The Monte Carlo Method: Versatility Unbounded In A Dynamic Computing World
Chattanooga, Tennessee, April 17-21,2005, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2005)

COMPARISON BETWEEN THE MONTE CARLO CODES MCNPX AND FLUKA WITHIN THE FRAMEWORK OF CALCULATIONS FOR THE TRADE EXPERIMENT

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ABSTRACT

The TRADE experiment, to be performed at the TRIGA nuclear reactor of the ENEA Casaccia Centre (Rome, Italy) consists in the coupling of an external proton accelerator to a spallation target to be installed in the central channel of the reactor kept in a sub-critical configuration. TRADE is meant to represent a major demonstration step of the Accelerator-Driven-Systems concept.

Monte Carlo calculations are needed for the radiation transport analysis of various aspects of the experiment. The Monte Carlo general purpose codes MCNPX and FLUKA have been applied, among other issues, to the analysis of the shielding configuration of the beam transport line and to the assessment of the radioactivity induced by the impact of the 140 MeV proton beam with the target. In the shielding analysis the dose rates due to the proton beam leakage along the transport line have been calculated for points beyond the barytic concrete shields. Various leakage angles with respect to the beam axis have been considered. The analysis of the induced radioactivity has involved the calculation of the type and amount of the residual nuclei produced by the spallation process within the tantalum target and of the evolution of such nuclei. The results obtained with MCNPX and FLUKA are compared and discussed.

Key Words: TRADE, MCNPX, FLUKA, activation, shielding

1 INTRODUCTION

Within the framework of the European Roadmap towards the experimental demonstration of an Accelerator-Driven-System (ADS), the separate components of an ADS (accelerator, target, sub-critical core) are being validated by means of several distinct experiments. To perform a preliminary coupling of the various components at power an experiment has been planned on the TRIGA reactor at the ENEA Casaccia Centre (Rome, Italy) a pool reactor of 1 MW thermal power. The TRADE (TRiga Accelerator Driven Experiment) project [1][2] is aimed at performing such a pilot experiment using a 140 MeV cyclotron.

The presence of a proton accelerator adds new radioprotection problems to such a system with respect to the traditional reactor. For instance the presence of beam losses under the normal operating conditions requires to provide a shielding structure along the Beam Transport Line (BTL) which carries the proton beam from the accelerator building to the spallation target inside the reactor core [3]. Another radioprotection problem is created by the spallation products generated inside the target. At the end of its life, the TRADE target must be removed and transported to a decay site; after a while, some samples will be eventually cut out and examined in suitably equipped laboratories. This set of operations has to be envisaged and performed assuring the safety of operators and minimizing the contamination of equipments, therefore a reliable calculation of the final activation of the target is required even before the design phase of the target and of the handling tools. Another calculation strictly connected with the target end-of-life activity is the target decay heat. Its knowledge becomes very important when studying some accidental scenarios. In case of complete fault of the target cooling system, the proton beam will be immediately interrupted but, without its forced cooling system, the target cooling must completely rely on the convective motions taking place inside the target container and their capability to exchange power through its wall to the TRIGA core because the mixing of water is prevented. This accidental case will be carefully simulated in the thermal-hydraulic experiments and, at this aim, the exact value of the decay heat must be preventively assessed by calculation.

The Monte Carlo method represents a tool of choice to handle such issues. The general purpose codes MCNPX (Los Alamos National Laboratory) [4][5] and FLUKA (INFN-Milan) [6][7] have been used to calculate the dose levels behind the BTL shields and the spallation products created in the target. Both of these issues strongly depend on the description of the proton-nucleus interactions in the intermediate energy range. However, while the calculation of the spallation products depend on all the possible reaction channels, those for the shielding refer only to the reaction channels involving neutron emission (as well as to neutron transport). On the other hand, the angular-energetic distributions of the emitted particles, which are important for the shielding, are less relevant for the spallation products, at least in this energy range.

The purpose of such an usage of two codes has been both to provide a check on the calculations and to assess the agreement between MCNPX and FLUKA.

2 SHIELDING CALCULATIONS

2.1 Configuration of the Beam Transport Line

The dose limit to be respected within the reactor hall is 50 μSv/h, under certain hypotheses of controlled access. The fraction of beam lost is assumed to be 1 nA/m along the BTL. Various leakage angles of the protons have been considered, ranging from 1 to 90 degrees with respect to the beam direction. The horizontal part of the BTL, the only one considered here, is shielded with barytic concrete of 140 cm thickness (Fig. 1 and 2).

