UNCERTAINTY METHODS IN ACTIVATION AND INVENTORY CALCULATIONS

Carlos J. Díez*, O. Cabellos, J.S. Martínez

Universidad Politécnica de Madrid (UPM)

First ANDES annual meeting

CIEMAT, Madrid (Spain), May 23 – 25, 2011

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*C.J. Díez e-mail: cj.diez@upm.es carlosjavier@denim.upm.es

Task 2.4 Covariances for activation, radioactive decay and fission yields

Task leader: UPM
Participants: UPM, NRG, NNL, CIEMAT

- For a number of important nuclides, complete activation data libraries with covariance data will be produced, so that **uncertainty propagation in fuel cycle codes** (in this case ACAB, FISPIN, ...) can be developed and tested.

- Eventually, fuel inventory codes should be able **to handle the complete set of uncertainty data**, i.e. those of nuclear reactions (cross sections, etc.), radioactive decay and fission yield data. For this, capabilities will be developed both to produce covariance data and to propagate the uncertainties through the inventory calculations.

- **Demonstrations on a realistic burn-up case** will be provided.

Deliverables and Milestones

Milestones:

- M2.2. Report on the usability of Monte Carlo uncertainty propagation in fuel cycle codes, and comparison with conventional approach (**31 May 2012**) (**UPM/UNED, NRG, CIEMAT**).
- M2.3. An upgraded ACAB code, which now will deal with cross-channel and cross-nuclide correlations (**31 May 2012**) (**UPM**)
- M2.4. New computational method for the use of covariance information of reaction, decay and fission yield data in an inventory calculation (**31 May 2012**)(**NNL**)

Deliverables:

- **D2.1.** Activation data libraries for Monte Carlo uncertainty propagation in fuel cycle code ACAB (**31 May 2011**) (**UPM**)
  by the end of June 2011 (according to the schedule)
- D2.5. Report with transmutation calculations for advanced reactors with new covariance data + updated sensitivity tables. (**31 May 2013**) (**NNL**)
- D2.6. Report on the impact of uncertainties of the fission product nuclear data on the inventory of the irradiated fuel for ACAB (**31 May 2013**) (**UPM**)

Abstract

ACTIVATION CALCULATIONS

Different error propagation techniques can be used:

- Sensitivity analysis
- Response Surface Method
- **Monte Carlo technique**

Then, in this paper, it is assessed the **impact of ND uncertainties on response functions in two applications:**

- Fission Pulse Decay Heat calculation (**FPDH**) (in collaboration with R. Mills)
- Conceptual design of European Facility for Industrial Transmutation (**EFIT**)

The complete set of **uncertainty data** for **cross sections** (EAF2007/UN), **decay data** and **fission yield data** (JEFF-3.1.1) are processed and used in **ACAB code**.

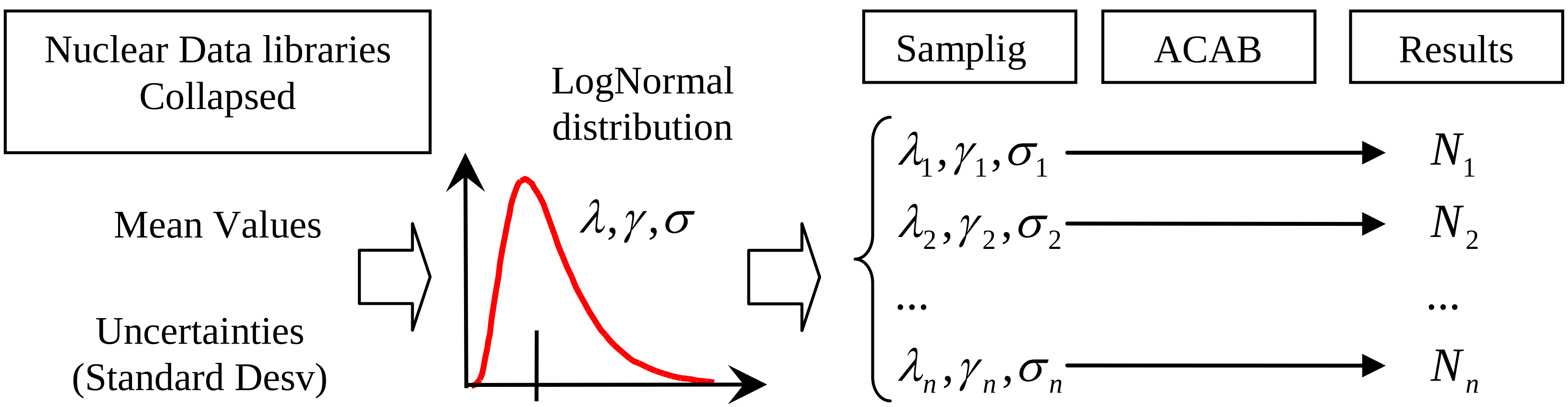
PART I Methodology to propagate ND uncertainties

Goal: "To analyse how ND uncertainties are transmitted to response functions"

$$\frac{dN}{dt} = [\lambda]N + \left[\sigma^{eff}\right]\cdot \Phi N + \left[(\gamma\sigma_{fiss})^{eff}\right]\cdot \Phi N = A \cdot N \quad \Longrightarrow \quad N_i = N_i(\lambda, \sigma, \gamma)$$

2) Monte Carlo Uncertainty Analysis (MC)

- To treat the global effect of all nuclear data uncertainties
- Without any approximation



Uncertainty data

➔ **Cross section from activation-oriented nuclear data libraries**

- **EAF2007-UN**

e.g.: $W^{180}(n,\gamma)$

E_{i+1}(eV)

```
W -180N,G                                                                    748033102
 7.41800E+4 1.7840E+02          0          0          0                     1748033102
 0.0000E+00 0.0000E+00          0        102          0                     1748033102
 0.0000E+00 0.0000E+00          0          1         10                     5748033102
 1.0000E-05 1.0000E+00 5.0000E+00 1.8404E-01 1.0140E+02 2.5000E-01748033102
 2.0000E+07 2.5000E-01 6.0000E+07 0.0000E+00                                 748033102
```

