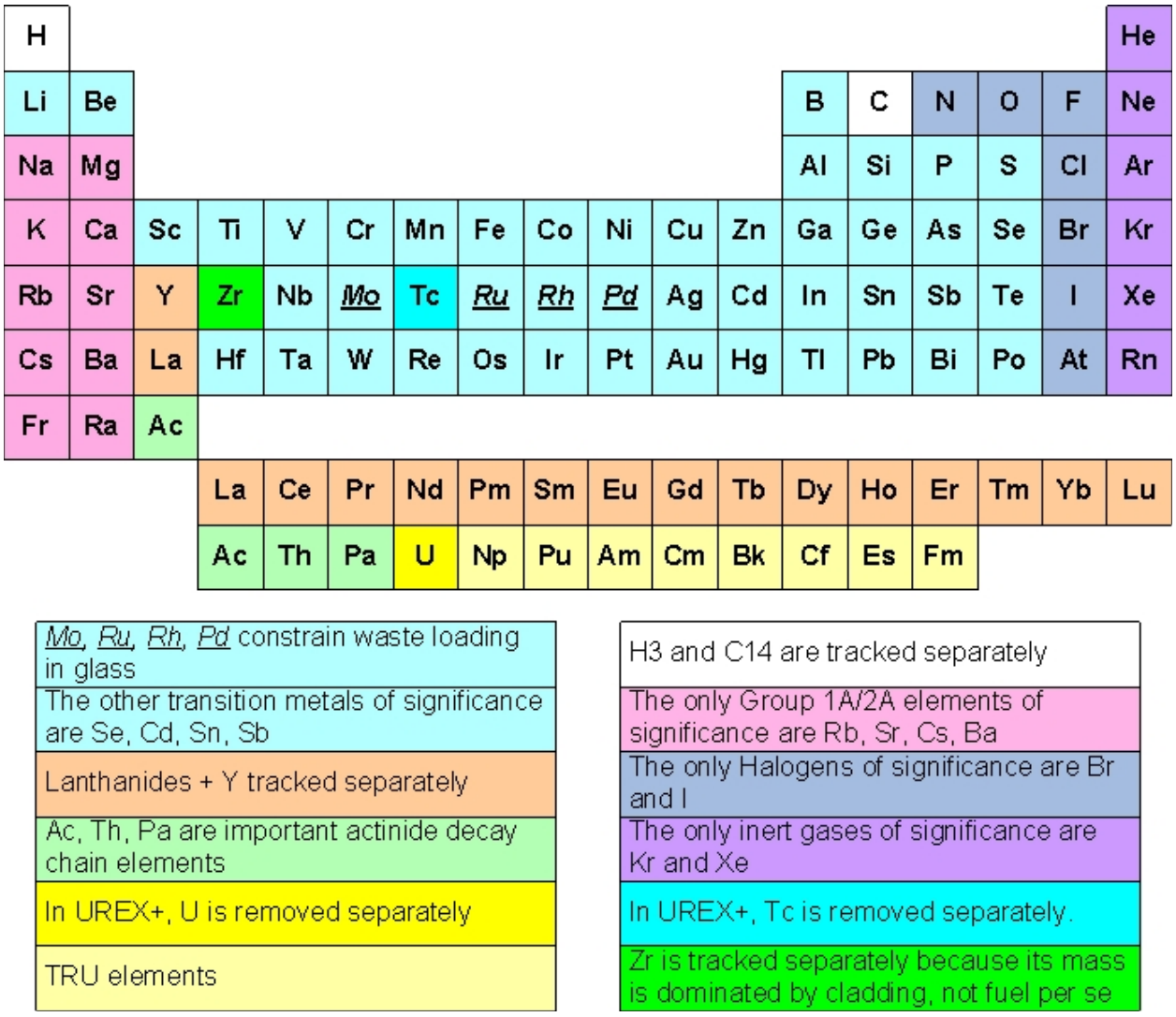

Figure 1-1. Periodic Table as seen from fuel cycle system analysis perspective

More recent examinations for four specific separation techniques (electrochemical, metal melt refining, aqueous, and AIROX) have shown that the best simplification of the Periodic Table is slightly different than that shown in Figure 1-1.[Piet2010] The difference is not the radioactive isotopes, but how the other "stable" mass is allocated. For example, in AIROX, Group 1 and Group 2 behave differently whereas they behave the same in aqueous separation. Therefore, the allocation of stable mass needs to be done somewhat differently.

We have not and will not update the Transmutation Library for each variation of the chemical groupings relative to Figure 1-1. There are two approaches analysts may use in such instances. First, go back to the ~1000-isotope data files (when they exist) and re-collapse them to the chemical groups that are needed. Second, the fission product chemical distribution does not vary much among cases (especially for those of the same reactor/fuel type) and so one can re-allocate stable masses to new chemical groups using allocation rules derived from cases in which ~1000-isotope data files do exist.

1.4 Types of Transmutation Analyses

Transmutation calculations are performed for different reasons. We nonetheless recognize that once available, data are often used for other purposes. Too often, a data set is obtained and used without awareness of how the data were calculated and what approximations were made. So, to caution the reader in using data in the Library, we have developed a categorization of types of transmutation analyses, Table 1-2. The Library includes considerable information on how each case was calculated, see Section 2.

Table 1-2. Types of Transmutation Analyses

Type of Analysis	Implication to Library User	Definition	Typical Level of Effort	Examples
Fire drill	Not optimized, use with a grain of salt, may be only order of magnitude	Quick and dirty analysis to answer some ad hoc question	Hours or Days	
Exploratory	Not optimized	Analysis to determine the feasibility or possible performance of some new concept, helps identify whether more work is warranted and (if so) what might be its focus	Days or weeks	Feasibility of Tc transmutation
Parameter Scan	Results should give a good understanding of the impact of varying the parameters indicated but may not be optimal for other parameters	Analysis to identify and understand trends in design and performance that is typically performed for a planned study. Typically performed as a result of questions that are raised that require more detailed understanding.	Weeks or months	UOX cooling time Compare Pu, NpPu, NpPuAm, all TRU
Case Study	Results specific for that case, may not be representative of a broader strategy	Analysis of a very specified and specific case, little or no iteration	Weeks or months	2007 calculations of 1-tier and 2-tier scenarios
Design Study	Reasonably optimized per the objectives of that study, which may or may not be applicable to the Library user	Iterative analysis to produce a recommendation on the best design parameters, often performed for a specific project with various design objectives and criteria specified	Weeks or months	Target composition study for Fuels campaign

2. EXPLANATION OF TRANSMUTATION DATA IN LIBRARY

This section describes data associated with each transmutation case in the Library. We have divided the data into three sets:

- Table 2-1 Basic
- Table 2-2 Feed material such as enriched uranium, recycled Pu, recycled TRU.
- Table 2-3 Irradiation parameters such as burnup and fuel residence time, which are the two most important parameters for VISION. The block also includes the codes and cross section sets used in the calculation (if known).

Table 2-1. Basic Data

Data	Implication
Shorthand name	A way to reference this case
Reactor	Indicates the type of reactor, e.g., PWR or FR
Fuel	Indicates the type of fuel, e.g. UOX, MOX, FR-metal, or FR-oxide
Purpose of the calculation	See "Types of Analyses" (Table X)
Who did the reactor physics calculation?	Accountability and source for asking questions
Who input the data into this library?	Accountability and source for asking questions
Who reviewed the data?	Accountability and source for asking questions
Documentation	A citation that best describes the calculations for this case
Filename of source data	Text

Table 2-2. Feed Material Data

Data	Examples
Type of feed material	Enriched U, recycled Pu, recycled TRU
Reactor that produced feed material	PWR, SFR
Feed fuel type	UOX
Burnup of the feed material (MWth-day/kg-iHM)	51
Cooling time (CY) from discharge to separation	5 years
Separation technology	PUREX, UREX+1, echem (often this is inferred from what materials are found in the input fuel)
Cooling time (CY) of feed material after separation	2 years
Source of feed material data (give shorthand name or citation)	UOX to MOX-Pu (another recipe in library) Stillman2004a (a citation)

Table 2-3. Irradiation Parameters

Data	Implications and examples
Recycle pass (0=once through, 1=first recycle pass)	
Core condition (initial load, equilibrium, or retirement discharge)	
Discharge burnup (MWth-EFPD/kg-iHM) - used in VISION	Used in VISION
TRU conversion ratio (reported by reactor physics calculation)	0.0 to about 1.7
TRU conversion ratio (approximation calculated in the Library based on time-average cross sections and initial masses)	See text below.
TRU "Class" conversion ratio (approximation to simulate REBUS)	See text below.
Fissile breeding ratio(approximation calculated in the Library based on time-average cross sections and initial masses)	See text below.
TRU destruction/production rate (kg/MWth-EFPD)	
Cycle length (CY)	Used in VISION
Cycle length (EFPY)	Not used in VISION
Capacity factor (EFPY/CY)	Used in VISION but VISION user may choose a different parameter
Number of batches	Used in VISION
Fuel residence time (CY)	cycle length x # batches
Fuel residence time (EFPY)	cycle length x # batches
Specific power level (Wth/g-iHM)	Useful to compare cases
Codes used	MC2-2, REBUS-3
Cross section data base used	ENDF/B-V
Scale	Infinite lattice, full core, etc.
Key physics assumptions	
1-group cross section set available?	If so, they are provided below the input and output recipes

Some important definitions are as follows:

- Conversion Ratio: Classically, this is the ratio of (fissile, plutonium, transuranic, etc.) production divided by (fissile, plutonium, transuranic, etc.) destruction if the ratio is less than unity.
- Breeding Ratio: Classically, this is the ratio of (fissile, plutonium, transuranic, etc.) production divided by (fissile, plutonium, transuranic, etc.) destruction if the ratio is greater than unity.

  Note: All call outs in the spreadsheet refer to either a conversion ratio or a breeding ratio as a convenience. In practice, if a row is labeled as a conversion ratio but the cell calculates a value greater than one then the value is a breeding ratio by classical definition. The reverse is true for rows labeled as breeding ratio. Therefore, the spreadsheet uses the following adjusted recipes.
- Transuranic Conversion Ratio (TRU CR): The ratio of transuranic production via (n,γ) reactions in U-236 and U-238, divided by the total fission rate by all transuranics, whether the ratio is above or below 1.0.

  Often, this has not been calculated by the original reactor physics analyst, and so we use this equation to approximate it.

$$\text{TRU Conversion Ratio} = \frac{\sigma_{n,\gamma}^{U^{236}} w^{U^{236}} + \sigma_{n,\gamma}^{U^{238}} w^{U^{238}}}{\sum_{Np^{237} \rightarrow Cf^{252}} \sigma_{fission}^{i} w^{i}}$$

- TRU "Class" conversion ratio: The sum of all (n,γ) reactions for U-236 through Cf-252, divided by the sum of all (n,γ) + (n,fission) reactions for Np-237 through Cf-252. This methodology compares the total source of Class 1 divided by the total sink of Class 1.

  Note: The term "Class" is jargon used in the REBUS-2 manual (R. Hosteny, ANL-7721, 1978). Class 1 is a user specified list of isotopes used as the "fissile" feed in its internalized blending calculation. Class 2 is a user specified list of isotopes used as the "fertile" feed in its internalized blending calculation.

  Often, this has not been calculated by the original reactor physics analyst, and so we use this equation to approximate it.

$$\text{TRU "Class" Conversion Ratio} = \frac{\sum_{U^{236} \to Cf^{252}} \sigma_{n,\gamma}^{i} w^{i}}{\sum_{Np^{237} \to Cf^{252}} \sigma_{n,\gamma}^{i} w^{i} + \sum_{Np^{237} \to Cf^{252}} \sigma_{fission}^{i} w^{i}}$$

- Fissile breeding ratio: The ratio of (n,γ)reactions for all fertile isotopes (even neutron number) that directly result in a fissile (odd neutron number) upon transmutation, divided by the sum of all (n,γ) + (n,fission) reactions of all fissile isotopes.

  Note: This definition is useful for enriched uranium fuels where the TRU breeding ratio is necessarily > 1 because the initial TRU loading is zero by default, but the conversion of fissile isotopes (including U-233 and U-235) is < 1, e.g., LWR once-through cases.

  Often, this has not been calculated by the original reactor physics analyst, and so we use this equation to approximate it.

$$\text{Fissile Breeding Ratio} = \frac{\sigma_{n,\gamma}^{U^{234}} w^{U^{234}} + \sigma_{n,\gamma}^{U^{236}} w^{U^{236}} + \sigma_{n,\gamma}^{U^{238}} w^{U^{238}} + \sigma_{n,\gamma}^{Pu^{238}} w^{Pu^{238}} + \sigma_{n,\gamma}^{Pu^{240}} w^{Pu^{240}} + \ldots}{(\sigma_{n,\gamma}^{U^{233}} + \sigma_{fission}^{U^{233}}) w^{U^{233}} + (\sigma_{n,\gamma}^{U^{235}} + \sigma_{fission}^{U^{235}}) w^{U^{235}} + (\sigma_{n,\gamma}^{Pu^{239}} + \sigma_{fission}^{Pu^{239}}) w^{Pu^{239}} + (\sigma_{n,\gamma}^{Pu^{241}} + \sigma_{fission}^{Pu^{241}}) w^{Pu^{241}} + \ldots}$$

3. EXPLANATION OF ISOTOPIC INFORMATION

Section 3 explains what isotope-specific information is in the Library and why.

3.1 Which Isotopes are Tracked?

Table 3-1 lists the 81 isotopes and elements tracked in the Library. The next subsection then indicates for each of the 81 items, (a) what isotopes and elements have to be included to determine the inventory at discharge (t=0), (b) which radioactive progeny have to be included when users assess heat, gamma, and dose, and (c) to which of the other 80 items the mass should be assigned when the tracked isotope decays.

Table 3-1. Tracked Isotopes and Chemical Elements

Isotope	Grouping	Type	Isotope	Grouping	Type
He4 (stable)		Decay products	H3	Other gases	Activation product
Pb206 (stable)	Transition metals		C14		
Pb207 (stable)			C-other		
Pb208 (stable)			Kr81	Inert gases (Group 18)	Fission products
Pb210			Kr85		
Bi209 (stable)			Inert gas other (Kr, Xe)		
Ra226	Radium (Group 2)		Rb	Group 1 & 2	
Ra228			Sr90 w/Y90 decay		
Ac227	Actinides		Sr-other		
Th228			Zr93 w/Nb93m decay	Zirconium	
Th229			Zr95 w/Nb95m decay		
Th230			Zr-other		
Th232			Tc99	Technetium	
Pa231			Tc-other		
U232	Uranium (actinide)	Uranium	Ru106 w/Rh106 decay	Glass constraining TM	
U233			Pd107		
U234			Mo-Ru-Rh-Pd-other		
U235			Se79	Other transition metals	
U236			Cd113m		
U238			Sn126 w/Sb126m/Sb126		
Np237	Neptunium	Trans-uranic elements (TRU)	Sb125 w/Te125m decay		
Pu238	Plutonium (actinide)		TM-other (Co-Se,Nb,Ag-Te)		
Pu239			I129	Halogens (Group 18)	
Pu240			Halogen-other (Br, I)		
Pu241			Cs134	Group 1 & 2	
Pu242			Cs135		
Pu244			Cs137 w/Ba137m decay		
Am241	Americium (actinide)		Cs-other		
Am242m			Ba		
Am243			Ce144 w/Pr144m/Pr144	Lanthanides (plus Y)	
Cm242	Curium (actinide)		Pm147		
Cm243			Sm146		
Cm244			Sm147		
Cm245			Sm151		
Cm246			Eu154		
Cm247			Eu155		

Cm248				Ho166m		
Cm250				LA-other plus Yttrium		
Bk249	Berkelium			Use column "grouping" when assessing chemical behavior of isotopes (element or group in the Periodic Table). Use "type" when referring to the origin of the isotope.		
Cf249	Californium (actinide)					
Cf250						
Cf251						
Cf252						

3.2 Rules for Collapsing Data to 81 Items

The inventory of short-lived isotopes is not tracked in the definition of long-lived parent isotope inventories at t=0, but, where relevant, decay parameters as heat, gamma, and dose from such isotopes should be included by users in the decay of longer-lived parents. With the rules below, there is no need for an "other" category for either actinides or fission products.

For each tracked isotope, we define which short-lived isotopes' mass (at t=0) is to be added to the mass of the tracked isotope at t=0, which short-lived radioactive progeny must be accounted for when the tracked isotope decays, and to which of the other 80 items the mass of the tracked isotope is assigned when it decays. For example, Sr90 illustrates progeny and decay rules. The mass of Y90 at t=0 is not included with the t=0 mass of Sr90, but we call this item Sr90/Y90 because one must remember to account for the decay energy of Y90 when Sr90 decays. And, the mass of Sr90 that decays is then assigned within subsequent VISION to Zr-other so that mass is conserved.

3.2.1 Actinide and Decay Chain Isotopes

We define this class of isotopes to include He, decay products, uranium, and TRU elements.

