Y. Celik, A. Stankovskiy, G. Van den Eynde - 28/05/2024

Advanced features of ALEPH2 depletion code applied to radioprotection of nuclear facilities

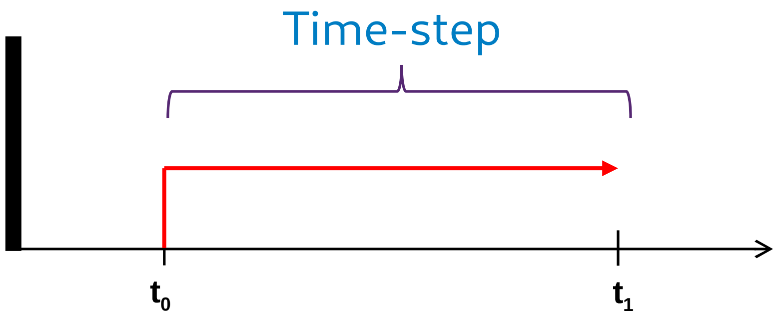
sck cen
Belgian Nuclear Research Centre

ALEPH2 – depletion code developed at SCK CEN since 2004

Features

- MCNP/PHITS as transport solver
- Advanced depletion solver based on RADAU5 Runge-Kutta algorithm
- Full consistency of nuclear data: same data are used for transport (MCNP) and depletion
- Multi-particle: transmutation of a nucleus by neutron, protons and photonuclear reactions
- Calculation of source terms
- Advanced treatment of secondary radiation
- Advanced predictor-corrector for thermal reactors simulation
- Simulation of contamination by compartment approach
- Parallelization: each depletable material is solved in own thread

ALEPH2 calculation flow



Integral flux in material *k*

$$\langle \varphi^k(\vec{r}) \rangle = \frac{1}{V}\int \varphi^k(\vec{r},E)\,dE$$

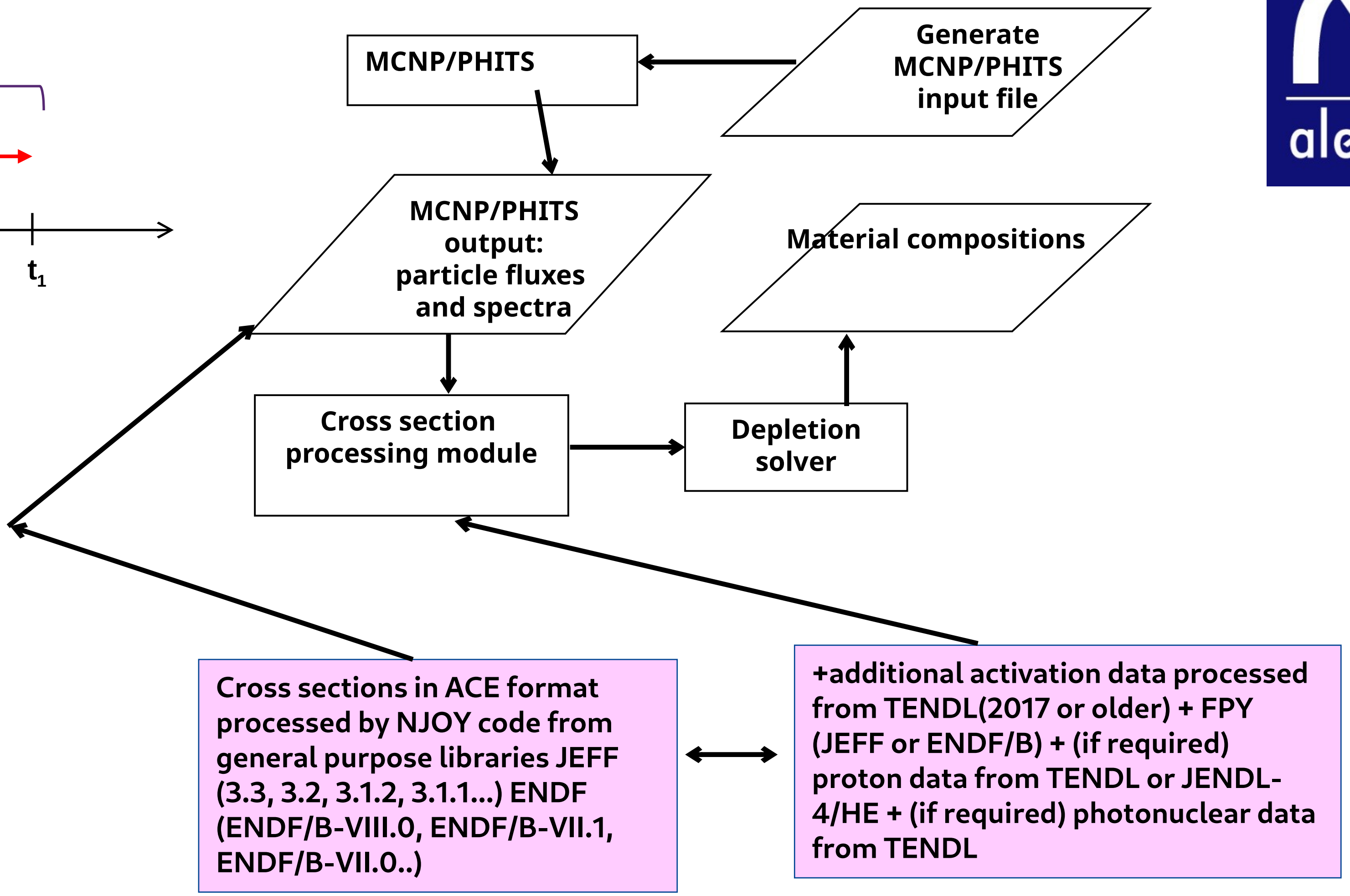
- Average cross section

  for reaction type *j* on nuclide *i*

$$\langle \sigma_{i,j}^k(\vec{r}) \rangle = \frac{\int \varphi^k(\vec{r},E)\sigma_{i,j}(E)\,dE}{\int \varphi^k(\vec{r},E)\,dE}$$

- Rate of reaction type *j* on nuclide *i*

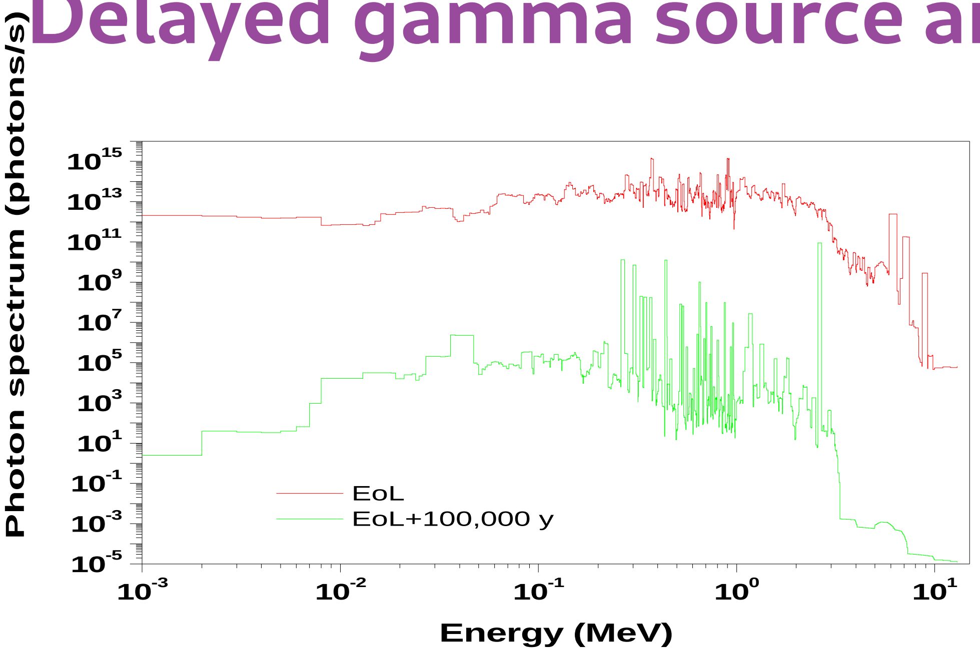
$$TR_{i,j}^k = \frac{N_i^k}{V}\int \varphi^k(\vec{r},E)\sigma_{i,j}(E)\,dE$$



From transport calculation (MCNP/PHITS output) ALEPH2 takes spectra in very fine energy group structure to account for self-shielding (~116,000 energy groups)

The spectra is used to collapse cross sections.