E_i (eV)

$\Delta^2_{I=1,EAF}$ (relative error, Δ)~ $\Delta_{I=1,EXP}= \Delta_{I=1,EAF}/3$

➔ **Fission yield from evaluated nuclear data library**

- **JEFF 3.1.1**

$\gamma_{Th232 \rightarrow H3, 400KeV} + 1\sigma_\gamma$

Th232

400 KeV

H3

```
 9.023200+4 2.300450+2          2          0          0          03486 8454    1
 4.0000E+05 0.0000E+00          1          0       3664          9163486 8454    2
 1.0010E+03 0.0000E+00 1.6073E-05 5.5423E-06 1.0020E+03 0.0000E+003486 8454    3
 4.9121E-06 1.6564E-06 1.0030E+03 0.0000E+00 7.0081E-05 2.2139E-053486 8454    4
```

Processing and collapsing of nuclear data

Collapsing method:

-Cross section: Conservation of reaction rate

$$Rate_{j\to i} = \int_E \sigma_{j\to i}(E)\cdot\phi(E)\cdot dE = \sigma_{j\to i}^{eff}\cdot\phi_T$$

-Uncertainties: Using "**Sandwich rule**" (*Propagation of Momentum, first order)*

$$\Delta^2 = \omega^T V \omega$$

➔ Cross section

$$\omega = [\frac{\phi_1}{\bar{\phi}}\frac{\sigma_1}{\sigma^{eff}},\cdots,\frac{\phi_G}{\bar{\phi}}\frac{\sigma_G}{\sigma^{eff}}]^T$$

➔ Fission yield

$$\omega = [\frac{\phi_1}{\bar{\phi}}\frac{\sigma_{1,fiss}}{\sigma_{fiss}^{eff}},\cdots,\frac{\phi_G}{\bar{\phi}}\frac{\sigma_{G,fiss}}{\sigma_{fiss}^{eff}}]^T$$

Advantages & Disadvantages of Monte Carlo Technique

➔ **Advantages**

- Collapsing to one energy group → Reduce amount of variables to sample
- No sensitivity coefficients should be calculated
- No approximation on equations → Take into account non-linear effects

➔ **Disadvantages**

- How to check if the phase space is well sampled ?
- Which PDFs should be taken ?
- Computational demanding

➔ **Monte Carlo Technique & Sensitivity Analysis are compatible**

APPLICATIONS:

A. Fission Pulse Decay Heat calculation

B. EFIT fuel cycle calculation

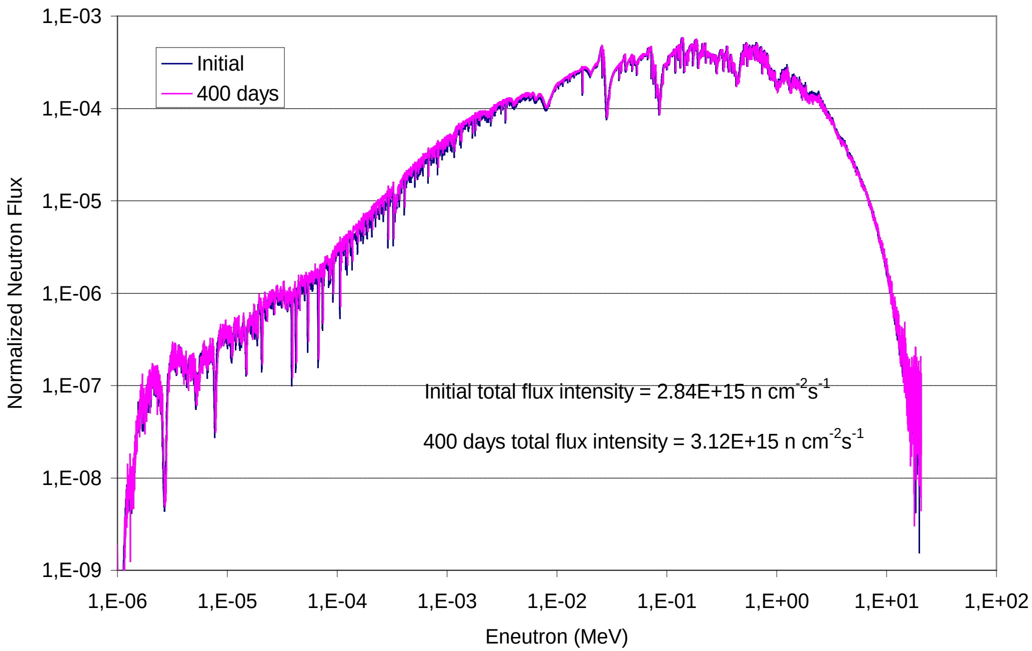
B. EFIT fuel cycle calculation

Reference system

- One of the preliminary conceptual designs of the **E**uropean **F**acility for **I**ndustrial **T**ransmutation (**EFIT**)

Coolant	**Pure Lead**
Thermal Power	**400 MWth**
Fuel	**(Pu, Am)O_2 + MgO**
Initial mass of actinides	**2.074 tonnes**

