Benchmark 15-A2 calculated with milonga

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1 Introduction

1. The benchmark ANL-7416-15A2 [2] was calculated using the milonga code.
2. The function of this benchmark is to test solutions of the neutronic depletion equations.
3. It is a infinite homogeneus nuclear reactor with isotopic concentrations given. At time zero, the neutron flux becomes nonzero.
4. The codes used were:

   wasora 0.4.117 (14dccdd2711f+ 2016-07-18 11:38 -0300) [3]

   wasora's an advanced suite for optimization & reactor analysis

   rev hash 14dccdd2711f7eea767f5b6a01aa509235e385e4

   last commit on 2016-07-18 11:38 -0300 (rev 272)

   compiled on 2016-07-18 21:00:58 by pablo@pablo (linux-gnu x86_64)

   with gcc (Debian 4.9.2-10) 4.9.2 using -O2 and linked against

   GNU Scientific Library version 1.16

   SUNDIALs Library version 2.5.0

   GNU Readline version 6.3

   wasora is copyright (C) 2009-2016 jeremy theler

   licensed under GNU GPL version 3 or later.

   wasora is free software: you are free to change and redistribute it.

   There is NO WARRANTY, to the extent permitted by law.
5. You also can use milonga [4] because it is a plugin of wasora.

2 Benchmark information

1. Solution of isotopic depletion equations at a point with constant flux and cross sections.

   $$\frac{d\mathbf{N}(t)}{dt} = \mathbf{A} \cdot \mathbf{N}(t) \tag{1}$$

   where

   $\mathbf{N}$ = vector of isotopic concentrations

   $\mathbf{A}$ = net production matrix coupling isotopes
2. The general ij^{th} entry in $\mathbf{A}$ (i.e., the production rate of isotope i form isotope j) is

   $$A_{ij} = Y_{ij} \sum_g \sigma^g_{fj} \Phi^g + \lambda_{ij} + \sum_g \sigma^g_{c_{ij}} \Phi^g \tag{2}$$

   where

   g = energy group index

   Y_{ij} = fission yield of isotope i from the fissioning of isotope j (Y_{ii} is defined as -1)

   σ^g_{fj} = microscopic fission cross section of isotope j in group g

   Φ^g = flux in group g

   λ_{ij} = decay constant for production of isotope i from the decay of isotope j (λ_{ii} is the negative of the decay constant)

   $\sigma^g_{c_{ij}}$ = microscopic capture cross section in group g for isotope j that produces i ($\sigma^g_{c_{ii}}$ is the negative of the capture cross section)

3. Constant two-group flux:

    3.1 Group 1 $= 6.1374 \cdot 10^{14} \frac{n}{cm^2\ s}$

    3.2 Group 2 $= 2.5078 \cdot 10^{14} \frac{n}{cm^2\ s}$

4. Fission product yields are defined in the Table 1.

5. Decay constants are defined in the Table 2.

6. The (n,2n) microscopic cross sections are defined in the Table 3.

7. The initial conditions are shown in the Table 4.

8. Microscopic cross sections are defined in Table 5.

9. The α and β^+ decay were not excluded from the depletion chain, see the Figure 1 and the Figure 2. So $\mathbf{A}$ is not a triangular matrix [2].

3 Expected results

1. The benchmark asks the following results:

    1.1 Variation of isotopic concentrations with time; 50-day concentrations.

    1.2 Calculational statistics.

4 Solutions available

1. Fourth-order Runge-Kutta of depletion: 15-A2-1 [2]

2. Matrix exponential method and finite difference solution: 15-A2-2 [2]

5 Solution

1. The Equation 2 is written differently as:

$$A_{ij} = Y_{ij}\boldsymbol{\sigma_{fj}} \cdot \boldsymbol{\Phi} + \lambda_{ij} + \boldsymbol{\sigma_{c_{ij}}} \cdot \boldsymbol{\Phi} \tag{3}$$

   where

$$\boldsymbol{\Phi} = \begin{bmatrix} 6.1374 \cdot 10^{14} \\ 2.5078 \cdot 10^{14} \end{bmatrix} \tag{4}$$

   $\boldsymbol{\sigma_{fj}}$ and $\boldsymbol{\sigma_{c_{ij}}}$ for $i = 13,\ j = 12$ are (from Table 5):

$$\boldsymbol{\sigma_{f,12}} = \begin{bmatrix} 14.403 \\ 348.89 \end{bmatrix}; \quad \boldsymbol{\sigma_{c_{13,12}}} = \begin{bmatrix} 9.8658 \\ 196.77 \end{bmatrix}$$

   note that $\boldsymbol{\sigma_{c_{i,12}}}$ is zero when $i \neq 13$. It means that ^{239}Pu becomes ^{240}Pu when it absorbs a neutron.

2. The β^+ and the α decay were appended to $\boldsymbol{\lambda}$. The ^{242}Am can decay by β^+ or β^-, so its decay constant is the sum of both ones.