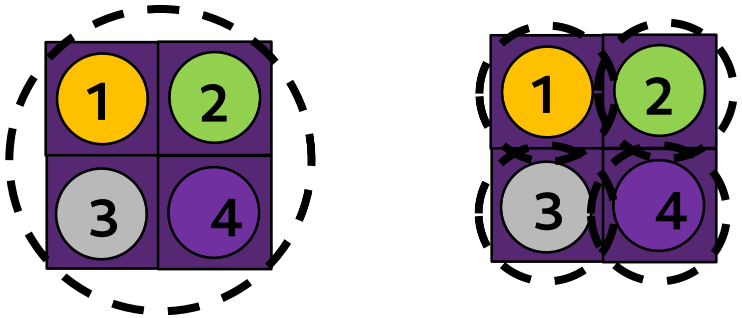
Delayed gamma source and spectra



From the vector of radioactive nuclides, ALEPH2 calculates gamma spectrum at each moment of time:

- 1500 energy bins from 1 keV to max photon energy (> 10 MeV)
- all major discrete gamma lines could be identified in the output photon spectra

The user has either to provide a virtual cylinder covering all cells with depletable materials, or a set of virtual materials covering each depletable material



Delayed photon spectra are distributed in these materials for subsequent transport calculation

(α,n) neutron source and spectra

2 options

Thick Target Yield

The number of neutrons Y_n produced by α-particles with energy E_α

$$Y_n(E_\alpha) = N_T \int_0^{E_\alpha} \frac{\sigma_{(\alpha,n)}(E)}{\left|\frac{dE}{dx}\right|} dE$$

N_T - atomic density of target nucleus (i.e. Oxygen in UO_2 fuels)
$\sigma_{(\alpha,n)}$ - neutron production cross sections on Oxygen nuclei
$\frac{dE}{dx}$ - stopping power of alphas ion materials (UO_2 fuel)

Limitations:

- stopping powers are given only for limited nuclei
- outgoing neutron spectra are unknown

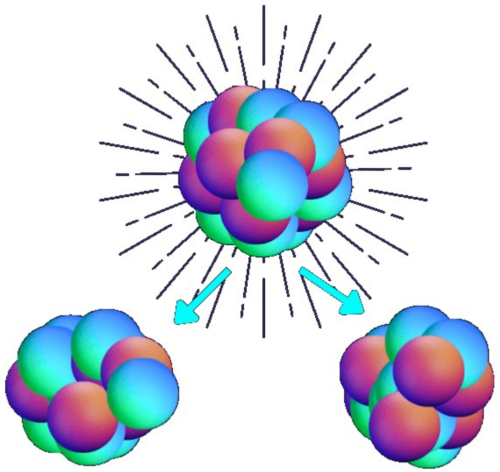
α-particle transport calculation

$$Y_n = N_k V_k \sum_i \int \sigma_{(\alpha,n),i}(E) \varphi_\alpha^k(E) dE$$

N_k - atomic density of material *k* (i.e. fuel)
$\sigma_{(\alpha,n),i}$ - neutron production cross sections on light nucleus *l* (e.g. Oxygen)
φ_α^k - flux of alpha-particles in material *k*

- α-particle spectra are treated by ALEPH2 in the same way as photon spectra (previous slide)
- Usually α-particle transport does not take long (limited range)
- Outgoing neutron spectra are calculated from the data libraries JENDL/AN-2005 (default) or TENDL
- This is most accurate approach

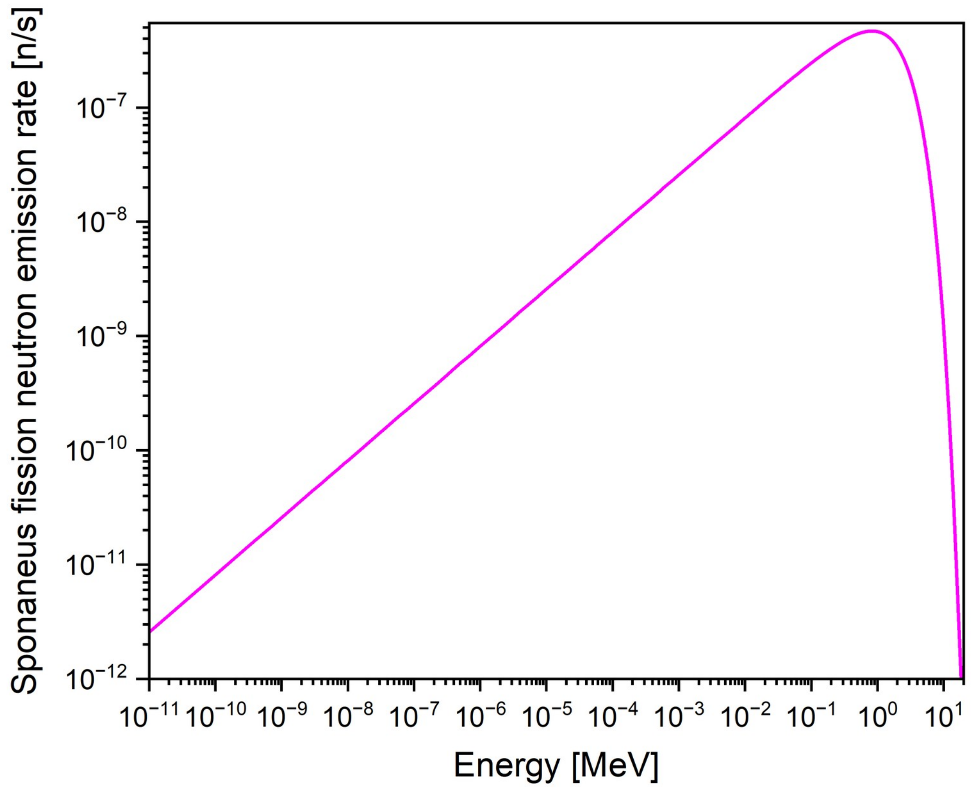
Spontaneous fission neutron source and spectra



Spectra generated from approximate formulas for Watt-like spectrum

$$\frac{dY_n}{dt}(E,t) = \sum_i N_i \lambda_i b_{spf,i} \bar{\upsilon}_i e^{-E/A_i} sinh\sqrt{B_i E}$$

Parameters $\bar{\upsilon}$, A and B are nuclide dependent



If the spectrum is given in decay data library, it is taken. However, in modern libraries the spectrum is given only for Cf-252. For other nuclides like Cm-244 (important for spent fuel characterization) approximate formulas are used.

