Multi-Reactor Transmutation Analysis Utility (MRTAU, α 1): Verification

Andrea Alfonsi
Samuel E. Bays
Cristian Rabiti
Steven J. Piet

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**Idaho National Laboratory
Idaho Falls, Idaho 83415**

<http://www.inl.gov>

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1. INTRODUCTION

The purpose of this laboratory report is to explain the status of MRTAU code, after further developments and an accurate verification through a code-to-code comparison of the entire set of nuclides with SCALE 6.0 (TRITON). The first part of this report gives an overview of the code, lists the most important input/output files and discusses the method of solution used. The second part will deal with results of verification and issues incurred.

1.1 CURRENT TASK

The current task has been focalized to the following steps:

- 1) expand the number of nuclides tracked in the code:

The isotopes introduced in MRTAU, not previously in the code, are summarized in the table below:

Table 1.1 – Nuclides added in MRTAU.

Actinides			
Pu-244	Cm-250		
Fission Products			
He-4	Zr-95	Nb-95	Nb-95m
Ag-110	I-135	Xe-135	Pm-146

- 2) Update to the most recent fission yield data available, ENDF/B VII, for the entire nuclide library;
- 3) Restyling of the input files (e.g., transmute.inp) and relative parts in the source code;
- 4) Verification of MRTAU through code-to-code comparison against SCALE 6.0 code.

The results of the task are explained in the following pages.

2. MULTI-REACTOR TRANSMUTATION ANALYSIS UTILITY

2.1 OVERVIEW

The Multi-Reactor Transmutation Analysis Utility (MRTAU) is a light-weight software, used to solve for isotopic evolution and depletion in fuel as it is exposed to a neutron flux in a nuclear reactor. The code also solves for isotopic evolution for radioactive decay outside of a reactor core. MRTAU is able to determine the isotopic composition of discharged fuel for any given reactor type for any number of recycles and has the capability to compute the fission product composition of it. The code tracks 29 actinides and 180 fission products. The isotopes are listed in the tables below:

Table 2.1 – List of Actinides tracked

ACTINIDES TRACKED					
U234	NP238 ¹	PU241	AM243	CM246	CF249
U235	PU236 ¹	PU242	CM242	CM247	CF250

¹ These isotopes are offered in output but not currently enlisted in any transmutation chain.

U236	PU238	PU244	CM243	CM248	CF251
U238	PU239	AM241	CM244	CM250	CF252
NP237	PU240	AM242M	CM245	BK249	

Table 2.2 – List of Fission Products tracked

FISSION PRODUCTS TRACKED								
HE-4	SE-82	ZR-95	PD107	SN117	TE130	PR141	GD153	TM169
ZN-66	KR-82	NB-95	AG107	SN118	XE130	ND143	GD154	TM171
ZN-67	KR-83	NB-95M	PD108	SN119	XE131	CE144	EU155	YB171
ZN-68	KR-84	MO-95	AG108M	SN119M	XE132	ND144	GD155	YB172
GA-69	KR-85	ZR-96	CD108	SN120	CS133	ND145	GD156	
ZN-70	RB-85	MO-96	AG109	SN121M	XE134	ND146	GD157	
GE-70	KR-86	MO-97	CD109	SB121	CS134	PM146	GD158	
GA-71	SR-86	MO-98	PD110	SN122	BA134	PM147	TB159	
GE-72	RB-87	RU-98	AG110 ²	TE122	I-135	SM147	GD160	
GE-73	SR-87	TC-99	AG110M	SB123	XE135	ND148	DY160	
GE-74	SR-88	RU-99	CD110	TE123	CS135	SM148	DY161	
AS-75	Y-89	MO100	CD111	SN124	BA135	SM149	DY162	
GE-76	SR-90	RU100	CD112	TE124	XE136	ND150	DY163	
SE-76	ZR-90	RU101	CD113	SB125	BA136	SM150	DY164	
SE-77	ZR-91	RU102	CD113M	TE125	CS137	SM151	HO165	
SE-78	ZR-92	Pd102	IN113	SN126	BA137	EU151	HO166M	
SE-79	ZR-93	RH103	CD114	TE126	BA138	SM152	ER166	
BR-79	NB-93	RU104	SN114	I-127	LA138	EU152	ER167	
SE-80	NB-93M	PD104	IN115	TE128	LA139	GD152	ER168	
KR-80	ZR-94	PD105	SN115	XE128	CE140	EU153	YB168	
BR-81	NB-94	RU106	CD116	I-129	CE142	SM154	ER170	
KR-81	MO-94	PD106	SN116	XE129	ND142	EU154	YB170	

2.2 INPUT/OUTPUT FILES

The MRTAU code is organized in order to be relatively easy to use and to allow the user to modify the source code effortlessly. The code organizational layout is provided in Appendix B. In the same way the input/output files are organized.

2.2.1 INPUT FILES

MRTAU has four important input files:

- Transmute.inp:
Allows the user to control the calculation procedure;
- Decay.dat:
Data file for decay constant and fission yields;
- Budep.inp:
Data file for burn-up-dependent cross sections derived from detailed reactor simulations by other sources (e.g., SCALE, MCNP, REBUS, etc.), numbers of calculation time steps per printed

² Ag110 is a very short-lived isotope ($T_{1/2}=24.6s$). Thus inclusion of this isotope in the transmutation of Ag109 by (n,γ) to Ag110 is bypassed due to numerical solution instability (discussed later). Thus, Ag109 (n,γ) is assumed to transmute directly into Cd110. Also, isomeric transition of Ag110m is assumed to go directly to Cd110.

time steps skipped in order to produce the output, number of transmutation and partitioning loops, number of burn-up intervals, transuranic enrichment, time designating beginning of life, time designating end of life, lower and upper time step boundary, total flux and the power history;

d) Mass.inp:

It is the file of the initial masses for each isotope.

Through these four files the user can control the entire calculation. The budep file also provides provisions for user defined decontamination factors per actinide and fission product isotope. This file also contains provisions for multi-recycle simulation (via the “number of transmutation and partitioning loops” option). By manipulation of the values in budep.inp, the user may run sensitivity studies of an original existing detailed reactor physics simulation to varying fuel cycle assumptions (e.g., alternate decay time between reactor passes). By manipulation of decay.dat, the user may perform sensitivity studies of transmutation performances given different half-life and yield assumptions. By manipulation of mass.inp, the user may test assumptions of depletion performance for alternate compositions given the exact reactor physics conditions of the assumed fixed cross-section and nuclear data sets in budep.inp and decay.dat. Examples of these input files are provided in Appendix C.