3. The (n,2n) reaction was added to $\boldsymbol{\sigma_{c_{ij}}}$ in this way:

$$^{A}Isotope + n \rightarrow ^{A-1} Isotope + 2n \tag{5}$$

Table 1: Fission product yield, [%]

Fission product	Fissioning isotope			
	^{235}U	^{238}U	^{239}Pu	^{241}Pu
^{135}I	6.17	5.78	6.93	6.26
^{135}Xe	0.24	0.22	0.27	0.24
^{149}Pm	1.13	2.1	1.3	1.2
^{147}Nd	2.36	2.8	2.05	2.2
Long-lived fission products	90.1	89.1	89.45	90.1

4. The results are shown in the Table 6 with a comparison with one of the results from the solution 15-A2-1 [2]. Note that the units were translated into $atom/cm^3$ and FP means fission products.

5. The diference in the Table 6 is among the milonga results and the [2] one.

6. The maximum difference was in the isotope ^{243}Cm. It is considered unimportant because the results of the isotope ^{242}Cm, from which ^{243}Cm appears, and the isotope ^{244}Cm, in which ^{243}Cm becomes, were similar in these results and in [2].

7. The time evolution of each isotope's numerical density can be seen in the Figure 3, the Figure 4, the Figure 5, the Figure 6, the Figure 7, the Figure 8, and the Figure 9.

6 milonga's input file

1. There are two keywords which are more or less new:

   rel_error: It sets the relative numerical error in each variable. If it is too small, the calculation could not converge and finish in a messge error.

   INITIAL_CONDITIONS_MODE FROM_VARIABLES: The IDA library needs the derivative of the vector being solved at time zero: $\dot{\mathbf{N}}(0)$. This keyword asks milonga calculate it. If it were not used, the user would have to initiate $\dot{\mathbf{N}}(0)$. If not, the calculation could not converge or give a message error.

7 Excercise

1. Print the matrices $\mathbf{Y}$, $\boldsymbol{\sigma_f}$, $\boldsymbol{\lambda}$, $\boldsymbol{\sigma_c}$ and $\mathbf{A}$.

