Time Evolution of Selected Actinides in TRIGA MARK-II Fuel

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Abstract

Study is made on the evolution of several actinides capable of undergoing fission or breeding available on the Malaysian Nuclear Agency (MNA) TRIGA MARK-II fuel. Population distribution of burned fuel in the MNA reactor is determined with a model developed using WIMS. This model simulates fuel conditions in the hottest position in the reactor, thus the location where most of the burn up occurs. Theoretical basis of these nuclide time evolution are explored and compared with the population obtained from our models. Good agreements are found for the theoretical time evolution and the population of Uranium-235, Uranium-236, Uranium-238 and Plutonium-239.

Abstrak

Kajian ini melihat evolusi beberapa nuklid yang mengalami pembelahan dan pembiakan nuklear yang terdapat pada bahan api TRIGA MARK-II di Agensi Nuklear Malaysia (MNA). Taburan populasi bahan api yang telah digunakan di reaktor MNA ditentukan menerusi model yang dibina menggunakan WIMS. Model ini cuba menghasilkan suasana dan keadaan yang serupa seperti di kawasan yang paling panas di reaktor tersebut, lantas kawasan yang paling tinggi pembakarannya. Teori asas evolusi masa untuk nuklid ini disiasat dan dibandingkan dengan hasil daripada model. Persamaan yang baik untuk nilai teori evolusi masa dengan populasi nuklid Uranium-235, Uranium-236, Uranium-238 dan Plutonium-239 telah diperolehi.

Keywords: Burnup, WIMS, modelling, data fitting, population, fissile materials, breeding materials, research reactor, fuel management, Bateman equation.

Introduction

The TRIGA MARK-II reactor at the Malaysian had been established since 1983 under the pseudonym PUSPATI and has a respectable history of research in the application of nuclear technology. This research reactor provides facilities for Neutron Activation Analysis (NAA), isotope productions, small angle neutron scattering (SANS) and numerous other services for use within the agency, universities and private companies. Study of fuel burnup is essential for fuel management and the provision of services. Common computer codes for calculating burnup are ORIGEN, WIMS and MCNPX[4][8][1]. WIMS are chosen due to its versatility in computation of various parameters and its ability to keep track the populations of various fission yields including fissile and breeding materials. Due to its deterministic nature, it is fairly easy and fast to implement.

Time evolution of the nuclides is studied in order to explore the processes involved in dictating the population of the said nuclides due to burnup. Actinides chosen for this study are ^{235}U, ^{236}U, ^{238}U and ^{239}Pu. WIMS [2] can generate the burnup population of those nuclides and fitted based on the equation developed later. The goodness of fit depends largely on the understanding of relevant physics. From the equations, we hope to glean informations on fission yield of TRIGA type fuel. For good estimation, we focus our attention on the B ring. Fuel elements in the B ring experience the most severe burnup and WIMS can calculate the hottest position on the fuel.

WIMS Model

The model is a typical TRIGA MARK-II $UZrH_{1.6}$ fuel of ^{235}U 20% enriched. The content of Uranium is 8.5 wt%, and the rest of the weight is due to the Hydrided Zirconium. The fuel is produced by

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heating ZrU alloy at high temperatures in hydrogen filled atmosphere. Fuel meat is cylindrical, with zirconium rod fitted at the centre bore, and the whole structure are enclosed with Stainless Steel 304 (SS-304) cladding. Geometry information required for WIMS output are illustrated in Table 1, showing a series of annulus from the central Zirconium rod, followed by the fuel meat, air gap, cladding and the surrounding water.Although the model is only 2D model of a single fuel, it is trivial to extract the required 3D information.