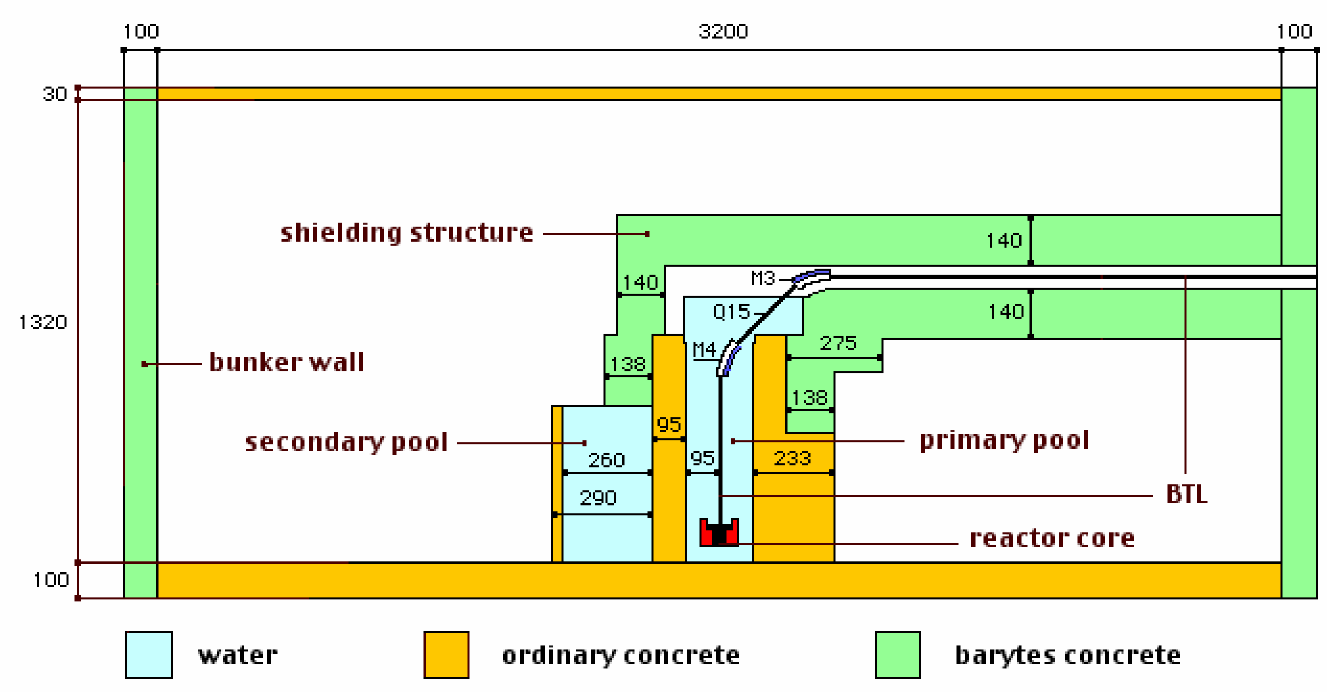

Figure 1. MCNPX model showing on the right the shielding configuration of the horizontal part of the Beam Transport Line (M4 and M3 are bending magnets and Q15 is a quadrupole). The dimensions are in cm.

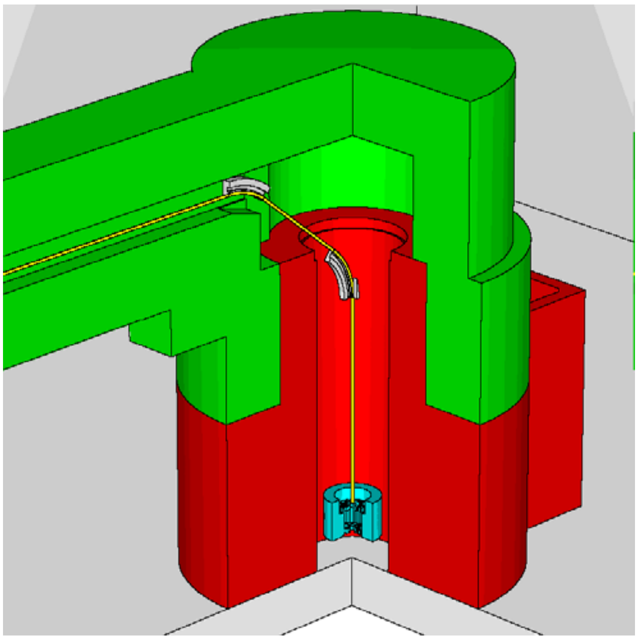

Figure 2. 3-D preliminary shielding configuration of the Beam Transport Line.