All isotopes in the decay chains with halflife greater than 0.5 years are tracked in VISION, with five exceptions: Np235, Np236, Pu236, Cf248, and Es254 for reasons explained in section 3.3. For these five exceptions and for all isotopes with halflife less than 0.5 years, the mass at discharge (t=0) is included with long-lived progeny that are tracked in VISION.

Table 3-2 lists the actinide chain isotopes, which isotopes' mass must be added to tracked isotopes at t=0 (discharge), which short-lived progeny isotopes' decay must be accounted for, and where the mass of the tracked isotopes is assigned when it decays. The five stable isotopes (He and the ends of the four decay chains) have no progeny and thus mass does not have to be reassigned, so those two columns are blacked out.

Table 3-2 makes more sense if you also look at figures 3-1 through 3-4, which show the four actinide chains. The second column in Table 2 indicates which short-lived isotopes are to be added to the VISION isotopes at discharge (t=0). All actinide chain isotopes are listed in either the first column (tracked) or second column (allocated to tracked isotopes at discharge). When tracked isotopes decay, the values per decay for heat, gamma, and dose must include the isotopes in the third column, e.g., when Pb210 decays the heat and gamma for Po210 and Bi210 must be incorporated by users as those isotopes are not tracked and are quite short-lived. The mass of tracked isotopes goes into the isotopes shown in the fourth column, e.g., Pb210 decays to Pb210 plus one He4.

Table 3-2. Actinide and Decay Chain Rules (color coded among the four decay chains)

Tracked Isotope or set of isotopes	Isotopes/elements to **combine with tracked isotope** to set inventory at discharge (t=0) (branching ratios in parentheses)	**Radioactive progeny** to include with heat, gamma, dose	**Next tracked isotope in chain** to where the mass is assigned when the tracked isotope decays
He4 (stable)			
Pb206 (stable)	Po210, Bi210		
Pb207 (stable)	Th227, Fr223, Ra223, Rn219, Po215, Pb211, Bi211, Po211, Tl207		
Pb208 (stable)	Ra224, Rn220, Po216, Pb212, Bi212, Po212, Tl208		
Pb210	Pa230 (9.5%), U230, Th226, Ra222, Rn218, Po214; Rn222, Po218, Pb214, Bi214, Po214	Po210, Bi210	Pb206 + 1x He4
Bi209 (stable)	Ra225, Ac225, Fr221, At217, Bi212, Po212, Tl209, Pb209		
Ra226		Rn222, Po218, Pb214, Bi214, Po214	Pb210 + 4x He4
Ra228		Ac228	Th228
Ac227		Fr223, Ra223, Rn219, Po215, Pb211, Bi211, Po211, Tl207	Pb207 + 5x He4
Th228	Ac228	Ra224, Rn220, Po216, Pb212, Bi212, Po212, Tl208	Pb208 + 5x He4
Th229	Pa229	Ra225, Ac225, Fr221, At217, Bi212, Po212, Tl209, Pb209	Bi209 + 5x He4
Th230	Pa230 (90.5%)		Ra226 + 1x He4
Th232			Ra228 + 1x He4
Pa231	U231, Th231		Ac227 + 1x He4
U232	Np236m (48%), Pu236 Np236 (12.7%), Pa232		Th228 + 1x He4
U233	Pa233, Th233		Th229 + 1x He4
U234	Th234, Pu234, Pa234m		Th230 + 1x He4
U235	Np235	Th231	Pa231 + 1x He4
U236	Np236 (87.3%) Np236m (52%)		Th232 + 1x He4
U238		Th234, Pu234, Pa234m	Th234 + 1x He4
Np237	U237, Pu237, Cm241 (1%)		U233 + 1x He4
Pu238	Np238		U234 + 1x He4
Pu239	U239, Np239		U235 + 1x He4
Pu240	U240, Np240		U236 + 1x He4
Pu241			Am241
Pu242	Am242 (17.3%)		U238 + 1x He4

Table 3-2. Actinide and Decay Chain Rules (color coded among the four decay chains)

Tracked Isotope or set of isotopes	Isotopes/elements to **combine with tracked isotope** to set inventory at discharge (t=0)	**Radioactive progeny** to include with heat, gamma, dose	**Next tracked isotope in chain** to where the mass is assigned when the tracked isotope decays
Pu244		Am244	Cm244
Am241	Cm241 (99%)		Np237 + 1x He4
Am242m		Np238 (0.5%)	Pu242 (17.21%), Cm242 (82.29%), Pu238 + 1x He4 (0.50%)
Am243	Pu243	Np239	Pu239 + 1x He4
Cm242	Am242 (82.7%)		Pu238 + 1x He4
Cm243			Pu239 + 1x He4 (99.8%) Am243 (0.2%)
Cm244	Am244, Cf248		Pu240 + 1x He4
Cm245	Am245, Pu245		Pu241 + 1x He4
Cm246	Pu246, Am246		Cm242 + 1x He4
Cm247		Pu243	Am243 + 1x He4
Cm248			Pu244 + 1x He4
Cm250	Cf-254	Pu246, Am246 (8%) Bk250 (6%)	Cm246 + 1x He4 (8%) Cf250 (6%)
Bk249	Es253, Es253, Cm249		Cf249
Cf249			Am245 + 1x He4
Cf250	Bk250, Es154	Pu246, Am246 (8%)	Cm246 + 1x He4
Cf251	Fm255, Es255, Bk251		Cm247 + 1x He4
Cf252			Cm248 + 1x He4