Table 1: Geometry Input for WIMS

Materials	Annulus (cm)
Zironium Rod	0.3175
Fuel Meat	1.8150
Air Gap	1.8240
Cladding	1.8770
Water	2.3859

WIMS takes information regarding material composition in terms of the atomic density of the materials in barns. From the density of each isotope in our material of interest, ρ_i is calculated by the formula,

$$N_i = \frac{0.6022\rho_i}{A_i} \text{ atoms. cm}^{-3} \text{ b}^{-1} \tag{1}$$

Each materials also sport different levels of temperature, such as 493 K in the fuel meat and 310 K elsewhere. These values does not need to be particularly realistic as it serves only to enable the code to calculate it consistently. Also required is the user judgment on the the materials spectrum. This spectrum enables the identification whether the material is treated as fuel (n=1), cladding (n=2), coolant (n=3) and moderator (n=4) for the purpose of resonance cross section evaluations and for use in preliminary calculation. Table 2 summarizes the information required for input in WIMS such as material composition, spectrum and temperature as we have just discussed. It must be noted that the given atom density for Plutonium is just an arbitrary assignment of values designed to prevent WIMS from crashing.

Table 2: Summary of materials composition and the relevant spectrum and temperature values. Material are identified by IDs (Zirconium Rod=1; Fuel Meat=2; Air Gap=3; Cladding=4; Water Surround=5).

Material	Temp.(K)	Spect.	Isotopes	WIMS ID	Atom Densities
1	310	2	Zirconium	91	0.042846
2	493	1	Zirconium	91	0.034143
			Hydrogen	2191	0.054641
			Uranium-235	235.4	0.000251
			Uranium-238	238.4	0.000990
			Plutonium-239	3239	1.0E-12
3	310	2	Nitrogen	14	0.0000001
4	310	2	Carbon	12	0.000316
			Manganese	55	0.001730
			Chromium	52	0.018274
			Nickel	58	0.008904
			Nitrogen	14	0.000339
			Iron	56	0.056844
5	310	3	Hydrogen	2001	0.066856
			Oxygen	16	0.033428

The calculation of burnup requires estimates on fission counts for each second in a centimetre cube of volume. This calculation proceed as follows. TRIGA MARK-II research reactor belonging to MNA has a total power of 1 MW which currently accommodate 115 fuel elements (including fuel follower control rods). The average power contribution of each element is

$$\bar{P} = \frac{1000 \text{ kW}}{115} = 8695.652173913 \text{ W element}^{-1} \tag{2}$$

Before proceeding, let us consider our methodology for extrapolating this 2D code for application on 3D problems as we had promised earlier in the introduction. The TRIGA MARK-II reactor core is a ring type reactor core, 6 rings in total not including the central thimble. Due to the radial variation of power, each ring contributes differently to the total reactor power. Power as well as burnup is thus higher nearer to the central thimble, in this case the B ring (nearest ring to central thimble) is higher than C ring and so on, with the lowest power contribution given by the G ring. This distribution of power are thus aptly called the pin peaking factor (PPF). PPF is calculated by dividing the power contribution of the fuel pin in question with the average power calculated by equation (2).

This property is not an exclusive property of the core in radial directions, as the same phenomena are also observed axially. The axial distribution of power is defined as the axial peaking factor(APF) [6]. APF calculation first require us to split the fuel into several sections. In this paper, we split our fuel into 11 sections and the APF of the section under question is due to the ratio of power contributed by that section with the average power in each section. Both APF and PPF parameters can be obtained through experimental design.

The study however relied on MCNP for the power calculation of each fuel pin and its axial contribution. Once both parameters, PPF and APF is obtained, 3D distribution of power may be obtained by multiplying PPF and APF. The combination of both peaking factors are conveniently termed as the combined peaking factor (CPF). Table 3 illustrates the APF, PPF and CPF of various fuel locations and its section in the reactor but we limit our calculation only up to F ring because the power concentration is very small and consist mostly of empty locations.

Table 3: APF, PPF and CPF values of various fuel position and its sections.

