Journal of Physics: Conference Series

ActiWiz 3 – an overview of the latest developments and their application

To cite this article: H Vincke and C Theis 2018 *J. Phys.: Conf. Ser.* **1046** 012007

IOP Conf. Series: Journal of Physics: Conf. Series **1046** (2018) 012007 doi:10.1088/1742-6596/1046/1/012007

ActiWiz 3 – an overview of the latest developments and their application

H Vincke[1] **and C Theis**[1]

[1] CERN, Geneva 23, CH-1211 Geneva, Switzerland

christian.theis@cern.ch

Abstract. In 2011 the ActiWiz code was developed at CERN in order to optimize the choice of materials for accelerator equipment from a radiological point of view. Since then the code has been extended to allow for calculating complete nuclide inventories and provide evaluations with respect to radiotoxicity, inhalation doses, etc. Until now the software included only pre-defined radiation environments for CERN's high-energy proton accelerators which were based on FLUKA Monte Carlo calculations. Eventually the decision was taken to invest into a major revamping of the code. Starting with version 3 the software is not limited anymore to pre-defined radiation fields but within a few seconds it can also treat arbitrary environments of which fluence spectra are available. This has become possible due to the use of ~100 CPU years' worth of FLUKA Monte Carlo simulations as well as the JEFF cross-section library for neutrons < 20 MeV. Eventually the latest code version allowed for the efficient inclusion of 42 additional radiation environments of the LHC experiments as well as considerably more flexibility in view of characterizing also waste from CERN's Large Electron Positron collider (LEP). New fully integrated analysis functionalities like automatic evaluation of difficult-to-measure nuclides, rapid assessment of the temporal evolution of quantities like radiotoxicity or dose-rates, etc. make the software a powerful tool for characterization complementary to general purpose MC codes like FLUKA. In this paper an overview of the capabilities will be given using recent examples from the domain of waste characterization as well as operational radiation protection.

1. Introduction

The ActiWiz code [1] was originally developed to optimize the selection of materials used at high-energy proton particle accelerators, with respect to their radiological hazard. In the second version, features were added which allowed for calculating and analyzing nuclide inventories either for irradiation scenarios included in ActiWiz or based on nuclide production terms originating from external sources [2].

All scenarios which were included in ActiWiz version 2.x (see Ref. [1] for details) are based on a large amount of FLUKA [3][4]simulations which were used to characterize the radiation fields and calculate the associated nuclide production terms. Eventually it was decided to undertake the effort to develop a completely new generation of ActiWiz, which would use arbitrary particle fluence spectra as input and subsequently could calculate the nuclide production terms by itself without the need for further Monte Carlo calculations. In a first step this allowed for efficient extension of the included radiation fields to the 4 major LHC experiments and more flexibility with respect to including future installations.

The calculations are carried out in a deterministic table-driven approach using specific pre-calculated nuclear libraries. In order to analytically calculate the production rate of a radionuclide, the energy as well as particle dependent production cross-section has to be known. Convolution of this function with particle fluence data allows for predicting the number of certain radionuclides produced in a specific radiation field. The disadvantage of this approach is that exhaustive knowledge of all possible isotope production channels is required in order to obtain a complete nuclide inventory. While this is feasible to some extent for some light target elements it becomes impractical and even impossible for compound materials. This problem is generally overcome by Monte Carlo codes using parametrized isotope production models included in their generalized intra-nuclear cascade descriptions. The obvious advantage is that the particle fluence data are calculated in parallel to the isotope production. However, depending on the problem set calculation times might be very long and impractical if radionuclide production in gaseous media or very thin material layers is to be studied. Especially in the domain of radiological characterization these aspects become relevant in order to verify if attention to coatings has to be paid from the radiotoxic point of view.

These are the cases where ActiWiz 3 can be used to complement Monte Carlo studies. In contrast to standard cross-sections it uses tables of nuclide production data which depend on particle type as well as energy. For protons, charged pions, photons as well as neutrons above 20 MeV these tables have been produced by spending ~100 CPU years' worth of FLUKA calculations bombarding thin targets of 85 different chemical elements. The data utilized for neutrons < 20 MeV are derived entirely from the evaluated JEFF cross-section library (version 3.1.1) [5] and include in addition energy dependent production data of isomeric states. The details of the preparation of these data libraries, containing ~17 million records, are beyond the scope of this paper and can be found in detail in Ref [6]. In contrast to ActiWiz 2 the new code now covers the complete periodic system of stable elements as well as a few radioisotopes as possible constituents of compound materials.