2.2 Calculation Method

2.2.1 MCNPX

The 2.5.d3 version has been used. Where available the LA150 data libraries [8] have been employed for the description of the nuclear interactions up to 150 MeV. For nuclides not present in LA150, the public library ENDF60 up to 20 MeV [9] has been used together with the cascade exciton model CEM2k [10] above 20 MeV. The flux-to-dose coefficients have been taken from [11] adopting the maximum values along the diameter of the ICRU sphere. The reduction of the variance has been carried out with the in-house optimiser DSA (Direct Statistical Approach) [12].

2.2.2 FLUKA

The April 2004 version has been used. In the energy range of interest for the present work, FLUKA employs the pre-equilibrium cascade model PEANUT [13]. Below 19.6 MeV the neutron interactions are described by means of data libraries [14]. Two user routines have been modified; the source routine, in order to have a leakage on a semi-conical surface, and the fluscw routine in order to multiply the scored fluence by the flux-to-dose coefficients. The same coefficients as in the MCNPX case have been used.

2.3 Results

In the MCNPX calculations exclusively a proton direction of 1 degree upward with respect to the beam direction has been considered, while in the FLUKA calculations also other angles up to 90 degrees and a direction on a semi-conical surface have been treated. In the case of leakage on a semi-conical surface the results represent an upper limit to the more realistic case of leakage within a semi-conical volume. The results are presented in tables 1 and 2 and Fig. 3. The dose values are calculated on the upper surface of the shielding structure.

Table I. Neutron and gamma dose rate for a proton leakage direction 1 degree upward.

Neutron dose rate (µSv/h)		Gamma dose rate (µSv/h)	
MCNPX	FLUKA	MCNPX	FLUKA
20.7±0.6	21±5	0.160± 0.006	0.15±0.04

Table II. Neutron and gamma dose rate calculated with FLUKA for a proton leakage direction on a semi-conical surface.

Leakage angle (degrees)	Neutron dose rate (μSv/h)	Gamma dose rate (μSv/h)
1	17±4	0.13±0.04
15	20±5	0.14±0.04
30	27±7	0.19±0.05
45	35±8	0.24±0.05
90	62±9	0.42±0.08

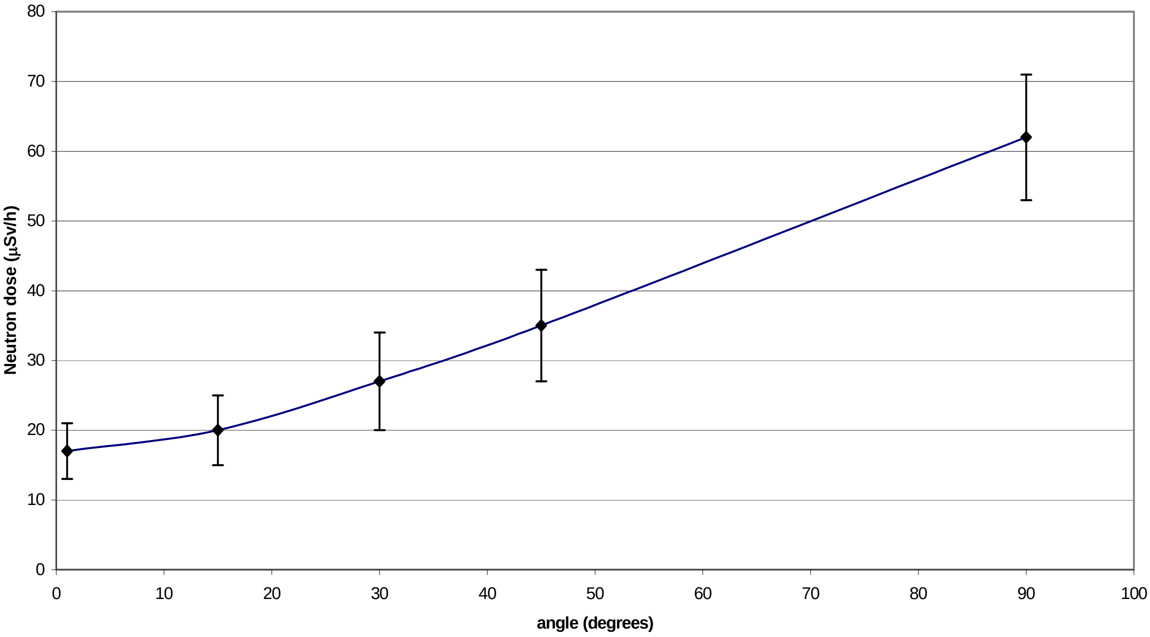

Figure 3. Variation of the neutron dose rate calculated with FLUKA with the angle of the beam losses.