Position	APF	B ring PPF=1.38	C ring PPF=1.24	D ring PPF=1.05	E ring PPF=0.83	F ring PPF=0.65
36.3682	0.6	0.828	0.744	0.63	0.498	0.39
32.9045	0.8	1.104	0.992	0.84	0.664	0.52
29.4409	0.99	1.3662	1.2276	1.0395	0.8217	0.6435
25.9773	1.14	1.5732	1.4136	1.197	0.9462	0.741
22.5136	1.24	1.7112	1.5376	1.302	1.0292	0.806
19.0500	1.28	1.7664	1.5872	1.344	1.0624	0.832
15.5864	1.25	1.725	1.55	1.3125	1.0375	0.8125
12.1227	1.17	1.6146	1.4508	1.2285	0.9711	0.7605
8.6591	1.03	1.4214	1.2772	1.0815	0.8549	0.6695
5.1955	0.84	1.1592	1.0416	0.882	0.6972	0.546
1.7318	0.66	0.9108	0.8184	0.693	0.5478	0.429

The hottest position in the B ring is at 19.05 cm from the bottom of the fuel, given by its CPF of 1.7664. In terms of Watt, this is equivalent to,

$$P_{B,x=19.05} = \text{CPF}_{x=19.05} \times \bar{P} = 1.7664 \times 8695.652173913 \text{ W} = 15360 \text{ W} \tag{3}$$

Power density is equivalent to,

$$\wp_W = \frac{P_{B,x=19.05}}{38.1\pi \ (1.815^2 - 0.3175^2)} = \frac{15360}{382.235235762} = 40.184678342 \text{ Wcm}^{-3} \tag{4}$$

Given that $1 \text{ W} = 1 \text{ Js}^{-1} = 6.24150974 \times 10^{18} \text{ eV s}^{-1}\text{cm}^{-3}$, we can rephrase equation (4) as

$$\wp_{eV} = 40.184678342 \times \left(6.24150974 \times 10^{18}\right) = 2.508130613 \times 10^{20} \text{ eV s}^{-1}\text{cm}^{-3} \tag{5}$$

Since a single fission produces 200 MeV of energy, the total amount fission in that section is

$$N_{fission} = \frac{\wp_{eV}}{200 \times 10^6} = 1.254065307 \times 10^{12} \tag{6}$$

This fission count is required for burnup calculation along with information on burnup time step and the total irradiation period. We supplied WIMS with an irradiation time of 1000 days, equivalent to the total operation time since 1983 at MNA reactor. The time step is 0.1 days, this time resolution is sufficient to observe most large scale process influencing the nuclide population.

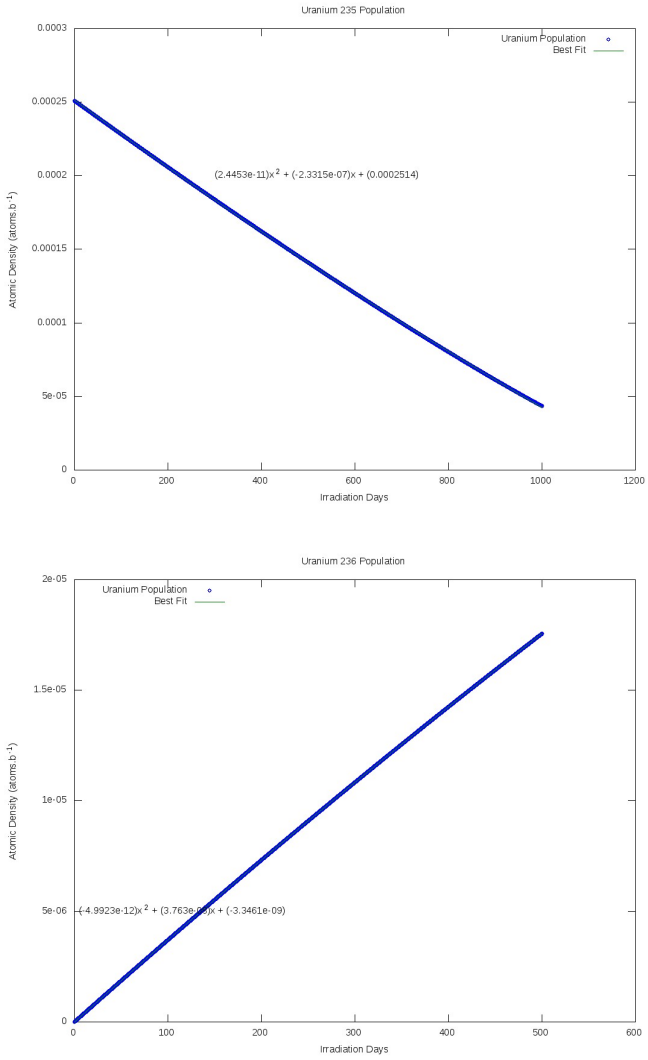

Figure 1: Population of Uranium 235 and Plutonium 236 as a function of Irradiation Time.