2.2.2 OUTPUT FILES

MRTAU provide several types of output file, but the most important are two:

a) Numbers.plot:

Results of the depletion calculation [Mass or atom basis against Time(days)];

b) Reaction.out:

A summary of the fuel condition from begin to the end of cycle.

2.3 THEORY

2.3.1 STATEMAN OF THE PROBLEM

The main equation used in MRTAU is the production/destruction equation. We can start, in order to simplify the reading, from the multi-group and spatial point wise form of this equation Eq. 1. Thus the energy and space variables are discretize with piecewise constant approximations (respectively g and h indexes).

$$\begin{aligned} \frac{dN_k^h(t)}{dt} = & \sum_{i=1}^{actinides} N_i^h(t) \sum_{g=1}^G \varphi^{h,g}(t) \sigma_{f,i}^{h,g} y_{i \rightarrow k}^g + \sum_{z=r}^{reactants} N_z^h(t) \sum_{g=1}^G \varphi^{h,g}(t) \sigma_{c,z}^{h,g} \gamma_{z \rightarrow k}^g \\ & + \sum_{j=n}^{parents} N_j^h(t) \lambda_j \alpha_{j \rightarrow k} - \lambda_k N_k^h(t) - N_k^h(t) \sum_{g=1}^G \varphi^{h,g}(t) \sigma_{a,k}^{h,g} \end{aligned}$$

Eq.1a where:

N_k^h is the atomic density of isotope k, in region h

$\varphi^{h,g}$ is the flux for energy group g, in region h

$\sigma_{f,i}^{h,g}$ is the microscopic fission cross section for isotope i, in energy group g, in region h

$\sigma_{c,z}^{h,g}$ is the microscopic capture cross section for isotope z, in energy group g, in region h

$\sigma_{a,k}^{h,g}$ is the microscopic absorption cross section for isotope k, in energy group g, in region h

λ_j is the radioactive decay constant of nuclide j

λ_k is the radioactive decay constant of nuclide k

$y_{i \rightarrow k}^g$ is the probability that a fission of isotope i will produce isotope k for a neutron in energy group g

$\gamma_{z \rightarrow k}^g$ is the probability that a neutron capture in nuclide z will produce isotope k for a neutron in energy group g

The final step to reach the equation that is the focus of this work is to eliminate the non linearity by assuming the fluxes constant within each time step. The constant value of the flux is the one corresponding to the nuclide densities at the previous time step. This scheme is in literature known as operator splitting since it decouples, by shifting the time, the different physical aspects of the problem (in this case production/destruction from neutron flux calculation)

To express the operator splitting we introduce an index that highlights the time step for which we are solving and from which the quantities are derived (subscript s). Equation 1a for time step Δt_s could be therefore written in the following form:

$$\begin{aligned} \frac{dN_{k,S}^h}{dt} = & \sum_{i=1}^{actinides} N_{i,S}^h \sum_{g=1}^G \varphi_{S-1}^{h,g} \sigma_{f,i}^{h,g} y_{i \rightarrow k}^g + \sum_{z=r}^{reactants} N_{z,S}^h \sum_{g=1}^G \varphi_{S-1}^{h,g} \sigma_{c,z}^{h,g} \gamma_{z \rightarrow k}^g + \sum_{j=n}^{parents} N_{j,S}^h \lambda_j \alpha_{j \rightarrow k} - \\ & \lambda_k N_{k,S}^h - N_{k,S}^h \sum_{g=1}^G \varphi_{S-1}^{h,g} \sigma_{a,k}^{h,g} \end{aligned} \quad \text{Eq.1b}$$

In Eq. 1b, the first summation is the production rate of isotope k due to the fission of all fissionable nuclides present. The second summation is the production rate of isotope k following a neutron capture and the third summation is the production rate of k due to the decay of a parent isotope. The fourth term is the loss rate due to radioactive decay and the final portion is the destruction rate as a result of neutron absorption. The operator splitting practically is performed as it follows:

- The flux must be found for the desired region using the transport or diffusion equations (performed externally to MRTAU).
- This flux is then used in Eq. 1 to determine the new isotropic concentrations.

- These new values are used to determine new material properties such as macroscopic cross section to calculate a new flux.
- This process is used to march over in time.
This mathematical treatment assumes that the space-energy-averaged flux can be considered constant over a sufficiently small time interval, Δt . Similarly, it is assumed that a single set of burn-up-dependent neutron cross sections can be used over the same time step. For a given time step, these assumptions are necessary if Eq. 1 is to be treated as a first-order, linear differential equation.

2.3.2 SOLUTION WITH THE MATRIX EXPONENTIAL MATRIX

Proceeding with the description of the MRTAU analytical model, for all nuclides N_k , Eq. 1b represents a coupled set of linear, homogeneous, first-order differential equations with constant coefficients. As such, Eq. 1 can be written in matrix notation as

$$\dot{\bar{N}} = -\bar{A}\bar{N} \quad \text{Eq. 2}$$

where:

$\bar{N}$ is a vector of nuclide concentrations;

$\bar{A}$ is the transition matrix containing decay/production constants plus absorption/fission cross section time the flux.

Given the nuclide concentration at t_{s-1} , $\bar{N}_{s-1}$ and assuming the neutronic flux constant for $t_{s-1} < t < t_s$ we can compute the exact nuclide density at t_s . Equation 2 has the solution:

$$\bar{N}_s = \exp(-\bar{A}_s \Delta t_s) \bar{N}_{s-1}. \quad \text{Eq. 3}$$

Analogous to a series expansion for the exponential function, the matrix exponential function, $\exp(\bar{A} \Delta t_s)$, appearing in Eq. 3, is defined as

$$\exp(-\bar{A}_s \Delta t_s) = \bar{I} - \bar{A}_s \Delta t_s + \frac{(\bar{A}_s \Delta t_s)^2}{2} + \dots = \sum_{m=0}^{\infty} (-1)^m \frac{(\bar{A}_s \Delta t_s)^m}{m!}, \quad \text{Eq. 4}$$

with $\bar{I}$ being the unit matrix. Equations 3 and 4 constitute the matrix exponential method. Under the assumption of constant flux within the time step the accuracy of the method is connected to the order of the Taylor development used in Eq. 4. A straightforward solution of Eq. 3 through the expansion in Eq. 4 require the storage of the complete transition matrix. Since MRTAU tracks only a few isotopes, when compared with other depletion codes (for example, ORIGEN-ARP^[1]), there is no need to use methods to reduce the size of the transmutation matrix.