This hybrid approach of using parametrized Monte Carlo based data as well as evaluated libraries resolves the shortcoming of having to provide explicit cross-section data as it implicitly includes all reaction channels predicted by a FLUKA simulation + the evaluated data from JEFF. Another advantage is that assessments with high statistical significance can be obtained in very short time, allowing for varying a multitude of parameters like material compositions with different trace elements or irradiation and cool-down scenarios. ActiWiz 3 is based on parallelized algorithms and allows for calculating the complete nuclide production data for 85 target elements within 2 seconds on a standard desktop computer (i7-2600 quad-core at 3.4 GHz).

However, it should be clearly stated that information on the particle fluence is the basic building block which is most often determined via Monte Carlo simulations. Therefore, it should be stressed that the code is not intending to replace Monte Carlo calculations but rather complements them specifically in view of radiological characterization. For this purpose a large number of out-of-the-box analysis functionalities and reports have been implemented, some of which will be discussed in the following sections.

2. Exemplary applications

2.1. Radiological characterization

While nuclide production data are the basis for any RP relevant assessment, eventually it is the nuclide inventory after a specific irradiation and cooling pattern that is of primary interest. For this purpose ActiWiz contains a built-up and decay engine operating at 512 bits floating point accuracy to avoid numerical pitfalls that can arise during the solution of the Bateman equations [2].

In general such a nuclide inventory needs to be put into relation with limits (e.g. clearance limits) or conversion functions (e.g. dose equivalent, inhalation dose, etc.) in order to become meaningful. For this purpose ActiWiz 3 already comes with a large set of such limits/conversion functions like Swiss, Austrian, Euratom, IAEA, US or Japanese clearance limits, and inhalation or ingestion dose conversion functions based on ICRP 72. This allows for easy assessment of for example the radiotoxicity of a material by calculating the sum of the activity with respect to the respective limit over all radionuclides. By default ActiWiz delivers reports relating nuclide activities in relation to any of the include limits/conversion functions. In addition to calculating hazard related quantities like the integral radiotoxicity, also the respective top contributing isotopes are determined.

2.1.1. Radiological relevance of thin coating layers

A typical case where the application of deterministic codes is advantageous over stochastic methods is the assessment of the radiotoxicity of thin layers. In the super conducting cavities of the Large Electron Positron collider (LEP SC cavities) the copper cavities contained a ~2 micro-meter thick Niobium layer. In order to remove such material from regulatory control one needs to assess the radiotoxic relevance of the Niobium layer which, due to its small thickness, becomes very challenging with Monte Carlo methods. This served as a practical example to demonstrate ActiWiz' capabilities for characterization. For this purpose a rough FLUKA model of a cavity assembly was built as depicted in Figure 1.