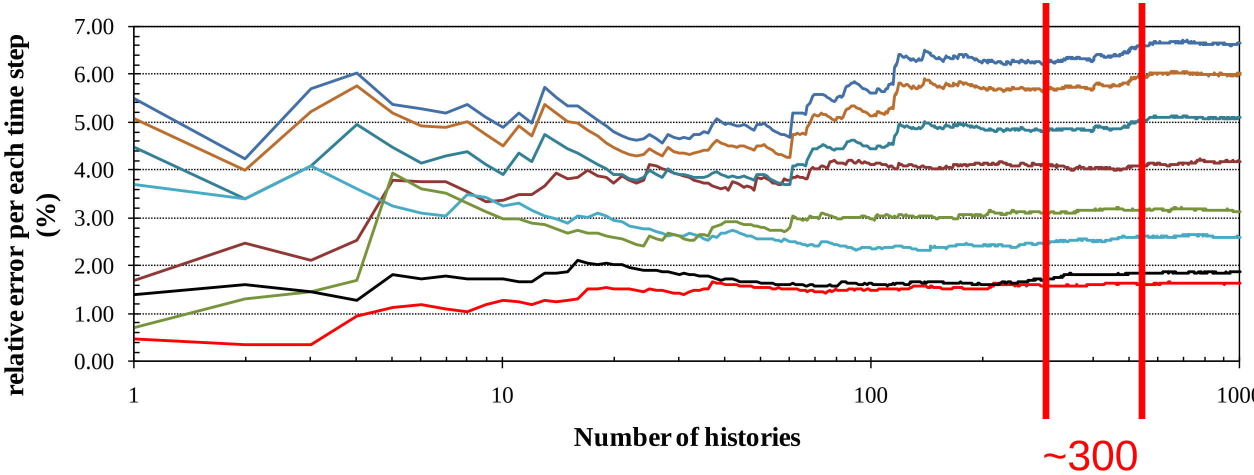
- **Constant neutron environment:**
  - neutron flux: 3.12 x 10^{15} n/cm^2 s
  - average energy <E> = 0.37 MeV



- **Calculations for discharge burn-up:**
  - 150 GWd/tHM (778 irradiation days)
  - 500 GWd/tHM (3225 irradiation days)

Calculations

- Histories launched:
  1000/DH case
  300/RTX case



Case studied

1. Decay heat

2. Radiotoxicity

   a. Inhalation dose

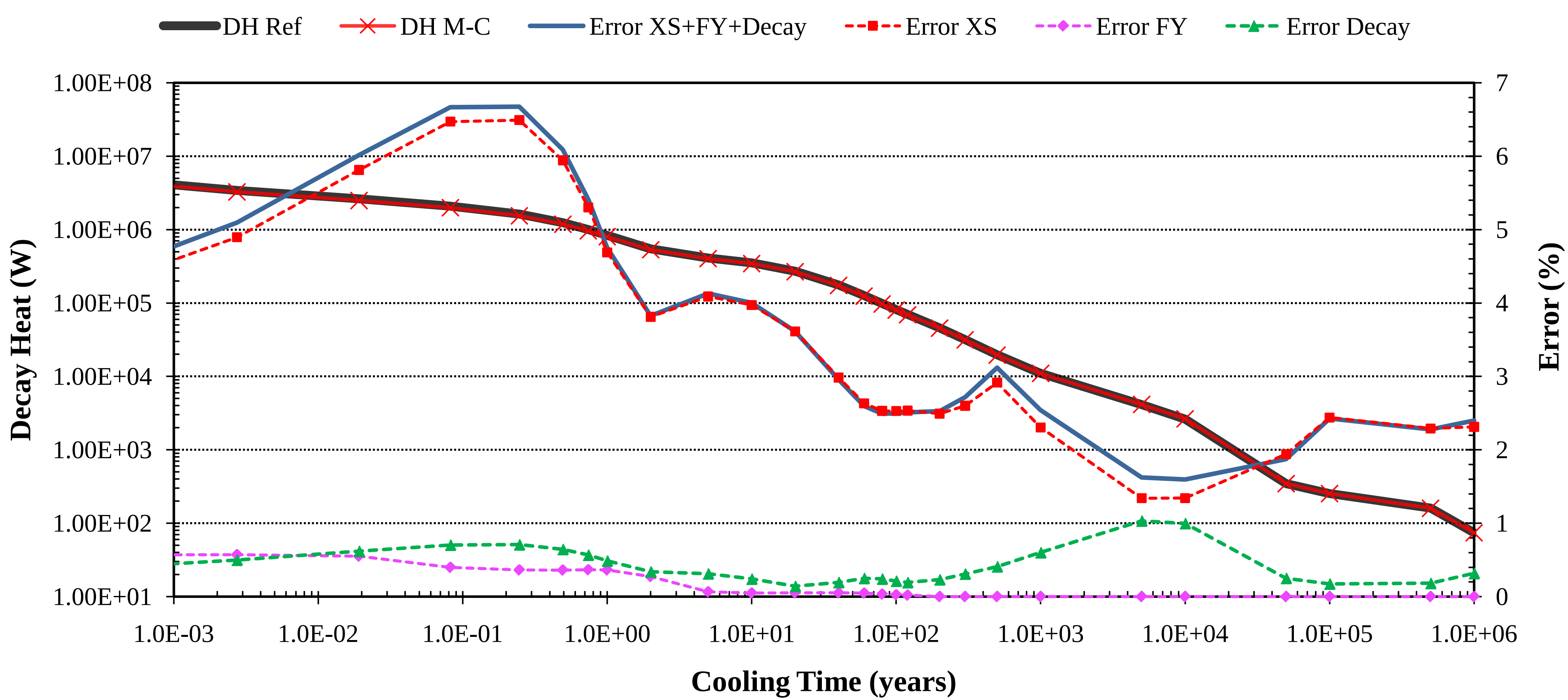
   b. Ingestion dose

All uncertainties are propagated:

