22.251 LAB Exercise 3
Spent Fuel Analysis with ORIGEN-2

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Introduction

- ORIGEN2 is a 0-D, one-group code written in FORTRAN 77 to compute the buildup, decay, and processing of radioactive materials
- focus on material composition, rely on the correct cross section library,
  - pros (various reactor types, fast execution, many isotopes …)
  - cons (Xsection library dependent, …)
- input file is the problem description and consists of different *cards* (three character identifier).
- file organization is complex - needs a batch file to run the code.
- key concept is so-called *Vector*, which stores the amount of all the nuclides. (12 output vectors + ~30 storage vectors)
- ID convention
  - NuclideID = 10000*Z+10*A+IS
  - ElementID = 10000*Z
  - example: O16 is 080160, U is 920000

Methodology

$$\frac{dX_i}{dt} = \sum_{j=1}^{N} l_{ij}\lambda_j X_j + \phi\sum_{k=1}^{N} f_{ik}\sigma_k X_k - \left(\lambda_i + \phi\sigma_i + r_i\right)X_i + F_i\,, \qquad i = 1, \ldots, N$$

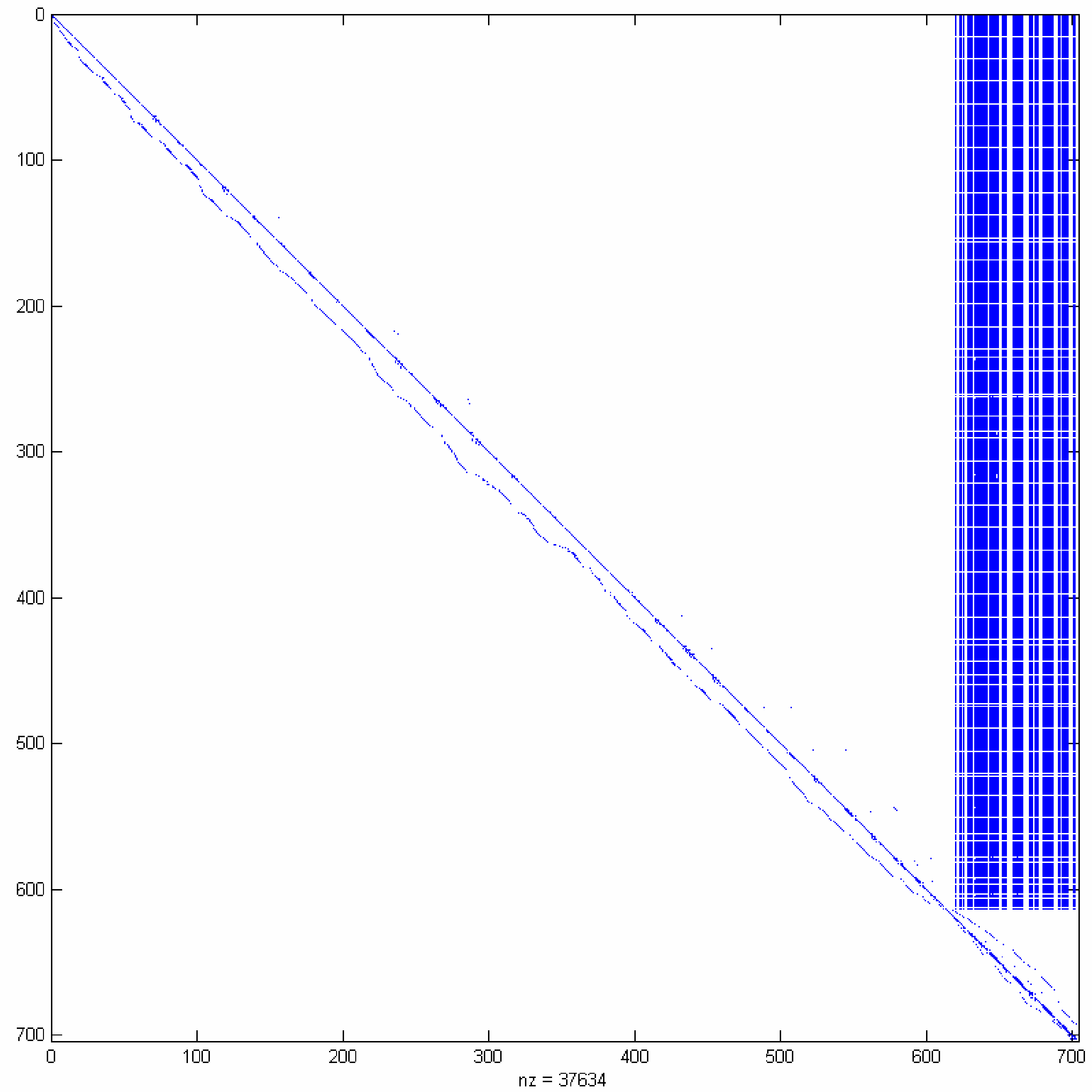
where

X_i = atom density of nuclide *i*;
N = number of nuclides;
l_{ij} = fraction of radioactive disintegration by nuclide *j* leading to formation of *i*;
λ_j = radioactive decay constant;
ϕ = position- and energy- averaged neutron flux;
f_{ik} = fraction of neutron absorption by nuclide *k* which leads to formation of nuclide *i*;
σ_k = spectrum-averaged neutron absorption cross section of nuclide *k*;
r_i = continuous removal rate of nuclide *i* from the system;
F_i = continuous feed rate of nuclide *i*.

Exponential of a Sparse Matrix

$$\dot{X} = AX$$

$$X(t) = exp(At)\ X(0)$$



Nuclides Classification

- Activation Products (AP) ~ 720 nuclides
  - usually used to handle structural materials (e.g., Zr), fuel impurities
  - nearly all naturally occurring nuclides
  - their neutron absorption products
  - their decay daughters
- Actinides (ACT) ~ 130 nuclides
  - include the actinide (heavy metal) isotopes, and their decay daughters
- Fission Products (FP) ~ 850 nuclides
  - nuclides produced by fission + their decay and capture products
- the nuclide *vector* is divided into the above 3 segments