8 References

[1] FDL licence. https://www.gnu.org/licenses/fdl-1.2-standalone.html

[2] ANL-7416-15A2. http://www.corephysics.com/benchmarks/anl7416_benchmark15.pdf

[3] Wasora code. https://bitbucket.org/wasora/wasora

[4] Milonga code. https://bitbucket.org/wasora/milonga/overview

Figure 1: Depletion chains for the actinides

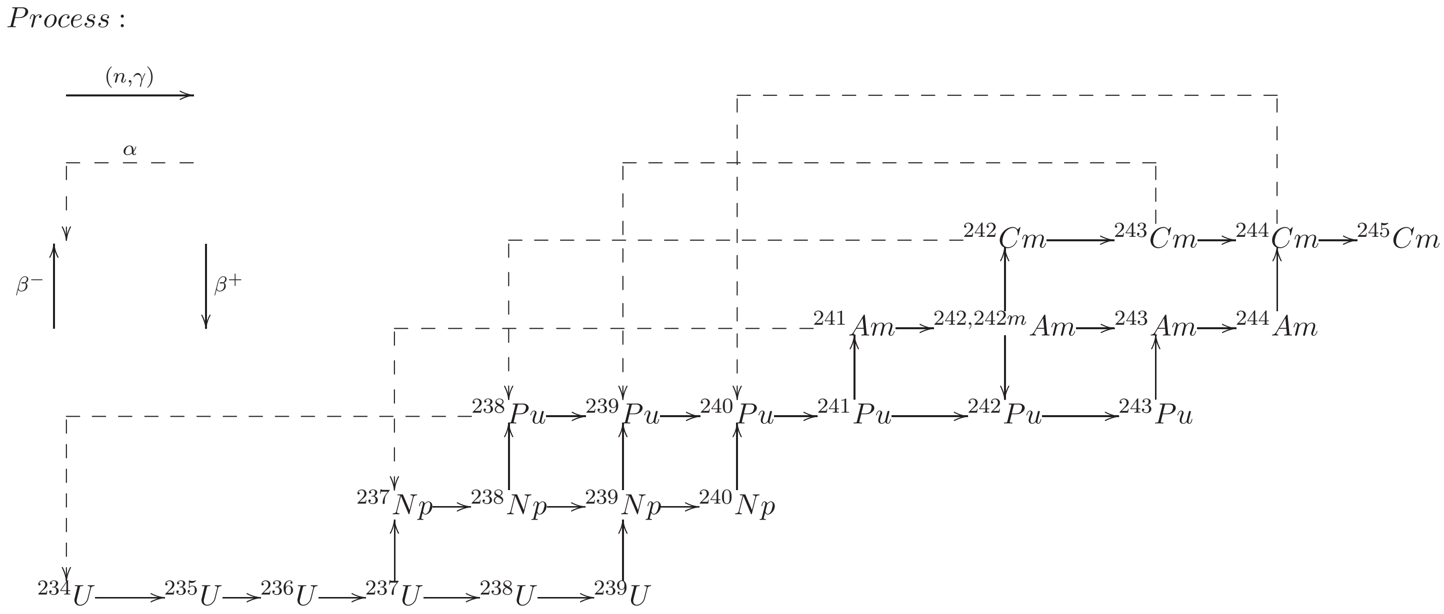

Figure 2: Depletion chains for the fission products

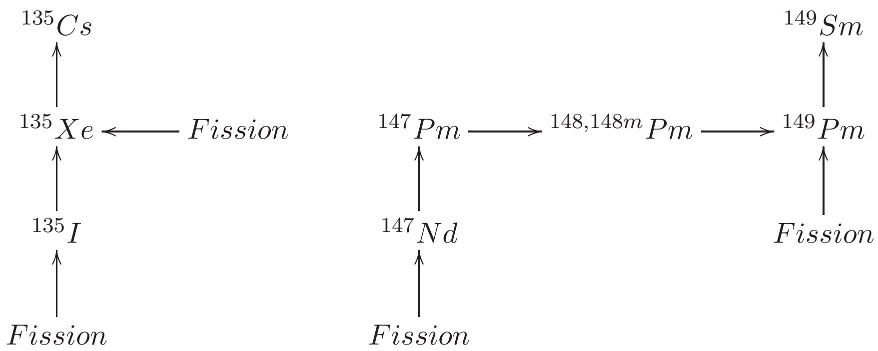

Table 2: Decay constants

Isotope	Emitted particle	Decay constant, s^{-1}
^{135}I	β^-	$2.874 \cdot 10^{-5}$
^{135}Xe	β^-	$2.093 \cdot 10^{-5}$
^{147}Nd	β^-	$7.228 \cdot 10^{-7}$
^{147}Pm	β^-	$8.289 \cdot 10^{-9}$
^{148}Pm	β^-	$1.488 \cdot 10^{-6}$
^{148m}Pm	β^-	$1.976 \cdot 10^{-7}$
^{149}Pm	β^-	$3.626 \cdot 10^{-6}$
^{237}U	β^-	$1.19 \cdot 10^{-6}$
^{239}U	β^-	$4.915 \cdot 10^{-4}$
^{238}Np	β^-	$3.82 \cdot 10^{-6}$
^{239}Np	β^-	$3.41 \cdot 10^{-6}$
^{240}Np	β^-	$1.583 \cdot 10^{-3}$
^{238}Pu	α	$2.55 \cdot 10^{-10}$
^{241}Pu	β^-	$1.68 \cdot 10^{-9}$
^{243}Pu	β^-	$3.886 \cdot 10^{-5}$
^{241}Am	α	$5.09 \cdot 10^{-11}$
^{242}Am	β^-	$9.93 \cdot 10^{-6}$
^{242}Am	β^+	$2.03 \cdot 10^{-6}$
^{244}Am	β^-	$4.44 \cdot 10^{-4}$
^{242}Cm	α	$4.91 \cdot 10^{-8}$
^{243}Cm	α	$6.86 \cdot 10^{-10}$
^{244}Cm	α	$1.25 \cdot 10^{-9}$

Table 3: (n,2n) Microscopic Cross Sections (Group 1 only)

Isotope	$\sigma[10^{-24} cm^2]$
^{235}U	0.002603
^{238}U	0.0043972
^{237}Np	0.00020144

Table 4: Initial conditions

Isotope	**Concentration** [atom/cm^3]
^{235}U	$0.74003\ 10^{20}$
^{238}U	$0.6936\ 10^{22}$

Table 5: Microscopic cross sections, [barns]