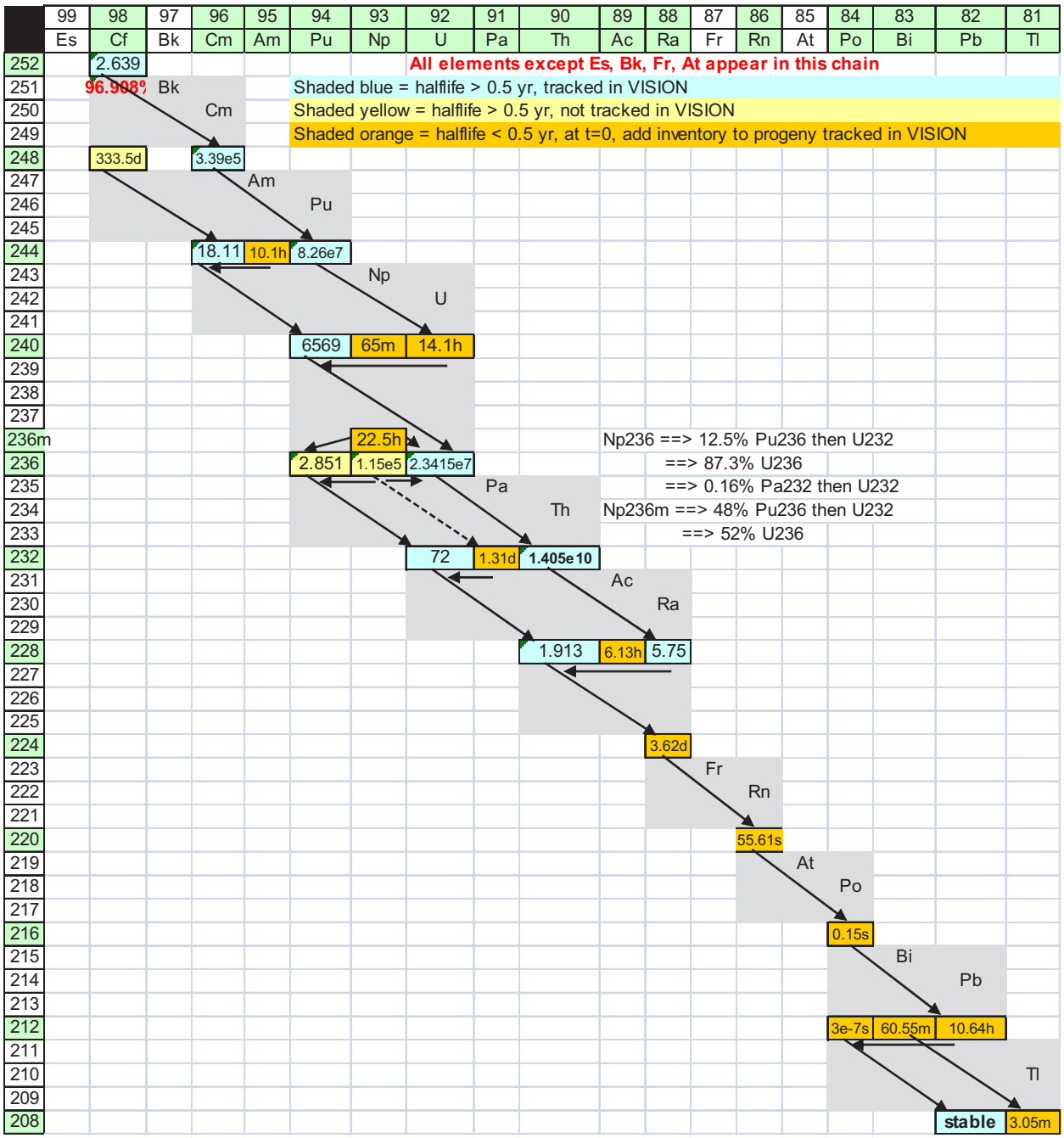

Figure 3-1. Decay chain for 4N isotopes

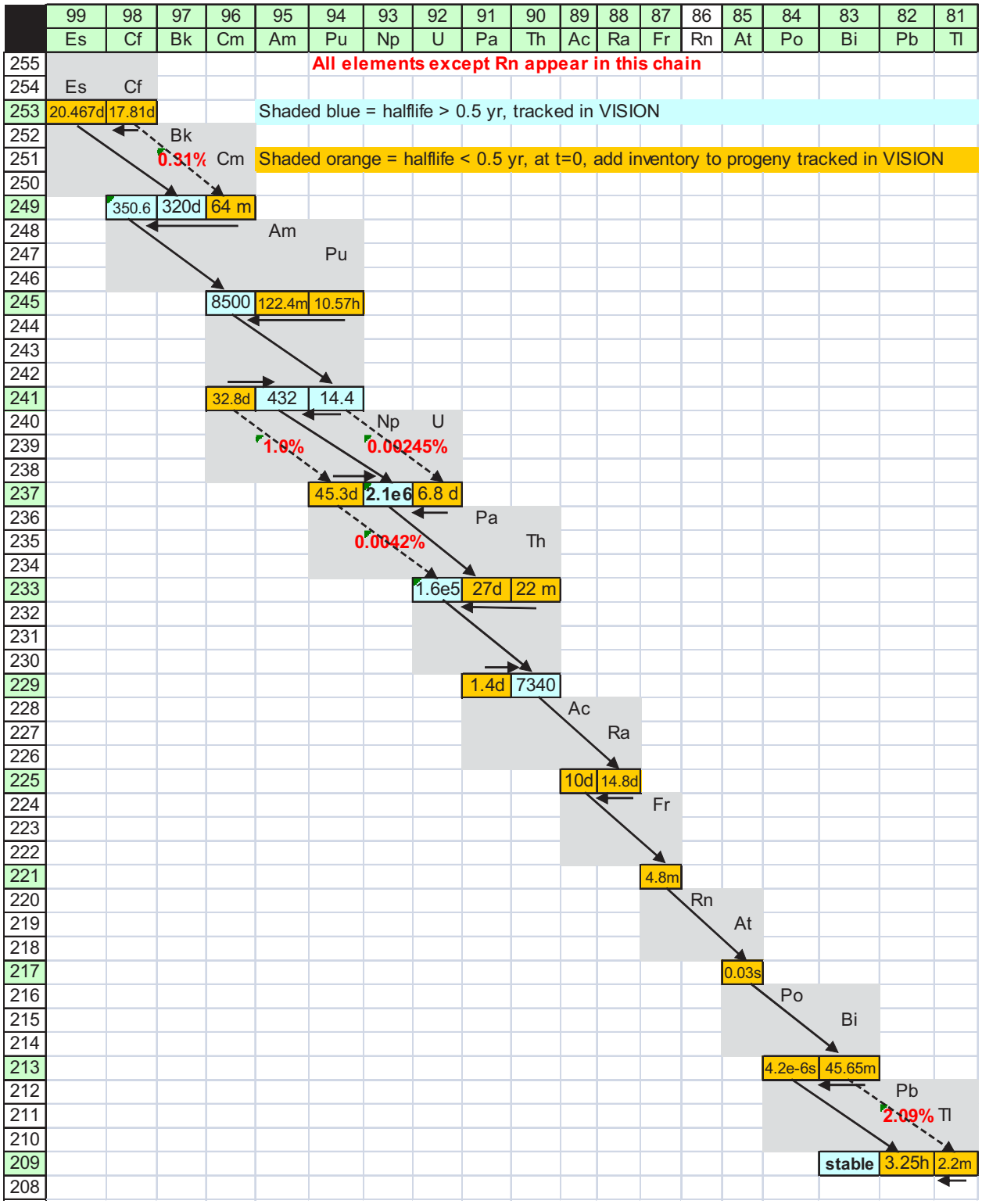

Figure 3-2. Decay chain for 4N+1 isotopes

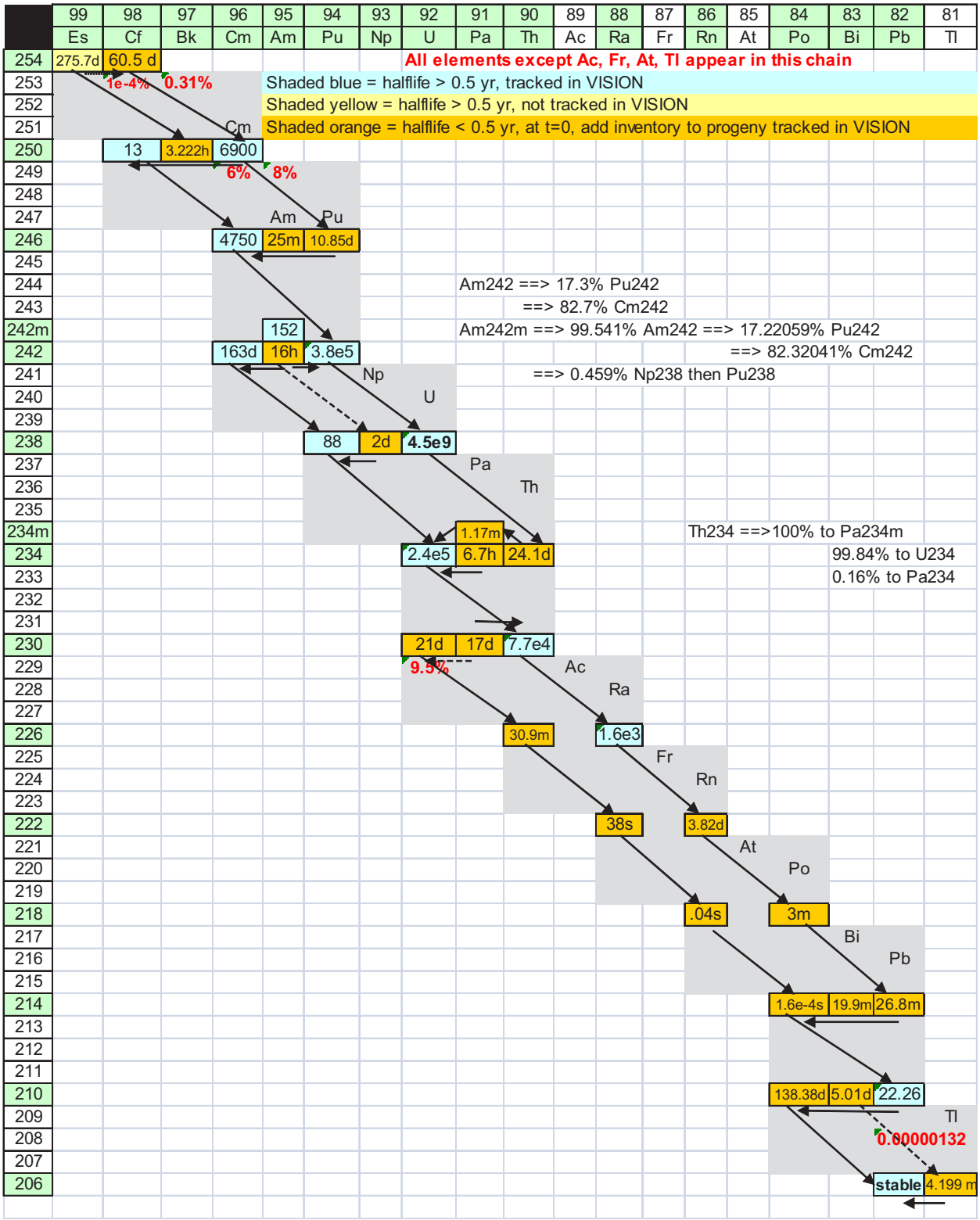

Figure 3-3. Decay chain for 4N+2 isotopes

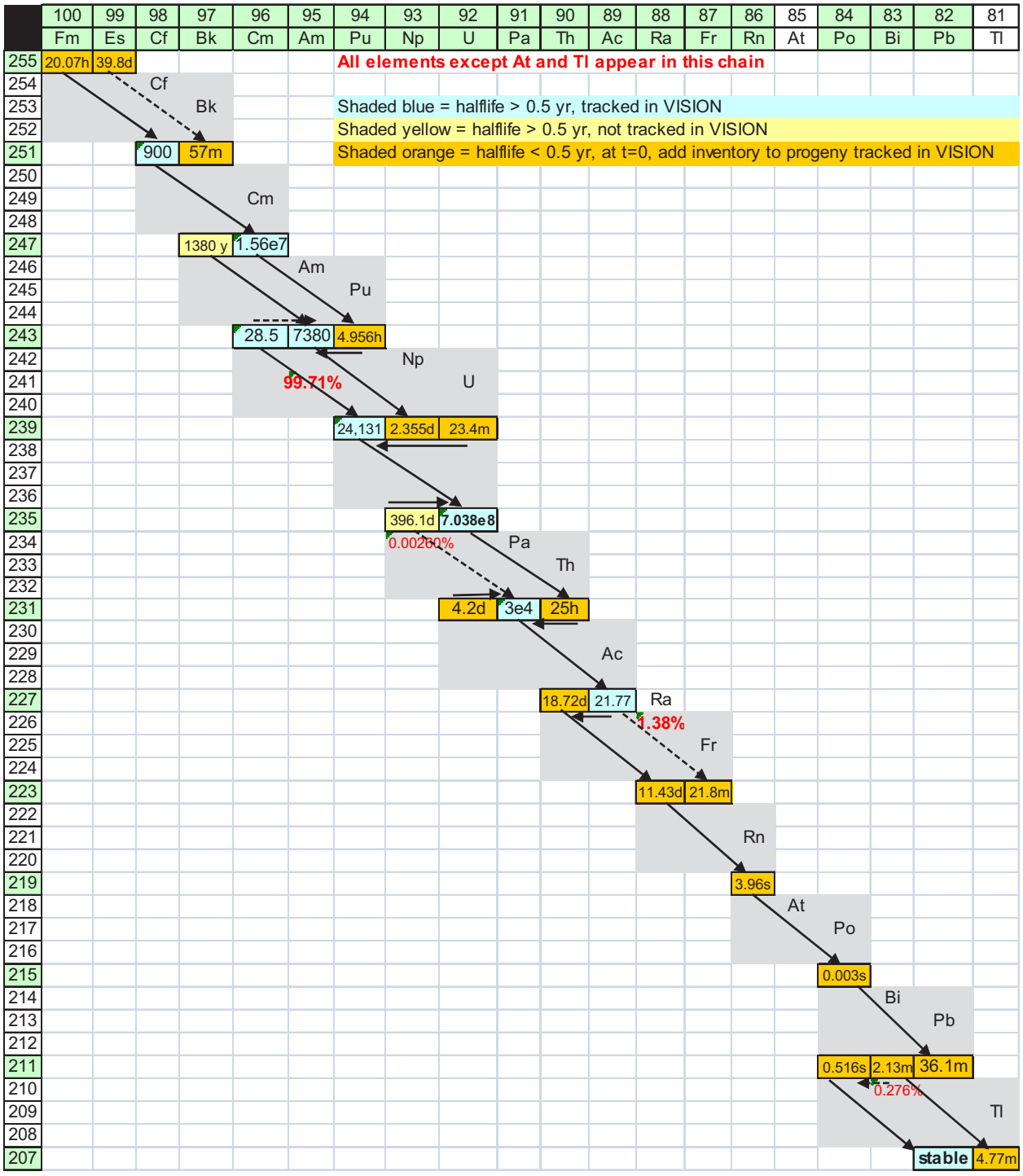

Figure 3-4. Decay chain for 4N+3 isotopes

Figure 3-5 shows the full chain of isotopes from thorium and up, this figure shows how the initial uranium in fuel builds to the various TRU isotopes via (n,γ) reactions and beta(-), constrained by (n,fission) and by alpha, beta(+), international transition, and neutron decay.[a]

Figure 3-6 shows the chain of isotopes with the short-lived isotopes removed; the chain is far simpler.

During transmutation calculations, the reactor physics calculations of course use the entire chain (figure 3-5) in all its complexity.

Calculations in models such as VISION use the simplified chain of figure 3-6 when assessing decay. Since VISION does not do any reactor physics and uses input/output recipes, the simplifications of figure 3-6 in (n,fission) and (n,γ) are irrelevant. VISION does not do any (n,fission) and (n,γ) calculations. Rather, in processing the output data with all isotopes, the mass in the short-lived isotopes of figure 3-5 are reallocated to long-term progeny so that only mass in the isotopes in figure 3-6 remain.

Why do figure 3-5 and 3.6 stop with Cf252? It is inadequate to answer that there is insufficient time (and neutrons) to push mass to Cf252 and beyond. In advanced fuel cycles we often analyze equilibrium cases from repeated recycling; so neutrons and time are not a hard limit *per se*. Figure 3-7 continues the actinide chain above Cf252 and shows two things. (Note that the color scheme in figure 3-7 differs from 3-5 and 3-6 because the purpose of the figure is different.) First, the halflives get shorter so that even if higher TRU isotopes are produced, they do not persist long enough to matter to fuel cycle assessments. The last isotope with halflife greater than 10 years (shaded red) is Cf251; the last isotope with halflife greater than 1 year (shaded orange) is Cf252. The last isotope with halflife greater than our threshold of 0.5 year (shaded yellow) is Es254. Later, in section 3.3.2, we note that in reactor physics calculations that do include Es254, the yield is extremely low even after 5 cycles of MOX-NpPuAm (2e-15). It apparently has not been included in FR equilibrium calculations but hand calculations with 1-group cross sections suggest that the fraction of Es254 in equilibrium with Cf252 is extremely low. Finally, note that the halflife of Fm258 is only 370 microseconds.

The other characteristic that limits movement beyond Cf252 is that progressively fewer isotopes have measurable beta(-) decay, which is the mechanism to move right in the diagram. None of the Fm isotopes (242 through 260) in the 8th Edition of the Table of Isotopes are reported as having beta(-) decay. For example, Fm257 (100.5 day) decays mostly (99.79%) by alpha to Cf253, with 0.21% via spontaneous fission, no beta(-) decay. Fm258 (370 microseconds), Fm259 (1.5 s), and Fm260 (4 milliseconds) decay via spontaneous fission, not beta decay, so even at equilibrium.

Thus, there does not appear to be a pathway to chemical elements beyond Fm (to the right of Fm in the diagram) based on simple neutron irradiation. Above mass 256, there are no isotopes reported in the 8th Edition of the Table of Isotopes of Cf or Es, i.e. to the left of Fm. The last (highest) reported Fm isotope is Fm260. So, we can be sure the TRU chain in a neutron environment stops at Fm260.

[a] Data from Edward M. Baum, Harold D. Knox and Thomas R. Miller, Nuclides and Isotopes, 16th Edition, Knolls Atomic Power Laboratory, 2002 and Richard B. Firestone et al, Table of Isotopes, Eighth Edition, John Wiley and Sons, 1999.

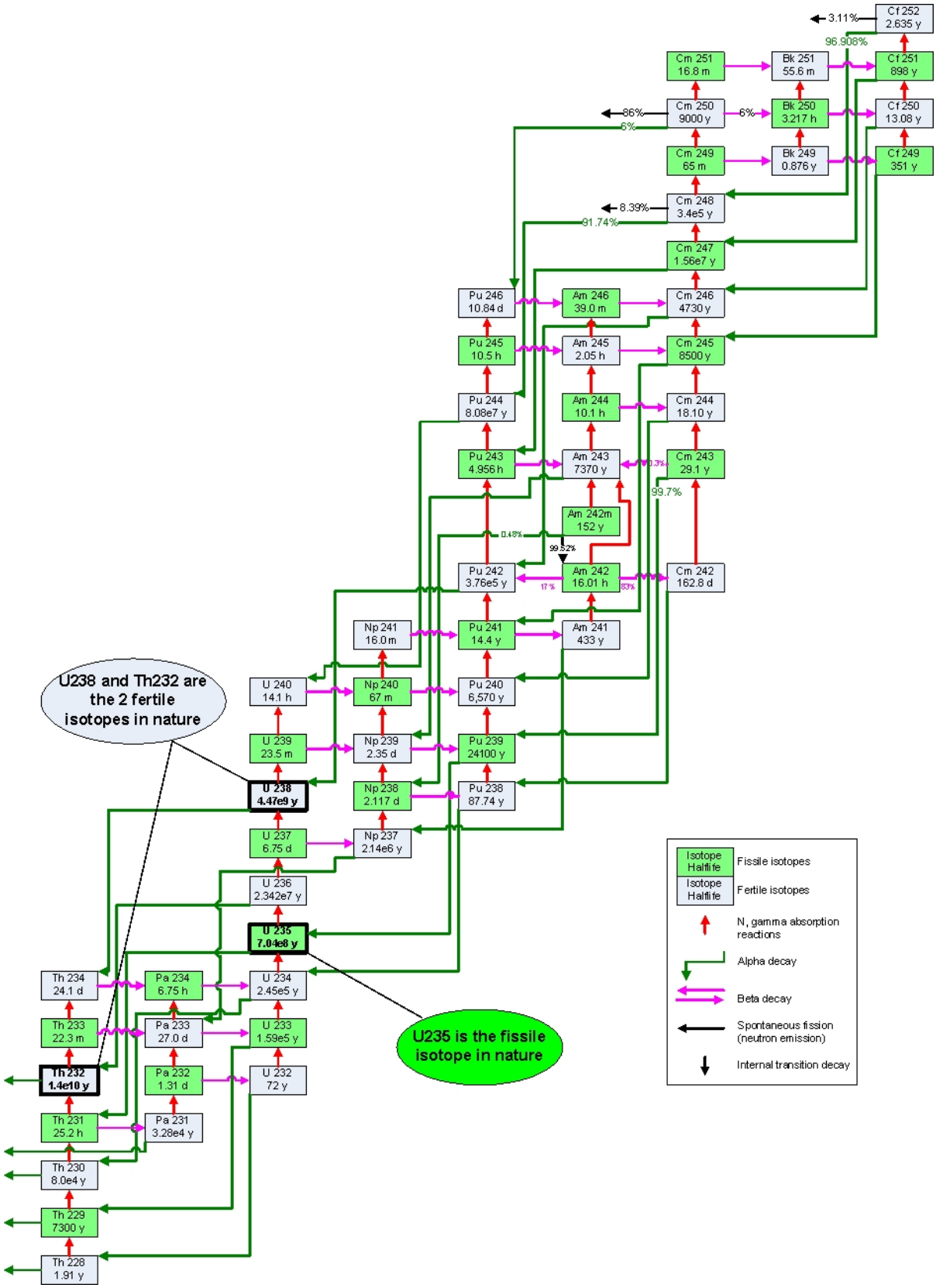

Figure 3-5. Accumulation of TRU elements from initial uranium (or thorium)

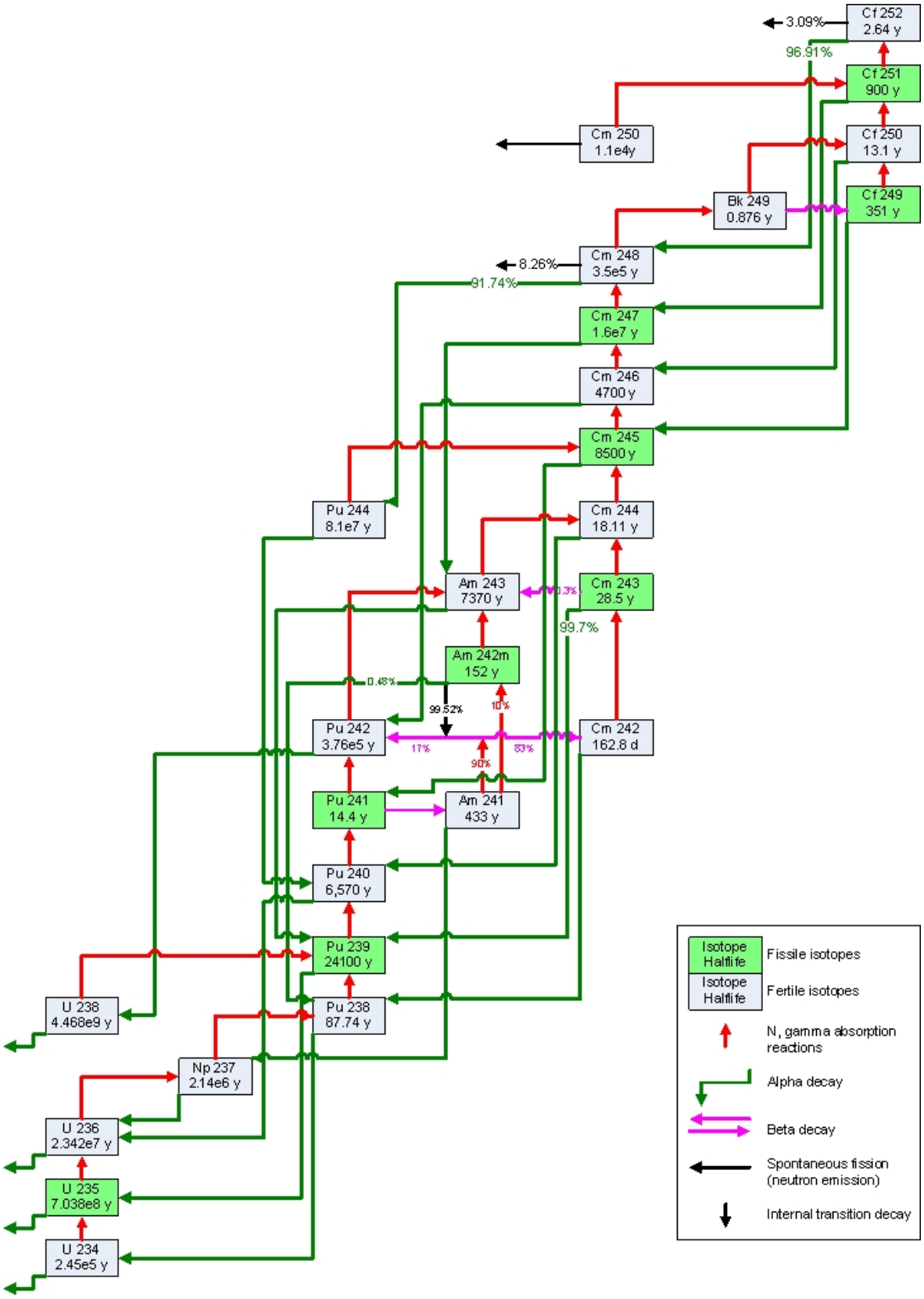

Figure 3-6. Accumulation of TRU elements from uranium (or thorium) with short-lived isotopes removed

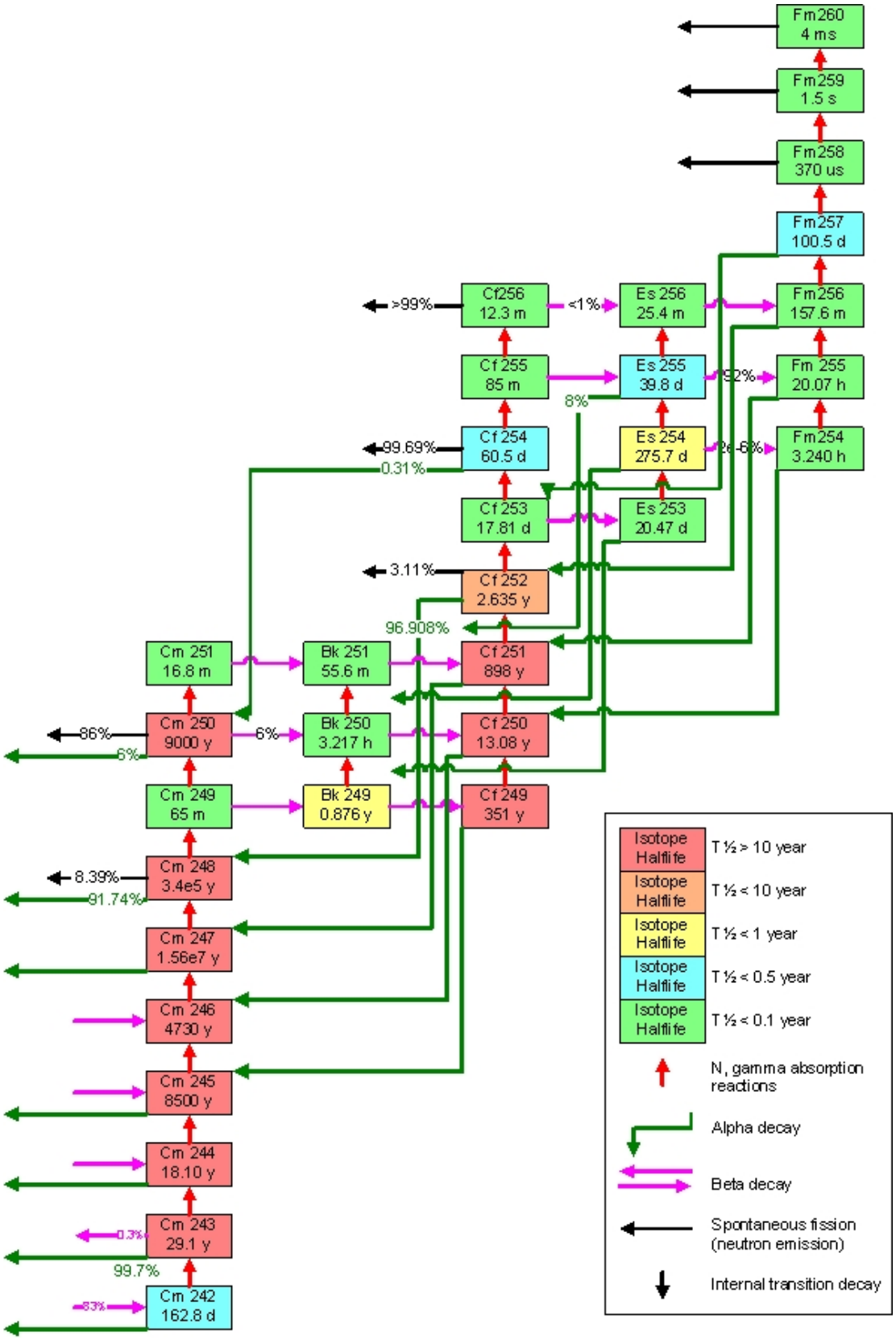

Figure 3-7. Top of the TRU chain in neutron absorbing environments, note different color scheme

3.2.2 Fission Product Isotopes

We define this class of isotopes to include H3 and fission products resulting from fission of actinide isotopes. We never track individual isotopes with halflife less than 0.5 year.