Compartment approach to simulate contamination

Compartment **1**: production of radioactivity → R_1 → Compartment **2**: (pipes etc.) → R_{n-1} → Compartment **k**: stack

Release rates towards next compartment

$$\begin{cases} \dfrac{dN_{1,i}(t)}{dt} = \sum_j \lambda_{j\to i}^{eff} N_{1,j}(t) - \lambda_i N_{1,i}(t) - R_{1,i} N_{1,i}(t) \\ \dfrac{dN_{2,i}(t)}{dt} = R_{1,i} N_{1,i}(t) + \sum_j \lambda_{j\to i} N_{2,j}(t) - \lambda_i N_{2,i}(t) - R_{2,i} N_{2,i}(t) \\ \quad \cdots \\ \dfrac{dN_{k,i}(t)}{dt} = R_{k-1,i} N_{k-1,i}(t) + \sum_j \lambda_{j\to i} N_{k,j}(t) - \lambda_i N_{k,i}(t) \end{cases}$$

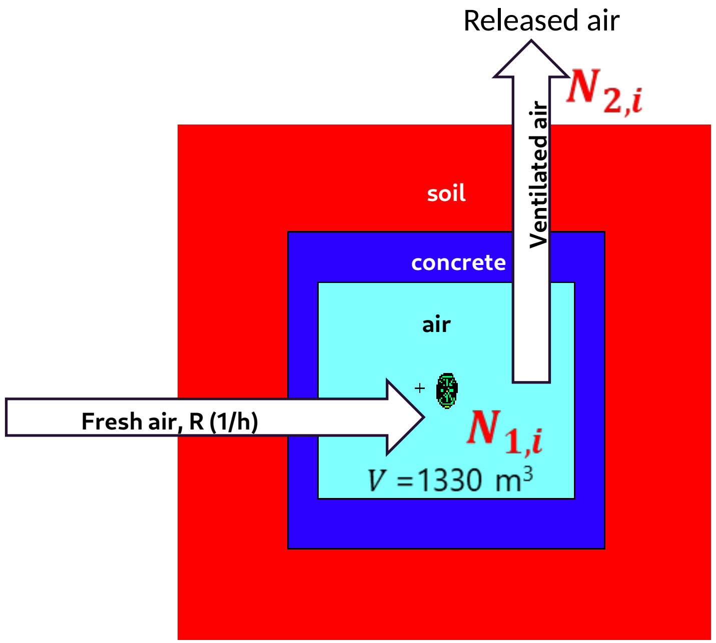
$$\lambda_{j\to i}^{eff} = b_{j\to i}\lambda_j + \sum_p \int \sigma_{j,p}(E)\varphi_p(E)dE$$

$$R(s^{-1}), = \frac{r \text{ (ventilation rate (cm}^3\text{/s))}}{v \text{ (volume of compartment (cm}^3\text{))}}$$

N_1, N_2 and N_3 are the inventories of the same nuclide in different compartments

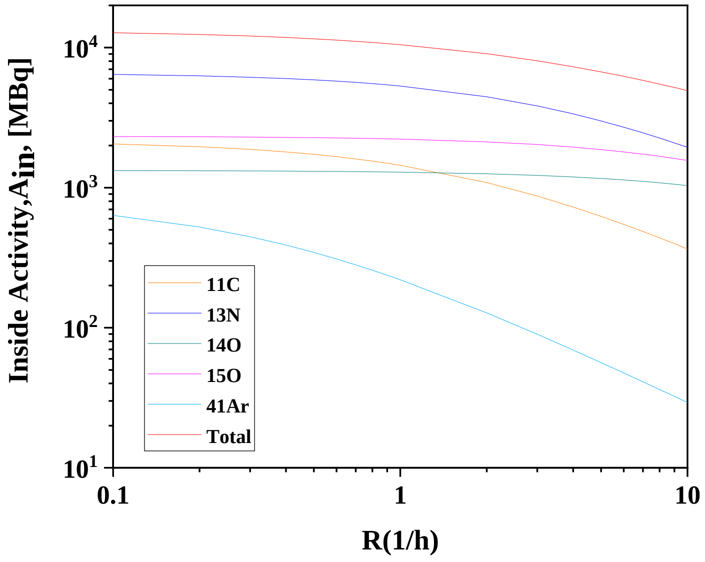
- At any moment of time, we know the source terms in each compartment
- Solving may be time consuming (if many materials are involved) but it is most accurate way
- Release rates should be known for each element. Sometimes they are simple ventilation rates applied to all elements in given compartment, this simplified the task

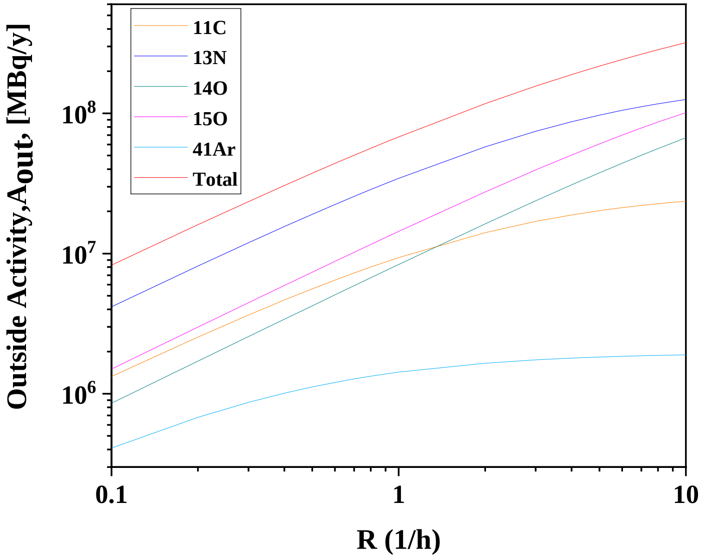
Application: MYRRHA Accelerator



10 W/m loss, 600 MeV p

- The activity of air inside the tunnel decreases with larger ventilation rate
- The activity releases to atmosphere per year increases with increasing ventilation rate.
- A lower ventilation rate is recommended to be used to decrease the activity release and therefore the total annual dose.





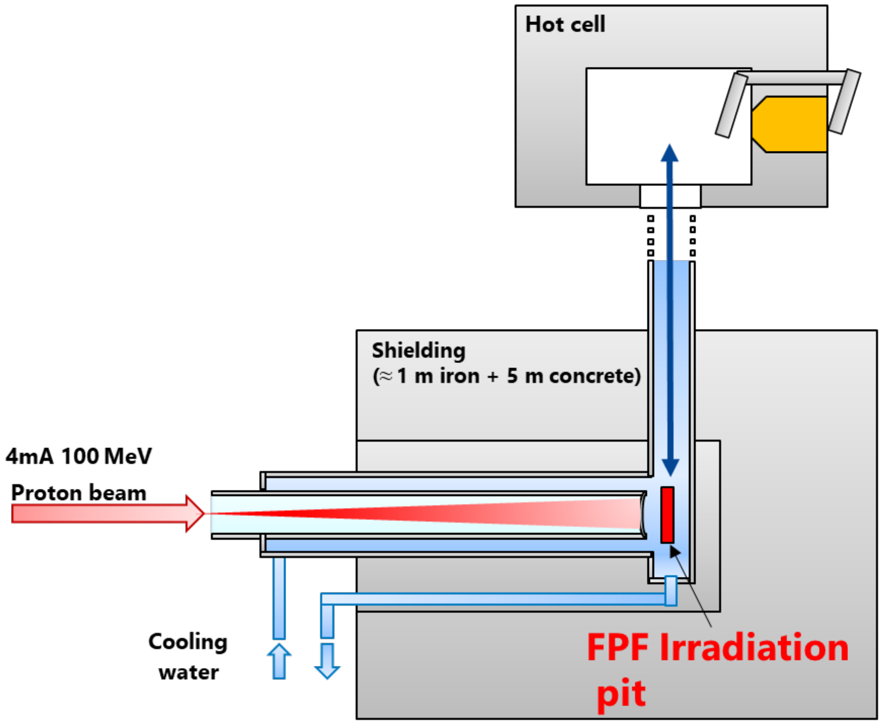
$$\frac{dN_{1,i}(t)}{dt} = \sum_j \lambda_{j\to i}^{eff} N_{1,j}(t) - \lambda_i N_{1,i}(t) - R_{1,i} N_{1,i}(t)$$

$$\frac{dN_{2,i}(t)}{dt} = R_{1,i} N_{1,i}(t) + \sum_j \lambda_{j\to i} N_{2,j}(t) - \lambda_i N_{2,i}(t)$$