Isotope	Isotope index	σ_{c_1}	σ_{c_2}	σ_{f_1}	σ_{f_2}	$\sigma^m_{(n,\gamma)_1}$	$\sigma^m_{(n,\gamma)_2}$
^{234}U	1	33.575	26.368	0.42744	0	0	0
^{235}U	2	5.9872	26.42	12.37	148.18	0	0
^{236}U	3	16.859	1.4399	0.16664	0	0	0
^{237}U	4	16.991	132.12	0.17139	0.55512	0	0
^{238}U	5	0.53258	0.73141	0.081338	0	0	0
^{239}U	6	0.40015	6.1613	0.27283	4.2009	0	0
^{237}Np	7	24.072	71.864	0.41867	0.009425	0	0
^{238}Np	8	5.2648	55.512	47.412	555.12	0	0
^{239}Np	9	26.341	16.654	0	0	0	0
^{240}Np	10	0	0	0	0	0	0
^{238}Pu	11	7.3125	119.91	1.5815	3.5496	0	0
^{239}Pu	12	9.8658	196.77	14.403	348.89	0	0
^{240}Pu	13	366.09	96.479	0.54033	0.016744	0	0
^{241}Pu	14	8.0305	152.24	29.986	352.73	0	0
^{242}Pu	15	51.82	5.1903	0.4346	0	0	0
^{243}Pu	16	11.03	21.649	28.382	49.96	0	0
^{241}Am	17	50.633	392.68	1.113	2.3817	6.7486	39.543
^{242}Am	18	2.3381	0	31.137	693.9	0	0
^{242m}Am	19	20.016	444.09	108.79	1776.4	0	0
^{243}Am	20	91.056	24.08	0.30784	0	0	0
^{244}Am	21	0	0	26.192	403.29	0	0
^{242}Cm	22	3.1202	1.7185	0	0.83267	0	0
^{243}Cm	23	9.9059	69.389	92.299	194.29	0	0
^{244}Cm	24	32.129	3.6915	1.5663	0.33307	0	0
^{245}Cm	25	4.8993	82.972	37.165	537.15	0	0
^{135}I	26	0	0	0	0	0	0
^{135}Xe	27	243.47	1064780	0	0	0	0
^{147}Nd	28	0	0	0	0	0	0
^{147}Pm	29	248.78	65.814	0	0	114.44	31.087
^{148}Pm	30	3368.4	420.09	0	0	0	0
^{148m}Pm	31	2921	7561.6	0	0	0	0
^{149}Pm	32	0	0	0	0	0	0
^{149}Sm	33	105.85	23387.4	0	0	0	0
Fission products	34	10.376	19.429	0	0	0	0

σ_{c_1} = capture in group 1 (all captures except fission and (n,2n); includes (n,γ) to excited state, if any).
σ_{c_2} = capture in group 2.
σ_{f_1} = fission in group 1.
σ_{f_2} = fission in group 2.
$\sigma^m_{(n,\gamma)_1}$ = (n,γ) to first excited state, group 1.
$\sigma^m_{(n,\gamma)_2}$ = (n,γ) to first excited state, group 2.

Table 6: Benchmark results

Isotope	milonga maximum Δt		15-A2-1 [2]	Difference [%]	
	1 hour	1 day	1 min	1 hour	1 day
^{234}U	4.29017 10^{14}	10^{14}	4.28817 10^{14}	4.66 10^{-2}	1.43
^{235}U	5.83315 10^{19}	10^{19}	5.83393 10^{19}	-1.34 10^{-2}	-4.1 10^{-1}
^{236}U	2.86193 10^{18}	10^{18}	2.86054 10^{18}	4.86 10^{-2}	1.48
^{237}U	3.5687 10^{16}	10^{16}	3.56768 10^{16}	2.86 10^{-2}	1.09
^{238}U	6.91915 10^{21}	10^{21}	6.91916 10^{21}	-1.45 10^{-4}	-4.19 10^{-3}
^{239}U	7.18361 10^{15}	10^{15}	7.18357 10^{15}	5.57 10^{-4}	-3.48 10^{-3}
^{237}Np	1.04823 10^{17}	10^{17}	1.04736 10^{17}	8.31 10^{-2}	2.78
^{238}Np	7.8119 10^{14}	10^{14}	7.80485 10^{14}	9.03 10^{-2}	2.96
^{239}Np	1.02944 10^{18}	10^{18}	1.02944 10^{18}	0	-3.89 10^{-3}
^{240}Np	1.32293 10^{13}	10^{13}	1.32292 10^{13}	-7.56 10^{-4}	-3.78 10^{-3}
^{238}Pu	4.42512 10^{15}	10^{15}	4.41854 10^{15}	1.49 10^{-1}	4.82
^{239}Pu	1.05792 10^{19}	10^{19}	1.05748 10^{19}	4.16 10^{-2}	1.33
^{240}Pu	9.96774 10^{17}	10^{17}	9.95892 10^{17}	8.86 10^{-2}	2.69
^{241}Pu	3.3467 10^{17}	10^{17}	3.34195 10^{17}	1.42 10^{-1}	4.45
^{242}Pu	1.64071 10^{16}	10^{16}	1.63736 10^{16}	2.05 10^{-1}	6.45
^{243}Pu	1.36631 10^{13}	10^{13}	1.36348 10^{13}	2.08 10^{-1}	6.5
^{241}Am	5.8755 10^{14}	10^{14}	5.8639 10^{14}	1.98 10^{-1}	6.29
^{242}Am	5.2204 10^{12}	10^{12}	5.20984 10^{12}	2.03 10^{-1}	6.43
^{242m}Am	5.06022 10^{12}	10^{12}	5.04819 10^{12}	2.38 10^{-1}	7.63
^{243}Am	4.58325 10^{14}	10^{14}	4.57037 10^{14}	2.82 10^{-1}	8.46
^{244}Am	6.37468 10^{10}	10^{10}	6.37996 10^{10}	-8.28 10^{-2}	8.08
^{242}Cm	4.51091 10^{13}	10^{13}	4.49667 10^{13}	3.17 10^{-1}	8.5
^{243}Cm	7.22665 10^{10}	10^{10}	9.50949 10^{10}	-2.40 10^{+1}	-1.64 10^{+1}
^{244}Cm	2.06679 10^{13}	10^{13}	2.06737 10^{13}	-2.81 10^{-2}	1.01 10^{+1}
^{245}Cm	2.43378 10^{11}	10^{11}	2.43318 10^{11}	2.47 10^{-2}	1.19 10^{+1}
^{135}I	8.82797 10^{15}	10^{15}	8.82738 10^{15}	6.68 10^{-3}	1.53 10^{-1}
^{135}Xe	9.14804 10^{14}	10^{14}	9.14753 10^{14}	5.58 10^{-3}	1.52 10^{-1}
^{147}Nd	1.21169 10^{17}	10^{17}	1.21154 10^{17}	1.24 10^{-2}	3.26 10^{-1}
^{147}Pm	2.01936 10^{17}	10^{17}	2.0181 10^{17}	6.24 10^{-2}	1.90
^{148}Pm	4.57349 10^{15}	10^{15}	4.57029 10^{15}	7 10^{-2}	2.11
^{148m}Pm	3.8698 10^{15}	10^{15}	3.86727 10^{15}	6.54 10^{-2}	2.09
^{149}Pm	1.99734 10^{16}	10^{16}	1.99679 10^{16}	2.75 10^{-2}	8.26 10^{-1}
^{149}Sm	1.19809 10^{16}	10^{16}	1.19776 10^{16}	2.76 10^{-2}	8.54 10^{-1}
FP	1.46224 10^{19}	10^{19}	1.45225 10^{19}	6.88 10^{-1}	2.41
Final time [days]	50.027	50.862	50	5.4 10^{-2}	1.72