- Individually
- All together

$\sigma, \quad \gamma, \quad \lambda$

Decay heat for *150 GWd/tHM*



Decay heat for *150 GWd/tHM*

Main contributors analysis

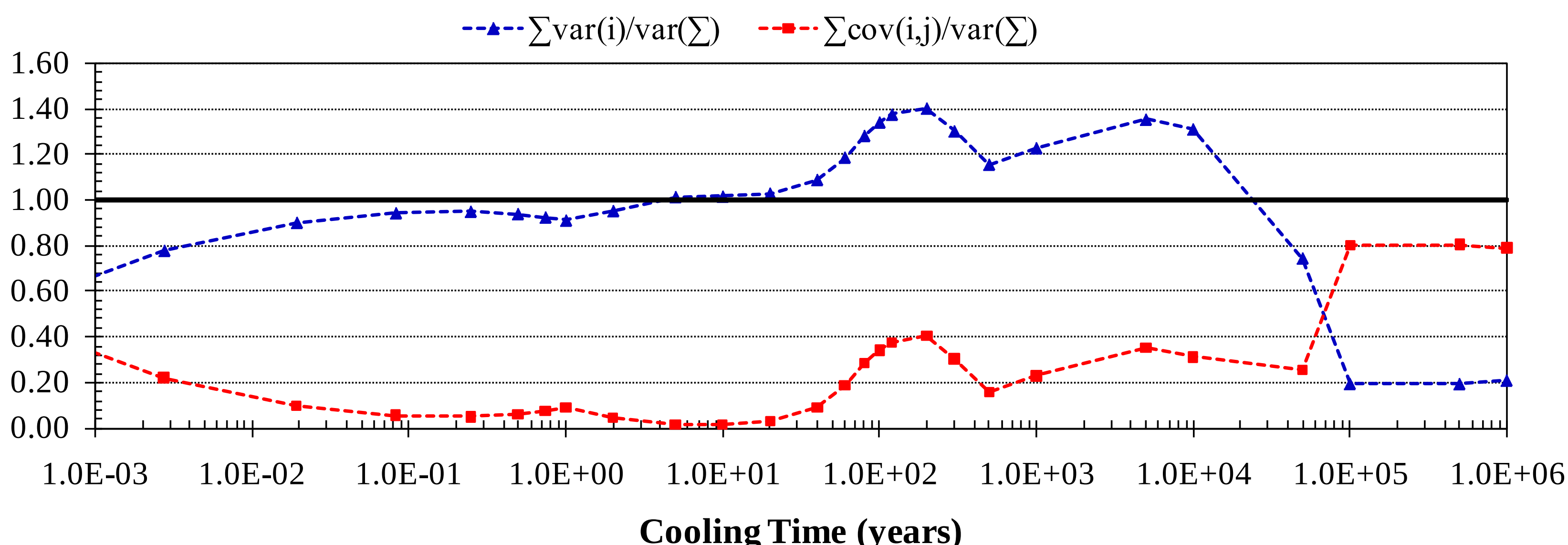
$$DH_{total} = \sum_{i=isotope} DH_i$$

$$\mathrm{var}(y) = \sum_{i=1}^{N} \mathrm{var}(y_i) + \sum_{i,j=1;i\neq j}^{N} \mathrm{cov}(y_i, y_j)$$

$$\Rightarrow$$

$$\sum_{i=1}^{N} \mathrm{var}(y_i) >> \sum_{i,j=1;i\neq j}^{N} \mathrm{cov}(y_i, y_j)$$

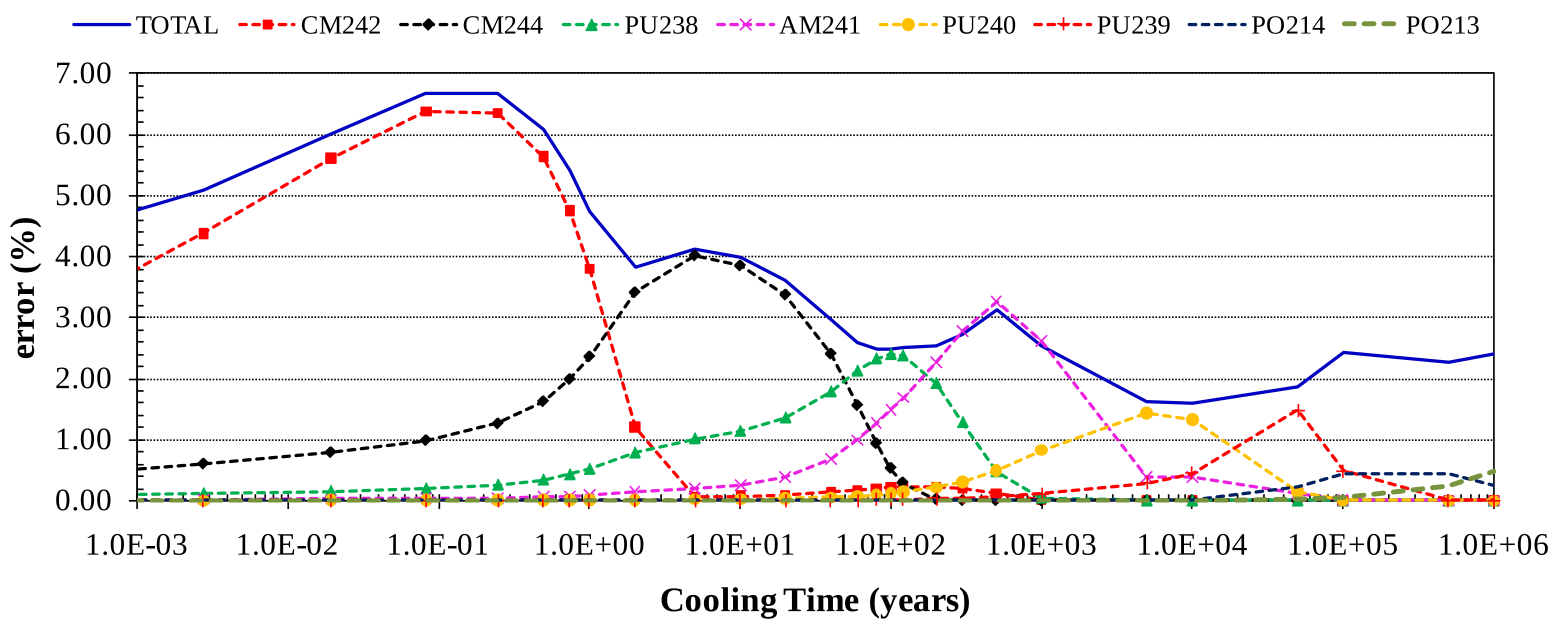
$$\frac{\sigma_x^2}{x^2} = \sum_{i=1}^{N} \frac{\sigma_{y_i}^2}{y_i^2} \cdot \frac{y_i^2}{x^2} = \sum_{i=1}^{N} error(y_i)^2 \cdot \frac{y_i^2}{x^2}$$