2.3.3 SPLITTING OF THE TRANSMUTATION MATRIX (A) IN THE ACTINIDE AND FISSION PRODUCT COMPONENTS

Equation 2 could be rewritten as it follows (we drop the time index from the A matrix and its component):

$$\begin{pmatrix} \dot{\bar{N}}_s^A \\ \dot{\bar{N}}_s^{Fp} \end{pmatrix} = \begin{pmatrix} -\bar{\bar{A}}_{A,A} & \emptyset \\ -\bar{\bar{A}}_{A,Fp} & -\bar{\bar{A}}_{Fp,Fp} \end{pmatrix} \begin{pmatrix} \bar{N}_s^A \\ \bar{N}_s^{Fp} \end{pmatrix},$$

Eq. 5

where A and Fp superscript/subscript stand for Actinides and Fission product respectively.

Given the fact that matrix is lower triangular it is convenient to solve actinides and fission product separately. For the actinides we have:

$$\bar{N}_s^A = \exp(-\bar{\bar{A}}_{A,A}\Delta t_s) \bar{N}_{s-1}^A \cong \bar{\bar{N}}_s^A = \left(\sum_{m=0}^M (-1)^m \frac{(\bar{\bar{A}}_{A,A}\Delta t_s)^m}{m!} \right) \bar{N}_{s-1}^A$$

Eq. 6

For the fission products the problem appears now as a source one (starting from Eq 5):

$$\dot{\bar{N}}_s^{Fp} = \bar{S}_s^{Fp} - \bar{\bar{A}}_{Fp,Fp} \bar{N}_s^{Fp}$$

Eq. 7

where

$$\bar{S}_s^{Fp} = -\bar{\bar{A}}_{A,Fp} \bar{N}_s^A$$

Eq. 8

The exact integration of Eq 7 leads to: $\bar{N}_s^{Fp} = \exp(-\bar{\bar{A}}_{Fp,Fp}\Delta t_s) \bar{N}_{s-1}^{Fp} + \bar{S}_s^{Fp} \frac{1 - \exp(-\bar{\bar{A}}_{Fp,Fp}\Delta t_s)}{\bar{\bar{A}}_{Fp,Fp}}$

Eq. 9

By introducing the expansion of the exponential we obtain:

$$\bar{N}_s^{Fp} = \left(\sum_{m=0}^{\infty} (-1)^m \frac{(\bar{\bar{A}}_{Fp,Fp}\Delta t_s)^m}{m!} \right) \bar{N}_{s-1}^{Fp} + \bar{S}_s^{Fp} \left(\sum_{m=1}^{\infty} (-1)^m \frac{(\Delta t_s)^m (\bar{\bar{A}}_{Fp,Fp})^{m-1}}{m!} \right)$$

Eq. 10

Due to further simplification in the MrTAU code the final equations have the following form:

$$\begin{cases} \bar{\bar{N}}_s^A = \left(\sum_{m=0}^2 (-1)^m \frac{(\bar{\bar{A}}_{A,A}\Delta t_s)^m}{m!} \right) \bar{N}_{s-1}^A \\ \bar{\bar{N}}_s^{Fp} = \left(\sum_{m=0}^2 (-1)^m \frac{(\bar{\bar{A}}_{Fp,Fp}\Delta t_s)^m}{m!} \right) \bar{N}_{s-1}^{Fp} + \bar{\bar{A}}_{A,Fp} \bar{\bar{N}}_s^A \Delta t_s \end{cases}$$

Eq. 11

It is important to note that the source term for the fission product is treated with a first order expansion so leading to a lower order than the overall second used in the inversion of the diagonal blocks of the matrix A. The effect of this further approximation is investigated in section (2.3.5).

2.3.4 CONSIDERATION ON THE STABILITY OF THE METHOD

Without seeking a fully exhaustive stability analysis we want to provide here a qualitative indication of possible stability problem of the method.

We can start from Equation 3 and 4. If we make the assumption that fluxes are not changing along the whole calculation (i.e. $\bar{\bar{A}}_s = \bar{\bar{A}}$, for $s = 1, \dots, S$) and the time step is constant (i.e. $\Delta t_s = \Delta t$, for $s = 1, \dots, S$) we can see that the recursive application of the algorithm lead to:

$$\bar{N}_s \cong \left(\sum_{m=0}^M (-1)^m \frac{(\bar{A}\Delta t)^m}{m!} \right) \bar{N}_{s-1} = \left(\sum_{m=0}^M (-1)^m \frac{(\bar{A}\Delta t)^m}{m!} \right)^s \bar{N}_0$$

Eq. 12

The last form indicates that every rounding off errors in the execution of the algorithm and the truncation error (in the Taylor development) tend to diverge if it is not satisfied:

$$\left\| \sum_{m=0}^M (-1)^m \frac{(\bar{A}\Delta t)^m}{m!} \right\| \leq 1$$

Eq. 13

This instability has been argument of several researches in the field. Codes like ORIGEN^[1] prescreen the A matrix to eliminate the isotope that with a large decay constant tend to increase the above norm. These isotopes are then treated with an ad hoc algorithm^[2].

When the stability criteria is failed the code might get into an instability range, producing an oscillation in the innitial composition of specific isotopes that propagates through associated decay chains. Since the terms in the matrix A contain the sum of the reaction rates (absorption and decay) for each nuclide, this problem is burdensome for the short-lived nuclides and, in particular, for those which have both big decay constant and big capture cross sections. This problematic instability could lead to complete failure of the calculation, even for nuclides not affected in the “instable” decay chain, if no appropriate countermeasures are taken. When the instability occurs, MRTAU forces the atomic density of the particular nuclide to become 0 for the current time step, in order to avoid the calculation failure for the rest of isotopes. Of course, that means that the build-up of the particular chain is at least partially incorrect.

An important and significant example is that of ¹³⁵I-¹³⁵Xe-¹³⁵Cs decay chain (Iodine, Xenon and Cesium). Iodine and Xenon have half life of 6.57 h and 9.10 h, respectively, and Xenon has big cross section of absorption as well. For that reason, the instability happens if the time step is not small enough. The following plots are for three different time-steps number (cycle length 5518 days):

- 200, that corresponds about to 27.5 days for each time step;
- 2000, that corresponds about to 2.75 days for each time step;
- 20,000, that corresponds about to 0.275 day for each time step.

Figure 2.1 – I135 chain MRTAU 200 time steps[x=mass(kg), y=time(days)]³.

Figure 2.2 – Xe135 chain MRTAU 200 time steps[x=mass(kg), y=time(days)]⁴.

³ MRTAU reports zero values for I135 for 200 time steps

⁴ MRTAU reports garbage data for Xe135 for 200 time steps

Figure 2.3 – Cs135 chain MRTAU 200 time steps[x=mass(kg), y=time(days)].⁵

Figure 2.4 – I135 chain MRTAU 2000 time steps[x=mass(kg), y=time(days)].⁶

⁵ MRTAU reports non-physical results for Cs135 for 200 time steps.