Figure 3: U numerical densities

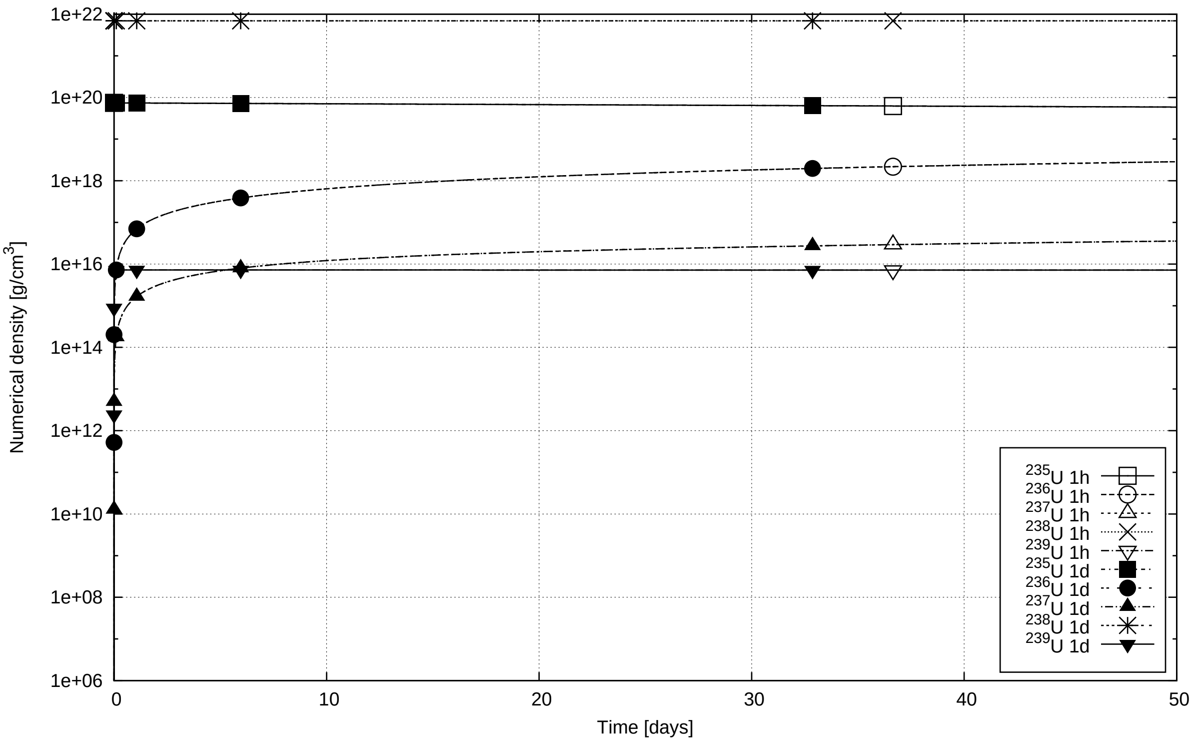

Figure 4: Pu numerical densities

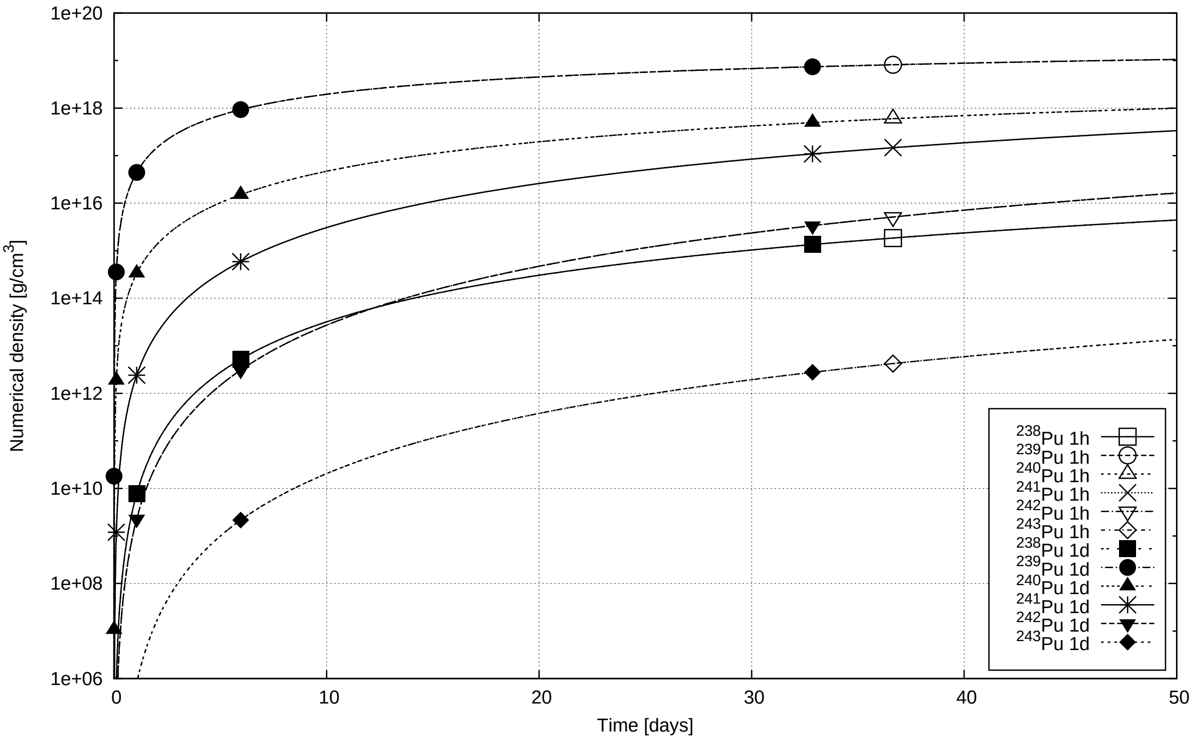

