

#### ActiWiz 3 – Getting ready for an activ(ated) future



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#### o Introduction

#### o Calculation of nuclide inventories

• Overview of ActiWiz 3

### Nuclear facility



#### Material activation



$$P_{i} = \sum_{j} \sum_{k} \nu_{j} \int_{0}^{\infty} \sigma_{j \to i,k}(E) \Lambda_{k}(E) dE$$

Total production rate of radio-nuclide  $P_i$  based on particle fluence  $\Lambda$  and a cross-section  $\sigma_{i \rightarrow i}$ 

- $\sigma_{j \rightarrow i,k}$  = probability to produce an isotope *i* from a chemical element *j* with particle type k
- Evaluation of (1) requires a-priori knowledge of all reaction channels:
  - Iron: > 300 isotopes
  - Silver: > 800 isotopes
  - Lead: > 2400 isotopes



Eq. (1) can only be used for very very simple cases or specific reactions 😕

#### Option 1: use Monte Carlo event generators to model $\sigma_{j \rightarrow i,k}$



#### Monte Carlo

#### <u>Pros:</u>

- Yields fluence + activation at the same time
- Takes geometry into account  $\rightarrow$  spatial distribution

#### <u>Cons:</u>

- Long calculation times & statistics can be difficult (e.g. thin coating layers)
- Requires additional analysis tools to treat raw data

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#### <u>Deterministic</u>

- Very fast & high statistical significance
- Analysis tools fully integrated

#### <u>Cons:</u>

Pros:

- Requires fluence spectra information
- No information on spatial distribution



ActiWiz does not intend to replace but to complement general purpose Monte Carlo codes with respect to radiological characterization

## ActiWiz 3 overview



## Nuclide inventory analysis



Nuclide	
inventory	

Radiotoxicity (EU, CH, US, A, Japan, IAEA limits)	γ emission spectra	dominating isotopes	isotope production sources
shielding	alpha/beta analysis	temporal evolution of dominating isotopes	inverse temporal extrapolation of hazard

Green = ActiWiz 2 Blue = added in ActiWiz 3

## Example analysis & reporting



More info: https://indico.esss.lu.se/event/560/session/29/contribution/20

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#### Quality assurance via code comparisons & benchmarks

### Quality assurance



none

Concealed bugs in the algorithms are too willingly blamed on different physics models (especially if the discrepancy is not fully understood)

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can be > 10%

tests Algorithm

Unit

x-checks

Physics results x-checks

### **Comparison with FLUKA**



#### Beam protection device TPSG

Isotope	Activity – FLUKA [Bq]	Activity – AW 3 [Bq]	Ratio FLUKA/AW3
Co-56	3.57E+05 +/- 1.0%	3.15E+05 +/- 1.3%	1.13 +/- 0.02
Co-58	5.98E+05 +/- 0.5%	5.75E+05 +/- 1.1%	1.04 +/- 0.01
Sc-46	6.53E+04 +/- 2.0%	4.86E+04 +-/ 0.8%	1.34 +/- 0.02
Co-57	4.82E+05 +/- 0.7%	4.41E+05 +/- 1.1%	1.09 +/- 0.01
Co-60	4.14E+03 +/- 1.6%	3.83E+03 +/- 1.2%	1.08 +/- 0.02
Zr-88	3.80E+04 +/- 3.8%	3.09E+04 +/- 1.0%	1.23 +/- 0.04
Mn-54	1.19E+05 +/- 1.6%	9.95E+04 +/- 0.9%	1.20 +/- 0.02
Fe-55	1.26E+05 +/- 0.8%	1.07E+05 +/- 0.8%	1.18 +/- 0.01
Y-88	4.54E+04 +/- 3.1%	3.59E+04 +/- 0.8%	1.26 +/- 0.03
Nb-91m	2.86E+04 +/- 2.6%	2.81E+04 +/- 1.2%	1.02 +/- 0.03
V-48	1.85E+04 +/- 1.5%	1.52E+04 +/- 1.1%	1.22 +/- 0.02

1 hour of irradiation & 4 months of cool-down

## Comparison to measurements

Spoil activation assessment for future civil engineering works at the HiLumi LHC:

- quantity of interest is the radiotoxicity = sum of activity over clearance limit
- in 2016 some concrete wall & soil samples were taken and analyzed
- particle fluence spectra calculated with FLUKA (detailed tunnel geometry)

$\sum_{i} \frac{a_i}{LE_i}$	Shutdown 2016/17 (~3 months cooling time)					
UPR	γ spectrometry measurements		Ac full	tiWiz 3		
concrete	0.12		0.5			
soil	0.008		0.016			
				Ca-45	809 79	
Ca-45 is a cannot be	pure $\beta$ emitter: seen with $\gamma$ -spec	Ca-45 Na-22 S-35	6 2	8% 8% 2%	Zn-65 Fe-55 S-35	39 39 19
					Mn-54	19



C. Adorisio, S. Roesler, *Induced activation studies for the LHC upgrade to High Luminosity LHC*, ARIA 2017 Workshop, Lund



### Comparison to measurements



Center for ion-beam therapy and research in Wr. Neustadt, Austria

• activation samples (Al, Cu, Steel) at known loss points





 nuclide inventory calculations based on a <u>generic</u> beam loss scenario of 160 MeV protons (medical beam operation) 160 MeV proton beam on iron cylinder (R= 50 cm, L= 155 cm) Volume for fluence scoring: red hollow cylinder (3 cm < r < 50 cm, l= 100 cm)