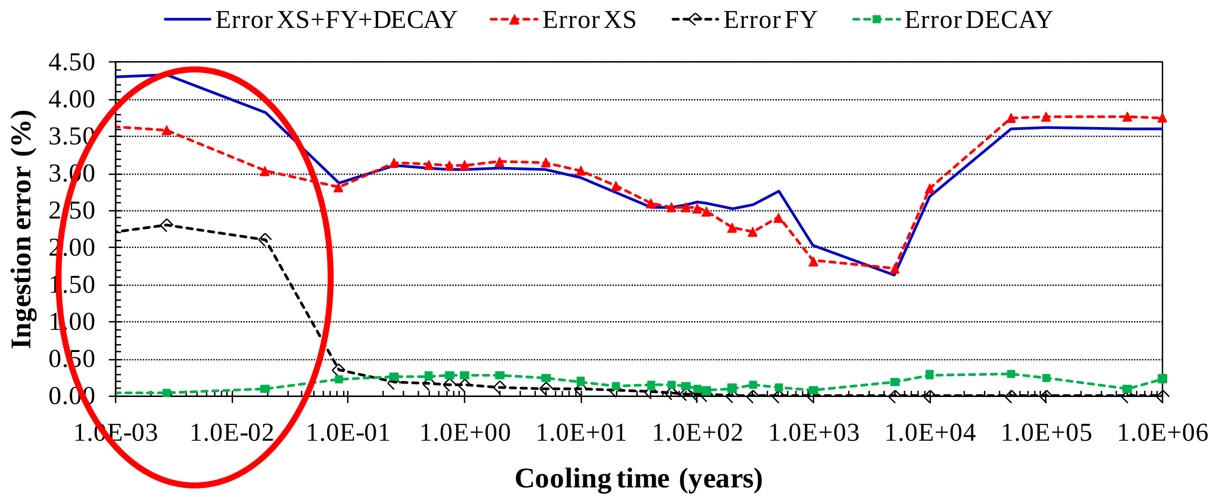
Decay heat for *150 GWd/tHM*

Main contributors

Cm242	Cm244	Pu238
Am241	Pu240	Pu239



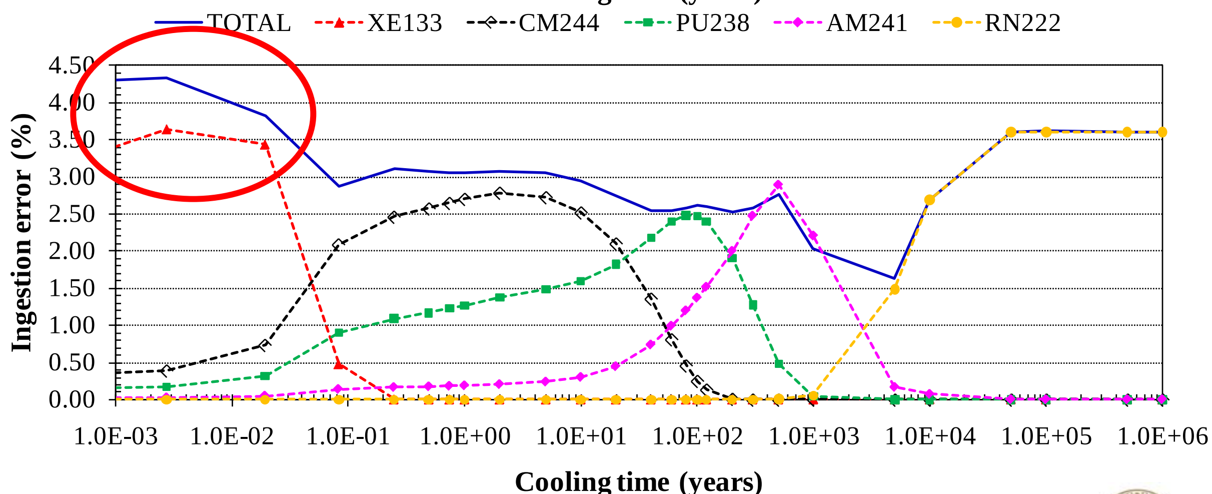
Radiotoxicity for *150 GWd/tHM*



Ingestion

Xe133	Cm244	Pu238
Am241	Rn222	

Due to FY / XS error



Differences between *150 GWd/tHM and 500 GWd/tHM*

Error varation because of burn-up discharge

	Decay Heat	Inhalation dose	Ingestion dose
150 GWd/tHM	6.67%	3.70%	4.33%
500 GWd/tHM	9.83%	9.04%	9.45%

↑t ↑burn-up => ↑ error

Main contributors in each burn-up discharge

	Xe133	Rn22	Pu238	Pu239	Pu240	Am241	Cm242	Cm244
150 GWd/tHM	Ing	Inh, Ing	DH, Inh, Ing	DH	DH, Inh	DH, Inh, Ing	DH	DH, Inh, Ing
500 GWd/tHM	Ing	Inh, Ing	DH, Inh, Ing	DH	DH, Inh	DH, Inh, Ing	-	DH, Inh, Ing

CONCLUSIONS

CONCLUSIONS

- **Monte Carlo technique for ND uncertainty propagation in activation calculations**
  - ***Pre-proccesing of nuclear data is needed:*** ***- Identifying uncertainties***
    - PDFs selection
    - Collapsing of nuclear data
  - ***Implemented on ACAB code***
- **Monte Carlo technique** VS **deterministic calculations / experimental data**
  - ***A good agreement is found between both***
- **PDFs dependence** is found in **FPDH calculation**, but **not in EFIT calculation**
- A method to identify **main contributors to error** is developed based on MC results
- **Importance of fission yield uncertainties depends on the applications and which response functions is studied**

THANK YOU FOR YOUR ATTENTION!!