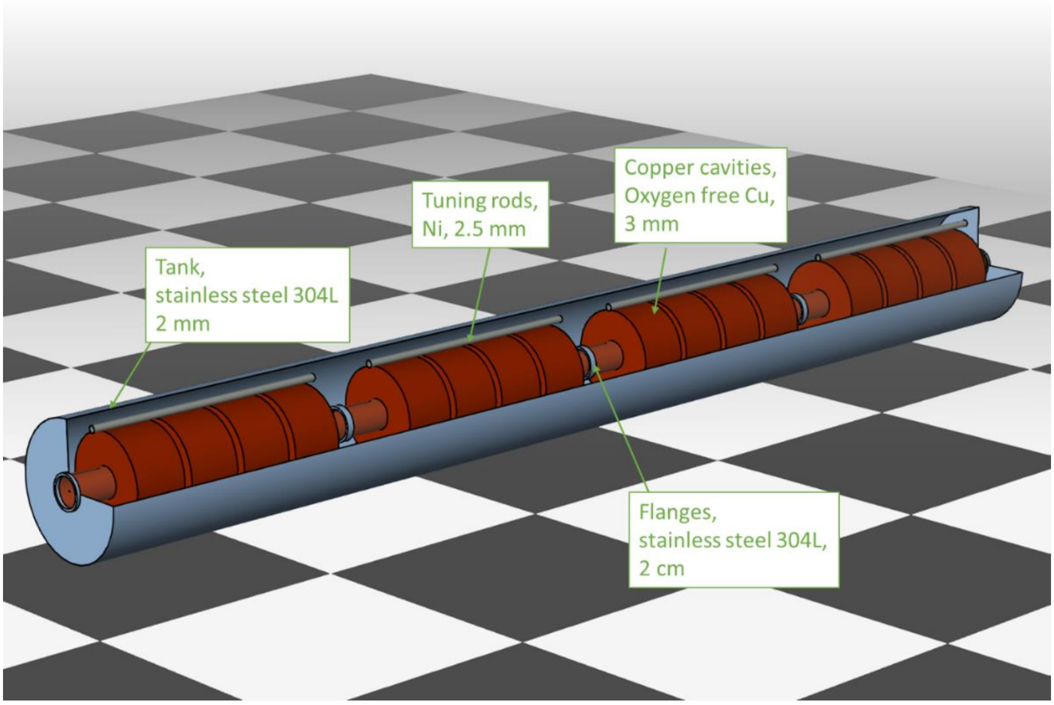

Figure 1 Visualization of the FLUKA geometry of a full SC cavity assembly consisting of 4 cavities with 4 cells each.

It should be noted that the geometry did not include the Niobium coating but only the copper cavities. Using FLUKA the impact of 105 GeV/c electrons at the entrance tube of an assembly was simulated and the ensuing particle spectra in the Copper tube at the beam impact as well as further down-stream have been recorded (see Figure 2 and Figure 3).

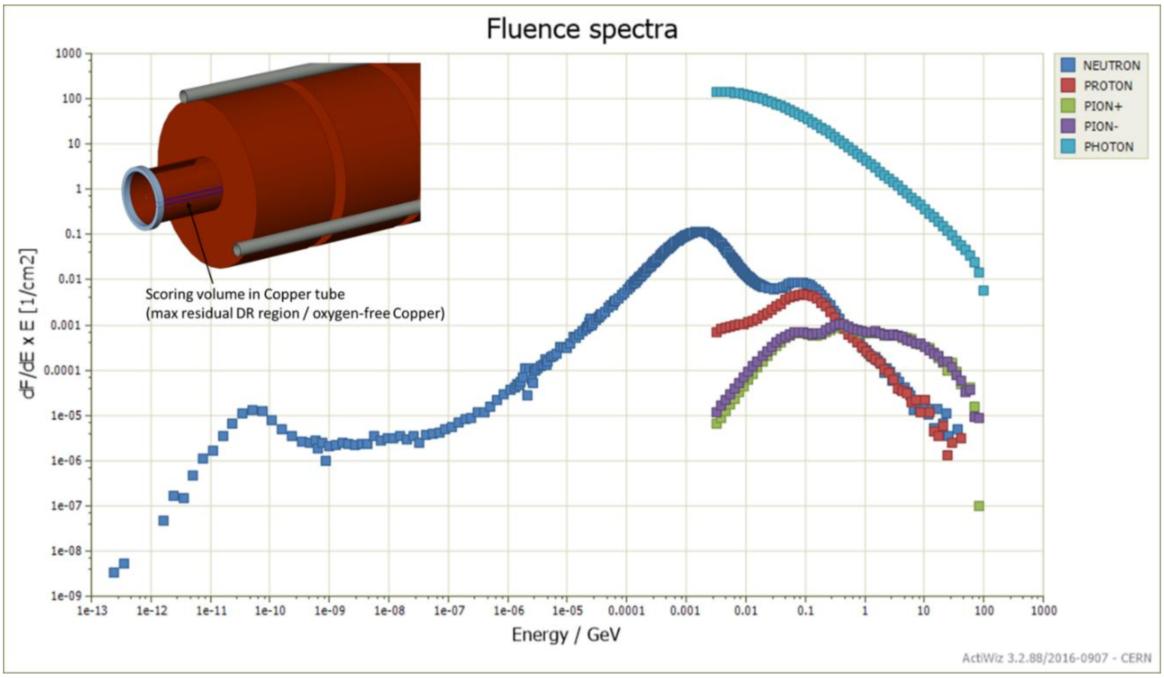

Figure 2 Particle fluence spectra in the Copper tube at the beam impact point. Error bars are generally smaller than 1%.