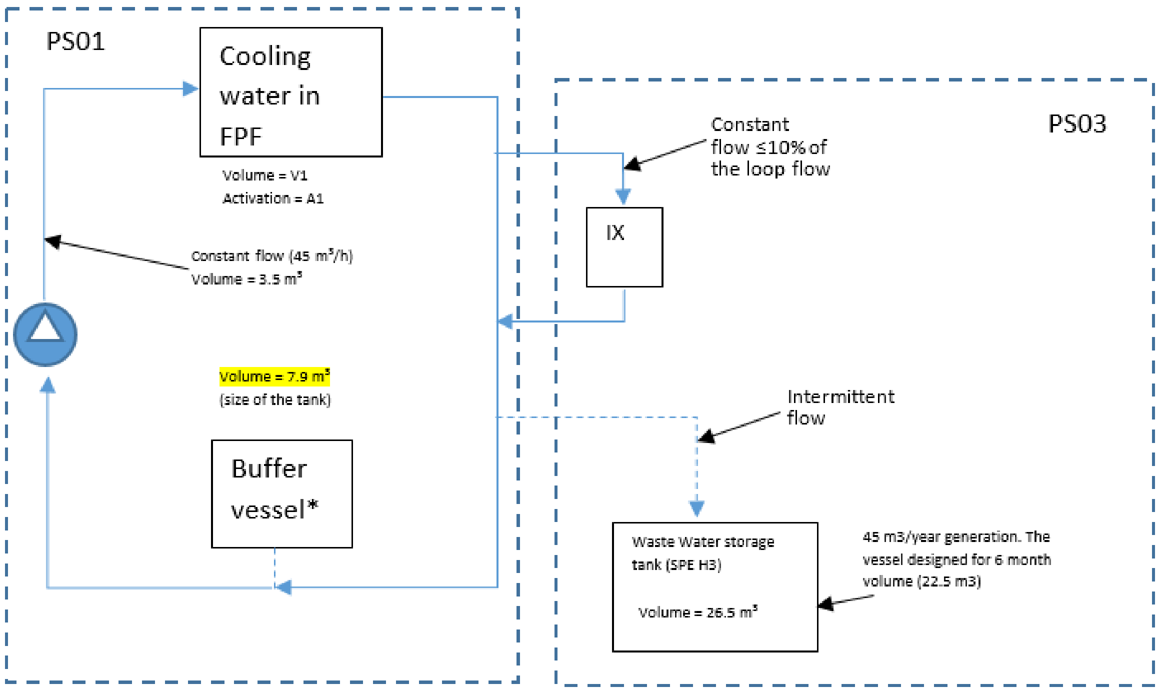
Activity release rate!

$$\boxed{RR(t) = R\langle A_1(t)\rangle[Bq \cdot s^{-1}]}$$

FPF (100 MeV, 4mA)



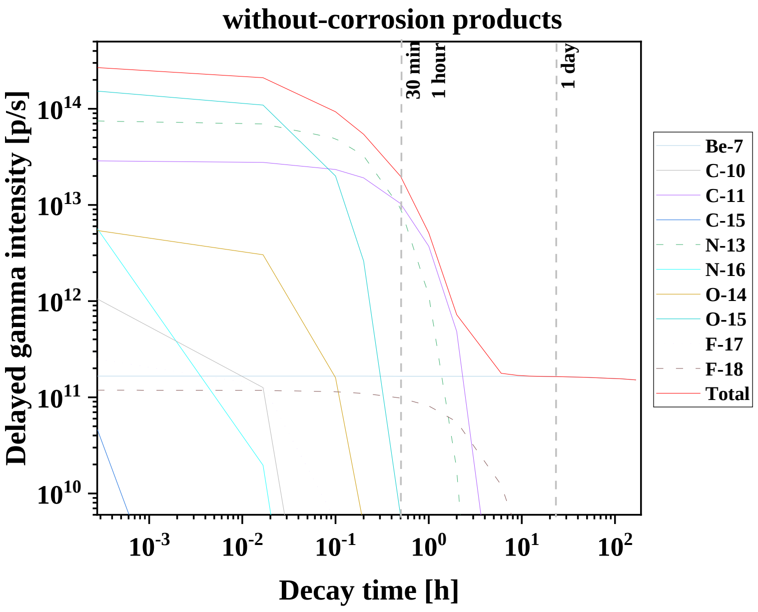
Simplified cooling water loop diagram

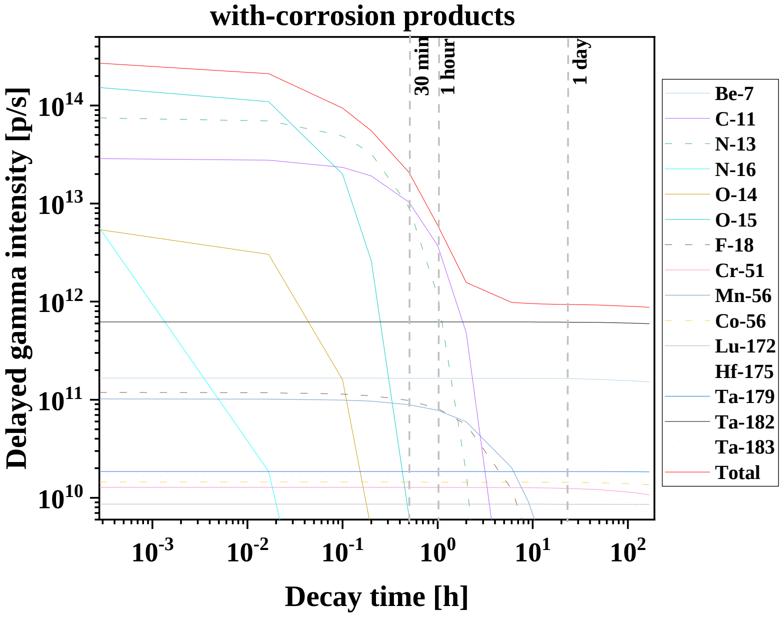


Material	A [Bq]	Volume [cm³]	Total Corrosion rate [µm/y]
Beam window	7.07E+09	3.15E-02	0.5
Ta beam dump	3.29E+11	2.31E-01	2 (0.5 x 4 layers)
Steel pipes	1.51E+11	4.48E+01	8.35 (1.67x5 pipes)
Pure cooling water	2.33E+14	1.53E+06	-

FPF (100 MeV, 4mA)

Nuclides	Half-life	Gamma decay energy [keV]	Percent yield per decay (%)	Delayed gamma intensity [p/s]	Average gamma decay Energy [keV]	Ambient dose conversion factor [pSv.cm²]
4-Be-7	53.22 d	477.604	10.44	1.659E+11	49.862	0.551
6-C-11	20.361 min	0.183* 511.0*	0.0002 199.5	2.873E+13	1019.445	5.266
7-N-13	9.965 min	0.277* 510.999*	3.356E-4 199.6	7.465E+13	1020.138	5.268
7-N-16	7.13 s	986.5 1755.0 1954.8 2741.5 2822.5 6048.2 6129.17 6915.5 7115.15 8869.2	0.0035 0.139 0.039999976 0.83999984 0.001299997 0.012999966 68.8 0.039999976 4.99999872 0.079999952	6.229E+12	4609.613**	14.680
8-O-14	1.177 min	0.392* 510.999* 1635.2 2312.59 3947.5	4.03E-04 199.756 0.052 99.388 0.00211	5.477E+12	3320.122	11.836
8-O-15	2.03 min	0.392* 510.999*	3.7275E-4 199.77	1.536E+14	1020.823	6.1632