⁶ MRTAU reports zero values for I135 for 2000 time steps.

Figure 2.5 – Xe135 chain MRTAU 2000 time steps[x=mass(kg), y=time(days)].⁷

Figure 2.6 –Cs135 chain MRTAU 2000 time steps[x=mass(kg), y=time(days)].⁸

⁷ MRTAU reports garbage results for Xe135 for 2000 time steps.

⁸ MRTAU reports non-physical results for Cs135 for 2000 time steps.

Figure 2.7 – I135 chain MRTAU 20000 time steps[x=mass(kg), y=time(days)].⁹

Figure 2.8 – Xe135 chain MRTAU 20000 time steps[x=mass(kg), y=time(days)].¹⁰

⁹ MRTAU reports very high error results for I135 for 20,000 time steps.

¹⁰ MRTAU reports descent agreement for Xe135 for 20,000 time steps.

Figure 2.9 – Cs135 chain MRTAU 20000 time steps[x=mass(kg), y=time(days)].¹¹

The instabilities for Xenon and Iodine lead the code to overestimate the build-up of Cesium. As can be seen in figures above, there is an obvious improvement going to smaller time-steps (bigger number of TS), reaching a good stability only for a number of time-steps more than 15,000 (at 20,000 TS we have a complete stability).

For the reason explained, it has been impossible adding to the code the precursors for Pu244 and Cm250, since Pu243 has a half-life about of 4.9 h and Cm249 about 1.1 h. This means that the code doesn't compute the build-up for those nuclides (response is ever 0).

The issue with numerical solution instability for the power/taylor series solution method of an exponential series is fairly well known^[3]. Given that MRTAU was originally envisioned as a fuel cycle tool and/or teaching tool, every effort has been made to avoid the need to include short-lived isotopes in the depletion chains. However, it was found during final proofing of the code that accuracy of certain isotopes, namely Cs135 ($T_{1/2}=2.3E6$ Yrs) is dependent on the accuracy of its parents I135 ($T_{1/2}=6.57$ hrs) and Xe135 ($T_{1/2}=9.14$ hrs). For most other isotope chains tracking short lived precursors can be avoided by assuming their production/destruction rates are dominated by beta decay and in secular equilibrium with the fission yield of that particular isomer, or term 1 in equation 1. For the I135, Xe135, Cs135 chain this assumption does not hold due to the large capture cross-section of Xe135 puts its destruction rate by n,γ on par with that by beta to Cs135. Thus, it must be included in the transmutation matrix. Other codes such as the ORIGEN family avoid numerical solution instability by solving scenarios such as the I135, Xe135, Cs135 scenario by solving these chains externally to the power series iteration technique^[1]. However, given the intent of MRTAU as a light-weight code, we decided to perform further research into solution techniques of the exponential matrix, other than power series iteration before continuing forward.

¹¹ MRTAU reports descent agreement for Cs135 for 20,000 time steps.

2.3.5 FISSION PRODUCT DEPLETION METHOD

The capability to track the fission products has been added to MRTAU last year. The FP depletion part of the code is performed by a subroutine that is called for each time-step after the computation of the actinides amount.

As explained in the previous section (2.3.3), the source term for the fission product is treated with a first order expansion so leading to a lower order than the overall second used in the inversion of the diagonal blocks of the matrix A.

This lack is not a great problem if it uses a big number of time-steps (i.e. 10,000 or over), since the second order term becomes “small”, if compared with the others; but it becomes an important source of error, running the code with the usual 200 time-steps. The influence of this “error” in the source code can be explained well with the example of ^{137}Cs .

Figure 2.10 – Cs137 SCALE against MRTAU 200,2000,20000 time steps[x=mass (kg), y=time (days)].

The 1st order series used leads the code to overestimate the build-up of ^{137}Cs , since not all the components needed to consider the actinide decay during the time-step are accounted. As can be seen in figure above, there is an obvious improvement going to smaller time-step (because the reason explained before), reaching a good matching already for 2000 time-steps.

3. CODE-TO-CODE COMPARISON

In this section the comparisons between SCALE 6.0 and MRTAU response will be presented for some important nuclides; all the comparison graphs are reported in the Appendix A.

3.1 CODE-TO-CODE COMPARISON

The verification of MRTAU code has been employed by comparison with the SCALE 6.0 calculation. The case used was a MOX (10% NpPu/HM, 50 MWD/kg) directly recycled from spent UO₂ (4.2% ²³⁵U/U, 50 MWD/kg, 5 years decay storage). The actinide mass input was the same for the two codes and the fluxes and cross sections used in MRTAU were extracted from the SCALE output thus eliminating these values from being a source of error. The table (3.1) summaries the initial conditions.

Table 3.1 – Initial conditions and parameters.

INITIAL FUEL MASS		GENERAL CONTROL PARAMATER	
Actinides	MASS(kg)	Reactor Passes (T&P Loops)	1
U-234	1.13E-12	Beginning of Life (days)	365.25
U-235	2.16E-02	End of Life (days)	1865.00
U-236	1.13E-12	Burn-up steps #	16
U-238	8.98E-01	Transuranic Enrichment(w/o)	10.00
NP237	4.19E-03	Spectrum type	thermal
NP238	1.13E-12		
PU236	1.13E-12		
PU238	1.97E-03		
PU239	4.12E-02		
PU240	1.96E-02		
PU241	7.27E-03		
PU242	5.78E-03		
PU244 through CF252	1.13E-12		

The comparisons have shown that MRTAU works well for about the 85% of the nuclides tracked, and for the rest there are certain reasons for which it presents some mismatching. In the following pages are reported graphs of some important nuclides for the “fuel cycle analysis”; the comparison for the entire set of isotopes tracked are given in the Appendix A.

Figure 3.1 – U235 SCALE against MRTAU 200,2000,20000 time steps[x=mass (kg), y=time (days)].

Figure 3.2 – U238 SCALE against MRTAU 200,2000,20000 time steps[x=mass (kg), y=time (days)].

Figure 3.3 – PU238 SCALE against MRTAU 200,2000,20000 time steps[x=mass (kg), y=time (days)].

Figure 3.4 – PU239 SCALE against MRTAU 200,2000,20000 time steps[x=mass (kg), y=time (days)].

Figure 3.5 –SR90 SCALE against MRTAU 200,2000,20000 time steps[x=mass (kg), y=time (days)].