C. Weixelbaumer, R. Wanzenböck, M. Deutsch, L. Jägerhofer, *Evaluation of induced activity and assessment of in-situ clearance procedures for MedAustron ion therapy accelerator components*, ARIA 2017 Workshop, Lund

## Comparison to measurements

Irradiation: 15 months, cooling: 14 days Quantity: relative contribution of activity (A) to the clearance level (CL)

Aluminium-alloy			
	% of CL contribution		
Nuclide	Meas.	Sim.	
Na-22	91.5 - 93	87	
Mn-54	7 - 8.5	10	

Copper			
	% of CL contribution		
Nuclide	Meas.	Sim.	
Co-60	69 - 72	42	
Co-58	18.5 - 19	38	
Mn-54	4.7 - 5	5	
Co-56	4.2 - 6.7	13	
Co-57	0.1 - 0.5	1	

Steel 1 (SFL)			
	% of CL contribution		
Nuclide	Meas.	Sim.	
Mn-54	69 - 69.5	72	
Co-58	14.5	2.5	
Co-60	8.1 - 8.6	0.5	
Co-56	6.7	20	
Co-57	0.5	0.5	
V-48	0.3 - 0.4	1.5	
Cr-51	0.1	< 0.5	

Steel 2 (SM1)			
	% of CL contribution		
Nuclide	Meas.	Sim.	
Mn-54	96.7 - 98.1	96	
V-48	1.7 - 3.1	1	
Cr-51	0.1 - 0.2	< 0.5	

 $\frac{\frac{A_i}{CL_i}}{\sum_i \frac{A_i}{CL}}$ 

Steel 3 (SM2)			
	% of CL contribution		
Nuclide	Meas.	Sim.	
Mn-54	99.6 - 99.7	96	
V-48	0.3 - 0.4	1	
Cr-51	0.1	< 0.5	

#### No dedicated simulation of beam loss but generic radiation scenario!

C. Weixelbaumer, R. Wanzenböck, M. Deutsch, L. Jägerhofer,

*Evaluation of induced activity and assessment of in-situ clearance procedures for MedAustron ion therapy accelerator components*, ARIA 2017 Workshop, Lund



## Summary

- ActiWiz 3 is a completely new generation of the code, including a large amount of built-in analysis functionality for radiological characterization
- Nuclear library based on JEFF 3.1.1 and 100 CPU years of generic FLUKA calculations
- Photonuclear reactions are now covered as well
- Energy range: thermal neutron energies up to 100 TeV
- Built-in radiation fields have been extended, including the LHC experiments
- Activation in arbitrary fields can be calculated, based on particle fluence spectra
- Together with FLUKA the ActiWiz 3 code has become one of the standard tools at CERN for radioactive waste characterization. It is also used for activation studies related to the design and material optimization of new facilities

Thank you

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#### Backup slides

### Analysis & reporting



How long do I have to wait for the residual dose rate to drop by X?



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# Nuclide inventory extrapolation

#### Typical questions:

- "how long do I have to wait to reduce the H\*(10) by a factor of X?"
- *"how much longer would I have to wait if I used the new LL values for clearance instead of the current LE clearance values"*?

Trivial for single isotopes but full inventories are considerably more complicated  $\rightarrow$  requires to solve the following equation for the time *t* efficiently(!):

$$\left(\sum_{i=1}^{M}\sum_{\substack{i \neq ields \\ i \neq k}} \frac{\lambda_l N_i^0}{LL_l} \prod_{j=1}^{l-1} \lambda_{j,j+1} \sum_{k=1}^{l} \frac{e^{-\lambda_k t}}{\prod_{\substack{p=1 \\ p \neq k}}^{l} (\lambda_p - \lambda_k)}\right) - \sum_{i=1}^{M} \frac{\lambda_i N_i^0}{LE_i} = 0 \qquad \text{with}$$

with nuclide concentration  $N(t = 0) = N^0$ 

ActiWiz 3 will provide this capability including full consideration of the temporal evolution of the nuclide inventory

# Analysis & reporting

For example: Stainless steel (304L) support irradiated in the PS. How long do I have to wait to reduce my dose rate by a factor of 10?

```
Selected hazard: H*(10) level
Current hazard: 5.99E-014, requested decrease: 0.1
Decreased hazard: 5.74E-015
after: 30878 s +/- 4.245% (= 8 hours, 2077 seconds)
Calculation time: 1.688 s
```



#### Brief feature summary



- Supports 85 different chemical elements as compound constituents
- High energy reactions based on FLUKA, low energy neutron reactions based on JEFF 3.1.1
- Creation of metastable states by low E neutrons based on evaluated data (JEFF)
- Decay engine limits numerical problems due to 170 digits accuracy (512 bits)

## Brief feature summary



• Multi-layer caching system for performance optimization of build-up & decay calculation



- calculation of the nuclide inventory of stainless steel for 55600 consecutive, different beam extractions (SPS case) in ~1.5 minutes with a precision of 170 significant digits

- 1 full year of SPS operation (>612.000 consecutive extractions) in ~15 minutes

• Now supports also loading of external radiation fields via rad. environment files

# Build-up & decay engine

- fully analytical solution without approximations, including also treatment of buildup
- allows for pairing irradiation & cooldown calculation in one step + modelling of complex irradiation/cooling patterns
- normalized partial solutions can be stored and reused in a 2-level cache → considerable speed-up in ActiWiz 3
- numerical issues treated by arbitrary precision arithmetics
   implemented with 512 bits significand ~ 170 digits