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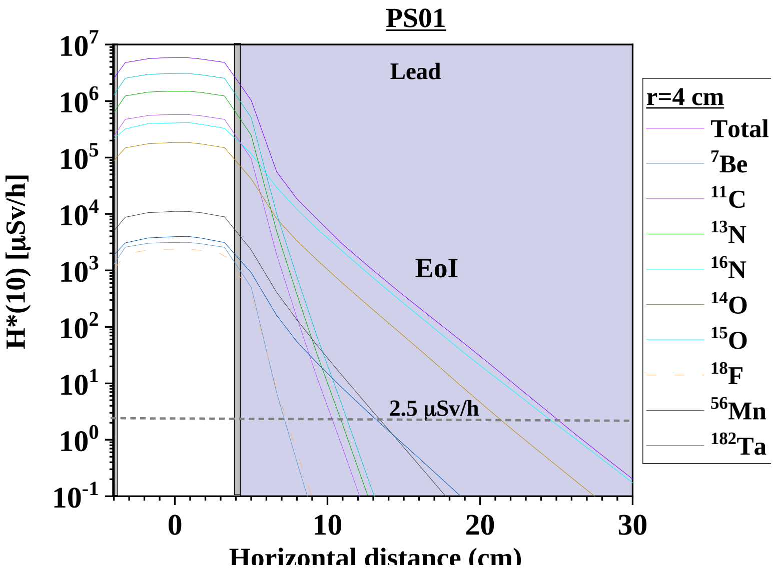

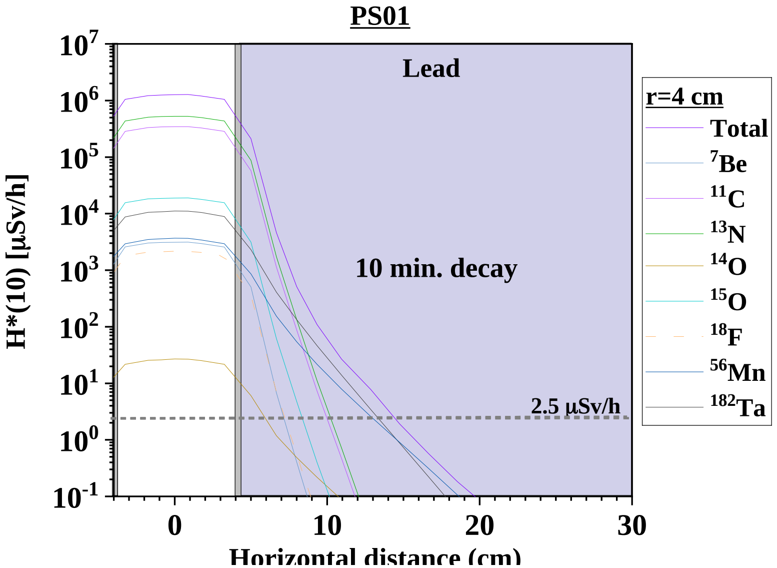

Application: RECUMO

A unique facility in Europa: RECUMO (Recovery of Uranium from Mo-99 Production)

More than 25% of medical radioisotopes are produced in BR2 research reactor of SCK CEN. These isotopes are then treated with a chemical process by the Institut National des Radioéléments (IRE) before they are administered to patients. The residues left behind by that chemical process still contain a number of substances that can be recovered. These residues are currently stored in special containers at IRE's site in Fleurus.

- Currently under construction at the SCK CEN site
- Commissioning in 2027
- The recovery is based on a chemical process
- After the recovery, the waste will be removed according to regulatory waste standards.

As part of the nuclear license, an ALARA study is required by the authorities before commissioning!

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Case	Cans in cases	Date Charge 1	Date Charge 2	Case	Cans in cases	Date Charge 1	Date Charge 2
	1 (bottom) /2/3/4 (top)	LL/MM/AAAA	JJ/MM/AAAA		1 (bottom) /2/3/4 (top)	LL/MM/AAAA	JJ/MM/AAAA
1	1	14/06/09	11/05/2015	9	1	7/07/04	21/12/2015
1	2	3/04/85		9	2	16/01/85	
1	3	4/05/87		9	3	10/03/86	
1	4	22/10/84		9	4	12/12/86	
2	1	5/12/83		10	1	1/06/93	
2	2	13/03/85		10	2	21/06/93	
2	3	22/05/85		10	3	3/05/93	
2	4	16/07/09	07/11/2013	10	4	20/02/07	18/08/2014
3	1	7/07/09	23/10/2013	11	1	17/08/10	22/05/2015
3	2	28/03/90		11	2	20/07/04	15/12/2015
3	3	18/04/90		11	3	7/06/06	09/01/2017
3	4	9/05/90		11	4	1/08/10	03/06/2015
4	1	25/07/84		12	1	30/11/10	08/02/2016
4	2	24/09/84		12	2	14/09/10	11/05/2015
4	3	29/04/85		12	3	30/01/06	27/01/2016
4	4	28/12/10	07/12/2016	12	4	20/02/06	15/01/2016
5	1	14/12/10	28/11/2016	13	1	8/10/09	26/08/2015
5	2	25/06/84		13	2	15/07/10	17/06/2015
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6	2	4/01/84		14	2	14/11/10	19/02/2016
6	3	7/11/83		14	3	31/03/11	23/07/2015
6	4	20/10/09	14/08/2015	14	4	17/06/10	10/07/2015
7	1	5/05/10	06/01/2016	15	1	31/05/04	23/03/2015
7	2	8/07/87		15	2	4/02/10	31/03/2014
7	3	2/05/86		15	3	31/10/10	02/03/2016
7	4	28/07/86		15	4	17/05/04	03/04/2015
8	1	17/04/87					
8	2	25/12/85					
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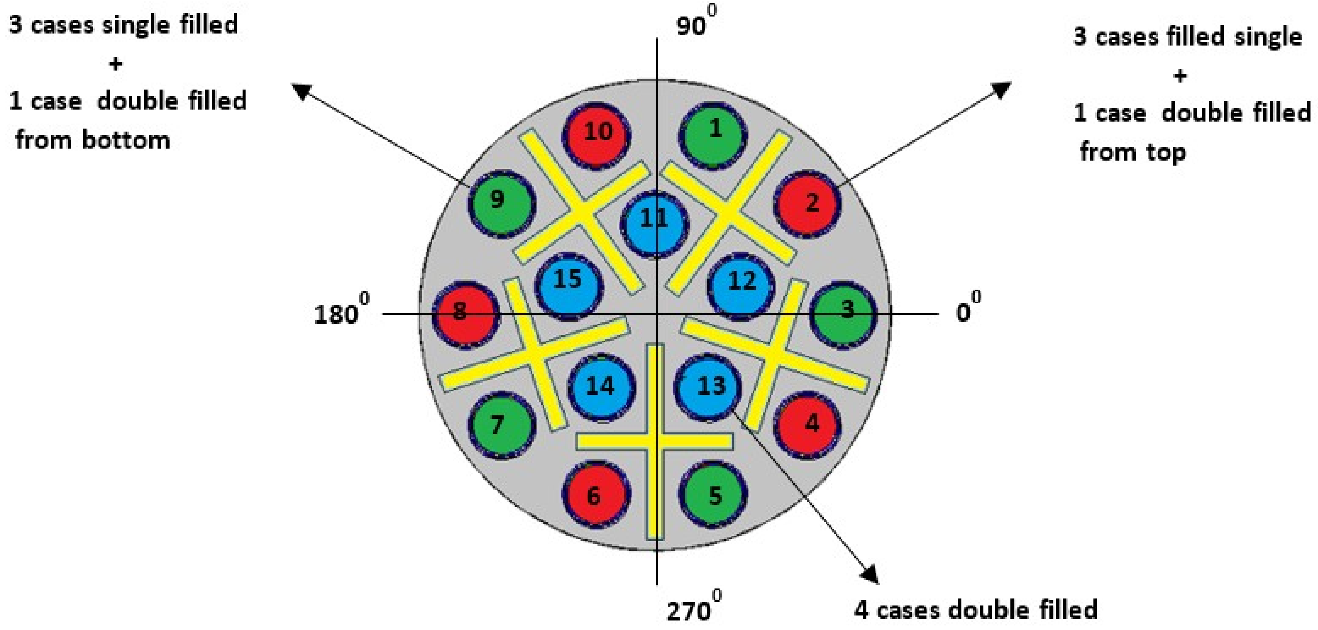
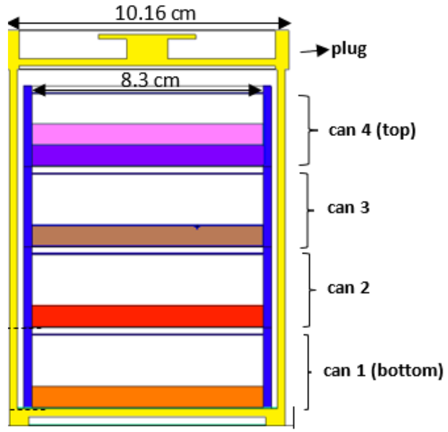