Figure 5: Np numerical densities

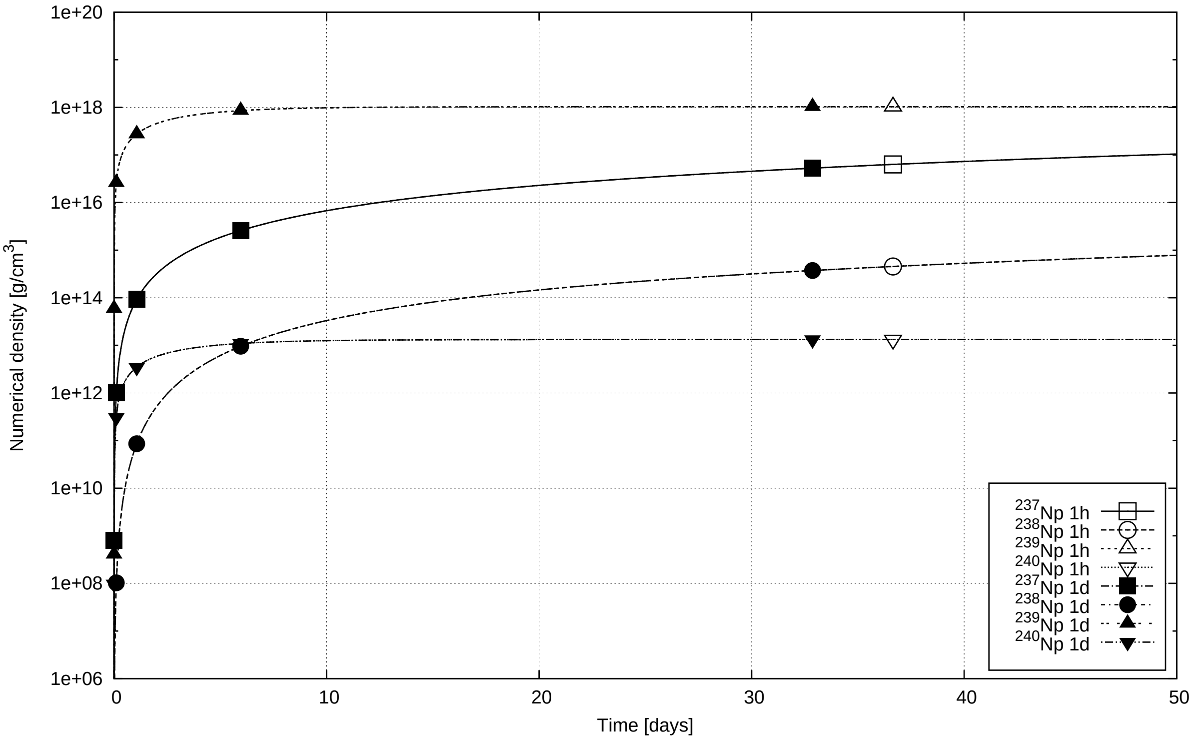

Figure 6: Am numerical densities

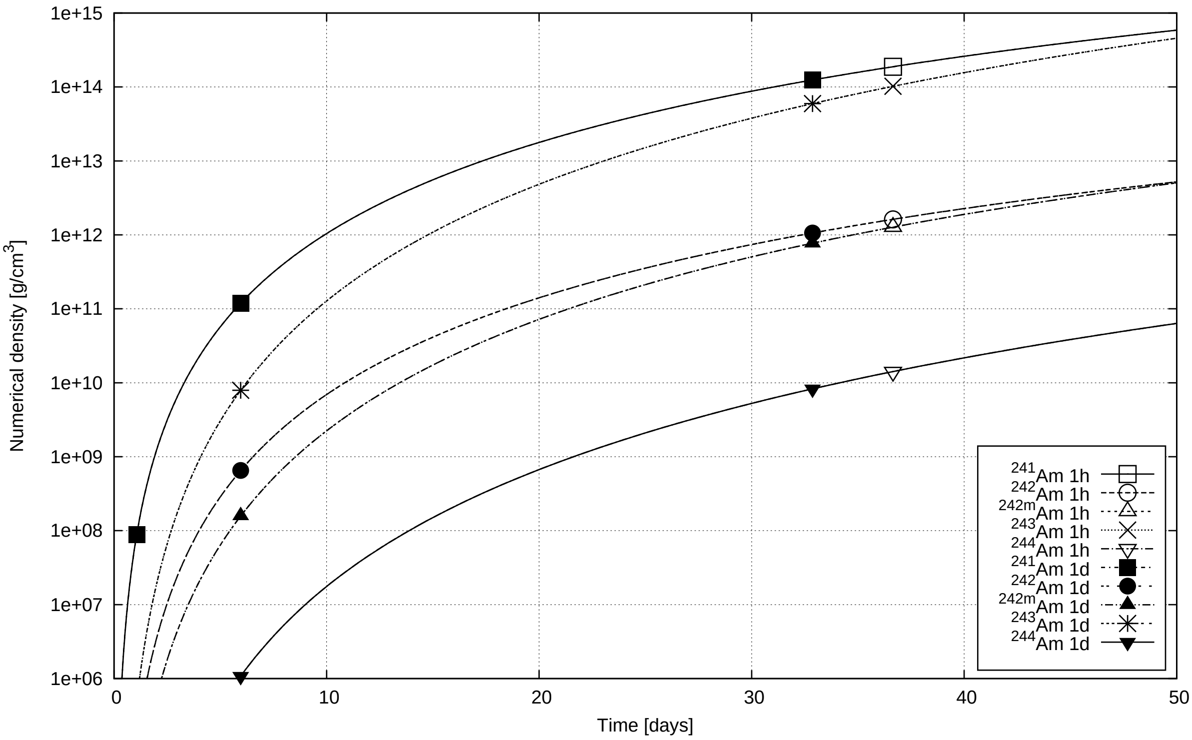