Table 3-3 lists the fission product isotopes, which isotopes' mass must be added to tracked isotopes at t=0 (discharge), which short-lived progeny isotopes' decay must be accounted for, and where the mass of the tracked isotopes is assigned when it decays. The five stable isotopes (helium and the ends of the four decay chains) have no progeny and thus mass does not have to be reassigned, so those two columns are blacked out. Table 3-3 is analogous to Table 3-2, except that Table 3-2 color codes isotopes by actinide decay chain and Table 3-3 color codes isotopes by chemical groups.

Table 3-3. Fission Product Rules (color coded by chemical group, same as Table 3-1)

Tracked Isotope or set of isotopes	**Isotopes/elements to include**	**Radioactive progeny** to include with heat, gamma, dose	**Stable progeny** to where the mass is assigned in VISION when the tracked isotope decays
H3			He (Inert gas other)
C14			N (Halogen-other)
C-other			
Kr81			Br (Halogen-other)
Kr85			Rb
Inert gas-other	Kr except Kr81 and Kr85, Xe		
Rb	All Rb isotopes		
Sr90		Y90	Zr-other
Sr-other	Sr except Sr90		
Zr93		Nb93m	Nb (TM-other)
Zr95		Nb95, Nb95m	Mo (Mo-Ru-Rh-Pd-other)
Zr-other	Zr except Zr93 and Zr95		
Tc99			Ru (Mo-Ru-Rh-Pd-other)
Tc-other			
Ru106		Rh106	Pd (Mo-Ru-Rh-Pd-other)
Pd107			Ag (TM-other)
Mo-Ru-Rh-Pd-other	All isotopes of these elements except Ru106 and Pd107		
Se79			Br (Halogen-other)
Cd113m			In (TM-other)
Sn126		Sb126m, Sb126	Te (TM-other)
Sb125		Te125m	Te (TM-other)
TM-other	Li, Be Co, Ni, Cu, Zn, Ga, Ge, As, Se Nb, Ag, Cd, In, Sn, Sb, Te		
I129			Xe (inert gas other)
Halogen-other	Br, I except I129		
Cs134, 135			Ba
Cs137		Ba137m	Ba
Cs-other	Cs except three isotopes above		
Ba	Ba		
Ce144		Pr144m, Pr144	LA-other
Pm147			LA-other

Sm146,147,151			LA-other
Eu154, 155			LA-other
Ho166m			LA-other
LA-other	Yttrium, LA except as above		

3.3 Completeness Checks

Appendices A and B analyze the illustrative case of UOX with 51 MWth-day/kg-iHM burnup with regard to how well the set of 81 tracked isotopes and chemical elements calculate mass and radiotoxicity. This subsection gives a summary with regard to mass.

3.3.1 Actinide and Decay Chain Isotopes

VISION development started in 2005. In the December 2005 VISION design planning and basis document, we identified six actinide isotopes with halflife greater than 0.5 year that we were nonetheless not put into VISION. The six exceptions have very low yields, see Table 3-4. There are only two additional isotopes with halflife greater than 0.1 year (but less than 0.5 year) that would be candidates for inclusion if we lowered the threshold from 0.5 to 0.1 year, namely Po210 and Pu237.

Table 3-4. December 2005 VISION Planning and Design Basis working document - Peak mass fraction of discarded decay chain isotopes at times within 300 years of start of simulation

Isotope	Halflife (years)	Peak mass fraction in UOX-51	Peak mass fraction in MOX-NpPuAm cycle 5 recipe	Peak mass fraction in MOX/CFR equilibrium recipe
Isotopes with halflives greater than 0.5 years, discarded because of low yield				
Np235	1.1	Not in ANL's reactor physics calculation		
Np236	1.2e5	3e-09	1e-07	5e-08
Pu236	2.9	6e-15	2e-13	2e-07
Bk249	0.9	9e-12		
Cf248	0.9	Not in ANL's reactor physics calculation		
Es254	0.8	1e-16	2e-15	Not in calculation

We re-examined this list to plan the Library, using additional criteria, primarily associated with looking at candidate isotopes from the perspective of their individual chemical elements. Four (Np236, Pu236, Cf248, Np235) are still not worth putting into VISION as all criteria indicate that they are insignificant, see Table 3-5. Bk249 and Es254 are found to be part of the main decay chains (4N+1 and 4N+2) and up to 100% of their respective chemical elements; the latter result arises because there are no other long-lived isotopes of those chemical elements. Additional analysis (not published here) of the role of Bk249 and Es254 play in the actinide transmutation matrix/chain suggests to add Bk249 but not Es254.

Table 3-5. Criteria To Determine Whether Actinides Need to be Added to Tracking List

Chain	Isotope	Halflife (year)	Maximum fraction of mass (between 1 and 1,000,000 years) relative to relevant individual chemical element (for UOX-51)	Maximum fraction (between 1 and 1,000,000 years) of radiotoxicity relative to relevant chemical element (for UOX-51)	Important to transition matrix calculations	Part of main decay chain (as opposed to side branch)
4N	Np236	2.85	≤ 4e-6 of Np-total	≤ 1e-6 of Np-total	No	No
	Pu236	1.15e5	≤ 3e-12 of Pu-total	≤ 4e-8 of Pu-total	No	No
	Cf248	0.91	Not in ANL's data	Not in ANL's data	No	No
4N+1	Bk249	0.88	Up to 100% of Bk 41% of Cf-total	≤ 27% of Cf-total ≤ 3e-9 of TRU-total	Yes	Yes
4N+2	Es254	0.75	Up to 100% of Es ≤ 6e-6 of Cf-total	≤ 3e-4 of Cf-total ≤ 3e-12 of TRU-total	No, it is at the top of the chain, <0.1% of Cf252 gets to Es254; Es254 not in ANL FR calc	Yes
4N+3	Np235	1.08	Not in ANL's data	Not in ANL's data	No	No

3.3.2 Fission Product Isotopes

Appendix A examines the completeness of the selection of isotopes with regard to radiotoxicity, i.e., if only the radiotoxicity of tracked isotopes is included, how much error in each of the element groups could occur relative to including all ~1000 isotopes.

Another question is how well for the fission product rules replicate the actual mass of the various streams between discharge and 100 years, which is the time period in which separation and waste form production can be expected. Table 3-6 provides the answer for the fission products from UOX-51. The behavior for UOX-51 should be representative because the yield among fission products does not vary greatly among fuels.

Such mass errors arise because the rules mean that VISION treats all the items that are not specific isotopes as "stable"; they don't decay. Even so, their mass can increase during VISION simulations if one of the tracked isotopes decays into them. But, the rules mean that short-lived isotopes' mass is kept in the location in which the isotopes are at t=0 (since such mass is treated as stable).

The first example is Sr89. Is mass is within Sr-other, which is considered stable. Since Sr89 actually decays, the rules will overestimate the mass of Sr between 0 and 100 years by as much as 0.44%. Sr89 decays into Y89, so the rules contribute to a slight overestimation of Group 1 and slight underestimation of lanthanide-other.

Y91 is not tracked, its mass is within lanthanide-other, which is treated as stable. So, the rules will overestimate the mass of lanthanides and underestimate Zr-other (Y91 decays to Zr91). Note that not tracking Sr89 and Y91 have opposite effects on lanthanide-other.

The worse cases are other-TM and halogens. The error in halogen mass is as much as 2.3%, caused by short-lived I131 decay into Xe131, since halogen-other (including I131) does not decay, it overestimates the true halogen-other mass.

The error in other-TM is mostly due to Nb95, which goes to Mo95, which is Mo-Ru-Rh-Pd-other.

We could, of course, further reduce these errors in the estimate of mass by tracking more isotopes, but we see no reason. There are larger uncertainties in other things, such as the basic reactor physics transmutation data.

Table 3-6. Maximum Error in Tracking Mass of Fission Products from UOX-51

	Maximum over estimate of mass	Key untracked isotopes	Maximum under estimate of mass	Key untracked isotopes
H3 and C14	0.00%		0.00%	
Inert	0.00%		-0.05%	I131
Group 1 and 2	0.44%	Sr89	0.00%	
Zr	0.00%		-0.72%	Y91
Tc	0.03%	Tc99m	0.00%	
Mo-Ru-Rh-Pd	0.00%		-0.33%	Nb95, Tc99m
Other TM	3.34%	Nb95	0.00%	
Halogens	2.27%	I131	0.00%	
Lanthanides	0.00%	Y91	-0.09%	Sr89
Total	0.00%		0.00%	

4. ARCHIVE OF DATA ON FCR&D PORTAL

All available isotopic data has been archived on the FCR&D data portal, contact Cindie Jensen at the INL for more information on location and access.

Table 4-1 shows how the archived data are organized. Each lowest tier folder contains archival data, in all cases, the files with set-of-81 data that were provided for inclusion into the Library. Where available, the same folder has the original full (~1000 isotopes) data for the same cases. That folder, or the one above (to the left) has the corresponding technical report describing the cases in question. Often, the same technical report appears in more than one place in the folder hierarchy. 2nd and 3rd tier folders often have related reports and data.

Table 4-1. Hierarchy of Storage Folders in the FCR&D Portal

1st tier	2nd tier	3rd tier	4th tier
Transmutation Data	Recipes 1-tier FR ANL	ANL-AFCI-177 Hoffman alternative feed	
		ANL-AFCI-177 Hoffman FR CR (replaced by ANL-AFCI-189)	
		ANL-AFCI-189 Hoffman FR CR	ANL-AFCI-189 Hoffman metal cases
			ANL-AFCI-189 Hoffman oxide cases
	Recipes 1-tier FR INL	INL-EXT-07-13236 Ferrer alternative feed material	Alt feed metal
			Alt feed oxide
			HEU to metal
			NpPu to metal
			RGPu to metal
			WGPu to metal
		INL-EXT-08-14034 Ferrer MA exclusion	1-tier 0.50 and 0.75 metal
			1-tier 0.50 and 0.75 oxide
		INL-EXT-08-14200 Ferrer cooling	LWR cooling time metal
			LWR cooling time oxide
			SFR cooling time metal
			SFR cooling time oxide
	Recipes 2-tier FR ANL	ANL-AFCI-177 Hoffman alternative feed	
	Recipes 2-tier FR INL	INL-EXT-07-13236 Ferrer alternative feed material	Alt feed metal
			Alt feed oxide
		INL-EXT-08-14034 Ferrer MA exclusion	2-tier 0.50 and 0.75 metal
			2-tier 0.50 and 0.75 oxide
		INL-EXT-08-14200 Ferrer cooling	LWR cooling time metal
			LWR cooling time oxide
			SFR cooling time metal
			SFR cooling time oxide
	Recipes 2-tier heterogeneous INL	INL-EXT-08-14831 Bays	
	Recipes ANL FR breeder		
	Recipes ANL impurities		

	Recipes comparisons		
	Recipes HWR ORNL		
	Recipes IMF ANL	ANL Heterogeneous IMF	
		ANL Homogeneous IMF	
	Recipes IMF INL	INL-EXT-07-12472 Asgari	UOX to IMF-Pu
			UOX to IMF-NpPu
			UOX to IMF-NpPuAm
			UOX to IMF-NpPuAmCm
		INL-EXT-07-12472-rev Pope	UOX to IMF-Pu
			UOX to IMF-NpPu
			UOX to IMF-NpPuAm
			UOX to IMF-TRU
		Goldman report	
	Recipes MOX ANL	ANL Hoffman MOX cases	
		ANL Kim MOX CORAIL	
	Recipes MOX INL	INL Asgari2007	
		INL-EXT-09-16091 Youinou	
	Recipes once through ANL	ANL ACR	
		ANL NGNP	
		ANL UOX correlation study	
	Recipes once through INL	INL Asgari2007	
	Recipes other reports ANL		
	Recipes other reports BNL		
	Recipes other reports INL		
	Recipes other reports ORNL		
	Recipes thorium INL		
	Recipes thorium other		
	Transmutation Library	Previous versions	
Transmutation Tools	Isotope Parameter and Decay Tool	Source data and Previous versions	

5. OTHER FEATURES

The Library has a few features in addition to the transmutation data described in sections 2 and 3. Those additional features are described below and include generic 1-group cross sections, various isotope parameters we have assembled from different sources, a correlation of fuel composition as a function of LWR UOX burnup between 33 and 100 MWth-day/kg-iHM, and a correlation of fuel composition as a function of fast reactor TRU CR between 0.00 and 1.00 for both metal and oxide fuel options.

5.1 1-Group Generic Cross Sections

This worksheet page of the Library has 1-group cross section data from ORIGEN-2.2 for the LMFBR fast breeder reactor, a PWR with uranium oxide at a burnup of 50 MWth-day/kg-iHM, a PWR with MOX-Pu fuel, and a PWR with MOX-EU-Pu. The difference between the last two is that the former is critical based on its Pu content, the latter uses enriched uranium to keep the Pu content lower because of void coefficient concerns.

Unlike the main data pages in the Library, this page has cross sections for "all" isotopes from H-1 through Es-254.

Data for the following reactions are provided: (n,fission), (n,γ) capture cross section, (n,2n) neutron multiplication, (n,α) He4 production, (n,p), (n,γ) going to the excited state (instead of the ground state), and (n,2n) going to the excited state instead of the ground state. The sum of these cross sections (not calculated) is the neutron absorption cross section.

The bottom of this page (row 590) has the subset of cross sections that are used on the main data pages for the tracked actinide isotopes. There are three special cases to note:

- (n,2n) cross section for Np-237 includes the (n,2n) to ground state and (n,2n) to excited state
- (n,γ) cross sections for Am241 and Am243 include (n,γ) to ground state and (n,γ) to excited state
- Non-zero guesses are included (and shaded orange) for some of the Pu244 and Cm250 cross sections.

Finally, for the tracked actinide isotopes, the ratio is given of the total neutron absorption cross section divided by simply the (n,fission) plus (n,γ) cross sections. In all cases, the ratio is in the range of 1.00 to 1.01, meaning that the total neutron absorption is given within 1% by simply the (n,fission) plus (n,γ) cross sections.

Note that the above statement is NOT true for all non-actinide isotopes. Most notably, the total neutron absorption by B-10 is dominated by (n,α), not by (n,γ) and the total neutron absorption by Be-9 is dominated by (n,2n) not by (n,γ).

5.2 Isotope Parameters

This worksheet page of the Library has a host of isotope-specific parameters, most notably:

- Atomic number
- Atomic mass
- Decay constant in 1/seconds and 1/years
- Halflife in seconds and years
- Specific activity in Bq/g and Ci/g
- The fraction of decays from ORIGEN-2.2 via beta, positron, internal transition, alpha, spontaneous fission.