The results show an excellent agreement between MCNPX and FLUKA. The assumption of a 90 degrees direction increases the neutron dose rate of a factor 3.6 with respect to the case of 1 degree.

3 SPALLATION PRODUCTS CALCULATIONS

3.1 Characteristics of the Proton Beam

The proton beam used in the simulations has an energy of 140 MeV and a current intensity of 285.7 μA. The radial profile has a truncated Gaussian shape with σ=0.88 and cut of the tail outside a radius of 43 mm.

3.2 Configuration of the Target

The experiment uses a tantalum target solution (Fig. 4) with a density of 16.48 g/cm^3 to generate the spallation neutrons for the sub-critical core. The volume is 622.5 cm^3 and the mass is 10.26 Kg.

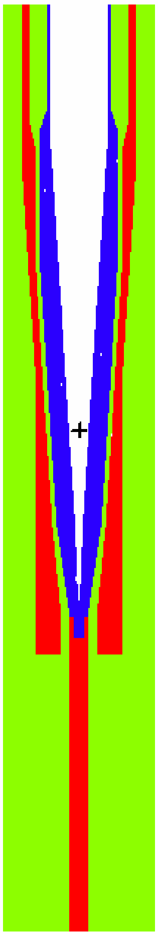

Figure 4. MCNPX model of the target. The blue area represents the tantalum. The proton beam enters from the upper opening.

3.3 Calculation Method

The accumulation and decay of the residual nuclei created in the target has been calculated by means of the code SP-FISPACT [15] using the data obtained with the Monte Carlo calculations. SP-FISPACT is an extension to energies higher than 20 MeV of FISPACT [16], an activation code designed for fusion applications for neutron energies below 20 MeV. The EAF-2001 libraries [17] used by FISPACT do not include all the residual nuclei calculated with MCNPX and FLUKA, yet the missing nuclei represent about the 1% of the total production.

3.3.1 MCNPX

MCNPX (together with the CEM-2k and Bertini [18] modules) has been used to calculate the the production of residual nuclei per primary proton excluding the nuclei created by neutrons with energy lower than 20 MeV. The obtained values have been furnished to SP-FISPACT which calculates the evolution (accumulation and decay) of the residual nuclei.

3.3.2 FLUKA

FLUKA has been used to calculate both the total residual nuclei production per primary proton and the production excluding the residual nuclei generated by neutrons below 19.6 MeV, the upper limit of the neutron transport library. These data have been furnished to SP-FISPACT to calculate the residual nuclei evolution. The data with cut below 19.6 MeV have been used for a comparison with those obtained with MCNPX with cut below 20 MeV. The FLUKA's source routine has been modified in order to sample the initial spatial co-ordinates of the source protons from a truncated Gaussian distribution, in accordance with the beam radial shape.

3.4 Results

The production of residual nuclei per primary proton in the Tantalum target is shown in Figures 5 and 6 as dependent on the mass number and in Figures 7-10 as dependent on the neutron number (for fixed charge numbers). The discrepancy generally decreases as far as the Z values become closer to Z=73 (the Tantalum target isotope).