  - about 1300 nuclides in total

Libraries

- Decay library - `DECAY.LIB` (specified in unit 9)
  - Provides a list of nuclides under consideration
  - Provides decay data
  - Nuclear compositions for naturally occurring elements
  - MPC values (Radiotoxicity coefficients)
- Cross Section & Fission Product Yield Data Library (also in unit 9)
  - key library for ORIGEN2,
  - one-group cross section is obtained using other sophisticated physics code by spectrum-averaging the cross section of each reaction type,
  - full list of libraries is on the next page
- Photon Data Library (3 libraries) (specified in unit 10)
  - provides number of photons per decay in 18-group structure
  - `GXH2OBRM.LIB` - Bremsstrahlung in water
  - `GXUO2BRM.LIB` - Bremsstrahlung in UO_2
  - `GXNOBREM.LIB` No Bremsstrahlung

Input Deck Organization (Unit 5)

Control cards defining input/output units;

miscellaneous initialization data changes;

ORIGEN2 commands(cards);

decay data library;

cross-section/fission yield data library;

photon data library;

initial nuclide composition & continuous feed and reprocessing rates;

substitute decay, cross-section, and fission-product yield data;

non-standard, flux-dependent reactions.

File Organizations

Unit number	Description
3	Substitute data for decay and cross section libraries (specified by `LIB`)
4	Alternate unit for reading material compositions
5	Card reader (specified in `MAIN` in call to `LISTIT`)
6	Principal output unit; usually directed to line printer (specified in `BLOCK DATA`, variables = `IOUT`, `JOUT`, `KOUT`)
7	Unit to write an output vector (used by `PCH` command)
9	Decay and cross section library (specified by `LIB` command)
10	Photon library (specified by `PHO` command)
11	Alternate output unit, usually directed to line printer
12	Table of contents for unit 6 above, usually directed to line printer (specified in `BLOCK DATA`, variables = `NTOCA`)
13	Table of contents for unit 11, usually directed to line printer (specified in `BLOCK DATA`, variables = `NTOCB`)
15	Print debugging information
16	Print variable cross section information
50	Data set used to temporarily store input read on unit 5 (specified in `BLOCK DATA`, variables = `IUNIT`)