Results and Discussion

Materials irradiated by neutrons are treated analytically through the Bateman equation [7] [9] for comparison with WIMS result. The Bateman equation for the purpose of this paper is usually described as a function of population change, dependent on the current isotope population, N_i, fission cross section, σ_f, neutron capture cross section, σ_c and its decay constant, λ.

$$\frac{d\,N_i}{dt} = \sigma_{c,i-1}N_{i-1}\Phi - \sigma_{c,i}N_i\Phi - \sigma_{f,i}N_i\Phi - \lambda N_i \tag{7}$$

Figure (1) describe the time evolution of Uranium-235 and Uranium-236 population in TRIGA fuels for 1000 days. The second order polynomial interpolation result are:

$$N(t) = (2.4453 \times 10^{-11})\,t^2 - (2.3315 \times 10^{-7})\,t + 0.0002514 \tag{8}$$

First order polynomial interpolation are fairly accurate if we limit the interpolation period to 300 days from the initial burnup.

$$N(t) = 0.00025072 - (2.2377 \times 10^{-7})\,t \tag{9}$$

Analytical solution for Uranium-235 are possible given the following WIMS result on thermal absorption macroscopic cross section $\Sigma_a(E)$ and the corresponding normalized neutron flux $\Phi(E)$.

$$\Sigma_a(E) = 1.2453 \times 10^{-1} \quad ; \quad \Phi(E) = 1.66524 \times 10^{-2}\,\mathrm{ns}^{-1}\mathrm{cm}^{-2} \tag{10}$$

For comparison with interpolated values, it is convenient to use microscopic absorption cross section and rephrase the flux in term of days, hence

$$\sigma_a(E) = \frac{\Sigma_a(E)}{N_0} = 496.14 \quad ; \quad \Phi(E) = \frac{1.66524 \times 10^{-2}\,\mathrm{ns}^{-1}\mathrm{cm}^{-2}}{8640s} = 1.9274 \times 10^{-6} \tag{11}$$

The relationship between σ_f and σ_c with σ_a are $\sigma_a = \sigma_f + \sigma_c$. We consider the case where the 235 isotope of Uranium are not increasing as a result of neutron capture of lighter isotopes. Due to the Uranium long decay time, we can also drop the decay term from our solution. By Laplace transform, the solution is

$$N_{235}(t) = N_{235}(0)\, e^{-\sigma_a \Phi\, t} = 0.000251\, e^{-\,9.5623\times 10^{-4}\, t} \tag{12}$$

Comparison with our polynomial interpolation can be made by the first and second order Taylor approximation of equation (12), leading us to the following expressions for first order polynomial,

$$\begin{aligned} N_{235}(t) &= N_{235}(0)\,(1 - \sigma_a \Phi\, t) && \text{(13a)} \\ &= 0.000251\left[1 - (9.5623 \times 10^{-4})\, t\right] \\ &= 0.000251 - \left(2.4001 \times 10^{-7}\right) t && \text{(13b)} \end{aligned}$$

and second order polynomial,

$$\begin{aligned} N_{235}(t) &= N_{235}(0)\left(1 - \sigma_a \Phi\, t + \frac{1}{2}\sigma_a^2 \Phi^2\, t^2\right) && \text{(14a)} \\ &= 0.000251\left[1 - (9.5623 \times 10^{-4})\, t + \frac{1}{2}(9.1438 \times 10^{-7})\, t^2\right] \\ &= 0.000251 - \left(2.4001 \times 10^{-7}\right) t + \left(1.1475 \times 10^{-10}\right)\, t^2 && \text{(14b)} \end{aligned}$$

Errors are due to the coarse time resolution and generating the data for the same period with even finer time resolution are beyond the capabilities of WIMS. Another source of error are due to fission from a variety of other isotopes. Since only the energy averaged cross section are given for the particular fuel zone, the contributions from a variety of other isotopes complicates the problem. For Uranium-235 however, we can rest assure that the contributions by other isotopes are minimal largely because of the larger population of Uranium-235.