Figure 3.6 –TC99 SCALE against MRTAU 200,2000,20000 time steps[x=mass (kg), y=time (days)].

Figure 3.7 –I129 SCALE against MRTAU 200,2000,20000 time steps[x=mass (kg), y=time (days)].

Figure 3.8 –PM147 SCALE against MRTAU 200,2000,20000 time steps[x=mass (kg), y=time (days)].

As can be seen above, the results from MRTAU match up closely with those of SCALE 6.0 for most of the isotopes. These nuclides are basically those which are not affected by the “problems” of the source

code exposed in the paragraphs (2.3.3) and (2.3.4). In general, depletion of actinides gives quite reasonable agreement with SCALE6.0. Possible errors among the fission products are given in the following section.

3.2 IDENTIFICATION OF THE POSSIBLE ERRORS

In this section we analyzed the possible errors for the radionuclides that should be checked in future work. The table below summarizes the causes for the isotopes that mismatch the SCALE calculation.

Table 3.2 – Identification possible problems.

Nuclide	Problem Type	Possible Cause	Nuclide	Problem Type	Possible Cause
HE-4	Underestimation	No precursors	SN114	Overestimation	IN113
ZN-66	Underestimation	No all precursors	SN115	Underestimation	Unknown
ZN-67	Underestimation	No all precursors	SN121M	Underestimation	No all precursors
ZN-68	Underestimation	No all precursors	XE135	Instability	Short-lived
GA-69	Underestimation	No all precursors	CS135	Overestimation	Instability Xe135
ZN-70	Underestimation	No all precursors	BA135	Overestimation	Instability Xe135
GE-70	Underestimation	No all precursors	XE136	Overestimation	Instability Xe135
KR-85	Underestimation	No all precursors	BA136	Overestimation	Instability Xe135
RB-85	Underestimation	No all precursors	PM146	Underestimation	No all precursors
SR-86	Underestimation	No all precursors	SM148	Overestimation	SCALE ENDF VI –
SR-87	Underestimation	No all precursors	SM149	Overestimation	MRTAU ENDF VII
MO-94	Underestimation	No all precursors	EU151	Underestimation	No all precursors
RU-98	Underestimation	No all precursors	GD152	Underestimation	No all precursors
RU-99	Underestimation	No all precursors	GD153	Underestimation	No all precursors
Pd102	Underestimation	No all precursors	GD154	Underestimation	No all precursors
RH103	Overestimation	Unknown	GD157	Underestimation	No all precursors
PD104	Underestimation	No all precursors	HO166M	Underestimation	No all precursors
CD108	Underestimation	No all precursors	ER170	Underestimation	No all precursors
CD109	Underestimation	No all precursors	YB170	Underestimation	No all precursors
AG110M	Underestimation	No all precursors	TM171	Underestimation	No all precursors
CD113M	Overestimation	Fission Yields	YB171	Underestimation	No all precursors
IN113	Overestimation	Cd113m			

Focussing the attention on the most important chains, the table above and the graphs in the Appendix A show that it is advisable not to use the code (in its current form) for the following chain:

- Cd;
- I135-Xe135-Cs135;
- Gd.

4. FUTURE WORK

The future work should be pointed on two different lines:

- 1) Calculation method;
- 2) Expansion of nuclides tracked.

The first task is necessary to solve the problem with the short-lived nuclides, that drive the code to instability. There are two possible ways forward in addressing this problem:

- Implement in the code a recursive formula to treat separately the short-lived isotopes, for example the Voondy's formula (Origen style)^[1];
- Change completely the solver of MRTAU, substituting it with one that doesn't present troubles with those nuclides, for example the CRAM method^{[5][6][7]}.

The second task is needed to track well the entire set of nuclides, including all precursors for each isotope.

Appendix A : Code-to-Code comparison – Graphs

In the following pages are listed the plots of the code-to-code comparison for the entire set of nuclides tracked by MRTAU. In the section of Actinides, Np238, Pu236, Pu244 and Cm 250 have not been reported since the response is ever 0 (for the last two no precursors). In the section of Fission Products He4 has not plotted since the underestimation is of 6 orders of magnitude (Only yield by ternary-fission). Production of Helium by alpha decay of actinides is performed using the fission gas production flag in transmute.inp.

In these graphs the vertical axis is “mass” in kilograms and the horizontal one is “time” in days.

Actinides

Figure A.1 – Code-to-Code comparison U234.

Figure A.2 – Code-to-Code comparison U235.

Figure A.3– Code-to-Code comparison U236.

Figure A.4– Code-to-Code comparison U238.

Figure A.5– Code-to-Code comparison NP237.

Figure A.6– Code-to-Code comparison PU238.

Figure A.7– Code-to-Code comparison PU239.

Figure A.8– Code-to-Code comparison PU240.

Figure A.9– Code-to-Code comparison PU241.

Figure A.10– Code-to-Code comparison PU242.

Figure A.11– Code-to-Code comparison AM241.

Figure A.12– Code-to-Code comparison AM242M.

Figure A.13– Code-to-Code comparison AM243.

Figure A.14– Code-to-Code comparison CM242.

Figure A.15– Code-to-Code comparison CM243.

Figure A.16– Code-to-Code comparison CM244.

Figure A.17– Code-to-Code comparison CM245.

Figure A.18– Code-to-Code comparison CM246.

Figure A.19– Code-to-Code comparison CM247.

Figure A.20— Code-to-Code comparison CM248.

Figure A.21— Code-to-Code comparison BK249.

Figure A.22– Code-to-Code comparison CF249.

Figure A.22– Code-to-Code comparison CF250.

Figure A.23– Code-to-Code comparison CF251.

Figure A.24– Code-to-Code comparison CF252.

Fission Products

Figure A.25– Code-to-Code comparison Zn66.

Figure A.26– Code-to-Code comparison Zn67.

Figure A.27– Code-to-Code comparison Zn68.

Figure A.28– Code-to-Code comparison Ga69.

Figure A.29– Code-to-Code comparison Zn70.

Figure A.30– Code-to-Code comparison Ge70.

Figure A.31– Code-to-Code comparison Ga71.

Figure A.32– Code-to-Code comparison Ge72.

Figure A.33– Code-to-Code comparison Ge73.

Figure A.34– Code-to-Code comparison Ge74.

Figure A.34— Code-to-Code comparison As75.

Figure A.35— Code-to-Code comparison Ge76.

Figure A.36– Code-to-Code comparison Se76.

Figure A.37– Code-to-Code comparison Se77.

Figure A.38– Code-to-Code comparison Se78.

Figure A.39– Code-to-Code comparison Se79.

Figure A.40– Code-to-Code comparison Br79.