Figure 7: Cm numerical densities

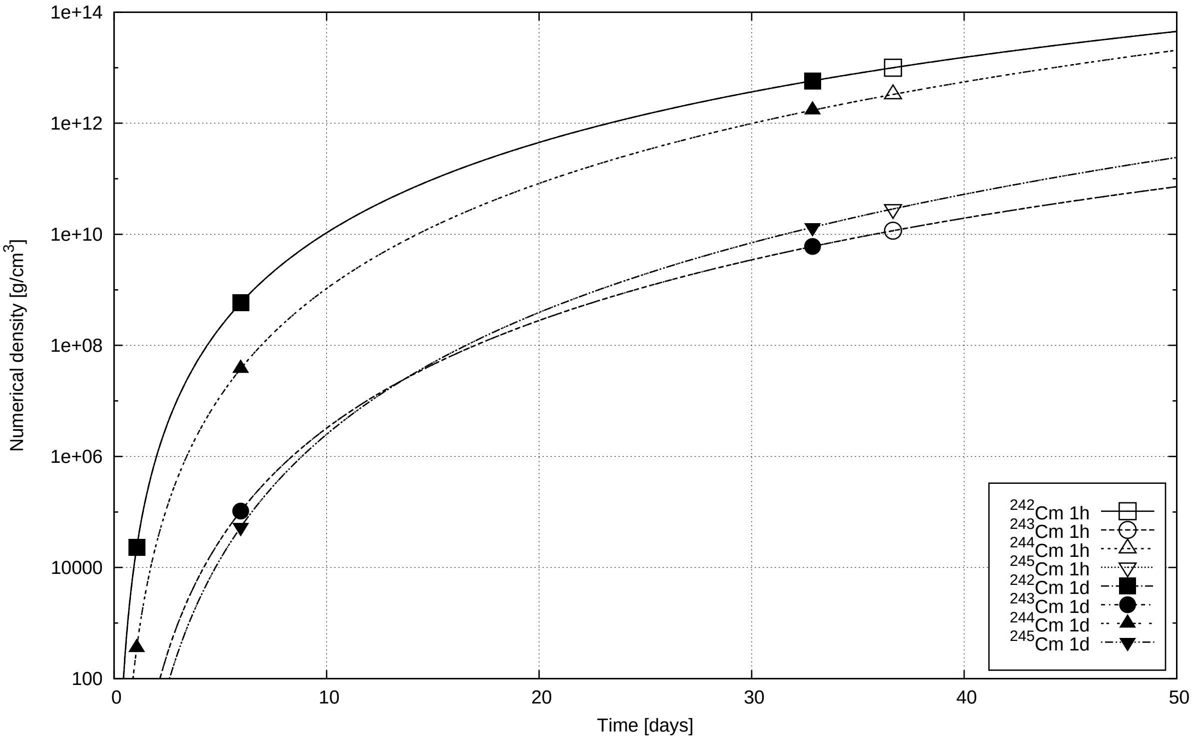

Figure 8: ^{135}I, ^{135}Xe and FP numerical densities