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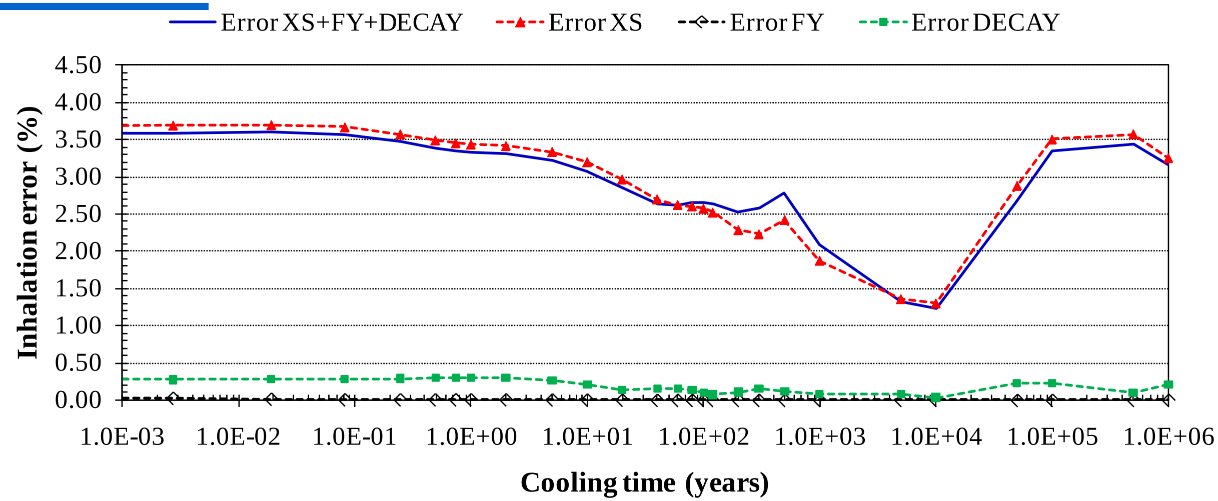
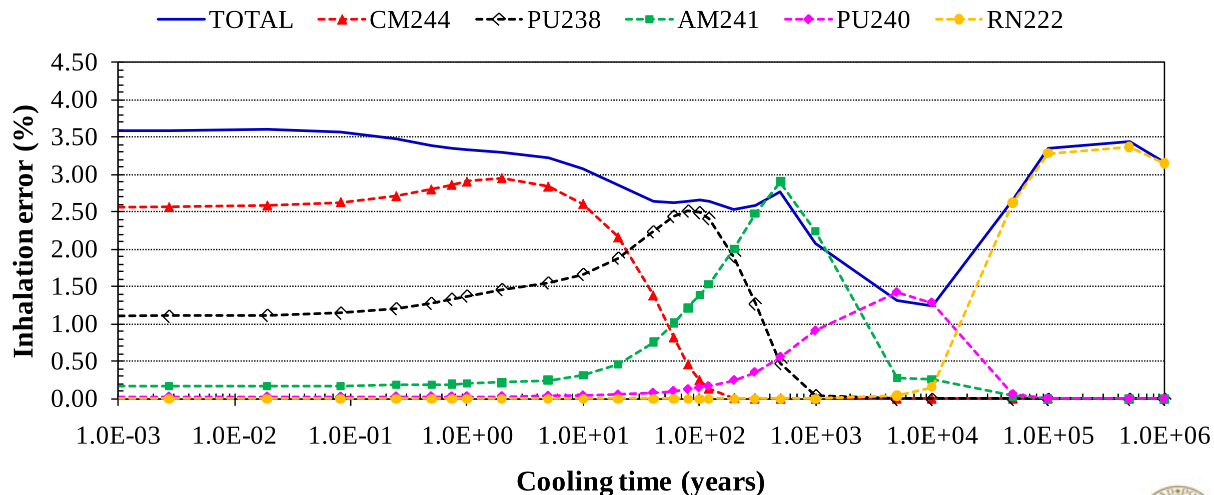
C.J. Díez e-mail: cj.diez@upm.es carlosjavier@denim.upm.es