Uranium-236 evolution can be calculated by similar procedure. We obtain the microscopic neutron capture cross section and the adjusted neutron flux at high energy,

$$\begin{aligned} \sigma_{c,235}(E') &= \frac{\Sigma_a(E')}{N_{0,235}} - \frac{\Sigma_f(E')}{N_{0,235}} = 25.234 && \text{(15a)} \\ \Phi(E') &= 4.4636 \times 10^{-6}\ \mathrm{n.days}^{-1}\mathrm{cm}^{-2} && \text{(15b)} \end{aligned}$$

Variation of Uranium-236 are due to neutron capture of Uranium-235, thus with regards to the Bateman equation, the differential equation may be written as

$$\frac{d\, N_{236}(t)}{dt} = \sigma_{c,235}(E')\Phi(E')N_{235}(t) \tag{16}$$

The solution for equation (16) is obtained by inserting our result for

$$N_{236}(t) = \left(2.8271 \times 10^{-8}\right)\, t - \left(1.3517 \times 10^{-11}\right) t^2 \tag{17}$$

Comparing this equation with the interpolation result of Uranium-236

$$N_{236}(t) = -\left(3.0604 \times 10^{-8}\right) + \left(3.7949 \times 10^{-8}\right)\, t - \left(5.5849 \times 10^{-12}\right)\, t^2 \tag{18}$$

The result is acceptable given the amount of uncertainty in our basic data. In our WIMS version, it does not calculate the transmutation of Uranium-237 from Uranium-236. As a consequence, there is no benchmark data for Uranium-237 and also no neutron capture of Uranium-237 which results in the formation of Uranium-238. For Uranium-238, the decay rate can be written simply as

$$\frac{d\,N_{238}(t)}{dt} = -\sigma_a \Phi N_{238} \tag{19}$$

The value σ_a, encompass all energies. Given the following data,

$$\sigma_a(E) = \frac{\Sigma_a(E)}{N_{238}(0)} = 125.79 \;;\; \sigma_a(E') = \frac{\Sigma_a(E')}{N_{238}(0)} = 9.2964 \tag{20a}$$

$$\Phi(E) = 1.9274 \times 10^{-6}\ \text{n.days}^{-1}\text{cm}^{-2} \;;\; \Phi(E') = 4.4636 \times 10^{-6}\ \text{n.days}^{-1}\text{cm}^{-2} \tag{20b}$$

We require σ_a and corresponding Φ for all energies [3] calculated by the formulation below

$$\sigma_a = \frac{\sigma_a(E)\Phi(E) + \sigma_a(E')\Phi(E')}{\Phi(E) + \Phi(E')} = 40.738 \tag{21a}$$

$$\Phi = \frac{\sigma_a(E)\Phi(E) + \sigma_a(E')\Phi(E')}{\sigma_a(E) + \sigma_a(E')} = 2.1019 \times 10^{-6}\ \text{n.days}^{-1}\text{cm}^{-2} \tag{21b}$$

The solution is

$$N_{238}(t) = 0.000990\ e^{-\left(8.5627\times 10^{-5}\right)t} \tag{22}$$

and could be approximated by

$$N_{238}(t) = 0.000990 - \left(8.4771 \times 10^{-8}\right) t + \left(3.6293 \times 10^{-12}\right) t^2 \tag{23}$$

Figure 2 shows the population of Uranium-238 and Plutonium-239 by WIMS and the interpolation of the result. For Plutonium isotopes, purely analytic solution are difficult to derive because the initial conditions for Plutonium are assumed to be zero. We could use some very small value but the result is very inaccurate. Initial values are essential in deriving the cross section. Arbitrary assignments of initial condition would give a random cross section. Alternatively, we could explore some semi-analytic techniques but such discussion are better served in a different paper. Hence, for Plutonium-239, the approach from hereon would be to solve its time evolution without any direct comparison with WIMS data.