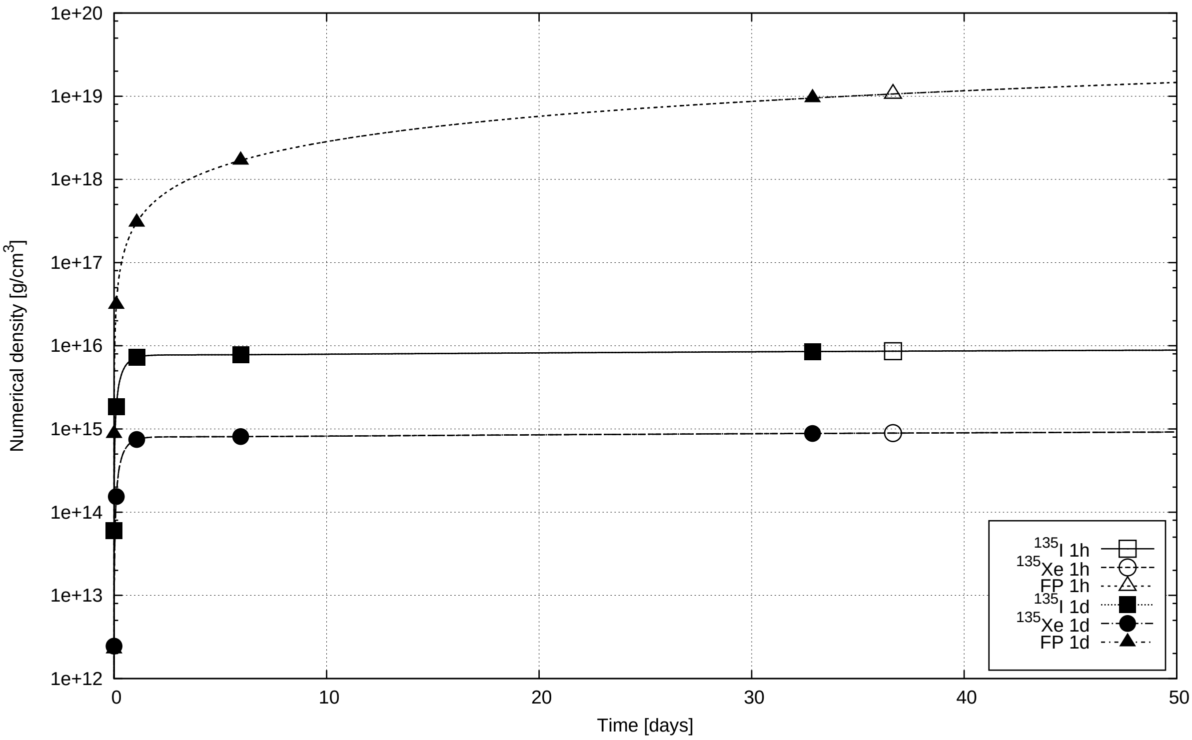

Figure 9: ^{147}Nd, ^{147}Pm, $^{148,\,148m}$Pm, ^{149}Pm and ^{149}Sm numerical densities