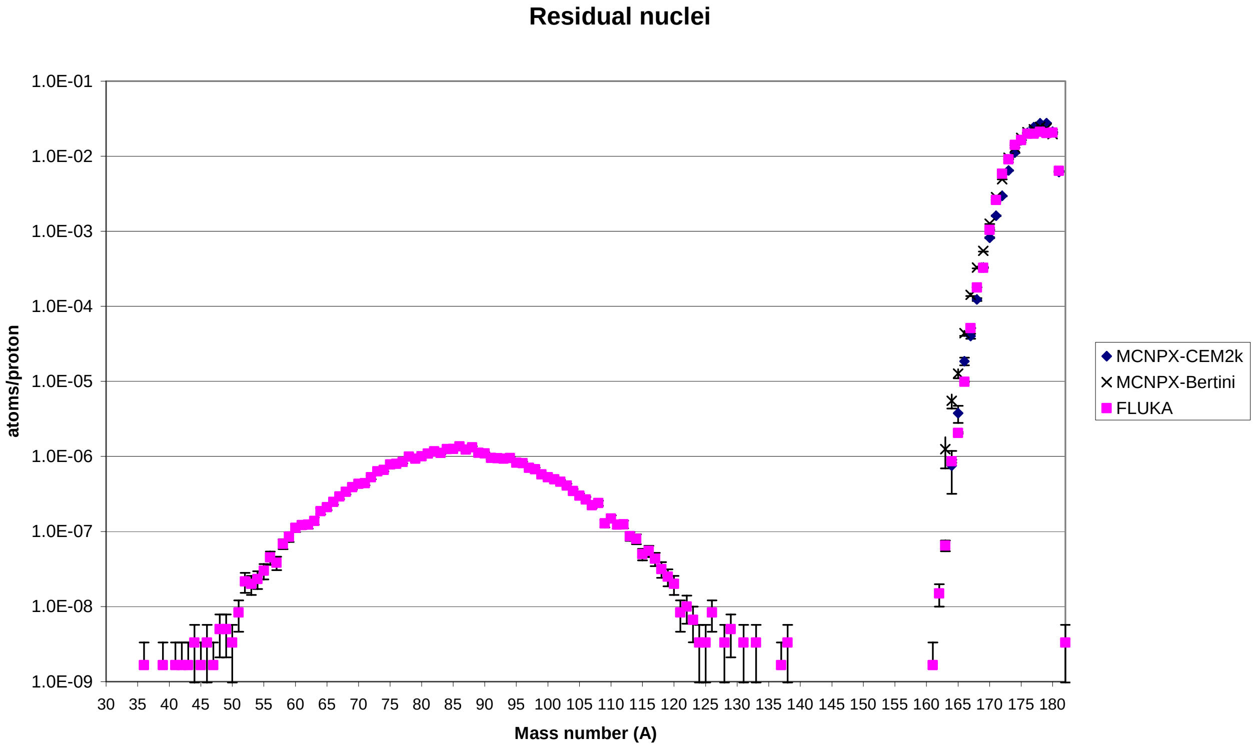

Figure 5. Residual nuclei calculated with MCNPX and FLUKA. The curve for A<140 represents the fission products (this curve has not been calculated with MCNPX).

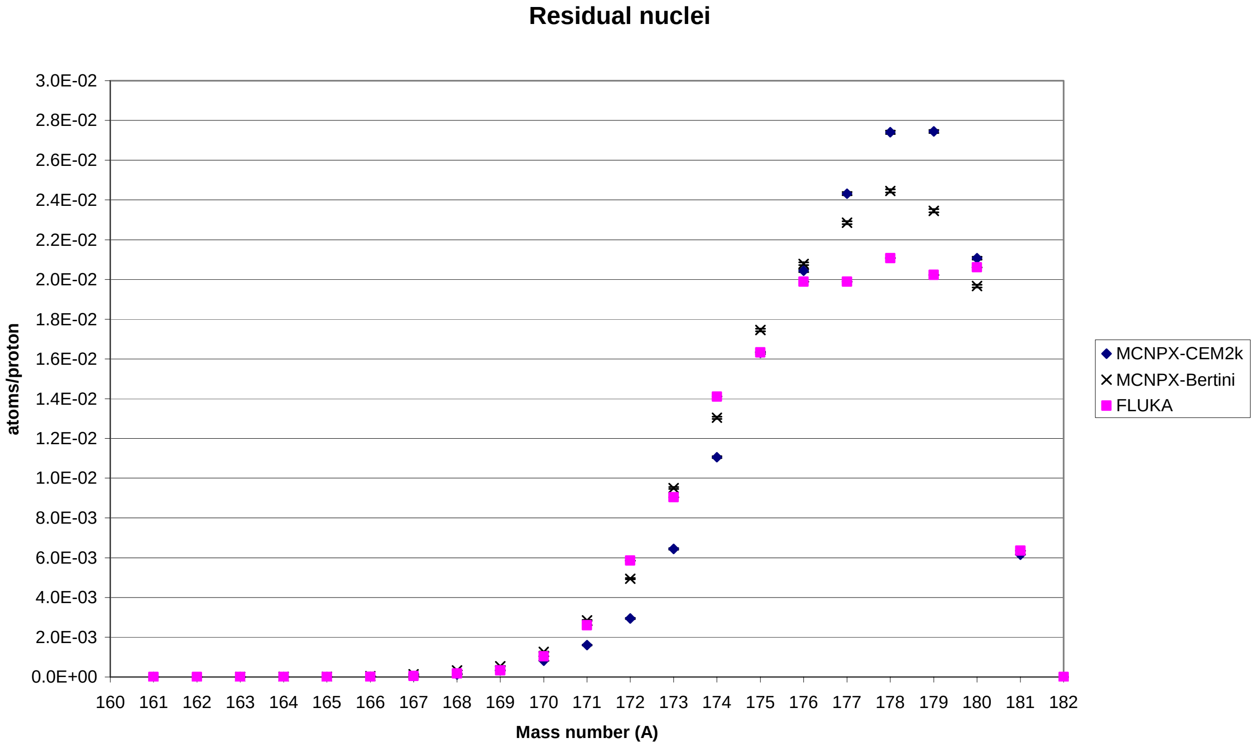

Figure 6. Residual nuclei of higher mass number. The production is shown on a linear scale.