Running Batch File

Under DOS/Windows environment, suppose input file `ref.inp` and ORIGEN2 is installed under `C:\` directory, then a batch file `(run.bat)` is needed to execute the ORIGEN2.

```
REM  prepare different units
copy ref.inp TAPE5.INP
copy c:\usr\codes\origen2\libs\decay.lib+c:\usr\codes\origen2\libs\PWRUE.lib tape9.inp
copy c:\usr\codes\origen2\libs\gxuo2brm.lib tape10.inp
c:\usr\codes\origen2\code\origen22
REM  combine and save files from run
copy tape12.out+tape6.out ref.OUT
REM  cleanup files
del tape*.inp
del tape*.out
```

Under UNIX environment (mightyalpha), batch file `(run.o22)` is

```
cp ref.inp TAPE5.INP
cat /codes/ORIGEN22/LIBS/DECAY.LIB /codes/ORIGEN22/LIBS/PWRUE.LIB > TAPE9.INP
cp  /codes/ORIGEN22/LIBS/GXUO2BRM.LIB TAPE10.INP
/codes/ORIGEN22/CODE/origen22
cat TAPE12.OUT TAPE6.OUT > PWRU5U8.OUT
rm TAPE*.*
```

Output Grouping (Unit 6)

Reactivity and burnup data;

Activation product segment (AP)

Table type #

Nuclide aggregation
Element aggregation
Summary isotope aggregation
Summary element aggregation

… … ;

Actinide segment (ACT) [same as AP];

Fission product segment (FP) [same as AP];

Neutron production rates:

(alpha, n), Spontaneous fission;

Photon production rates.

ref.inp (CASE 1)

```
-1
-1
-1
RDA    STANDARD PWR, 4.2% ENRICHED U, 50 MWd/kg
RDA    CROSS SECTION LIBRARY = PWRUE.LIB
BAS    ONE METRIC TON OF HEAVY METAL
CUT     5 1.0E-10   7 1.0E-10   9 1.0E-10   15 1.0E-10   -1
LIP     0 0 0
RDA       (DECAY.LIB)  (PWRUE.LIB)                    (PWRUE.LIB)
LIB     0    1 2 3     604 605 606    9   50   0   1       39
RDA     (PHOTON LIB)
PHO     101 102 103   10
TIT    INITIAL FUEL (4.2% ENRICHED U), 1 MT HEAVY METAL
INP     -1  1  -1  -1  1  1
MOV     -1  1  0  1.0
HED    1                                                   CHARGE
BUP
RDA    BURNUP CALC. BEGINS...
IRP      65.557  38.1347    1    2    4    2   BURNUP =  2.5 MWd/kgIHM
IRP     131.114  38.1347    2    3    4    0   BURNUP =  5.0 MWd/kgIHM
IRP     262.228  38.1347    3    4    4    0   BURNUP = 10.0 MWd/kgIHM
IRP     393.343  38.1347    4    5    4    0   BURNUP = 15.0 MWd/kgIHM
IRP     524.457  38.1347    5    6    4    0   BURNUP = 20.0 MWd/kgIHM
IRP     655.571  38.1347    6    7    4    0   BURNUP = 25.0 MWd/kgIHM
IRP     786.685  38.1347    7    8    4    0   BURNUP = 30.0 MWd/kgIHM
IRP     917.799  38.1347    8    9    4    0   BURNUP = 35.0 MWd/kgIHM
IRP    1048.913  38.1347    9   10    4    0   BURNUP = 40.0 MWd/kgIHM
IRP    1180.028  38.1347   10   11    4    0   BURNUP = 45.0 MWd/kgIHM
IRP    1311.142  38.1347   11   12    4    0   BURNUP = 50.0 MWd/kgIHM
RDA    BURNUP CALC. END...
BUP
```

ref.inp (CASE 1)