- The energy of decay (MeV/decay) from ORIGEN-2.2, converted also to W/kg
- Natural isotopic abundance from ORIGEN-2.2
- Ingestion and inhalation dose conversion factors from ICRP 72 (rem/ci), converted also to Sv/kg
- Recommended concentration guide limits (Ci/cc) for air (inhalation) and water (ingestion) from ORIGEN-2.2, converted also to units of g/cc.
- Photon energy of decay (MeV/day) from ORIGEN-2.2, converted also to W/kg.
- Spontaneous neutron emission from ORIGEN-2.2, converted to N/s per kg in column AW. Columns AX, AY, and AZ contain N/s per kg data from TOPS2000, ANL-AFCI-132, and from AAA. The suggested value to be used is shown in column BA.
- The neutron yield per neutron-induced fission from ORIGEN-2.2. These values are the same for thermal and fast reactor cases; the same as listed in section 5.1.
- Isotope concentration limits regarding near-surface burial. Columns BF and BG provide the values in the official 10CFR61 regulation with and without the regulation's factor of 10 credit (i.e. higher limit) for waste in a durable metal waste form as opposed to any waste, which could be anything. Column BH has a few values extracted from NUREG-0782, which was the technical report that preceded 10CFR61. Columns BI and BJ have the values from S. Fetter et al, with and without the 10x credit for being in the stable metal waste form. Column BK has the value suggested to be used, in units of Ci/m^3-waste. Finally, the Ci/m^3-waste value in column BK is converted to kg/m^3-waste in column BL.
- Finally, columns BN to BQ have dose values at 1-meter distance from an LWR fuel assembly.[Bays2009] Column BN is the neutron emission dose. Column BO is the (alpha,n) dose that exists because of reactions with oxygen in the fuel. Column BP is the gamma dose. The final column is the sum of these three contributions to dose, converted to the units of Sv/hour.

5.3 Correlation of LWR UOX Burnup

There are three types of tools to adjust recipes in simulation tools such as VISION because of the inevitable mismatch between the isotopic mix of what is available in a given time step, and a detailed reactor physics calculation:

- Higher density of cases so that the deviation between available material composition and a case is minimized; assembly of the Library gives us a better assessment of this "case" density.
- Correlations of input/output recipes for UOX as a function of burnup and for FR fuel as a function of FR TRU conversion ratio. When completed, the Library will include those correlations developed by A. M. Yacout, and future correlations as they are developed.
- 1-group cross section perturbation approach for adjusting recipes, not addressed in the Library.

At present, we have two correlations [Yacout2008] that allow adjustment of input/output recipes as a continuous function of parameters: UOX as function of burnup between 33 and 100 MWth-day/kg-iHM and fast reactor (both metal and oxide) as a function of TRU conversion ratio between 0.00 and 1.00. Both use 4^{th} order polynomial fits to a set of transmutation calculations, hence five coefficients for each isotope for input and for output.

The worksheet page, LWR burnup correlations, has the 4^{th} order polynomial correlation coefficients for LWR UOX. The original calculations were done in 2008.[Yacout2008] E. Hoffman updated the calculations of the correlation coefficients to the set of 81 isotopes we now track. (The spreadsheet used

to calculate these correlation coefficients is on the FCR&D data portal in a subfolder under the Transmutation Library.) The coefficients are given in columns B through F. To calculate an input/output recipe, put the desired burnup into cell H6.

This page has other information. Using values for reactor capacity factor (cell H7), fuel residence time (cell H8), and other parameters in cells M3 to N15, a set of calculations were done for fuel comsumption/year, required U235 enrichment, the ratio of natural uranium to enriched uranium (NU/EU), the consumption of uranium ore/year, and the number of enrichment SWUs/year. These are graphed further down the page.

5.4 Correlation of TRU CR

The worksheet page, FR CR correlations, as the 4th order polynomial correlation coefficients for fast reactors in the range of CR=0.00 to CR=1.00. The original calculations were done in 2008.[Yacout2008] E. Hoffman updated the calculations of the correlation coefficients to the set of 81 isotopes we now track. (The spreadsheet used to calculate these correlation coefficients is on the FCR&D data portal in a subfolder under the Transmutation Library.)

There is a complication in these correlations beyond those for LWR UOX. The burnup, cycle length, and fuel residence times each vary with TRU CR and therefore there are correlations for those parameters in addition to the input and output mass fractions.

There are four sets of correlation coefficients:

- Fast reactor metal fuel, startup cycle, i.e., the first recycle of LWR used fuel into the fast reactor
- Fast reactor metal fuel, equilibrium cycle, i.e., the equilibrium composition after many recycles
- Fast reactor oxide fuel, startup cycle, i.e., the first recycle of LWR used fuel into the fast reactor
- Fast reactor oxide fuel, equilibrium cycle, i.e., the equilibrium composition after many recycles

To calculate an input/output recipe, burnup, cycle length, and fuel residence time, put the desired TRU CR into cell AC2.

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Appendix A

Radiotoxicity from UOX-51

We considered radiotoxicity as a major way of selecting which isotopes to study. The basis was the output recipe data for UOX at 51 MWth-day/kg-iHM burnup. The radiotoxicity of each of the ~1000 isotopes was calculated by dividing the inventory of each isotope at each time step in the output file by the maximum permission concentration in the ORIGEN2.2 data base. The units are unimportant (but are cc-water/tonne of used fuel); the issue is the relative contribution of isotopes. A slightly better calculations of radiotoxicity is used in VISION and other assessments, the ingestion dose factor is used instead of the maximum permission concentration. Here, we use the concentration values because they are available for more isotopes.

A-1. Actinide and Decay Chain Isotopes

With five exceptions, we include all isotopes with halflife greater than five years. As described in Section 3, those five exceptions (Np235, Np236, Pu236, Cf248, and Es254) are so low in mass that they cannot contribute significantly to radiotoxicity.

The shortest-lived isotope that *is* tracked is Cm242 (0.45 year), which we included to be cautious even though it is less than 0.5 year. The next shortest-lived isotope is Po210 (0.38 year), it is toward the end of a long decay chain and is in equilibrium (or less) with Pb210 (22.26 years). So, in such cases, we do not "lose" any radiotoxicity by including the radiotoxicity of Po210 with Pb210, i.e., by effectively assuming that the shorter-lived progeny is in equilibrium with the longer-lived parent.

Table A-1 compares the raw discharged mass for UOX at 51 MWth-day/kg-iHM burnup versus the mass of the 81 isotopes once short-lived mass is allocated to the 81. Consider U232. Inclusion of its parent isotopes (48% of Np236m, 12.7% of Np236, Pu236, Pa232) increases the discharged inventory of U232 by 32%. This case is probably the worst approximation in the current method, but is nonetheless acceptable. It is acceptable because U232 never appears as a significant isotope in our studies to date, its mass is very low. (Note that this result for a thorium fuel cycle may change!) Figure 3-1 shows why the approximation is relatively poor. Two of the parent isotopes exceed the 0.5 year threshold, Pu236 (2.851 year) and Np236 (1.1e5 years). At discharge, the masses are U232 (1.04e-3 ppm), Np236 (2.63e-3 ppm), Pa232 (3.24e-6 ppm), Pu236 (1.27e-9 ppm), and Nb236m (zero). Allocation of 12.7% of Np236 to U232 increases the adjusted U232 by 32% whereas in reality, long-lived Np236 would mostly stay as Np236.

The other isotopes with a significant adjustment are Pb210 and the four stable termination points of the decay chains. Recall that the short-lived parents of such isotopes are included when longer-lived parents decay. The discharge inventory of the parents of those five isotopes has decayed before fuel cycle operations begin. The longest-lived parent of those five isotopes that is not tracked are as follows:

Pb208 (Chain 4N) - Ra224 (3.62 day = 0.010 years), mass at discharge = 4.40e-8 ppm

Bi209 (Chain 4N+1) - Ra225 (14.8 day = 0.041 years), mass at discharge = 3.52e-11 ppm

Pb210 (Chain 4N+2) - U230 (21 day = 0.057 years), mass at discharge = 6.12e-12 ppm

Pb206 (Chain 4N+2) - Po210 (138.38 day = 0.379 years), mass at discharge = 2.39e-12 ppm

Pb207 (Chain 4N+3) - Th227 (18.72 day = 0.051 years), mass at discharge = 7.01e-11 ppm

So, except for Po210, the very low mass of the short-lived isotopes have more than ten halflives of decay in the first year after discharge; so reallocation at t=0 is a fine approximation; they quickly become in equilibrium with their longer-lived parents, which matches the approximation used in section 3. The discharge inventory of Po210 is too low to matter. By 10 years, it has grown to 1.82e-11 ppm, necessarily lower than its parent Pb210 (22.26 year halflife, 3.10e-9 ppm at 10 years). There values are insignificant.

Table A-1. Impact of Allocating Short-lived Actinide Isotopes to the Set of 81

	Raw data at discharged	Adjusted data by allocating short-lived isotopes per Table 3-2	Magnitude of adjustment
He4 (stable)	9.47E-07	9.47E-07	0.00%
Pb206 (stable)	5.57E-18	8.10E-18	45.23%
Pb207 (stable)	1.69E-15	1.80E-15	6.66%
Pb208 (stable)	3.69E-12	3.74E-12	1.34%
Pb210	1.88E-16	1.95E-16	3.59%
Bi209 (stable)	6.61E-16	7.44E-16	12.53%
Ra226	9.79E-14	9.79E-14	0.00%
Ra228	2.75E-20	2.75E-20	0.00%
Ac227	3.10E-14	3.10E-14	0.00%
Th228	8.48E-12	8.48E-12	0.00%
Th229	2.73E-12	2.73E-12	0.00%
Th230	2.63E-09	2.63E-09	0.00%
Th232	4.17E-10	4.17E-10	0.00%
Pa231	9.25E-10	9.27E-10	0.31%
U232	1.04E-09	1.37E-09	32.50%
U233	2.21E-09	2.23E-09	0.95%
U234	1.72E-04	1.72E-04	0.00%
U235	7.65E-03	7.65E-03	0.00%
U236	5.71E-03	5.71E-03	0.00%
U238	9.21E-01	9.21E-01	0.00%
Np237	6.09E-04	6.19E-04	1.65%
Pu238	2.91E-04	2.93E-04	0.63%
Pu239	6.07E-03	6.15E-03	1.45%
Pu240	2.91E-03	2.91E-03	0.00%
Pu241	1.76E-03	1.76E-03	0.00%
Pu242	8.64E-04	8.64E-04	0.00%
Pu244	2.86E-08	2.86E-08	0.00%
Am241	6.44E-05	6.44E-05	0.00%
Am242m	8.53E-07	8.53E-07	0.00%
Am243	1.98E-04	1.99E-04	0.10%
Cm242	2.59E-05	2.60E-05	0.53%
Cm243	7.71E-07	7.71E-07	0.00%
Cm244	8.56E-05	8.58E-05	0.21%
Cm245	5.72E-06	5.72E-06	0.00%
Cm246	7.30E-07	7.30E-07	0.00%
Cm247	9.97E-09	9.97E-09	0.00%
Cm248	7.69E-10	7.69E-10	0.00%
Cm250	4.28E-18	4.28E-18	0.00%
Bk249	9.15E-12	9.16E-12	0.12%
Cf249	1.65E-12	1.65E-12	0.00%
Cf250	2.04E-12	2.05E-12	0.52%
Cf251	9.87E-13	9.87E-13	0.00%
Cf252	6.58E-13	6.58E-13	0.00%
Total	0.947263	0.947364	0.01%

A-2. Fission Product Isotopes

Figure A-1 shows the radiotoxicity of the various groups of elements. The two groups with lowest radiotoxicity are H3/C14 and the inert gases, which have the highest mobility in the environment. So, they have to be assessed even though their radiotoxicity is so low. The two plateaus in the H3/C14 curve are H3 (12 year) and C14 (5715 years). The inert gas curve is first dominated by several short-lived Xe isotopes followed by two plateaus from Kr85 and Kr81. After a few very short-lived Tc isotopes, the Tc curve is simply Tc99. The highest radiotoxicity comes from remaining four groups, Group 1A, halogens, transition metals, and lanthanides.

The following subsections go into more detail on those groups with several potentially important isotopes; there is no further discussion of H3/C14 and Tc99.

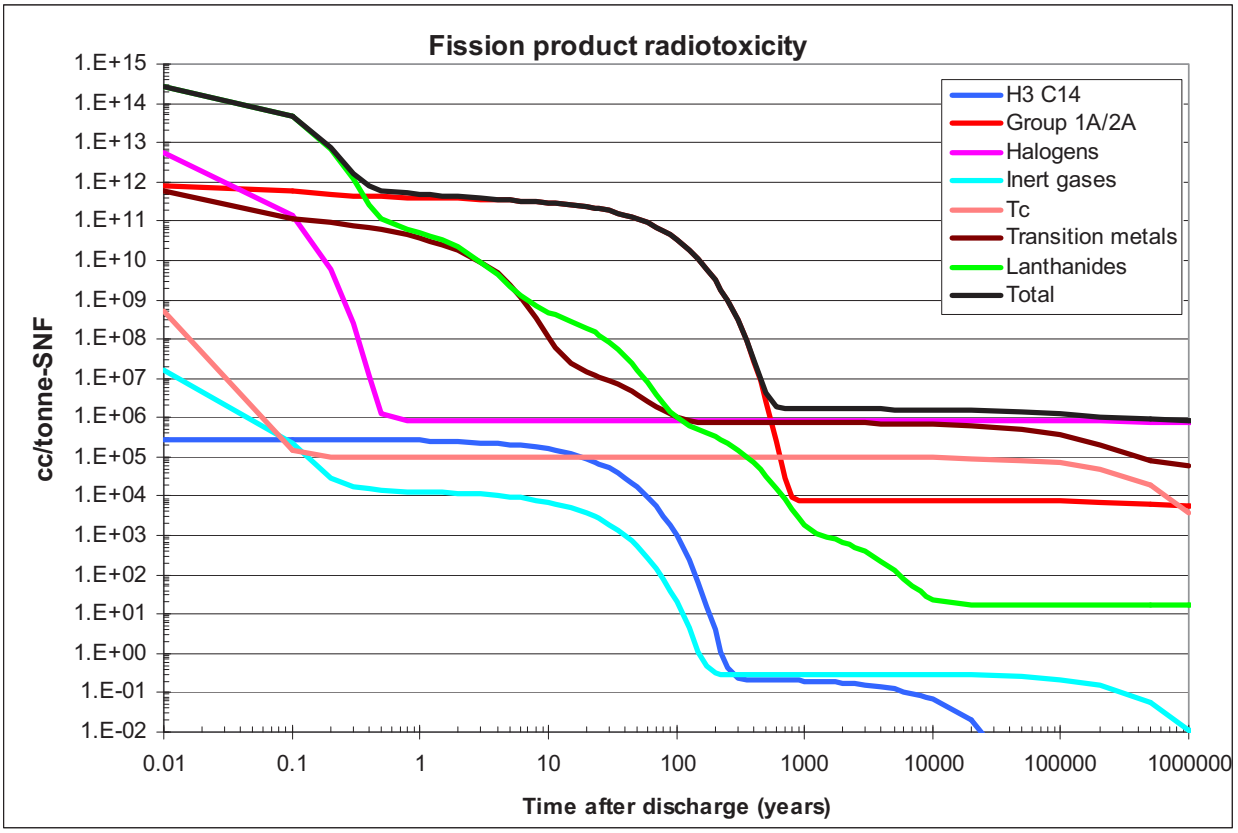

Figure A-1. Radiotoxicity of fission product radiotoxicity from UOX-51.

A-2.1 Group 1A/2A

The important elements of group 1A/2A are Rb, Sr, Cs, and Ba. Figure A-2 shows the radiotoxicity of the most important isotopes. These four isotopes comprise 99.6% of group 1A/2A radiotoxicity at 1 year, and 99.9% ≥ 1.2 years. These results are quite adequate for our purposes. The next most important isotopes, which are not tracked, are Rb86 (18.65 days) and Sr89 (50.52 days). If these were included, the set would comprise 99.9% of Group 1A/2A radiotoxicity ≥ 0.3 years. (Inclusion of Sr89 would slightly reduce the error in the mass assessments of Group 1A/2A and lanthanide-other, see section 3.3.)

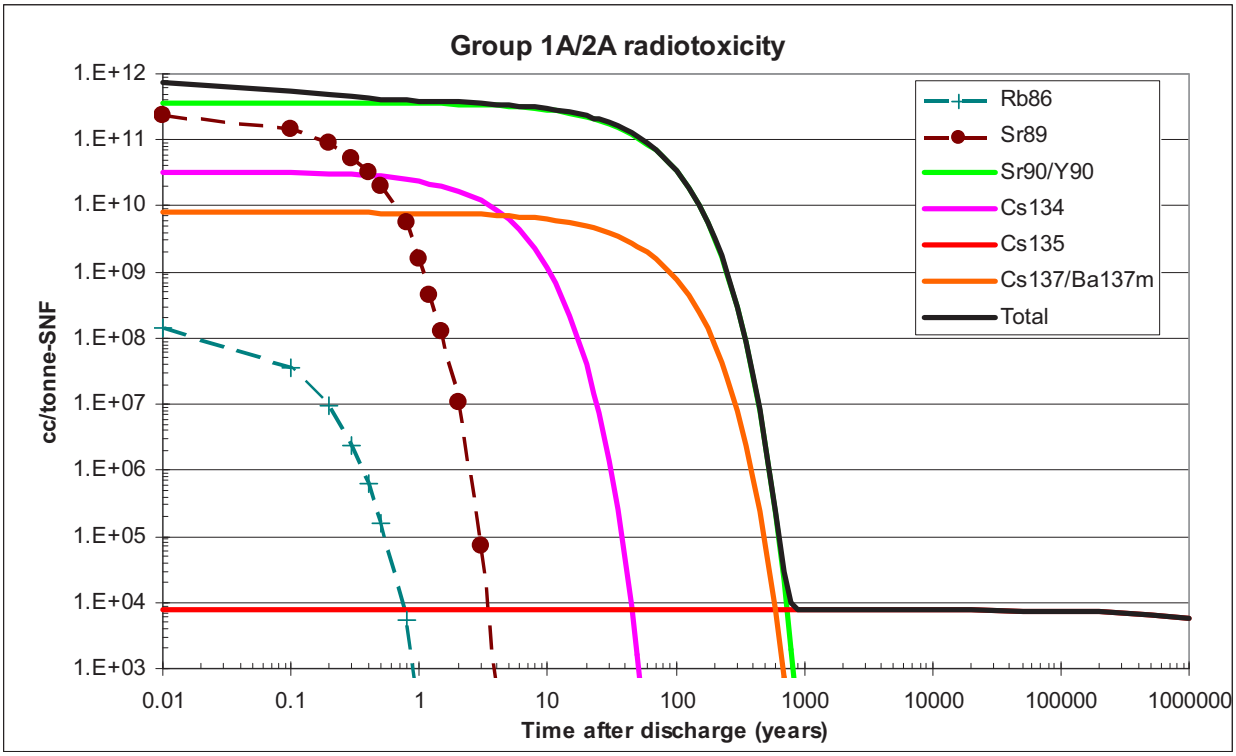

Figure A-2. Radiotoxicity of Group 1A/2A fission products from UOX-51. (Tracked isotopes shown via solid lines, untracked isotopes shown with dashed lines.)