Loading:

-Odd numbers (in green) double filled from bottom

-Even numbers (in red) double filled from top

-The canisters with numbers between 11 and 15 (in blue) are filled double at each position



Case	Cans in cases 1 (bottom) /2/3/4 (top)	Date Charge 1 LL/MM/AAAA	Date Charge 2 JJ/MM/AAAA	Case	Cans in cases 1 (bottom) /2/3/4 (top)	Date Charge 1 LL/MM/AAAA	Date Charge 2 JJ/MM/AAAA
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8	2	25/12/85					
8	3	24/11/86					
8	4	24/02/10	21/10/2015				

11.86 years

34.37 years

4.29 years

Time of dose rate measurement: **24/04/2021**

The source terms of HEU residue per gram of U-235

Nuclide	Bq/g	Nuclide	Bq/g	Nuclide	Bq/g
26-Fe-55	2.67E+07	47-Ag-110m	1.34E+05	61-Pm-147	1.53E+10
27-Co-60	3.84E+06	48-Cd-113m	1.36E+06	62-Sm-151	1.49E+08
30-Zn-65	2.73E+06	50-Sn-119m	6.00E+05	63-Eu-152	7.03E+04
38-Sr-89	3.18E+03	50-Sn-123	3.49E+05	63-Eu-154	2.77E+07
38-Sr-90	9.19E+09	50-Sn-126	1.67E+04	63-Eu-155	1.64E+08
39-Y-90	9.19E+09	51-Sb-124	1.28E+00	64-Gd-153	7.71E+02
39-Y-91	5.28E+04	51-Sb-125	3.07E+08	65-Tb-160	4.10E+00
40-Zr-93	2.14E+05	51-Sb-126	2.34E+03	90-Th-231	7.99E+04
40-Zr-95	2.31E+05	51-Sb-126m	1.67E+04	91-Pa-233	5.60E+03
41-Nb-93m	3.62E+04	52-Te-125m	7.53E+07	92-U-234	3.09E+06
41-Nb-95	5.11E+05	52-Te-127	3.93E+05	92-U-235	7.99E+04
41-Nb-95m	1.96E+03	52-Te-127m	3.99E+05	92-U-236	4.86E+04
43-Tc-99	7.39E+03	53-I-129	2.91E+02	92-U-238	8.36E+02
44-Ru-103	6.02E+00	55-Cs-134	7.00E+05	93-Np-237	5.60E+03
44-Ru-106	1.00E+09	55-Cs-137	4.69E+07	94-Pu-238	1.40E+06
45-Rh-103m	6.01E+00	56-Ba-137m	4.43E+07	94-Pu-239	6.14E+05
45-Rh-106	1.00E+09	58-Ce-144	9.81E+09	94-Pu-240	7.98E+04
46-Pd-107	1.69E+03	59-Pr-144	9.81E+09	94-Pu-241	3.20E+06
47-Ag-110	1.79E+03	59-Pr-144m	1.40E+08	95-Am-241	1.65E+04

Time of dose rate measurement: **24/04/2021**

1 container : 15 cases x 4 cans (one double or 2 doubled)

In total, there are 90 residues (active materials) that have different delayed photon sources. Each source is separately generated for each active material.