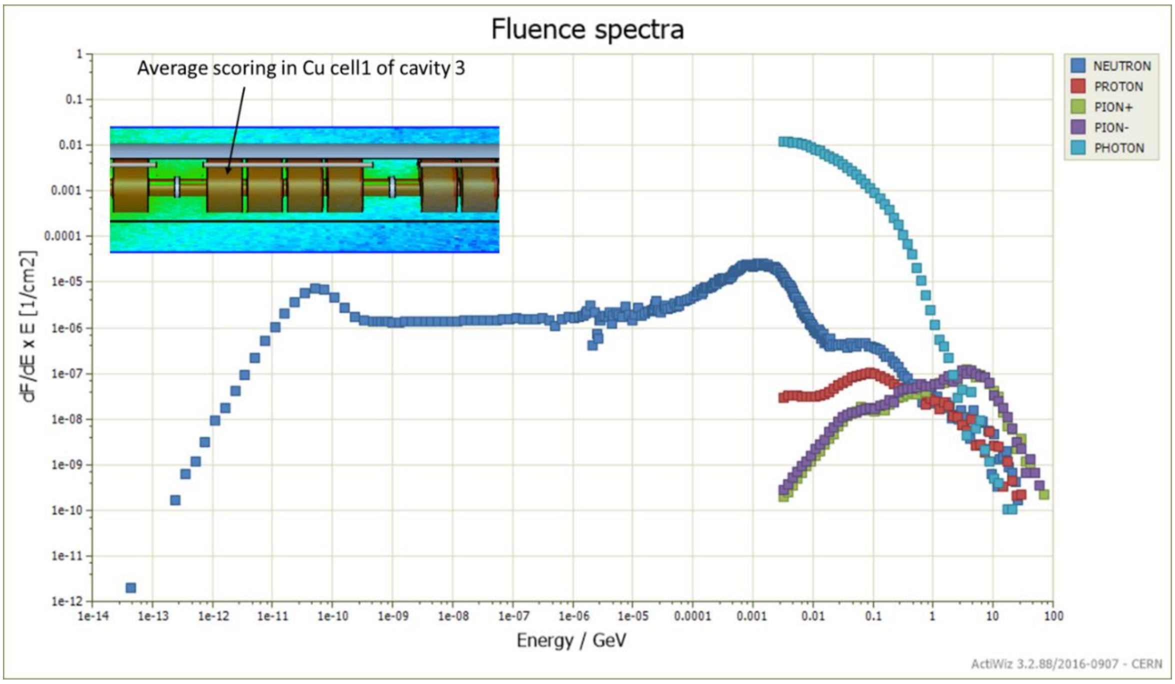

Figure 3 Particle fluence spectra for the “Cu-cell” volume downstream of the beam impact point. Error bars are generally smaller than 1%.

Using the fluence spectra shown above the nuclide inventory for Copper OFE as well as Niobium have been calculated assuming 5 years of irradiation and 15 years of cool-down. Table 1 shows the obtained sum of all nuclide activities over their respective clearance values using different sets of limits.

Table 1 Ratio of the radiotoxicity of Copper vs. Niobium for the different positions as well as different clearance limits.

	Copper vs. Niobium		
	CERN design clearance limit	LE – Swiss clearance limit	LL – future Swiss clearance limit (draft)
Beam impact :			
Copper vs Niobium	14	7	13
Downstream:			
Copper vs Niobium	3	3	3

It can be seen that the radiotoxicity of the Copper always outweighs the one of Niobium by at least a factor of 3 up to a factor of 14. Therefore, one can deduce that the Niobium layer can be neglected in any further assessment with respect to the clearance of the Copper, notwithstanding that the total mass of Niobium is negligible in comparison to the base material Copper.

2.1.2. Criticality of chemical constituents

In addition to an isotope based assessment ActiWiz also analysis the contribution to the respective hazard (clearance threshold, dose rate, etc.) by the different chemical constituents of a chemical compound. This is possible as the code provides information on the proportion of how much each chemical element contributes to the production of a specific isotope. Future versions of the code will also provide details differentiating between direct production as well as production via decay chains.