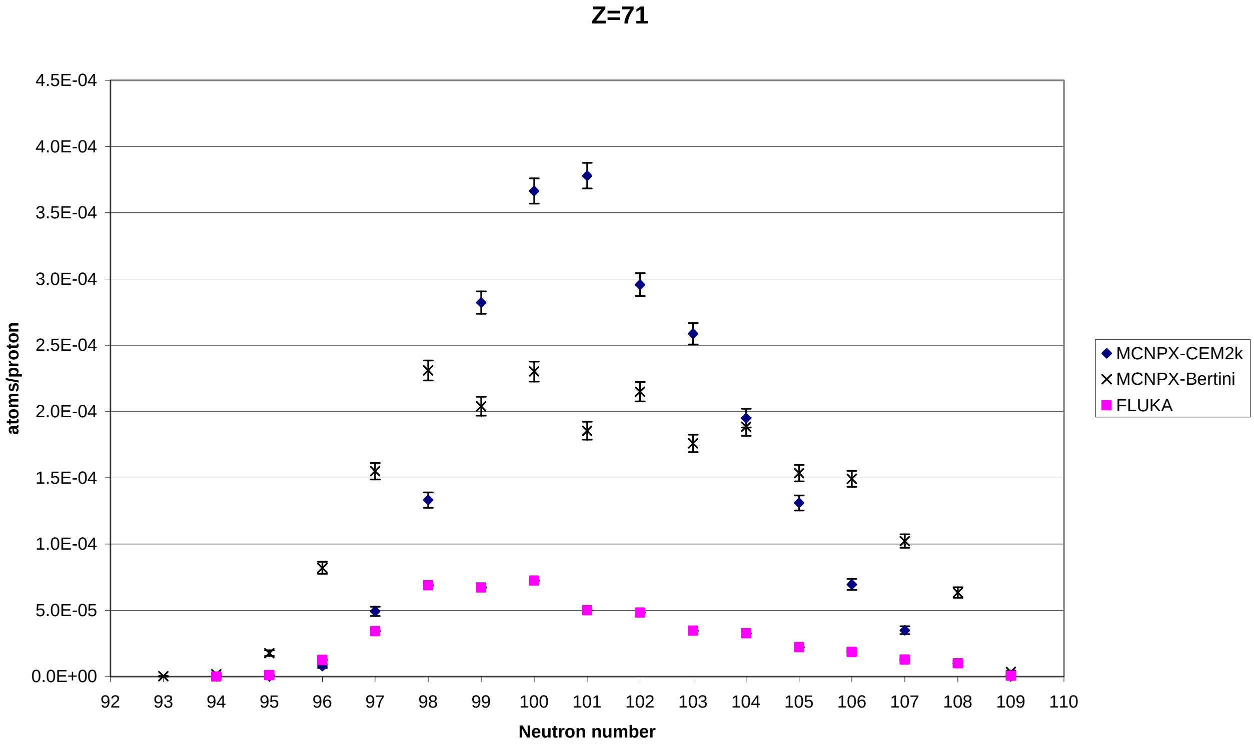

Figure 7. Residual nuclei with Z = 71 (Lutetium).