- continued

```
MOV     12 1 0 1.0
HED     1       FUEL DIS
RDA     DISCHARGED FUEL IS DECAYING...
DEC        0.1      1      2      5      2
DEC        0.215    2      3      5      0
DEC        0.462    3      4      5      0
DEC        1.0      4      5      5      0
DEC        2.15     5      6      5      0
DEC        4.62     6      7      5      0
DEC        10.0     7      8      5      0
DEC        21.5     8      9      5      0
DEC        46.2     9     10      5      0
DEC        100.    10     11      5      0
DEC        215.    11     12      5      0
OPTL       4*8  7   8   7   8   7   5*8  7   9*8
OPTA       4*8  7   8   7   8   7   5*8  7   9*8
OPTF       4*8  7   8   7   8   7   5*8  7   9*8
OUT       12     1      -1     0
DEC        462.    12      1      5      0
DEC         1.0     1      2      7      0
DEC        2.15     2      3      7      0
DEC        4.62     3      4      7      0
DEC        10.0     4      5      7      0
DEC        21.5     5      6      7      0
DEC        46.2     6      7      7      0
DEC        100.     7      8      7      0
DEC        215.     8      9      7      0
DEC        462.     9     10      7      0
DEC        1000.   10     11      7      0
OUT       11     1      -1     0
END
  2 922350 42000.    922380 958000.  0        0.0
URANIUM 4.2%
0
```

List of Libraries

Name	NLIB(5)	NLIB(6)	NLIB(7)	NLIB(12)	Description
PWRU.LIB	204	205	206	1	^{235}U enriched UO_2, with a burnup of 33 MWd/kg
PWRPUU.LIB	207	208	209	2	^{235}U enriched UO_2 in a self-generated Pu recycle reactor
PWRPUPU.LIB	210	211	212	3	Pu-enriched UO_2 in a self-generated Pu recycle reactor
PWRDU3TH.LIB	213	214	215	7	ThO_2-enriched with denatured ^{233}U
PWRPUTH.LIB	216	217	218	8	Pu-enriched UO_2
PWRU50.LIB	219	220	221	9	^{235}U enriched UO_2, with a burnup of 50 MWd/kg
PWRD5D35.LIB	222	223	224	10	ThO_2-enriched with makeup, denatured ^{235}U
PWRD5D33.LIB	225	226	227	11	ThO_2-enriched with recycled, denatured ^{233}U
PWRUS.LIB	601	602	603	38	3.2 w/o ^{235}U fuel, 3-cycle PWR to achieve 33 MWd/kg
PWRUE.LIB	604	605	606	39	4.2 w/o ^{235}U fuel, 3-cycle PWR to achieve 50 MWd/kg
BWRU.LIB	251	252	253	4	^{235}U enriched UO_2
BWRPUU.LIB	254	255	256	5	^{235}U enriched UO_2 in a self-generated Pu recycle reactor
BWRPUPU.LIB	257	258	259	6	Pu-enriched fuel in a self-generated Pu recycle reactor
BWRUS.LIB	651	652	653	40	3.0 w/o ^{235}U fuel, 4-cycle BWR to achieve 27.5 MWd/kg axial varying moderator density considered
BWRUS0.LIB	654	655	656	41	3.0 w/o ^{235}U fuel, 4-cycle BWR to achieve 27.5 MWd/kg, constant axial moderator density
BWRUE.LIB	657	658	659	42	3.4 w/o ^{235}U fuel, 4-cycle BWR to achieve 40 MWd/kg
CANDUNAU.LIB	401	402	403	21	CANDU, natural uranium
CANDUSEU.LIB	404	405	406	22	CANDU, slightly enriched uranium
					LMFBR: Early oxide, LWR-Pu/U/U/U:
EMOPUUUC.LIB	301	302	303	18	Core
EMOPUUUA.LIB	304	305	306	19	Axial blanket
EMOPUUUR.LIB	307	308	309	20	Radial blanket
					LMFBR: Advanced oxide, LWR-Pu/U/U/U
AMOPUUUC.LIB	311	312	313	12	Core
AMOPUUUA.LIB	314	315	316	13	Axial blanket
AMOPUUUR.LIB	317	318	319	14	Radial blanket
					LMFBR: Advanced oxide, recycle-Pu/U/U/U
AMORUUUC.LIB	321	322	323	15	Core
AMORUUUA.LIB	324	325	326	16	Axial blanket
AMORUUUR.LIB	327	328	329	17	Radial blanket
					LMFBR: Advanced oxide, LWR-Pu/U/U/Th
AMOPUUTC.LIB	331	332	333	32	Core
AMOPUUTA.LIB	334	335	336	33	Axial blanket
AMOPUUTR.LIB	337	338	339	34	Radial blanket
					LMFBR: Advanced oxide, LWR-Pu/Th/Th/Th
AMOPTTTC.LIB	341	342	343	29	Core
AMOPTTTA.LIB	344	345	346	30	Axial blanket
AMOPTTTR.LIB	347	348	349	31	Radial blanket
					LMFBR: Advanced oxide, recycle ^{233}U/Th/Th/Th
AMO0TTTC.LIB	351	352	353	35	Core
AMO0TTTA.LIB	354	355	356	36	Axial blanket
AMO0TTTR.LIB	357	358	359	37	Radial blanket
					LMFBR: Advanced oxide, 14% denatured ^{233}U/Th/Th/Th
AMO1TTTC.LIB	361	362	363	23	Core
AMO1TTTA.LIB	364	365	366	24	Axial blanket
AMO1TTTR.LIB	367	368	369	25	Radial blanket
					LMFBR: Advanced oxide, 44% denatured ^{233}U/Th/Th/Th
AMO2TTTC.LIB	371	372	373	26	Core
AMO2TTTA.LIB	374	375	376	27	Axial blanket
AMO2TTTR.LIB	377	378	379	28	Radial blanket
FFTFC.LIB	381	382	383	0	LMFBR: Fast Flux Test Facility (FFTF) Pu/U
					Clinch River Breeder Reactor (CRBR):
CRBRC.LIB	501	502	503	0	Core
CRBRA.LIB	504	505	506	0	Axial blanket
CRBRR.LIB	507	508	509	0	Radial blanket
CRBRI.LIB	510	511	512	0	Internal blanket
THERMAL.LIB	201	202	203	0	0.0253-eV cross section library