One example where this analysis functionality becomes useful is the characterization of stainless steel. Activation levels of this material after cool-down periods of several months are mainly driven by the amount of Cobalt impurities. However, this information is often unknown, which might pose a considerable problem for any further radiological characterization.

For the purpose of illustration we return to the example of the LEP SC cavities studying the nuclide inventory of stainless steel 304L (assuming 0.1 weight % of Co impurities) at the entrance flange of a cavity assembly as well as the outer cavity tank (see Figure 1). In this context the point of interest was not the radiotoxicity but rather the chemical element mainly responsible for the production of Co-60.

Table 2 Analysis of the dominant radionuclides found with the used stainless steel composition at different locations ("Flange" and "Tank"). In addition, the respective chemical elements are stated which give rise to the production of these radioisotopes [7].

Flange	**Rel. contribution to the radiotoxicity based on CERN's design limits**	**Source**
Co-60	45%	COBALT: 3.96%, IRON: 0.01%, NICKEL: 96.03%
Fe-55	28%	COBALT: 0.01%, IRON: 98.09%, MANGANESE: 0.01%, NICKEL: 1.89%
Tank	**Rel. contribution to the radiotoxicity based on CERN's design limits**	**Source**
Co-60	91%	COBALT: 94.55%, NICKEL: 5.45%
Fe-55	9%	IRON: 99.63%, NICKEL: 0.37%

As can be seen from Table 2 in the vicinity of the beam impact point ("Flange") or along the beam impact trajectory the actual Cobalt content of stainless steel plays a negligible role as the production of

Co-60 originates from Nickel. In contrast to Cobalt, Nickel has a rather well defined content (11 – 15%) as it is an intentional additive in stainless steel.

2.1.3. Criticality of difficult-to-measure (DTM) nuclides

The radiotoxicity of a specific material is defined as the total sum of the activity of each radioisotope with respect to its clearance limit. However, not all radioisotopes can be measured easily, either because they are pure alpha or beta emitters (e.g. Po-210) or have gamma lines which have a very low intensity (e.g. Fe-55). In order to evaluate the fraction of difficult-to-measure (DTM) isotopes contributing to a specific hazard quantity, like radiotoxicity or inhalation dose etc., ActiWiz automatically provides a detailed reporting function. For this purpose the nuclide inventory is processed and all isotopes are listed which are either pure alpha/beta emitters or have gamma lines only which are below 20 keV and/or if the integral intensity of the complete gamma spectrum is below 10^{-4}. A typical example of such a report is given in **Error! Reference source not found.**.

Table 3 Exemplary alpha/beta analysis (excerpt only!) of a nuclide inventory of Indium, irradiated close to the beam-pipe in the Large Hadron Collider for 180 days and 1 hour of cooling.

Difficult to measure nuclides (DTM)

Selected hazard: Radiotoxicty based on CERN's design limits

Id	rel. contribution to hazard [%]	$t_{1/2}$ [s]	Classification	Decay info
H-3	3.19000E-05	3.89E+08	pure alpha/beta	100% β^-
Be-10	1.21000E-10	5.05E+13	pure alpha/beta	100% β^-
C-14	1.34000E-07	1.80E+11	pure alpha/beta	100% β^-
Si-31	1.15000E-06	9432	integral gamma intensity < 1.00E-002	100% β^-
Cd-109	3.81000E-02	4.00E+07	integral gamma intensity < 1.00E-002	100% β^+(m)
Cd-113	5.99000E-18	2.43E+23	pure alpha/beta	100% β^-
Cd-114	0.00000E+00[1]	1.89E+25	pure alpha/beta	100% 2 β^-
In-100	0.00000E+00[1]	5.9	pure alpha/beta	96.1% β^+, 1.95% β^+, p, 1.95% β^+,p (m)
…	…	…	…	…

Total contribution to hazard = 33.6%, which equals = 5.634330E-004 Bq/unit (13.6% of total activity)

Data as such as those provided in the table above allows for providing a frame of reference of the criticality of radionuclides which cannot be measured by gamma-spectroscopy. ActiWiz 3 also provides such tables automatically for a set of fixed cooling periods (short term like 1 day up to long term like 30 years) in order to determine the maximum cool-down period beyond which the

---

[1] There is no contribution to the radiotoxicity as no clearance value is available for In-100 and Cd-114.

contribution of DTM nuclides become overwhelming. For elements like Indium such an analysis is critical as their contribution to the radiotoxicity can reach 99% after a few years of cooling.