Figure A.41– Code-to-Code comparison Se80.

Figure A.42– Code-to-Code comparison Kr80.

Figure A.43– Code-to-Code comparison Br81.

Figure A.44– Code-to-Code comparison Kr81.

Figure A.45– Code-to-Code comparison Se82.

Figure A.46– Code-to-Code comparison Kr82.

Figure A.47– Code-to-Code comparison Kr83.

Figure A.48– Code-to-Code comparison Kr84.

Figure A.49– Code-to-Code comparison Kr85.

Figure A.50– Code-to-Code comparison Rb85.

Figure A.51– Code-to-Code comparison Kr86.

Figure A.52– Code-to-Code comparison Sr86.

Figure A.53– Code-to-Code comparison Rb87.

Figure A.54– Code-to-Code comparison Sr87.

Figure A.55– Code-to-Code comparison Sr88.

Figure A.56– Code-to-Code comparison Y89.

Figure A.57– Code-to-Code comparison Sr90.

Figure A.58– Code-to-Code comparison Zr90.

Figure A.59– Code-to-Code comparison Zr91.

Figure A.60– Code-to-Code comparison Zr92.

Figure A.61– Code-to-Code comparison Zr93.

Figure A.62– Code-to-Code comparison Nb93.

Figure A.63– Code-to-Code comparison Nb93m.

Figure A.64– Code-to-Code comparison Zr94.

Figure A.65– Code-to-Code comparison Nb94.

Figure A.66– Code-to-Code comparison Zr95.

Figure A.67– Code-to-Code comparison Nb95.

Figure A.68– Code-to-Code comparison Nb95m.

Figure A.69– Code-to-Code comparison Mo95.

Figure A.70– Code-to-Code comparison Zr96.

Figure A.71– Code-to-Code comparison Mo96.

Figure A.72– Code-to-Code comparison Mo97.

Figure A.73– Code-to-Code comparison Mo98.

Figure A.74– Code-to-Code comparison Ru98.

Figure A.75– Code-to-Code comparison Ru99.

Figure A.76– Code-to-Code comparison Tc99.

Figure A.77– Code-to-Code comparison Mo100.

Figure A.78– Code-to-Code comparison Ru100.

Figure A.79– Code-to-Code comparison Ru101.

Figure A.80— Code-to-Code comparison Ru102.

Figure A.81— Code-to-Code comparison Pd102.

Figure A.82– Code-to-Code comparison Rh103.

Figure A.83– Code-to-Code comparison Ru104.

Figure A.84– Code-to-Code comparison Pd104.

Figure A.85– Code-to-Code comparison Pd105.

Figure A.86– Code-to-Code comparison Ru106.

Figure A.87– Code-to-Code comparison Pd106.

Figure A.88– Code-to-Code comparison Pd107.

Figure A.89– Code-to-Code comparison Ag107.

Figure A.90– Code-to-Code comparison Pd108.

Figure A.91– Code-to-Code comparison Ag108m.

Figure A.92– Code-to-Code comparison Cd108.

Figure A.93– Code-to-Code comparison Ag109.

Figure A.94– Code-to-Code comparison Cd109.

Figure A.95– Code-to-Code comparison Pd110.

Figure A.96– Code-to-Code comparison Ag110m.

Figure A.97– Code-to-Code comparison Cd110.

Figure A.98– Code-to-Code comparison Cd111.

Figure A.99– Code-to-Code comparison Cd112.

Figure A.100– Code-to-Code comparison Cd113.

Figure A.101– Code-to-Code comparison Cd113m.

Figure A.102– Code-to-Code comparison In113.

Figure A.103– Code-to-Code comparison Cd114.

Figure A.104– Code-to-Code comparison Sn114.

Figure A.105– Code-to-Code comparison In115.

Figure A.106– Code-to-Code comparison Sn115.

Figure A.107– Code-to-Code comparison Cd116.

Figure A.108– Code-to-Code comparison Sn116.

Figure A.109– Code-to-Code comparison Sn117.

Figure A.110– Code-to-Code comparison Sn118.

Figure A.111– Code-to-Code comparison Sn119.

Figure A.112– Code-to-Code comparison Sn119m.

Figure A.113– Code-to-Code comparison Sn120.

Figure A.114– Code-to-Code comparison Sn121m.

Figure A.115– Code-to-Code comparison Sb121.

Figure A.116– Code-to-Code comparison Sn122.

Figure A.117– Code-to-Code comparison Te122.

Figure A.118– Code-to-Code comparison Sb123.

Figure A.119– Code-to-Code comparison Te123.

Figure A.120— Code-to-Code comparison Sn124.

Figure A.121— Code-to-Code comparison Te124.

Figure A.122– Code-to-Code comparison Sb125.

Figure A.123– Code-to-Code comparison Te125.

Figure A.124— Code-to-Code comparison Sn126.

Figure A.125— Code-to-Code comparison Te126.

Figure A.126– Code-to-Code comparison I127.

Figure A.127– Code-to-Code comparison Te128.

Figure A.128– Code-to-Code comparison Xe128.

Figure A.129– Code-to-Code comparison I129.

Figure A.130– Code-to-Code comparison Xe129.

Figure A.131– Code-to-Code comparison Te130.

Figure A.132– Code-to-Code comparison Xe130.

Figure A.133– Code-to-Code comparison Xe131.

Figure A.134— Code-to-Code comparison Xe132.

Figure A.135— Code-to-Code comparison Cs133.

Figure A.136— Code-to-Code comparison Xe134.

Figure A.137— Code-to-Code comparison Cs134.

Figure A.138– Code-to-Code comparison Ba134.

Figure A.139– Code-to-Code comparison I135.

Figure A.140– Code-to-Code comparison Xe135.

Figure A.141– Code-to-Code comparison Cs135.

Figure A.142– Code-to-Code comparison Ba135.

Figure A.143– Code-to-Code comparison Xe136.

Figure A.144– Code-to-Code comparison Ba136.

Figure A.145– Code-to-Code comparison Cs137.

Figure A.146– Code-to-Code comparison Ba137.

Figure A.147– Code-to-Code comparison Ba138.

Figure A.148– Code-to-Code comparison La138.

Figure A.149– Code-to-Code comparison La139.

Figure A.150– Code-to-Code comparison Ce140.

Figure A.151– Code-to-Code comparison Pr141.

Figure A.152– Code-to-Code comparison Ce142.

Figure A.153– Code-to-Code comparison Nd142.

Figure A.154– Code-to-Code comparison Nd143.

Figure A.155– Code-to-Code comparison Ce144.

Figure A.156– Code-to-Code comparison Nd144.