Radiotoxicity for *150 GWd/tHM*

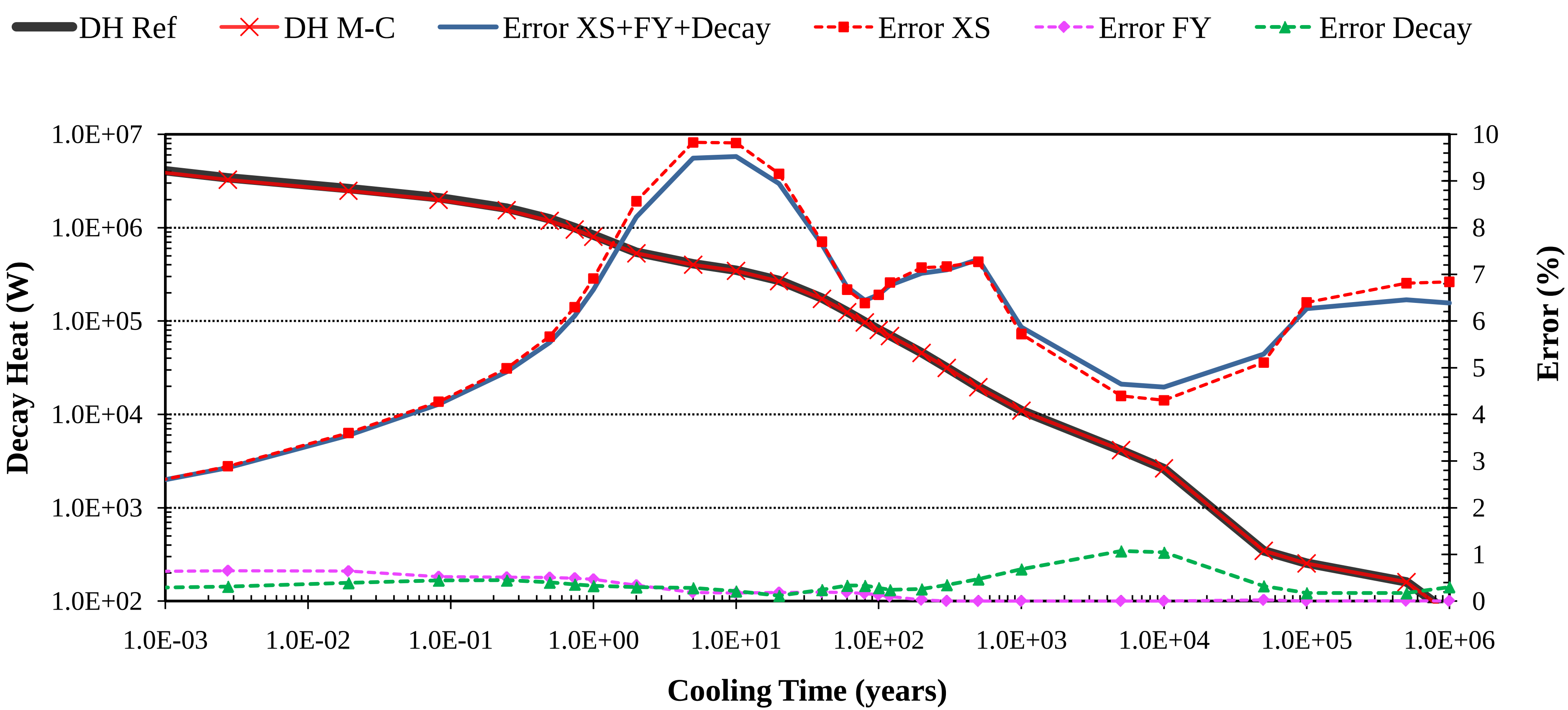


Inhalation

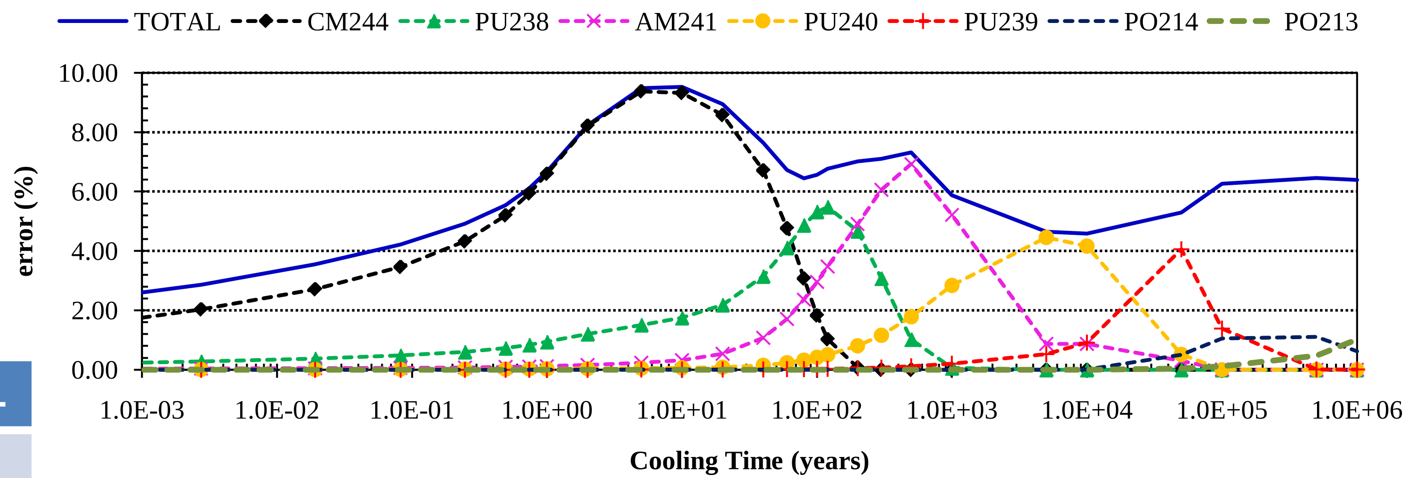
Cm244	Pu238	Am241
Pu240	Rn222	



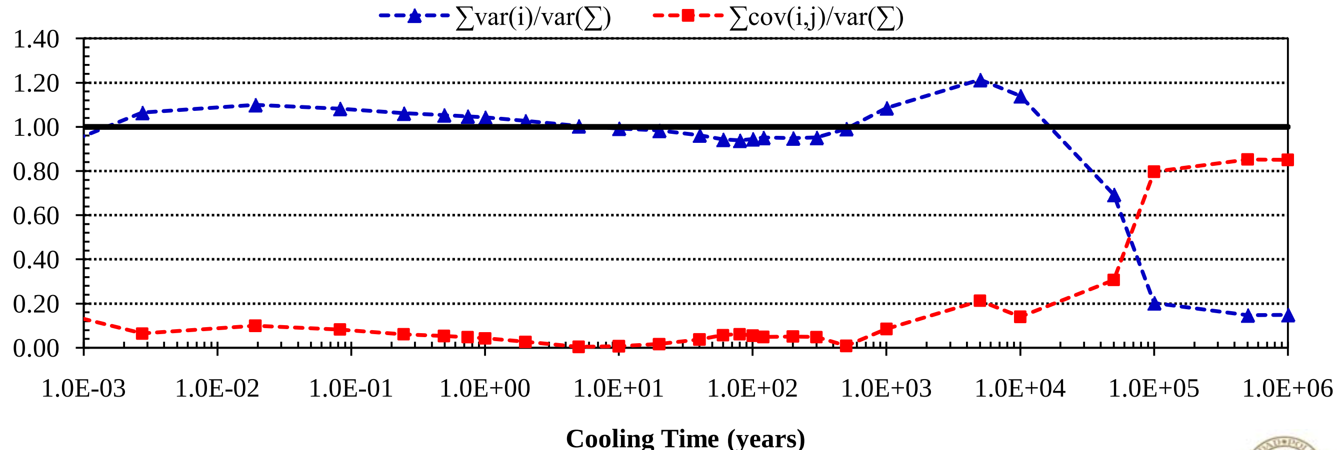
Decay heat for *500 GWd/tHM*



Decay heat for *500 GWd/tHM*



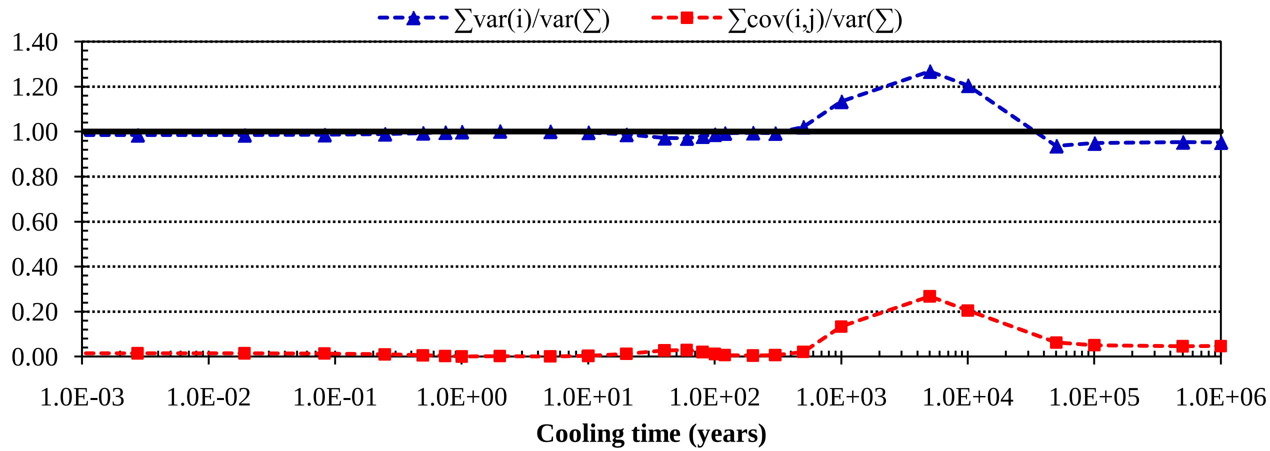