decay only problem

$$\frac{d}{dt}N_i(t) = \lambda_{j\to i}N_j(t) - \lambda_i N_i(t)$$

The source terms of HEU residue per gram of U-235

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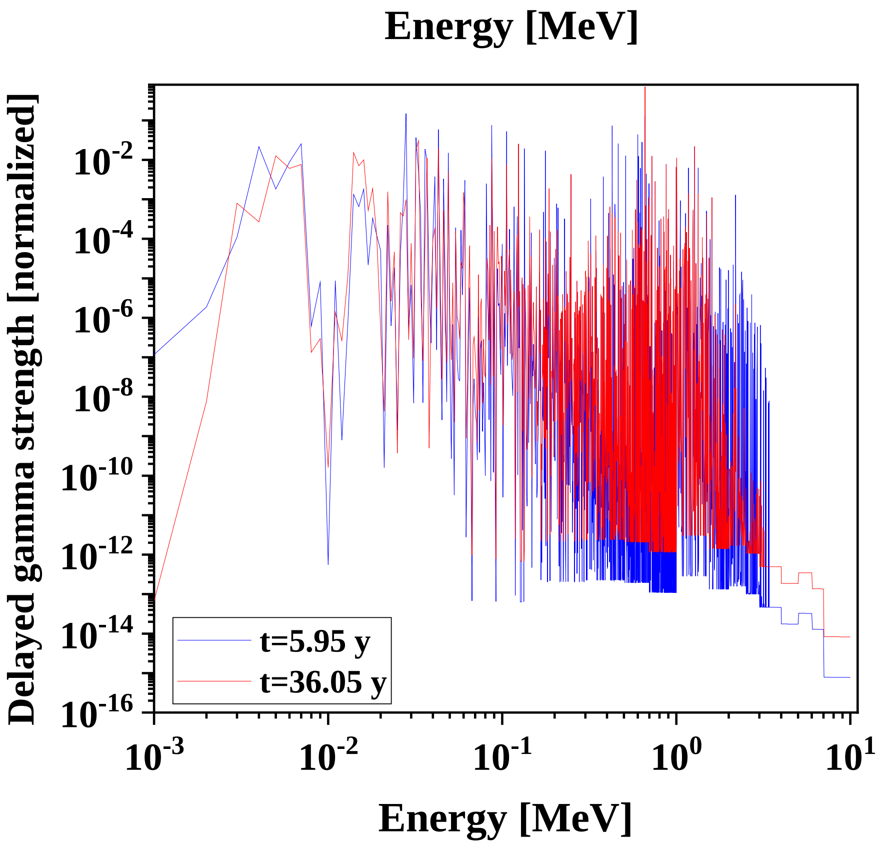
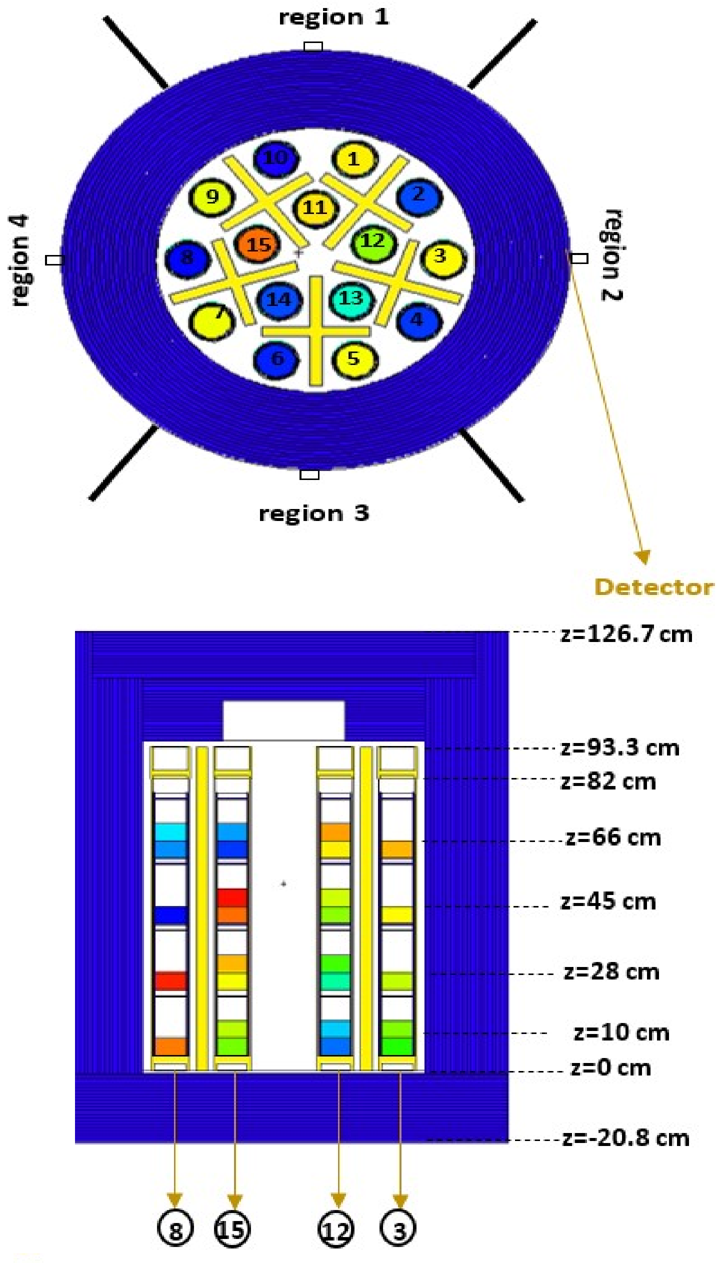
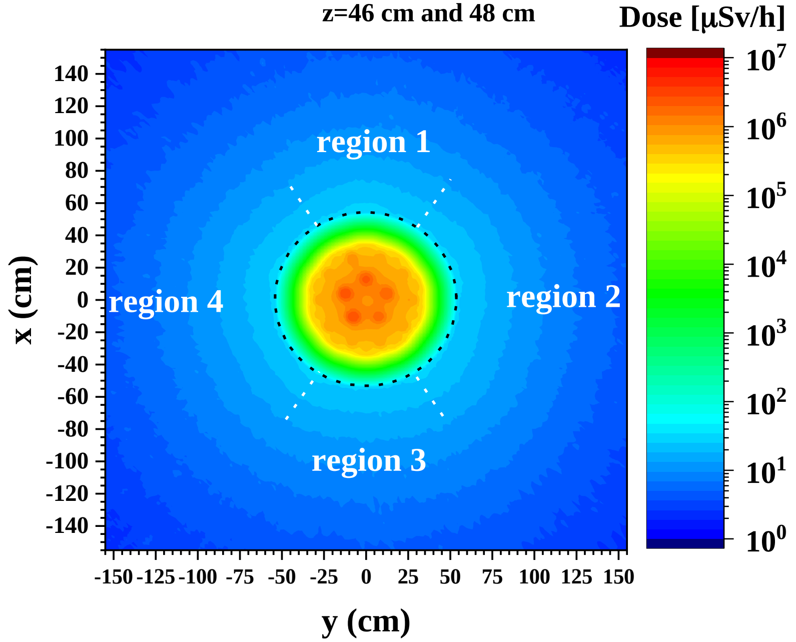
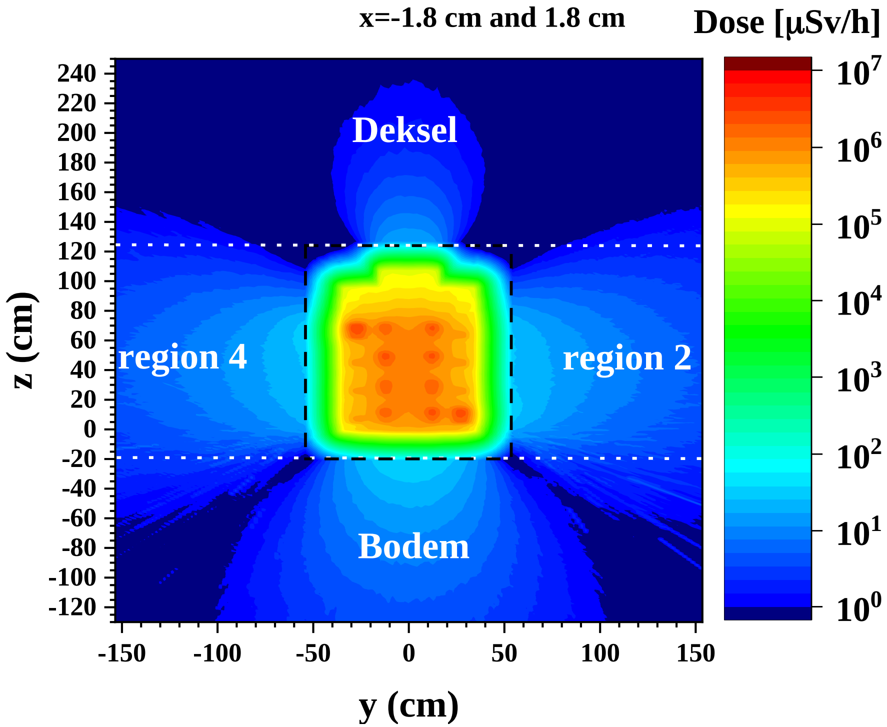
38-Sr-90	9.19E+09	50-Sn-126	1.67E+04	63-Eu-155	1.64E+08
39-Y-90	9.19E+09	51-Sb-124	1.28E+00	64-Gd-153	7.71E+02
39-Y-91	5.28E+04	51-Sb-125	3.07E+08	65-Tb-160	4.10E+00
40-Zr-93	2.14E+05	51-Sb-126	2.34E+03	90-Th-231	7.99E+04
40-Zr-95	2.31E+05	51-Sb-126m	1.67E+04	91-Pa-233	5.60E+03
41-Nb-93m	3.62E+04	52-Te-125m	7.53E+07	92-U-234	3.09E+06
41-Nb-95	5.11E+05	52-Te-127	3.93E+05	92-U-235	7.99E+04
41-Nb-95m	1.96E+03	52-Te-127m	3.99E+05	92-U-236	4.86E+04
43-Tc-99	7.39E+03	53-I-129	2.91E+02	92-U-238	8.36E+02
44-Ru-103	6.02E+00	55-Cs-134	7.00E+05	93-Np-237	5.60E+03
44-Ru-106	1.00E+09	55-Cs-137	4.69E+07	94-Pu-238	1.40E+06
45-Rh-103m	6.01E+00	56-Ba-137m	4.43E+07	94-Pu-239	6.14E+05
45-Rh-106	1.00E+09	58-Ce-144	9.81E+09	94-Pu-240	7.98E+04
46-Pd-107	1.69E+03	59-Pr-144	9.81E+09	94-Pu-241	3.20E+06
47-Ag-110	1.79E+03	59-Pr-144m	1.40E+08	95-Am-241	1.65E+04

Time of dose rate measurement: 24/04/2021







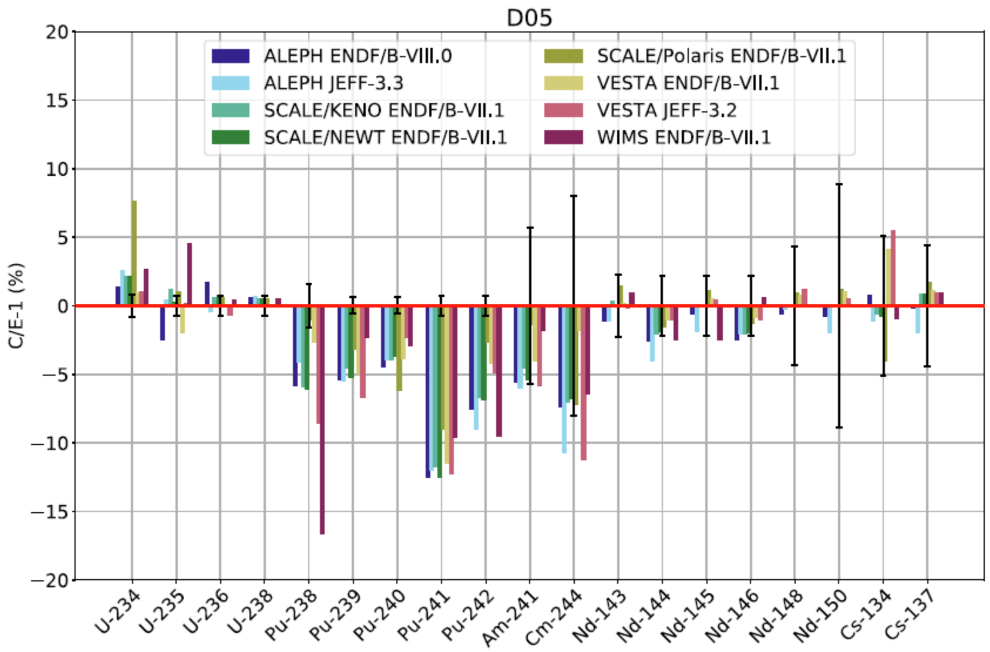


	C/E	
	contact	@100 cm
Reg. 1	1.03	1.00
Reg. 2	0.90	1.00
Reg. 3	0.90	1.00
Reg. 4	0.93	1.00