Figure A.157– Code-to-Code comparison Nd145.

Figure A.158– Code-to-Code comparison Nd146.

Figure A.159– Code-to-Code comparison Sm147.

Figure A.160– Code-to-Code comparison Nd148.

Figure A.161– Code-to-Code comparison Sm148.

Figure A.162– Code-to-Code comparison Sm149.

Figure A.163– Code-to-Code comparison Nd150.

Figure A.164– Code-to-Code comparison Sm150.

Figure A.165– Code-to-Code comparison Sm151.

Figure A.166– Code-to-Code comparison Eu151.

Figure A.167– Code-to-Code comparison Sm152.

Figure A.168– Code-to-Code comparison Eu152.

Figure A.169– Code-to-Code comparison Gd152.

Figure A.170– Code-to-Code comparison Eu153.

Figure A.171– Code-to-Code comparison Gd153.

Figure A.172– Code-to-Code comparison Sm154.

Figure A.173– Code-to-Code comparison Eu154.

Figure A.174– Code-to-Code comparison Gd154.

Figure A.175– Code-to-Code comparison Eu155.

Figure A.176– Code-to-Code comparison Gd155.

Figure A.177– Code-to-Code comparison Gd156.

Figure A.178– Code-to-Code comparison Gd157.

Figure A.179– Code-to-Code comparison Gd158.

Figure A.180– Code-to-Code comparison Tb159.

Figure A.181– Code-to-Code comparison Gd160.

Figure A.182– Code-to-Code comparison Dy160.

Figure A.183– Code-to-Code comparison Dy161.

Figure A.184– Code-to-Code comparison Dy162.

Figure A.185– Code-to-Code comparison Dy163.

Figure A.186– Code-to-Code comparison Dy164.

Figure A.187– Code-to-Code comparison Ho165.

Figure A.188– Code-to-Code comparison Ho166m.

Figure A.189– Code-to-Code comparison Er166.

Figure A.190– Code-to-Code comparison Er167.

Figure A.191– Code-to-Code comparison Er168.

Figure A.192– Code-to-Code comparison Tm169.

Figure A.193– Code-to-Code comparison Er170.

Figure A.194– Code-to-Code comparison Yb170.

Figure A.195– Code-to-Code comparison Tm171.

Figure A.196– Code-to-Code comparison Yb171.

Figure A.197– Code-to-Code comparison Yb172.

Appendix B: MRTAU Process

Flow chart describing the MRTAU process

Appendix C: MRTAU Inputs

Mass.inp

Actinide Mass		
ISOT	ATOM_WT	MASS(KG)
U-234	2.3404E+02	1.1340E-12
U-235	2.3504E+02	2.1620E-02
U-236	2.3605E+02	1.1340E-12
U-238	2.3805E+02	8.9840E-01
NP237	2.3705E+02	4.1890E-03
NP238	2.3805E+02	1.1340E-12
PU236	2.3605E+02	1.1340E-12
PU238	2.3805E+02	1.9730E-03
PU239	2.3905E+02	4.1180E-02
PU240	2.4005E+02	1.9610E-02
PU241	2.4106E+02	7.2680E-03
PU242	2.4206E+02	5.7820E-03
PU244	2.4406E+02	1.1340E-12
AM241	2.4106E+02	1.1340E-12
AM242	2.4206E+02	1.1340E-12
AM243	2.4306E+02	1.1340E-12
CM242	2.4206E+02	1.1340E-12
CM243	2.4306E+02	1.1340E-12
CM244	2.4406E+02	1.1340E-12
CM245	2.4507E+02	1.1340E-12
CM246	2.4607E+02	1.1340E-12
CM247	2.4707E+02	1.1340E-12
CM248	2.4807E+02	1.1340E-12
CM250	2.5009E+02	1.1340E-12
BK249	2.4907E+02	1.1340E-12
CF249	2.4907E+02	1.1340E-12
CF250	2.5008E+02	1.1340E-12
CF251	2.5108E+02	1.1340E-12
CF252	2.5208E+02	1.1340E-12

Fission Product Mass		
ISOT	ATOM_WT	MASS(KG)
He-4	4.0026E+00	0.0000E+00
Zn-66	6.5926E+01	0.0000E+00
Zn-67	6.6927E+01	0.0000E+00
Zn-68	6.7925E+01	0.0000E+00
Ga-69	6.9926E+01	0.0000E+00
Zn-70	6.9925E+01	0.0000E+00

Ge-70 6.9924E+01 0.0000E+00
Ga-71 7.0925E+01 0.0000E+00
Ge-72 7.1922E+01 0.0000E+00
Ge-73 7.2924E+01 0.0000E+00

...

...

...

Budep.inp

```
-----
10 $ Number of cadulation timesteps per printed timesteps skipped in order to produce output
1 $ Number of Transmutation and Partitioning Loops
16 $ Number of BU Intervals
10.0 $ User Defined BOL Transuranic Enrichment (w/o)
365.25 $ Time Designating Beginning of Life (d)
1865.0 $ Time Designating End of Life (d)
1 $ Apply Separation Efficiencies at Lower Bound of the BU Interval (1) / Apply Separation Efficiencies for Entire BU Interval (2)
1 $ Use initialized U vector every cycle (1) / Use reproessed U vector only (2)
1 $ Use blended TRU approach every cycle (1) / Use reproessed TRU vector only (2)
LBND Lower Time Step Boundary (d)
0.000E+00 3.653E+02 3.654E+02 4.486E+02 5.319E+02 6.153E+02 7.403E+02 8.653E+02 9.903E+02 1.115E+03 1.240E+03 1.365E+03 1.490E+03 1.615E+03 1.740E+03 1.865E+03
UBND Upper Time Step Boundary (d)
3.653E+02 3.654E+02 4.486E+02 5.319E+02 6.153E+02 7.403E+02 8.653E+02 9.903E+02 1.115E+03 1.240E+03 1.365E+03 1.490E+03 1.615E+03 1.740E+03 1.865E+03 5.518E+03
FLUX Total Flux (cm^-2*s^-1)
2.563E+14 2.563E+14 2.616E+14 2.648E+14 2.674E+14 2.705E+14 2.742E+14 2.778E+14 2.815E+14 2.852E+14 2.889E+14 2.926E+14 2.964E+14 3.001E+14 3.039E+14 8.976E+09
PHIST Manually Provided Power History (%)
0.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 0.000E+00
ISOT CAPT XSEC (b)
U-234 1.699E+01 1.697E+01 1.682E+01 1.657E+01 1.636E+01 1.612E+01 1.587E+01 1.566E+01 1.547E+01 1.531E+01 1.517E+01 1.505E+01 1.495E+01 1.486E+01 1.478E+01 1.474E+01
...
ISOT FISS XSEC (b)
U-234 5.944E-01 5.944E-01 5.945E-01 5.942E-01 5.939E-01 5.935E-01 5.930E-01 5.925E-01 5.920E-01 5.914E-01 5.909E-01 5.903E-01 5.898E-01 5.892E-01 5.887E-01 5.883E-01
...
ISOT N,2N XSEC (b)
U-234 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
...
ISOT Separation Efficiencies (%)
U-234 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00 1.000E+00
...
ISOT Uranium Transurancic $External Feed Vectors (Used if Blending Option Invoked)
U-234 1.000E-10 0.000E+00
...
Fission Product Block
ISOT n,g XSEC (b)
HE-4 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
ZN-66 4.781E-02 4.782E-02 4.757E-02 4.757E-02 4.769E-02 4.786E-02 4.809E-02 4.833E-02 4.859E-02 4.885E-02 4.913E-02 4.938E-02 4.973E-02 5.005E-02 5.037E-02 5.060E-02
...
ISOT n,g* XSEC (b)
HE-4 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
ZN-66 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
...
ISOT n,2n XSEC (b)
HE-4 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
ZN-66 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
...
ISOT n,alpha XSEC (b)
HE-4 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
ZN-66 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
...
ISOT n,p XSEC (b)
HE-4 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
ZN-66 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
...
ISOT Separation Efficiency
HE-4 0.00
ZN-66 0.00
```