Cm244	Pu238	Am241
Pu240	Pu239	

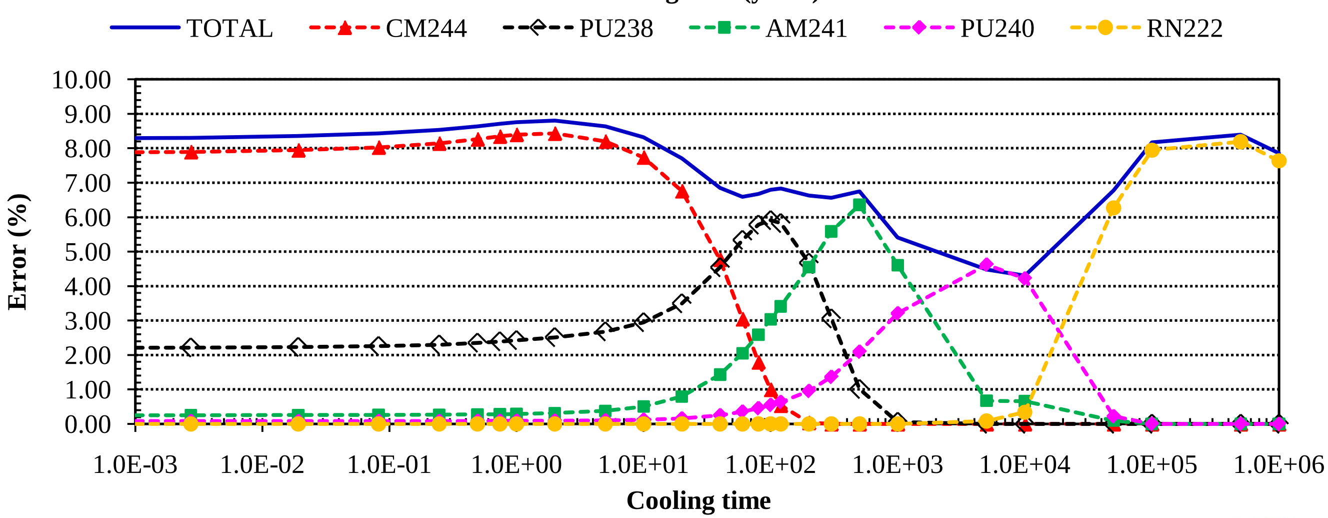


Radiotoxicity for *500 GWd/tHM*

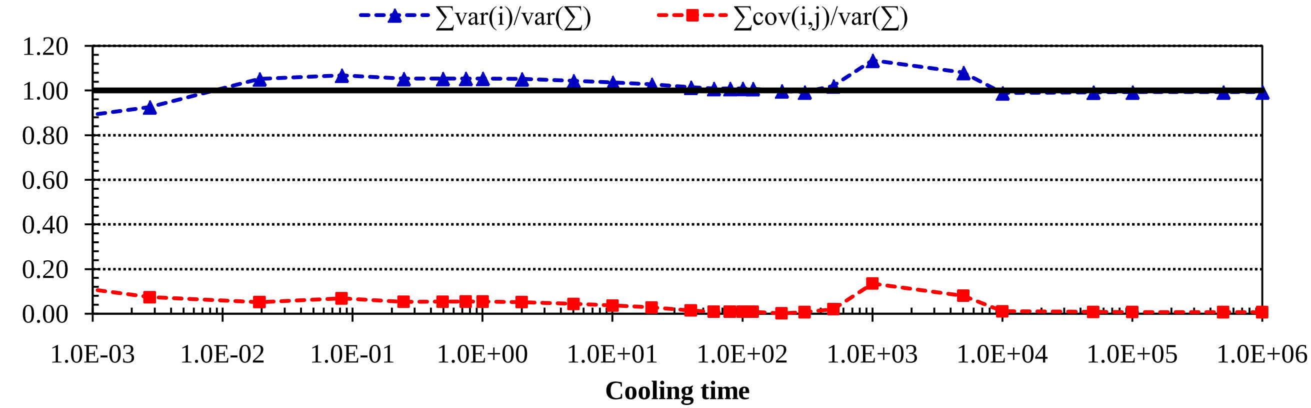
Inhalation

Cm244	Pu238	Am241
Pu240	Rn222	





Radiotoxicity for *500 GWd/tHM*



Ingestion

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