The increment of Plutonium-239 population by neutron capture of Uranium-238 and its depletion as the result of absorption is illustrated by the following differential equation

$$\frac{d\,N_{239}(t)}{dt} = N_{0,238} e^{\sigma_{c,238}\Phi\, t} - \sigma_{a,239}\Phi N_{239}(t) \tag{24}$$

thus the time evolution for Plutonium-239 is

$$N_{239}(t) = \frac{N_{0,238}}{\sigma_{a,239}\Phi + \sigma_{c,238}\Phi}\left[e^{\sigma_{c,238}\Phi\, t} - e^{-\sigma_{a,239}\Phi\, t}\right] + N_{239}(0) e^{-\sigma_{a,239}\Phi\, t} \tag{25}$$

Interpolating two or more exponential terms is difficult using the usual method by least square fit of logarithmically transformed data. Our approach for the fitting of Plutonium isotopes are based on the modified Prony method[5]. Plutonium-239 Prony interpolation result is

$$N_{239}(t) = \left(7.5788 \times 10^{-6}\right)\ e^{\left(5.9911\times 10^{-5}\right)t} - \left(7.7183 \times 10^{-6}\right)\ e^{-0.002932\, t} \tag{26}$$

As we can see, by re-arranging equation (25) we obtain similar form with our interpolation,

$$N_{239}(t) = \frac{N_{0,238}}{\sigma_{a,239}\Phi + \sigma_{c,238}\Phi}\ e^{\sigma_{c,238}\Phi\, t} - \left[\frac{N_{0,238}}{\sigma_{a,239}\Phi + \sigma_{c,238}\Phi}\ - N_{239}(0)\right] e^{-\sigma_{a,239}\Phi\, t} \tag{27}$$

It gives an excellent fit for Plutonium-239 however it must be noted that the Prony method approach to fitting is based on parameter prediction instead of the usual error minimization, thus it is mathematically ill defined. Further transmutation is difficult to express analytically and will result in an expression with multiple exponential terms. Even with the Prony method, a satisfactory solution is difficult to obtain. Our attempts with the Prony method to fit other Plutonium isotopes produce complex values (cosine function), inconsistent with our problem. We summarize our result in Table 4. We will not discuss the derivation for the rest of the Plutonium isotope because the derivation requires semi-analytical approach aptly explored in a different paper.