Output Tables

Table 4.3. Description of ORIGEN2 output table

Table number	Description of table	Units
1	Isotopic composition of each element	atom fraction
2	Isotopic composition of each element	weight fraction
3	Composition	gram-atoms
4	Composition	atom fraction
5	Composition	grams
6	Composition	weight fraction
7	Radioactivity (total)	Ci
8	Radioactivity (total)	fractional
9	Thermal power	watts
10	Thermal power	fractional
11	Radioactivity (total)	Bq
12	Radioactivity (total)	fractional
13	Radioactive inhalation hazard	m^3 air
14	Radioactive inhalation hazard	fractional
15	Radioactive ingestion hazard	m^3 water
16	Radioactive ingestion hazard	fractional
17	Chemical ingestion hazard	m^3 water
18	Chemical ingestion hazard	fractional
19	Neutron absorption rate	neutrons/sec
20	Neutron absorption rate	fractional
21	Neutron-induced fission rate	fissions/sec
22	Neutron-induced fission rate	fractional
23	Radioactivity (alpha)	Ci
24	Radioactivity (alpha)	fractional
25	(alpha,n) neutron production	neutrons/sec
26	Spontaneous fission neutron production	neutrons/sec
27	Photon emission rate	photons/sec
28	Set test parameter ERR	-