A-2.2 Halogens

I 129 by itself is more than 99.9% of total halogen radiotoxicity for all times greater than 0.8 years. So, no other isotopes need to be tracked. The next most important halogen isotopes are I 131 and I 132; their inclusion would achieve >99.9% at all times greater than 0.1 years. See figure A-3. All the Br isotopes are very short lived.

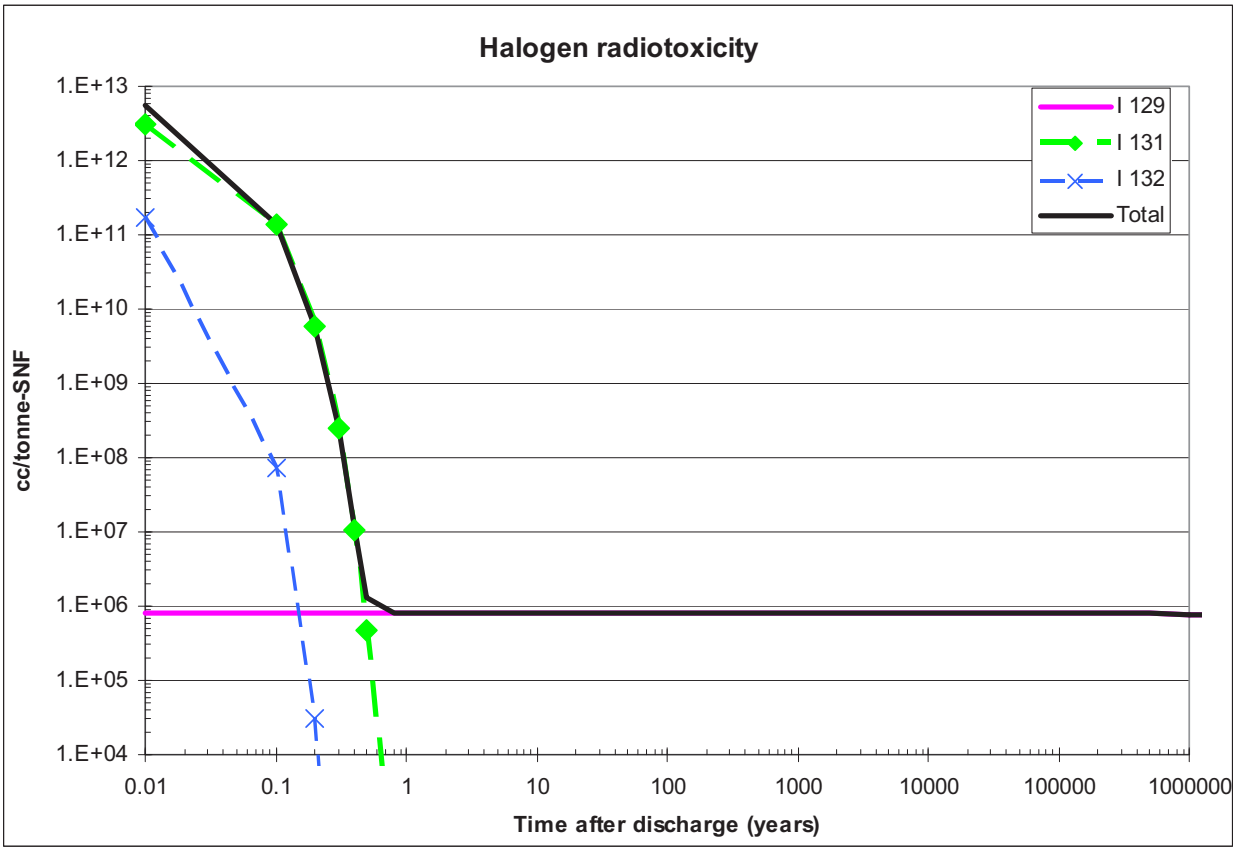

Figure A-3. Radiotoxicity of halogen fission products from UOX-51. (Tracked isotopes shown via solid lines, untracked isotopes shown with dashed lines.)

A-2.3 Inert Gases

Figure A-4 shows the radiotoxicity of inert gas fissions products from UOX-51. The two dominant isotopes are Kr81 and Kr85. They comprise 99.7% of radiotoxicity at 1 year after discharge and 99.9% ≥1.2 years. The next most important isotopes, which are untracked, are Xe isotopes. The longest-lived Xe isotope is Xe127 (36.4 days). With including Xe127, we would obtain 99.7% of total inert gas radiotoxicity ≥ 0.3 years and 99.9% ≥ 0.4 years. With all four Xe isotopes, we would obtain 99.9% ≥ 0.1 years, but this would be overkill.

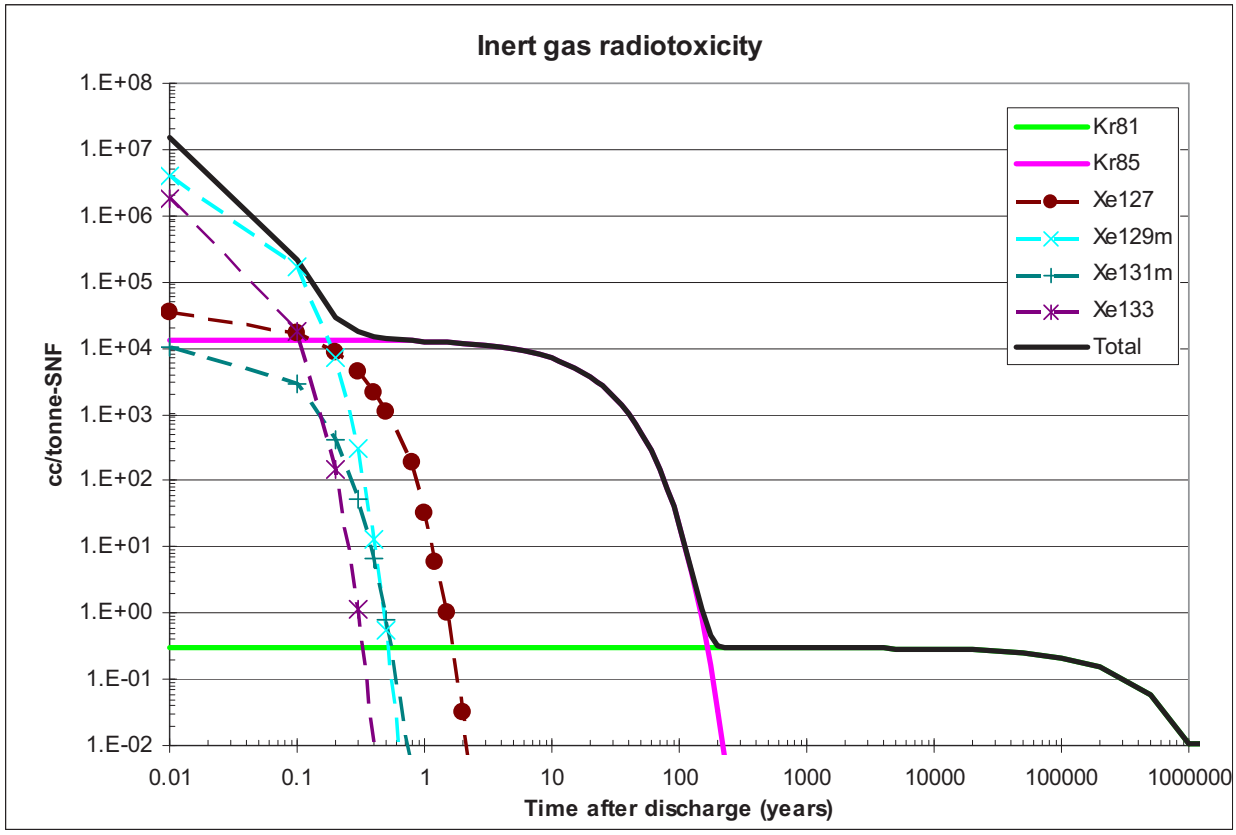

Figure A-4. Radiotoxicity of inert gas fission products from UOX-51. (Tracked isotopes shown via solid lines, untracked isotopes shown with dashed lines.)

A-2.4 Transition Metals

The hodge-podge of elements included in our class of transition metals is perhaps the most difficult to identify isotopes to track. To get to 99.9% for times ≥ 1.0 years would require tracking 14 isotopes shown in figure A-5. This seemed excessive considering that transition metals are not viewed as a stand-alone waste form. Tracking only eight isotopes provides 97.4% of radiotoxicity for times t ≥ 1.0 years and that is deemed adequate. The figure shows that the closest untracked isotope (i.e. closest to the "total" curve) is Sn121m. Indeed, were Sn121m to be included, the 99.9% of the radiotoxicity of the transition metals would be included for all times ≥ 4 years and 98.8% at 1 year. To get to 99.9% for all times between 1 and 1 million years would require tracking five additional isotopes (Ag110m, Sn119m, Sn123, Te127/Te127m).

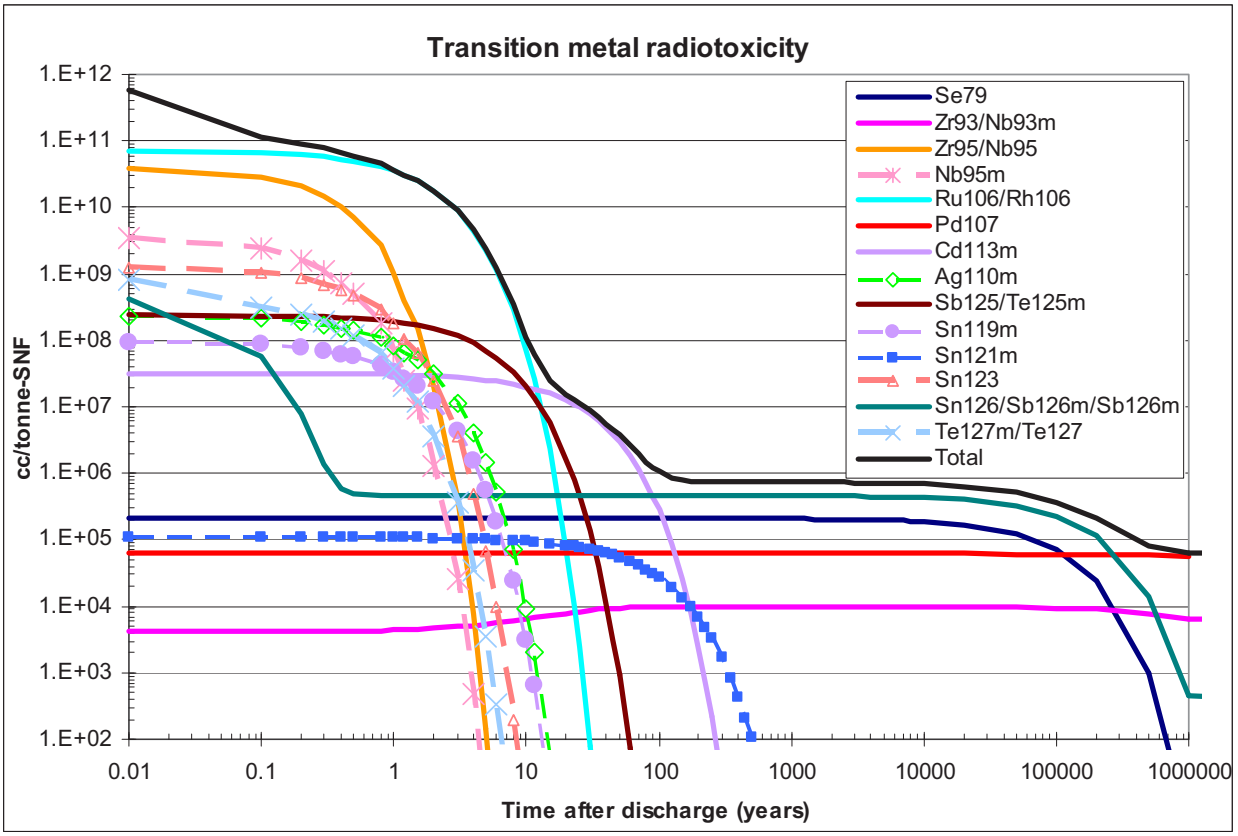

Figure A-5. Radiotoxicity of transition metal fission products from UOX-51. (Tracked isotopes shown via solid lines, untracked isotopes shown with dashed lines.)

A-2.5 Lanthanides

For our purposes, the lanthanides include the actual lanthanide elements in the Periodic Table plus yttrium. Yttrium adds no significant isotopes other than Y90, which is a short-lived progeny of Sr90 and therefore its radiotoxicity is included with Sr90. Yttrium inclusion does add some mass to the lanthanides, the issue of Y91 mass is discussed in section 3.3. Figure A-6 shows the radiotoxicity of lanthanide isotopes, excluding Y90. The eight tracked isotopes comprise 99.9% of lanthanide radiotoxicity at all times between 1 and 1 million years. If one wanted to extend that time period down to 0.01 years, Pr143 would have to be included.

Inclusion of Eu155 was a borderline case. Without it, the tracked isotopes are still 96.8% of total radiotoxicity for times ≥ 1 year. So, perhaps we are overcautious in including Eu155.

Inclusion of Sm147 was also a borderline case; indeed some transmutation calculations do not include it. Without it, the tracked isotopes are still 99.4% of total radiotoxicity. Because it is such a long-lived isotope and we will perform other assessments in addition to radiotoxoicity, e.g., 10CFR61-type assessments for near-surface disposal acceptability, we include Sm147 where the transmutation data exist.

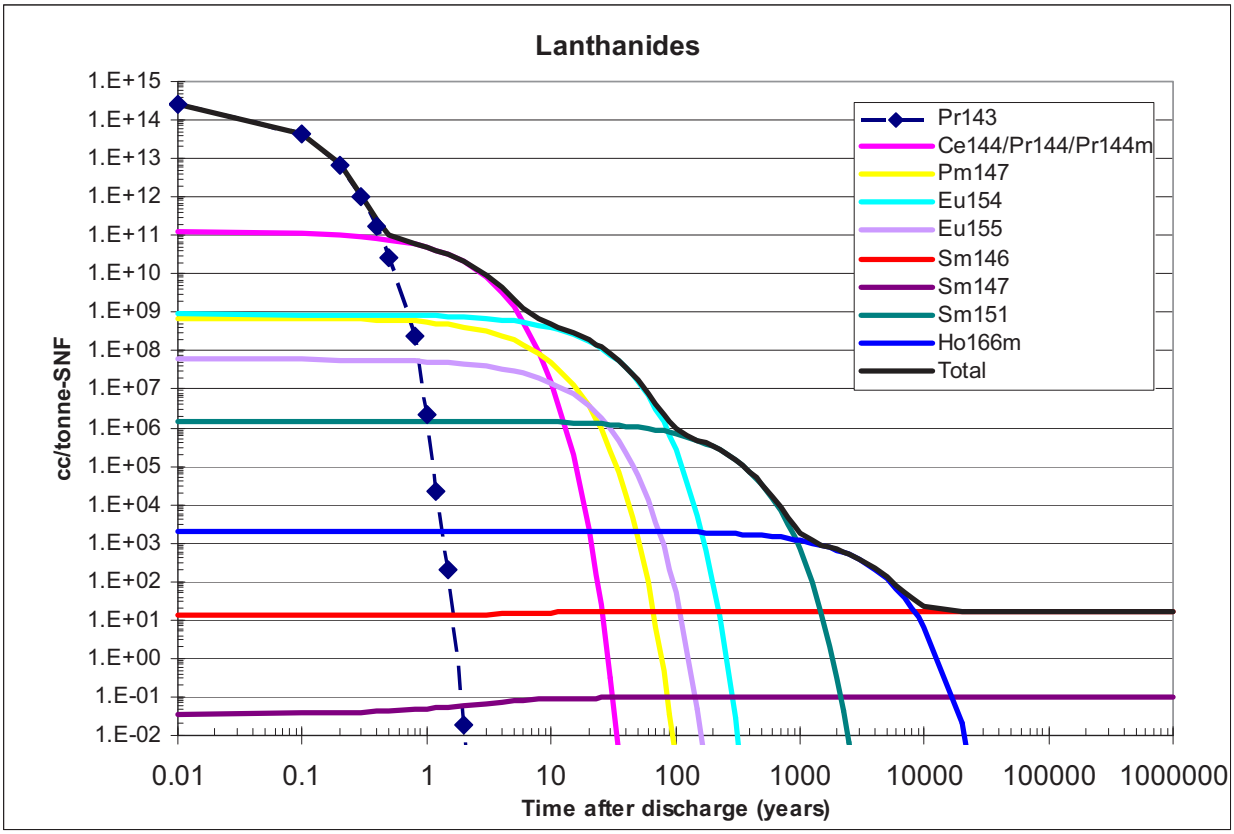

Figure A-6. Radiotoxicity of lanthanide fission products from UOX-51. (Tracked isotopes shown via solid lines, untracked isotopes shown with dashed lines.)