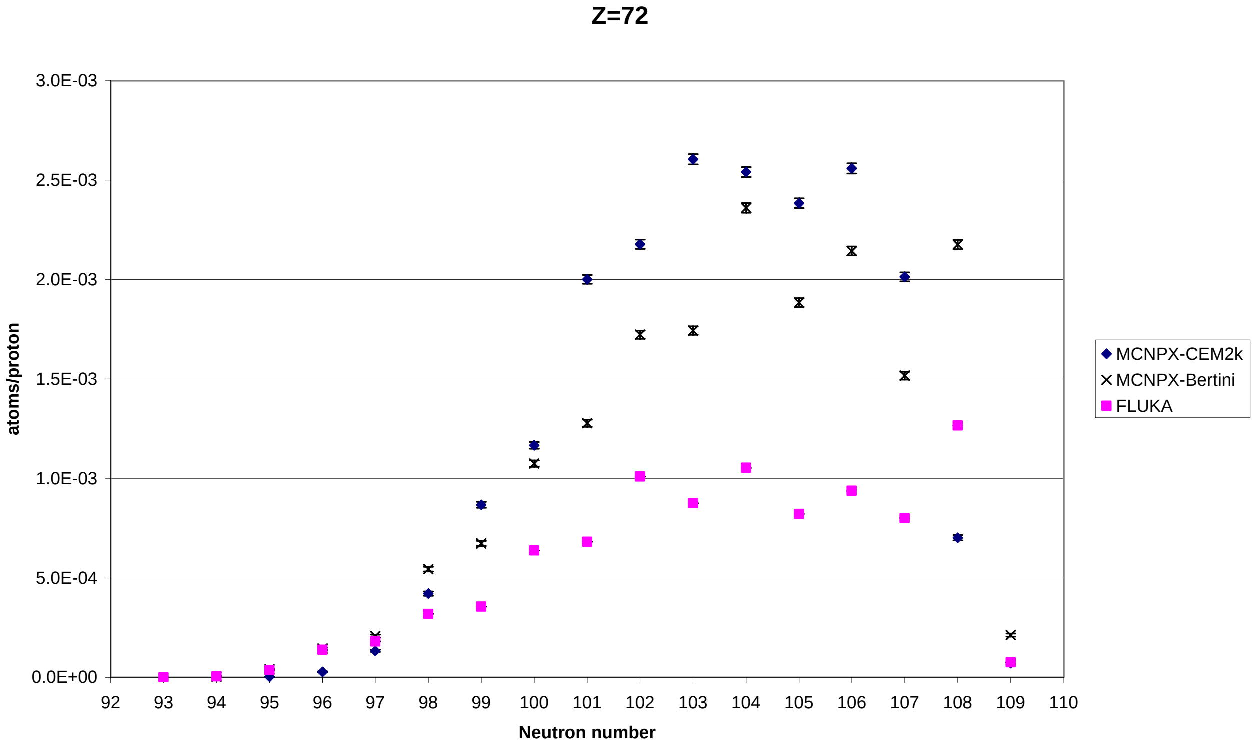

Figure 8. Residual nuclei with Z = 72 (Hafnium).