2.2. Operational radiation protection

Maintenance periods at CERN are often directly preceded by machine development periods during which beam intensities can often vary. In operational Radiation Protection it is sometimes of interest to know up to which extent these deviations from normal operation can influence the nuclide inventory and related quantities like the radiotoxicity or clearance-level of samples. For this purpose the build-up and decay engine implemented in ActiWiz can treat also subsequent patterns of irradiation and cooling periods.

2.2.1. Complex irradiation & cooling patterns

As detailed in [2] ActiWiz implements a fully analytic solution to the Bateman differential equations which describe the build-up and subsequent decay of radioisotopes. Yet, this approach is not free from numerical pitfalls due to the limited floating point accuracy provided on today's CPU architecture. To overcome this shortcoming high-precision arithmetics with 512 significant bits are being utilized, which of course comes at the cost of performance.

The decay engine in ActiWiz is natively parallelized and will automatically utilize all cores using dynamic thread scheduling for maximum efficiency. Yet, the performance loss of switching from native double precision to arbitrary precision with 256 or 512 bits (~170 digits significant) results in a runtime penalty of about one order of magnitude or more. Yet, another possibility for optimization becomes apparent when analyzing the nature of the algorithm in more detail as some of the calculations involved in solving the Bateman equations can be considered repetitive if written in canonical form. This gives rise to the possibility of implementing a cache using a common "mailboxing technique". A more technical explanation is beyond the scope of this paper and can be found in Ref. [8].

In order to demonstrate the power of this concept the nuclide inventory of stainless steel has been determined considering one full month of SPS operation, modeling 55600 consecutive extraction and cool-down pairs (see Figure 4). In order to make the task somewhat more challenging the irradiation as well as the cool-down time have been randomly varied. While the overall period of 35 seconds had been retained, the irradiation time varied between 9 and 10 seconds, whereas the associated cool-down period was fixed at either 26 or 25 seconds. Such variations would be encountered if the duty and super-cycle of the accelerators were not integer numbers (e.g. 9,3 seconds) while the accuracy of the logging system's time stamps would be fixed to 1 second.