Appendix B

Masses from UOX-51

Like Appendix A, we assessed the behavior of mass on the basis of UOX at 51 MWth-day/kg-iHM burnup.

B-1. Actinide and Decay Chain Isotopes

For actinide and decay chain isotopes, why did we feel we had to include virtually all isotopes with halflife greater than 0.5 year? The answer stems from the complexity of the behavior within the decay chains as illustrated in the following text and graphs. We assess the actinide and decay chains by each chain individually.

B-1.1 Chain 4N

Figure B-1 shows the mass of all tracked isotopes in chain 4N. It is complex. To better see what is happening, consider figures B-2 and B–3, which divide the chain into isotopes above and below mass 236 as U236 is the longest-lived isotope in the chain.

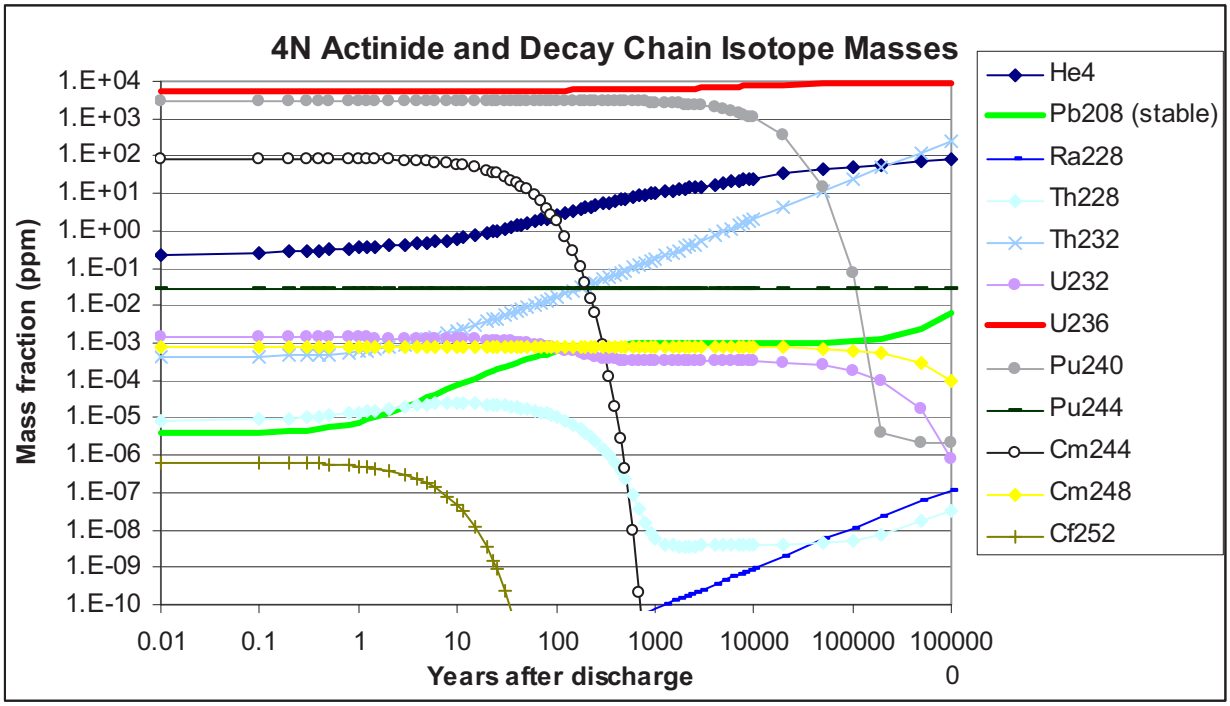

Figure B-1. Mass of 4N actinide and decay chain isotopes

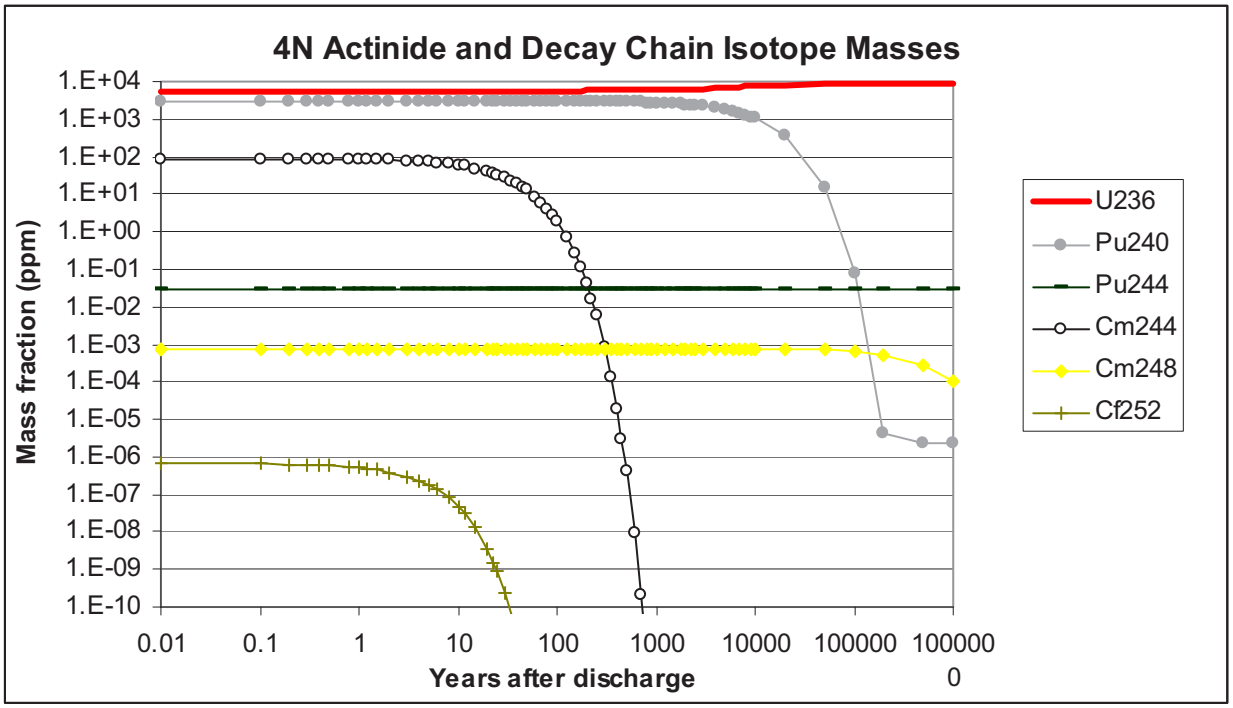

Figure B-2. Mass of 4N actinide and decay chain isotopes, only isotopes with mass ≥ 236

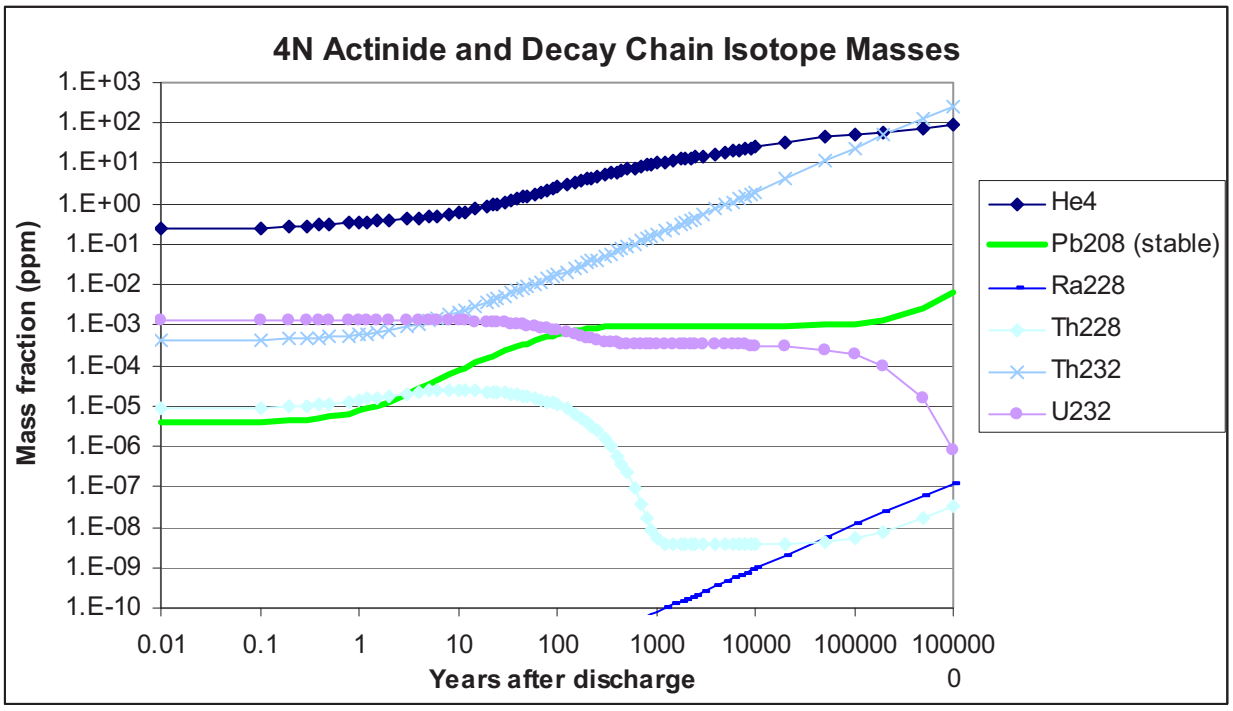

Figure B-3. Mass of 4N actinide and decay chain isotopes, only isotopes with mass less than 236

Figure B-2 shows that the actinide portion of the 4N chain decays back to uranium over time, with the exception of very long-lived Pu244, which fortunately is very low in mass (and radiotoxicity). The inventory in discharged UOX of Pu240 falls from its initial value until it reaches the level at which it is in equilibrium with Pu244 decay at about 200,000 years.

Figure B-3 shows the steady accumulation of decay chain isotopes. The end of the chain (Pb208) has only grown to very low values even at 1,000,000 years. U232 behavior is anomalous (it decreases instead of increases) because it is outside the mainline of the 4N decay chain fed from U236, see figure 3-1. So, U232 decays from its initial reactor-discharge value without replenishment from above. Th228 is where the two branches of the decay chain merge. It initially increases slightly as U232 decays into it, then stabilizes with U232 and declines as U232 does; finally, it again stabilizes and increases slightly as the mainline branch feeds it.

B-1.2 Chain 4N+1

Figure B-4 shows the 4N+1 decay chain isotopes with mass ≥ 237, Np237 is the longest lived member of this chain. Pu241 decays, increasing the inventory of progeny Am241; then both decay into Np237, increasing it. Am241 and Pu241 decline until they are in equilibrium with Cm245 and all three decline together. Bk249 and Cf249 have such small yields that their decay into Cm245 and below does not matter. (Bk249 decay slightly increases the inventory of progeny Cf249, which then decays.)

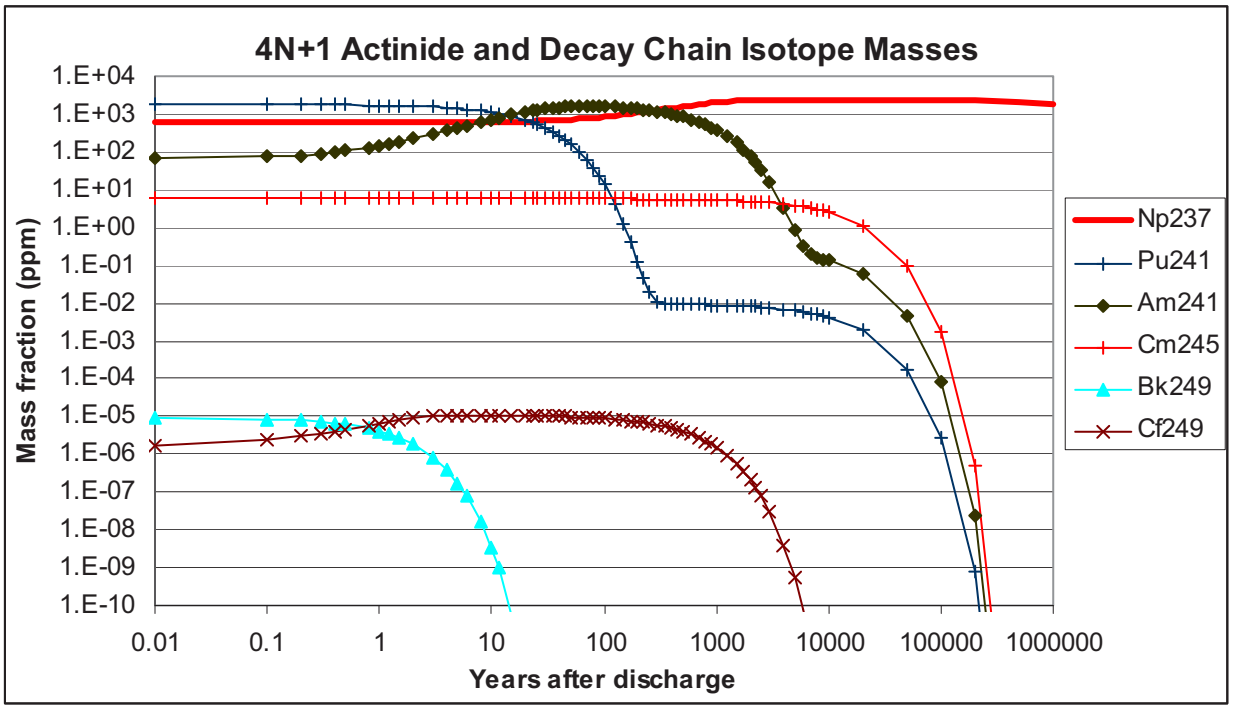

Figure B-4. Mass of 4N+1 actinide and decay chain isotopes, only isotopes with mass ≥ 237

Figure B-5 shows the bottom half of the 4N+1 chain, which shows simple and straightforward behavior. The end point of the chain (Bi209) has reached ~1000 ppm of total UOX mass by 1 million years as this is a decay chain not found in nature.

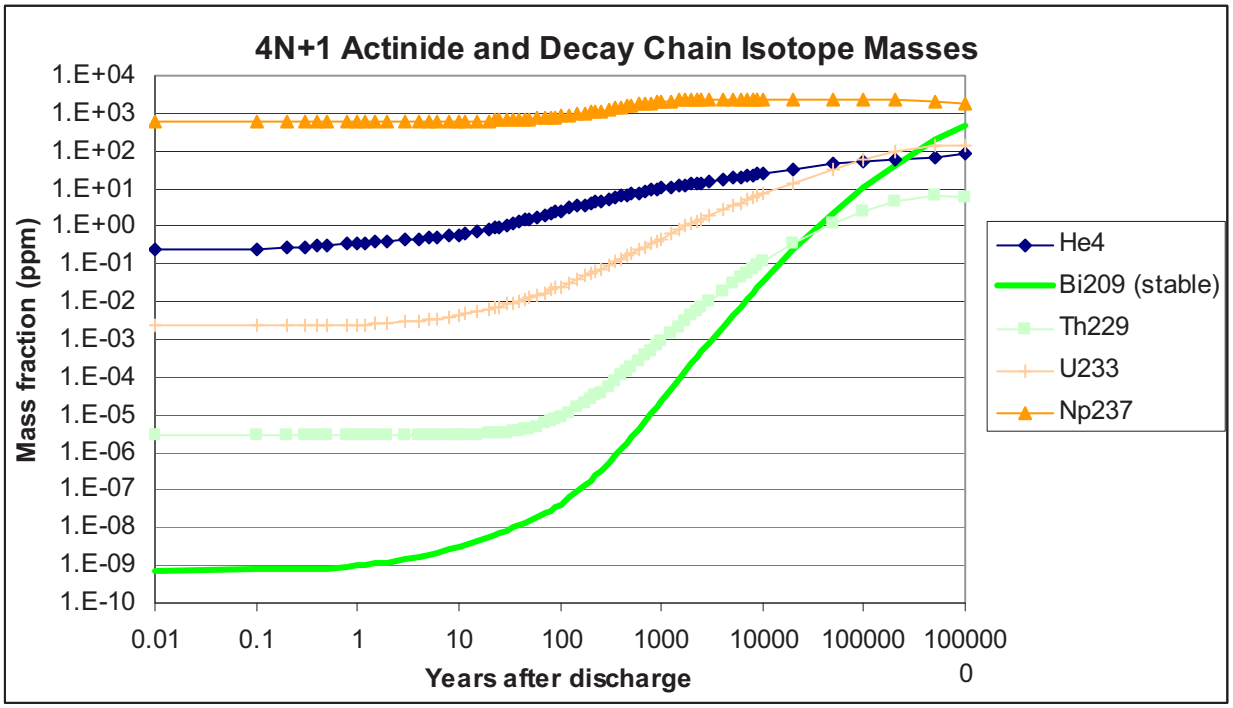

Figure B-5. Mass of 4N+1 actinide and decay chain isotopes, only isotopes with mass ≤ 237

B-1.3 Chain 4N+2

Figure B-6 shows the top half of the 4N+2 decay chain. All isotopes above U238 decay back to it. Short-lived Cm242 decays quickly but eventually reaches equilibrium with parent Am242m and then decays in conjunction with Am242m. Pu242 is relatively long-lived and has decayed relatively little by a million years.