Application: Spent Fuel Characterization

REGAL

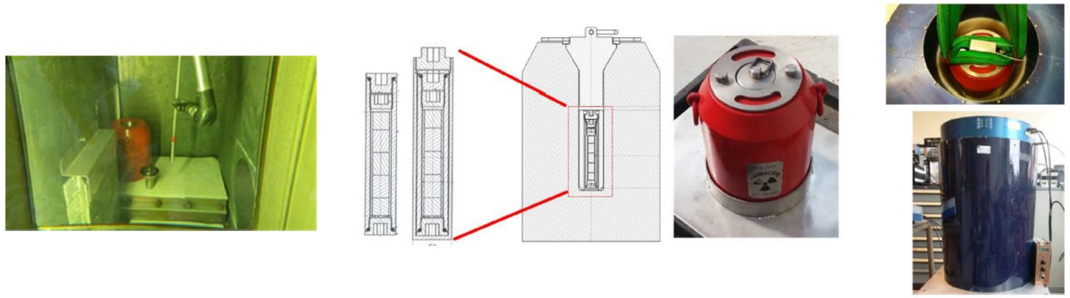
- PIE of UO_2 and low BU $(U,Gd)O_2$ (~50 & ~12 GWd/tHM) samples



Source: J. Eysermans *et al. REGAL International Program: Analysis of experimental data for depletion code validation*. Ann. Nucl. Energy 172 (2022) 109057

EURAD

- Absolute n-emission measurements



S_{sf} = 678 (12) $s^{-1}g^{-1}$ $\quad$ $S_{\alpha n} / S_{sf}$ = 0.039 (18)

Code	Library	Nuclide inventory, N_X/N_U			BU	S_{sf}	S_{α}/S_{sf}
		$^{148}Nd \times 10^{-4}$	$^{137}Cs \times 10^{-3}$	$^{244}Cm \times 10^{-5}$	MWd/kg	$s^{-1}g^{-1}$	
ALEPH2	JEFF-3.3	9.740	2.225	6.290	53.25	640.1	0.020

Source: P. Schillebeeckx *et al. An absolute measurement of the neutron production rate of a spent nuclear fuel sample used for depletion code validation*. Front. Energy Res. 11 (2023)

Conclusions

- ALEPH2 Monte Carlo depletion code uses MCNP/PHITS for spectral calculations, RADAU5 for the evolution calculations and NJOY for the nuclear data processing.
- Nuclear data consistency: the same data is used by ALEPH2 and MCNP/PHITS codes.
- Wide range of applications: from single pin to complex models such as ADS (MYRRHA designed at SCK CEN).
- Output of radioactive source terms, decay heat, yield of delayed radiation, etc.
- It has been validated using experimental data in the framework of many European projects.

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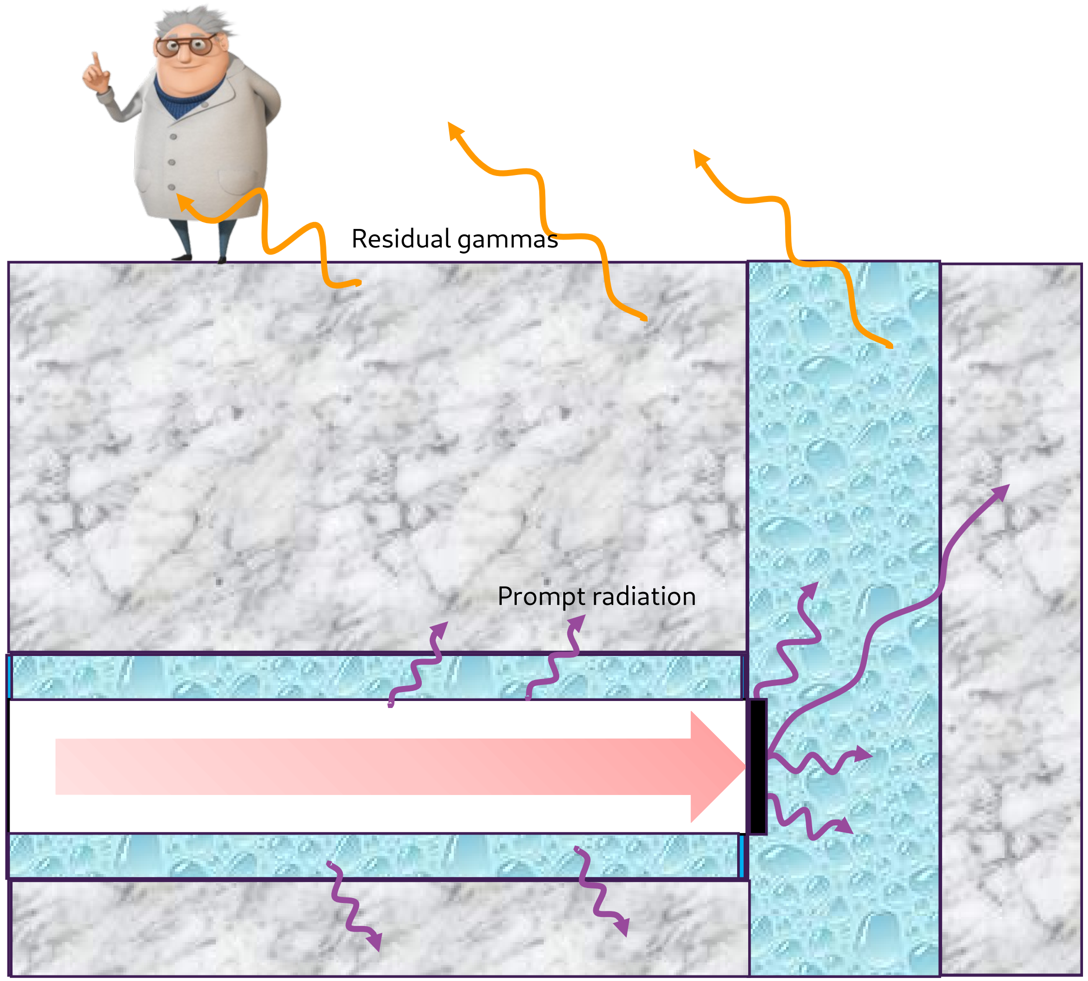
ALEPH2 automated calculation of residual doses



A single ALEPH2 run, but preparatory work is required to provide geometry locations of cells in order to tune the source for efficient sampling

First particle transport calculation is performed to get proton/neutron/photon field in which materials get activated.

↑

Vector of radioactive nuclides is obtained at the end of time step. ALEPH2 assumes uniform distribution of activated material in each user-defined cell

↑

Very fine energy group structure is used to represent the spectrum of delayed gamma-rays in each user-defined cell

↑

Combined source of gamma-rays is formed over all user-defined cells with probabilities proportional to total intensities in the cells

↑

2nd transport calculation (photons only) is performed and dose rates at detector positions are obtained