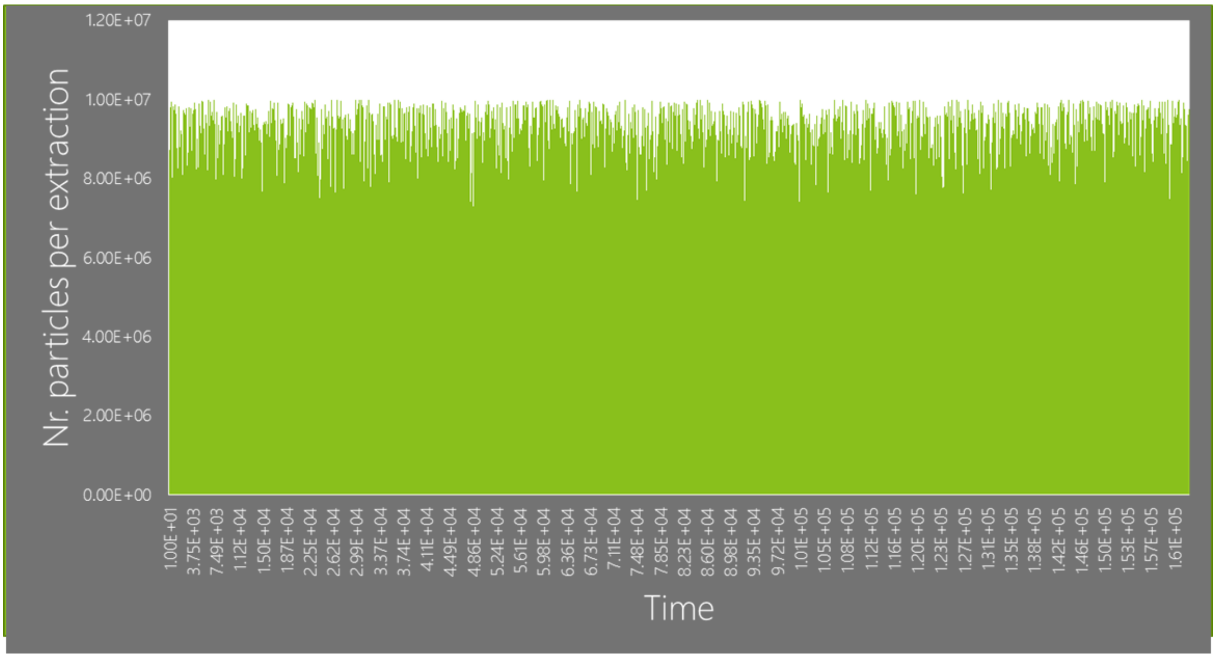

Figure 4 Exemplary data of 1 month of SPS operation, consisting of 55600 subsequent irradiation and cool-down pairs.

Using a standard desktop PC (i7-2600 quad-core at 3.4 GHz) the calculation could be performed in 93 seconds. While this example is extreme and somewhat academic, it serves to illustrate the potential of the implemented solution.

2.2.2. A practical application of an irradiation pattern

During the preparation of a maintenance stop of the Large Hadron Collider in 2016 it was discussed to reduce the beam intensity by a factor of about ~1/750 with respect to the nominal collision rate during the last four days (Thursday – Sunday) prior to the stop (Monday). However, it could not be excluded that at least on one day the intensity would not be raised again to nominal levels. In this specific case the interest was to determine the effect on the radiotoxicity of the C_6F_6 coolant used in the LHCb RICH detector. For this purpose four different scenarios have been evaluated modeling different irradiation/cooling patterns depicted in Figure 5. In all scenarios 6 months of continuous operation have been assumed as a basis followed either by four days of nominal operation, four days of low intensity operation or 3 days of low intensity operation interspersed with one day of nominal intensity.

For the purpose of modeling such time patterns ActiWiz provides a simple scripting language which allows for using mathematical expressions and variables (e.g.: 3 * day + 2 * hours – 5 * minutes). Within about twenty minutes it was possible to model and run a full study of four different scenarios yielding the results shown in Table 4.