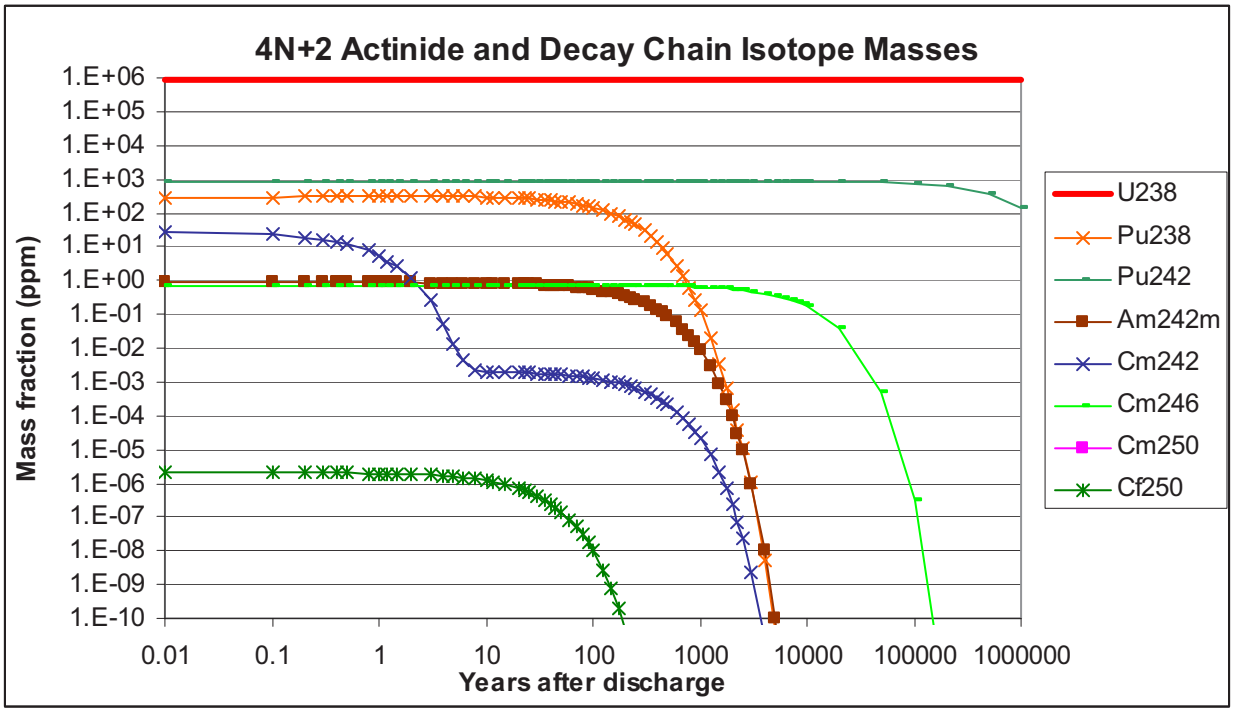

Figure B-6. Mass of 4N+2 actinide and decay chain isotopes, only isotopes with mass ≥ 238

Figure B-7 shows the bottom half of the 4N+2 decay chain. Decay chain 4N+2 has a mainline (figure 3-3) through U238 and a side branch including Cm242 and Pu238. The two branches merge at U234. So, U234 increases as the Cm242/Pu238 side branch decays. Then, the side branch empties and U234 stabilizes and then decays. After a million years, it will eventually decay back to its low equilibrium value relative to the remaining branch, fed by U238. Until then, U234 and its progeny in figure B-7 will actually be at higher levels than equilibrium with U238. So, this chain is the one chain where the decay products of uranium can be higher than found in nature.

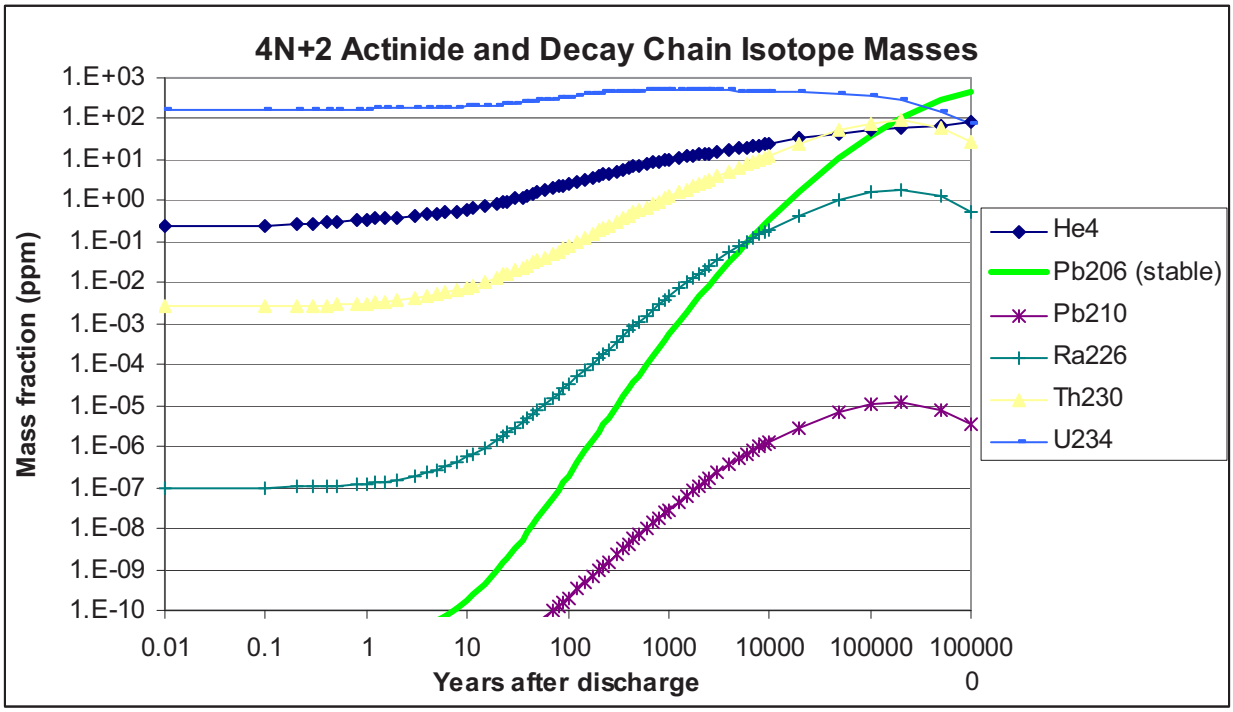

Figure B-7. Mass of 4N+2 actinide and decay chain isotopes, only isotopes with mass less than 236

B-1.4 Chain 4N+3

Figure B-8 shows the top half of chain 4N+3. The shorter-lived isotopes above U235 decay, increasing the inventory of U235. Cm247, however, is so long-lived that eventually Am243 (and later Pu239) fall to the equilibrium value relative to Cm247.

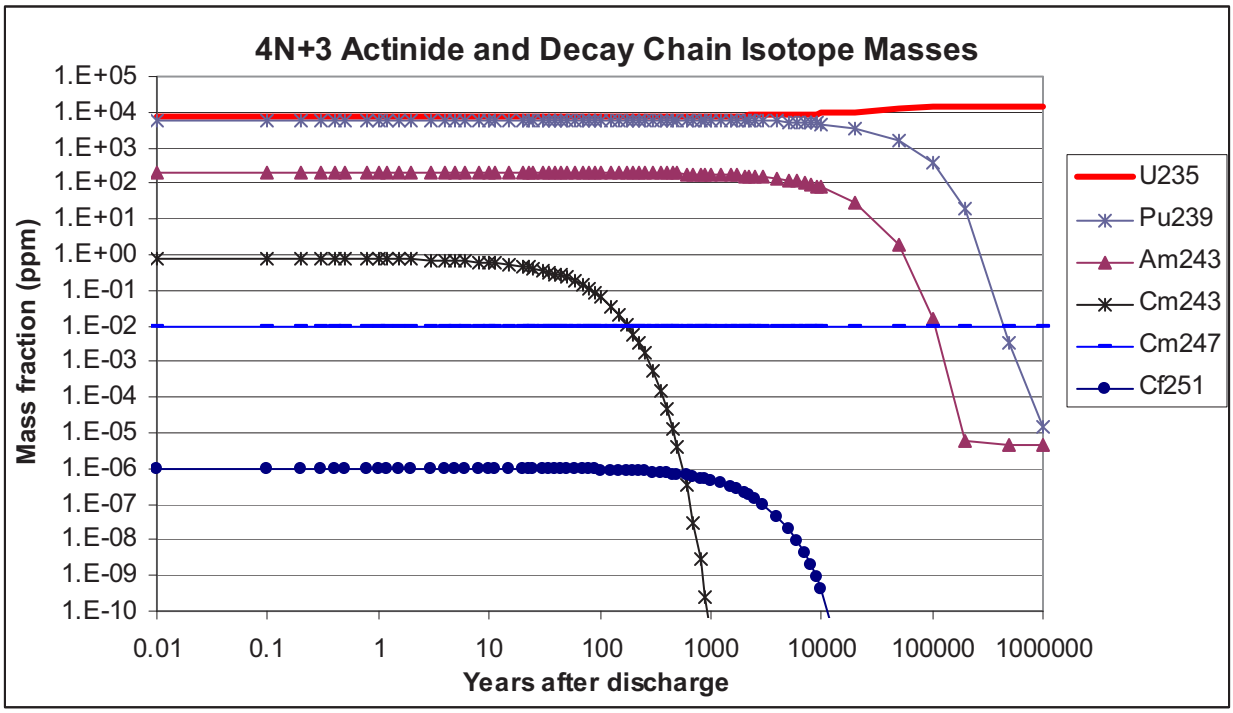

Figure B-8. Mass of 4N+3 actinide and decay chain isotopes, only isotopes with mass ≥ 235

Figure B-9 shows the bottom half of chain 4N+3, showing simple and straightforward behavior.

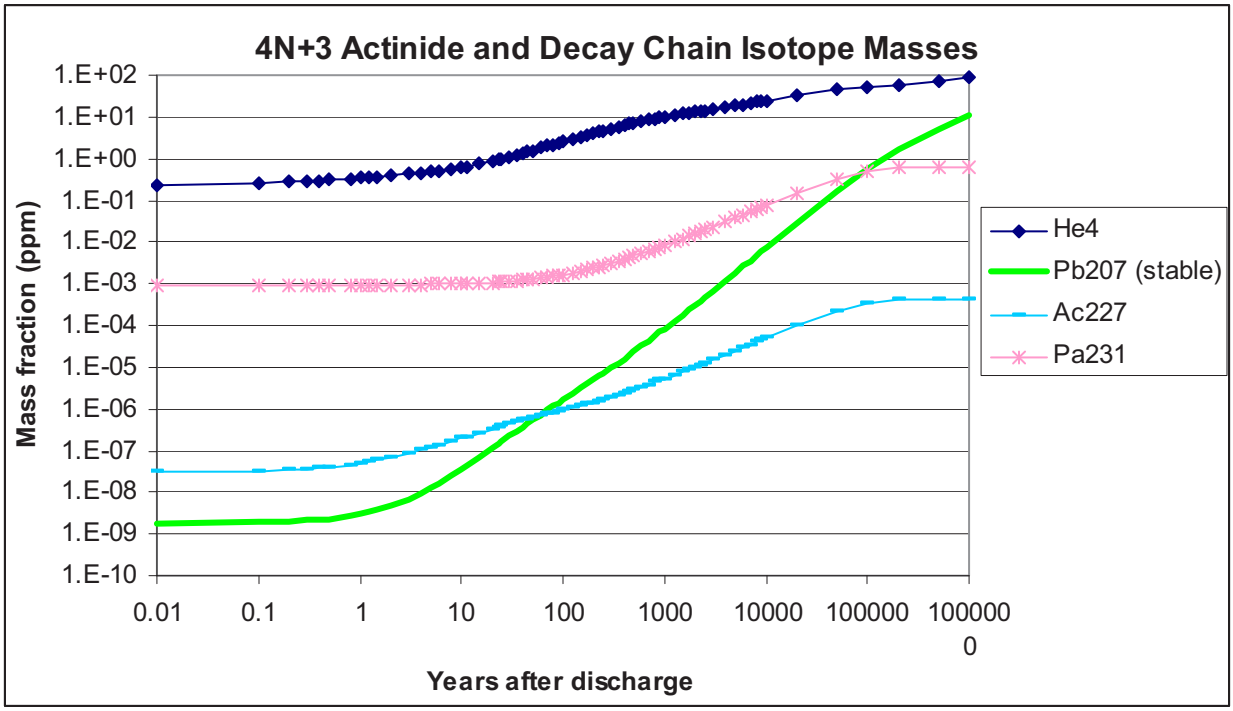

Figure B-9. Mass of 4N+3 actinide and decay chain isotopes, only isotopes with mass < 235

B-2. Fission Product Isotopes

The behavior of actinide and decay chain isotopes is so complex that we essentially have to include all isotopes with halflife greater than 0.5 years. Those less than 0.5 years are represented as being in equilibrium with longer-lived parents.

Fission product behavior is simpler. Section 3.3 summarized the maximum mass error caused by the rules for treating short-lived isotopes. Here is additional explanation of that analysis.

Method 1 - using the full ~1000 isotope output for UOX-51, determine the mass of each chemical group (inert gases, halogens, etc.). This merely requires summation of all the isotopes of that chemical group at each time step from 0 to 1 million years. So, this accounts for all the decay of all isotopes in and out of that group.

Method 2 - approximate the mass as a result of the rules for collapsing the data to the set of 81 isotopes and chemical elements.

- For XX-other, use the t=0 mass, i.e., treat XX-other as stable.
- For tracked isotopes in the chemical group, include the mass of those isotopes at each time step.
- For tracked isotopes outside the group that decay into it, include the delta of the mass of that isotope at t=0 versus the mass remaining, i.e., add to the chemical group's mass, the mass that has decayed.

For illustration, consider inert gases. At t=0,

- Kr81 is 4.22e-5 ppm
- Kr85 is 3.45e1 ppm
- Inert-gas other (including such short lived isotopes as Kr81m) is 8.56e3 ppm

So, the total inert-gas mass is 8.60e3. In both methods, the mass declines as Kr81 and Kr85 decay, but the approximation (method 2) misses the decline due to decay of untracked isotopes. In both methods, the mass of inert gas increases from decay of H3 to He and I129 to Xe129, but the approximation misses the increase from decay of untracked isotopes into inert gases.

By definition, the mass error is always 0% at t=0. In the inert gas case, by 0.1 years, the mass error has become -0.04%. This increases slightly to -0.05% at 0.4 years and stays there. The dominant cause of that mass error is I131 (8.02 days), which is not tracked. So, at shutdown, its mass of 7.5 ppm is included with the mass of inert-gas-other and left there, whereas in reality it decays to Xe131 eventually increasing the mass of inert gases by 0.09%. This would cause method 2 to underestimate inert gases by 0.09% except there are some short-lived isotopes that go in the opposite direction (out of inert gases) so that the net error is 0.05% instead of 0.09%.

I131 also causes the inventory of halogens to be overestimated by 2.27%.

Table 3-6 shows that worst case is TM-other, which is overestimated by as much as 3.34%. The primary cause is Nb95. (The Nb95 created by decay of parent Zr95 is included in method 2, but the Nb95 present at t=0 is included in TM-other.) Nb95 decays with 34.99 day halflife, to method 2 misses the fact that the t=0 Nb95 mass eventually becomes Mo-Ru-Rh-Pd. This contributes to overestimating TM-other by 3.34% and underestimating Mo-Ru-Rh-Pd by 0.33%.