add

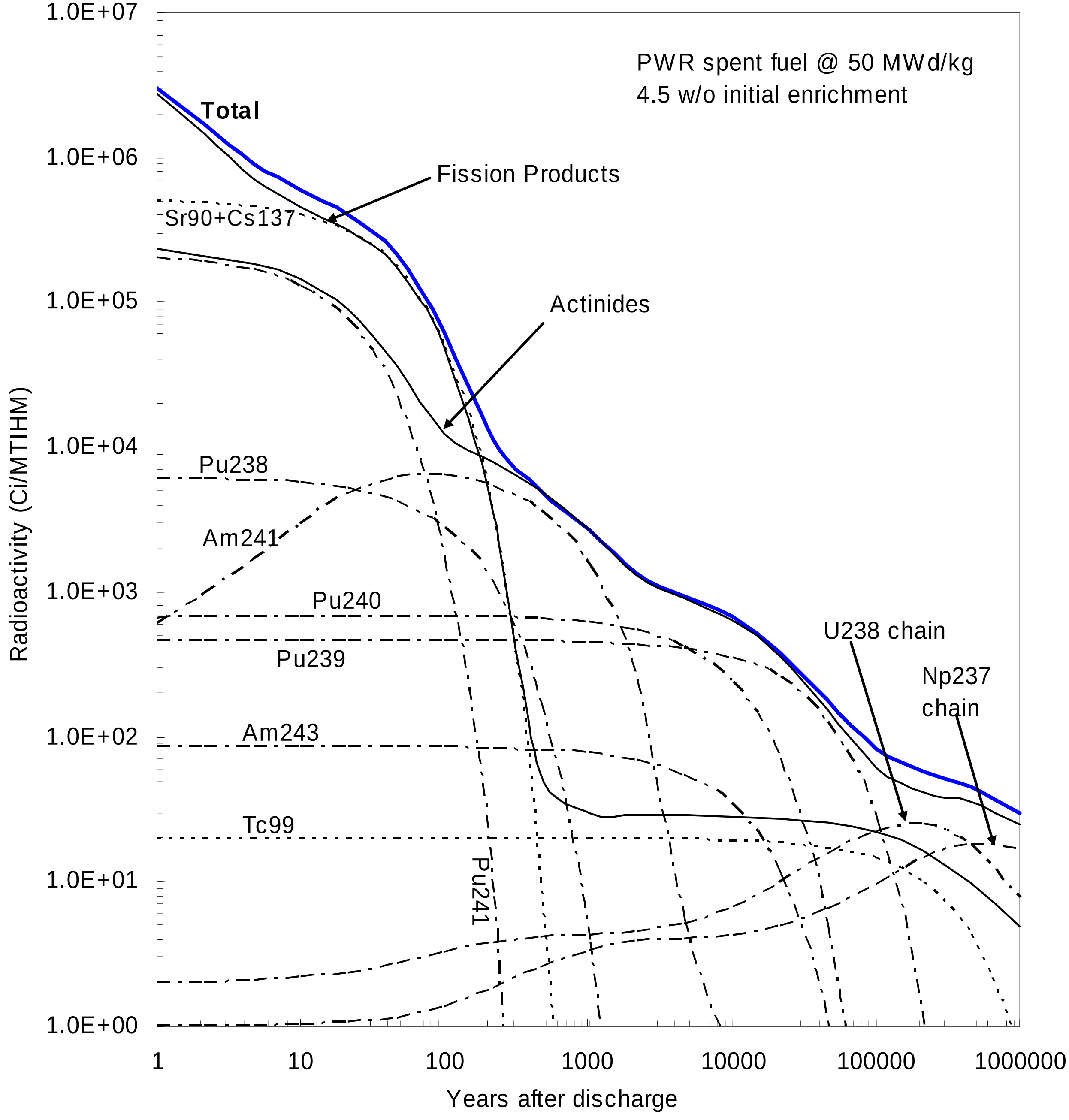
Table 4.2. Time unit designation

1 =	seconds
2 =	minutes
3 =	hours
4 =	days
5 =	years
6 =	stable
7 =	10^3 years (kY)
8 =	10^6 years (MY)
9 =	10^9 years (GY)

Table 4.6. Specification of output table types to be printed

NOPTL(I) NOPTA(I) NOPTF(I)	Table type printed		
	Nuclide	Element	Summary
1	Yes	Yes	Yes
2	Yes	Yes	No
3	Yes	No	Yes
4	No	Yes	Yes
5	Yes	No	No
6	No	Yes	No
7	No	No	Yes
8	No	No	No

Example



PWR spent fuel @ 50 MWd/kg
4.5 w/o initial enrichment
Total
Fission Products
Sr90+Cs137
Actinides
Pu238
Am241
Pu240
Pu239
Am243
Tc99
Pu241
U238 chain
Np237 chain
Radioactivity (Ci/MTIHM)
1.0E+07
1.0E+06
1.0E+05
1.0E+04
1.0E+03
1.0E+02
1.0E+01
1.0E+00
1
10
100
1000
10000
100000
1000000
Years after discharge

22.251 Systems Analysis of the Nuclear Fuel Cycle
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