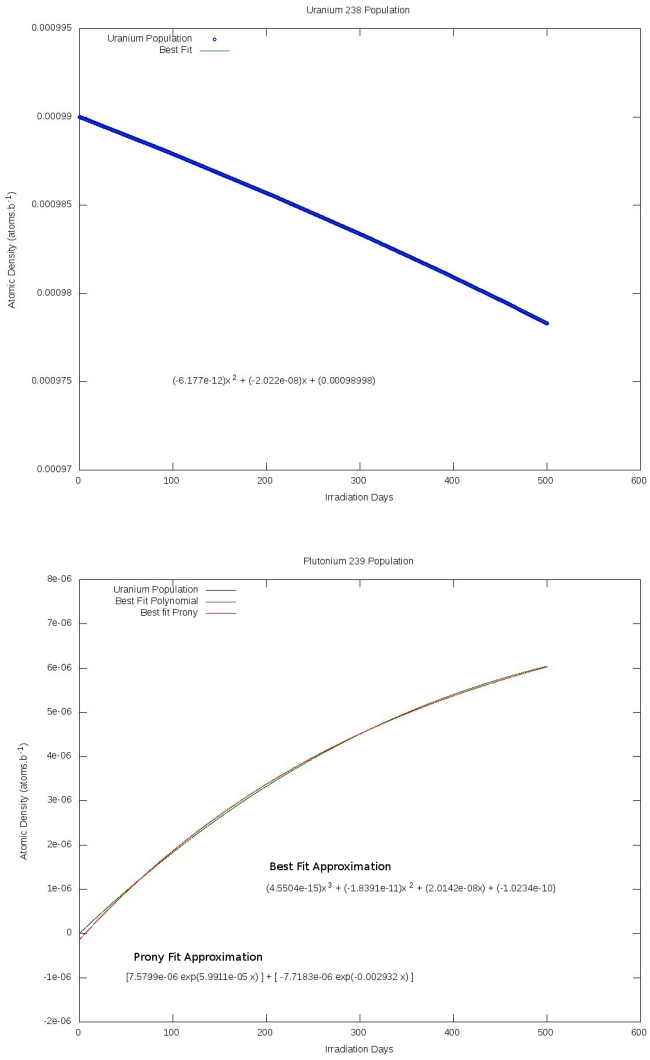

Figure 2: Population of Uranium 238 and Uranium 239 as a function of Irradiation Time.

Conclusion

This paper developed a WIMS pincell model and extract the burnup information for the hottest location. Our attention focus upon the time evolution of selected Uranium and Plutonium isotopes. We select Uranium-235, Uranium-236, Uranium-238 and Plutonium-239 as our study samples, and the data are interpolated. Polynomial coefficients provide useful information for comparison with analytical models. The analytical models are build based off the average cross section and average flux from our WIMS output. The approach was successful for Uranium-235, Uranium-236 and Uranium-238. It solves the Bateman equation for each nuclide. Afterwards, Taylor approximation of the said nuclide are performed to obtain the power series representation of our Bateman equation solution. The polynomial coefficient could then be compared with our power series. The examination reveals agreement between analytical method and WIMS within reasonable errors. Most of the errors are due to discretization errors and the energy averaging procedure.

Plutonium however are produced only after the initial irradiation. Solving for Plutonium required however a whole different technique. For this reason, we do not proceed in the previous fashion. Instead, we decide to merely display the interpolation of our results. We do however produce similar form in our derivation for Plutonium-239 and the interpolation by Prony method. Unfortunately, the Prony

Table 4: Time Evolution Results of: [1] Polynomial Interpolation [2] Analytical Derivation [3] Prony Interpolation

Isotope	Time Evolution	
^{235}U	$(2.4453 \times 10^{-11})\, t^2 - (2.3315 \times 10^{-7})\, t + 0.0002514$	[1]
	$0.000251 - (2.4001 \times 10^{-7})\, t + (1.1475 \times 10^{-10})\ t^2$	[2]
^{236}U	$(3.0604 \times 10^{-8}) + (3.7949 \times 10^{-8})\ t - (5.5849 \times 10^{-12})\ t^2$	[1]
	$(2.8271 \times 10^{-8})\ t - (1.3517 \times 10^{-11})\, t^2$	[2]
^{238}U	$(-6.177 \times 10^{-12})\, t^2 - (2.022 \times 10^{-8}) + 0.00098998$	[1]
	$0.000990 - (8.4771 \times 10^{-8})\, t + (3.6293 \times 10^{-12})\, t^2$	[2]
^{239}Pu	$(4.5504 \times 10^{-15})\, t^3 - (1.8391 \times 10^{-11})\, t^2 + (2.0142 \times 10^{-8})\, t - (1.0234 \times 10^{-10})$	[1]
	$(7.5788 \times 10^{-6})\ e^{(5.9911 \times 10^{-5})t} - (7.7183 \times 10^{-6})\ e^{-0.002932\, t}$	[3]

method are unable to interpolate for Plutonium-240, Plutonium-241 and Plutonium-242, giving us cosine solutions; contrary to our expectations. This is due to the parameter prediction nature of the Prony method, different from the usual interpolation based on error minimizations. Since there is no recourse in validating our derivation, we decide to drop any derivations for the other Plutonium isotopes. Future endeavor will focus upon semi-analytic derivations and sampling more energy groups for better agreement between theory and WIMS result. Inevitably, complete independence of WIMS result for deriving our solutions are explored given enough time and familiarity with neutron transport theory.

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