Decay.dat

```
-----
Actinides
BETA BETA PLUS ALPHA Kr Yield Xe Yield
U-234 0.000E+00 0.000E+00 0.979E-01 1.324E-01 1.902E-01
U-235 0.000E+00 0.000E+00 3.120E-17 1.324E-01 1.902E-01
U-236 0.000E+00 0.000E+00 9.379E-16 1.324E-01 1.902E-01
U-238 0.000E+00 0.000E+00 4.915E-18 9.117E-02 2.023E-01
NP237 0.000E+00 0.000E+00 1.026E-14 9.117E-02 2.023E-01
NP238 0.000E+00 0.000E+00 3.790E-06 9.117E-02 2.023E-01
PU236 0.000E+00 0.000E+00 7.703E-09 1.324E-01 1.902E-01
PU238 0.000E+00 0.000E+00 2.503E-10 9.117E-02 2.023E-01
PU239 0.000E+00 0.000E+00 9.109E-13 6.014E-02 2.099E-01
PU240 0.000E+00 0.000E+00 3.353E-12 5.646E-02 1.973E-01
PU241 1.525E-09 0.000E+00 0.000E+00 4.234E-02 1.988E-01
PU242 0.000E+00 0.000E+00 5.833E-14 4.234E-02 1.988E-01
PU244 0.000E+00 0.000E+00 2.744E-16 4.234E-02 1.988E-01
AM241 0.000E+00 0.000E+00 5.081E-11 4.234E-02 1.988E-01
AM242 1.189E-10 2.487E-11 7.225E-13 4.234E-02 1.988E-01
AM243 0.000E+00 0.000E+00 2.976E-12 4.234E-02 1.988E-01
CM242 0.000E+00 0.000E+00 4.924E-08 4.234E-02 1.988E-01
CM243 0.000E+00 2.002E-12 7.685E-10 4.234E-02 1.988E-01
CM244 0.000E+00 0.000E+00 1.213E-09 4.234E-02 1.988E-01
CM245 0.000E+00 0.000E+00 2.584E-12 4.234E-02 1.988E-01
CM246 0.000E+00 0.000E+00 4.642E-12 4.234E-02 1.988E-01
CM247 0.000E+00 0.000E+00 1.408E-15 4.234E-02 1.988E-01
CM248 0.000E+00 0.000E+00 6.312E-14 4.234E-02 1.988E-01
CM250 2.118E-13 0.000E+00 4.766E-13 4.234E-02 1.988E-01
BK249 2.507E-08 0.000E+00 0.000E+00 4.234E-02 1.988E-01
CF249 0.000E+00 0.000E+00 6.258E-11 4.234E-02 1.988E-01
CF250 0.000E+00 0.000E+00 1.679E-09 4.234E-02 1.988E-01
CF251 0.000E+00 0.000E+00 2.446E-11 4.234E-02 1.988E-01
CF252 0.000E+00 0.000E+00 8.304E-09 4.234E-02 1.988E-01
Fission Products
BETA BETA EXT POSIT POSIT EXT ALPHA INT TRAN
He-4 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
Zn-66 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
...
Thermal Fission Yield
U235 FY U238 FY Pu239 FY Pu240 FY Pu241 FY Pu242 FY Cm245 FY
He-4 1.702E-03 0.000E+00 2.192E-03 0.000E+00 1.860E-03 0.000E+00 4.700E-03
Zn-66 7.219E-10 0.000E+00 2.210E-09 1.600E-09 1.670E-09 4.970E-10 1.040E-08
...
Fast Fission Yield
U235 FY U238 FY Pu239 FY Pu240 FY Pu241 FY Pu242 FY Cm244 FY
He-4 1.700E-03 1.488E-03 2.190E-03 2.781E-03 1.860E-03 2.370E-03 4.700E-03
Zn-66 0.000E+00 0.000E+00 3.070E-14 1.070E-14 0.000E+00 0.000E+00 1.900E-12
...
```

Transmute.inp

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4    $ PHYS INPUT: Use MC2 and flux.out (2) / Use user supplied xsec.inp & flux.inp (3) / Use budep.inp (4)
2    $ MASS INPUT: Use user supplied mass.inp (2)
2    $ CALC INPUT: Specify Calculation: UtoCf Only Depletion (1) / UtoCf+FP Depletion (2) / Just Print BOEC Physics Data (3)
2    $ POWC INPUT: Perform Depletion using: Constant Flux Depletion (1) / Constant Power Depletion (2)
2    $ POLY INPUT: Specify Order of Taylor Series Polynomial Approximation
1    $ GASC INPUT: Calculate Helium using: No Gas Calc (1) / Integrated Activity (2) / Numerical Integration (3)
1    $ SPEC INPUT: Use physics data for: Thermal Spectrum (1) / Fast Spectrum (2)
2    $ PLOT INPUT: Create .plot files: No (1) / Yes-Mass (2) / Yes-Number (3)
3    $ EXTRA PLOT: Provide additional plot data (including end of cycle data): No (1) / Yes (2) / Create .csv file (3)
5.518E+03 $ Total Problem Time (days)
200    $ Number of Time Steps for Depletion Calculation (Max 10,000)
```

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