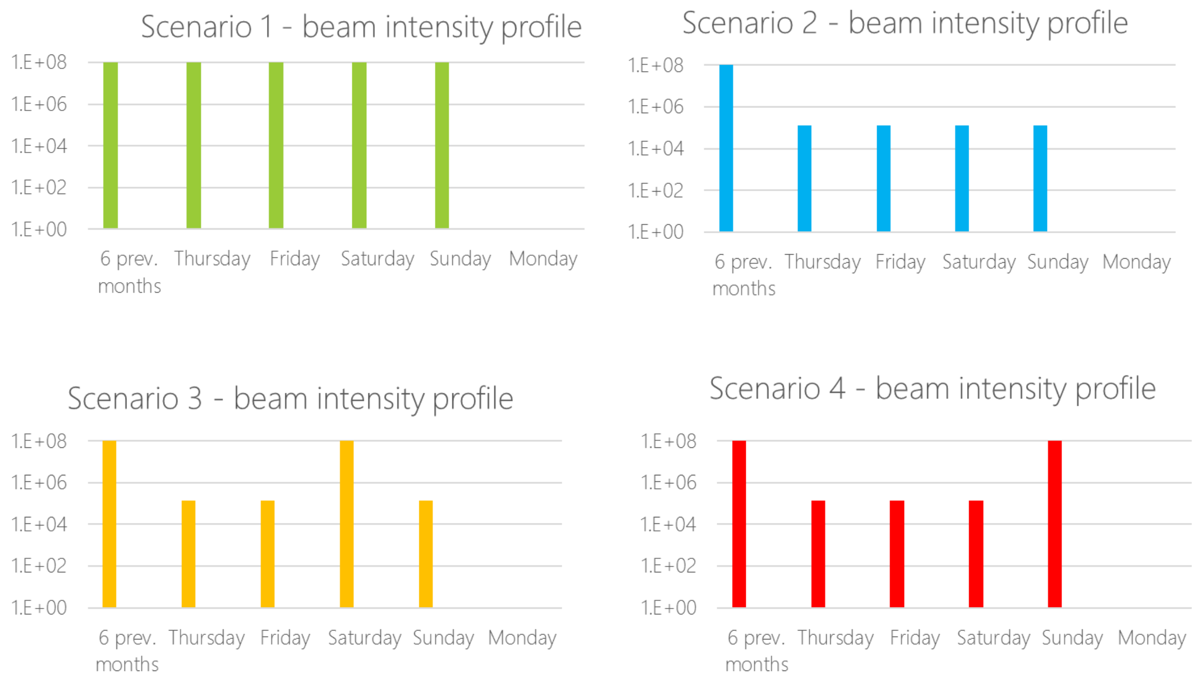

Figure 5 Four different irradiation / cooling scenarios prior to a maintenance stop of the LHC (Monday). In all scenarios 6 months of continuous operation have been assumed as a basis followed either by four days of nominal operation, four days of low intensity operation or 3 days of low intensity operation interspersed with one day of nominal intensity.

Table 4 Sum of the activity/clearance limit of the C_6F_6 coolant at LHCb's RICH detector as a function of the irradiation & cooling pattern prior to the machine stop.

Nominal intensity	Low intensity	Nominal intensity	Low intensity	Cooling	Activity / Swiss clearance limit
6 months	-	4 days	-	1 hour	0.0263
6 months	4 days	-	-	1 hour	0.00365
6 months	2 days	1 day	1 day	1 hour	0.0037
6 months	3 days	1 day	-	1 hour	0.0261

As can be seen only one day of low beam intensity is sufficient to decrease the radiotoxicity by a factor of about 7. Consequently, activation in the coolant is driven mainly by short-lived isotopes.

3. Summary and conclusions

This paper provides a brief overview of the ActiWiz 3 code which, in contrast to its predecessor, is not limited anymore to the assessment of nuclide inventories for CERN's high energy proton accelerators. Using particle fluence spectra for neutron, protons, charged pions as well as photons the software can assess nuclide inventories for compound materials exposed to arbitrary radiation fields within a few seconds. In addition the tool provides a large number of integrated analysis functionalities and out-of-the-box reports suitable for radiological characterization studies. In this paper features like the analysis of the radiotoxicity of thin Niobium coating as well as a radiation field dependent assessment of the criticality of knowing the exact amount of Cobalt impurities in stainless steel have been illustrated. For this purpose the LEP super conducting cavities haven been used as an exemplary case. Furthermore, features like the automatic evaluation of the importance of difficult to measure nuclides have been briefly discussed before concluding with an exemplary application in operational RP for the preparation of maintenance works. As such the code complements the use of general purpose Monte Carlo codes like FLUKA as far as the rapid calculation and analysis of nuclide inventories is concerned.

References

[1] Vincke H and Theis C 2014 ActiWiz – optimizing your nuclide inventory at proton accelerators with a computer code *Proceedings of the ICRS12 conference, Nara, Japan, Progress in Nuclear Science and Technology* **4** 228-232

[2] Theis C and Vincke H 2015 The use of ActiWiz in operational radiation protection *Proceedings of the SATIF-12 conference at Fermilab 2014, Nuclear Science Report NEA/NSC/R* **3**

[3] Fassò A, Ferrari A, Ranft J and Sala P R 2005 FLUKA: a multi-particle transport code, *CERN Yellow Report, INFN/TC_05/11, SLAC-R-773*

[4] Battistoni G, Muraro S, Sala P R, Cerutti F,Ferrari A, Roesler S, Fassò A and Ranft J 2007 The FLUKA code: Description and benchmarking *Proceedings of the Hadronic Shower Simulation Workshop 2006, Fermilab 6--8 September 2006, M. Albrow, R. Raja eds., AIP Conf. Proc.* **896** 31-49

[5] Koning A, Forrest R, Kellett M, Mills R, Henrkisson R and Rugama Y 2009 The JEFF-3.1.1. nuclear data library *JEFF Report* **22**

[6] Vincke H and Theis C 2017 Mass production of nuclide production data used in the ActiWiz3 code *CERN Technical Note* **CERN-RP-2016-220-REPORTS-TN, EDMS 1761230**

[7] Theis C and Vincke H 2016 The LEP superconducting cavities – a practical example of how to use ActiWiz 3 for radiological characterization *CERN Technical Note* **CERN-RP-2016-170-REPORTS-TN, EDMS 1719831**

[8] Theis C and Vincke H 2016 ActiWiz 3 – an overview of the concepts, architecture & new features *CERN Technical Note* **CERN-RP-2016-117-REPORTS-TN, EDMS 1706010**