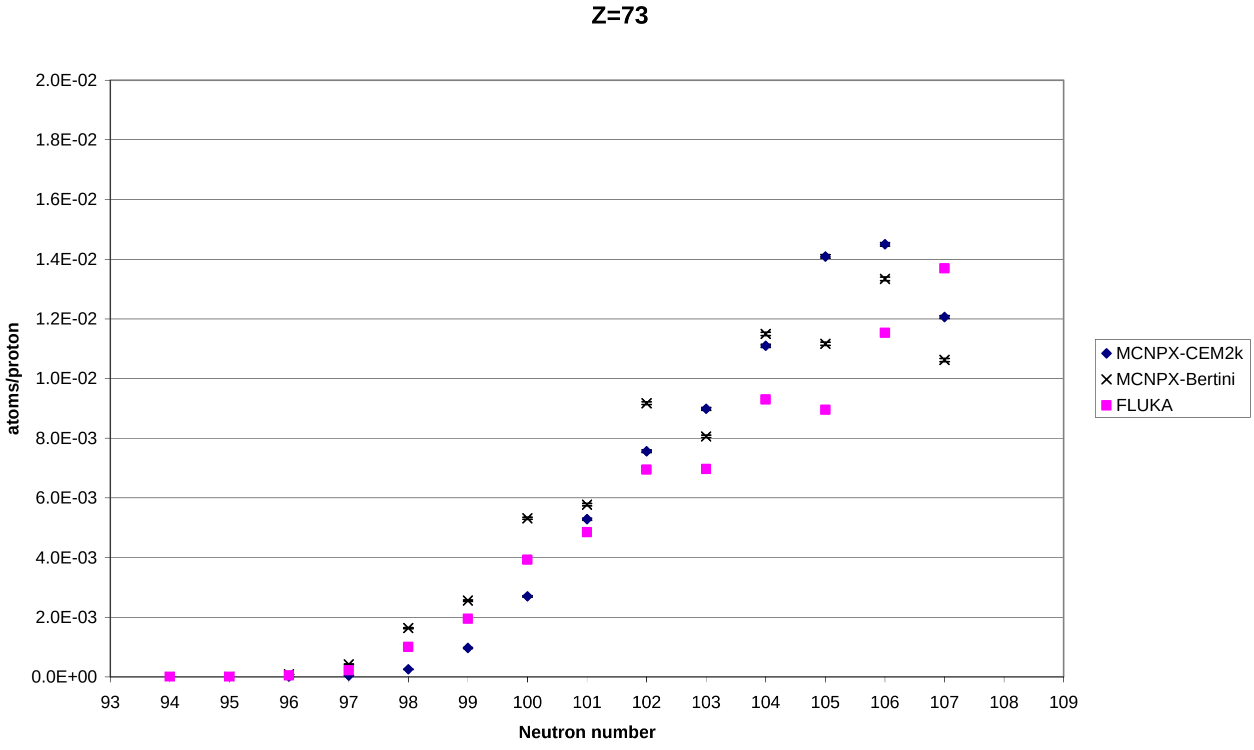

Figure 9. Residual nuclei with Z = 73 (Tantalum).

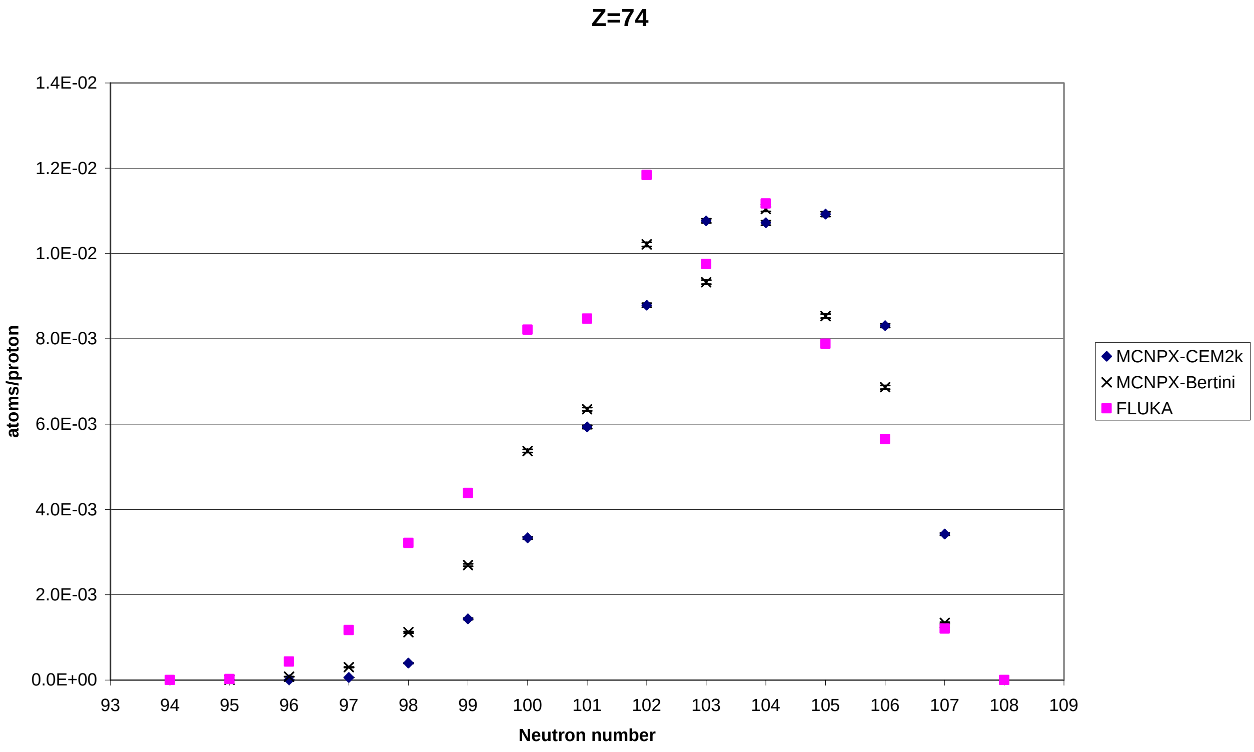

Figure 10. Residual nuclei with Z = 74 (Tungsten).

Generally speaking, the discrepancy between FLUKA and MCNPX is high for the isotopes whose production rate is low and thus less relevant. This is shown in Fig. 11, where the ratio of the results of MCNPX and FLUKA (MCNPX/FLUKA or FLUKA/MCNPX) is plotted as a function of the production rate. For the atoms whose production rate is about 1E-2 atoms/proton the discrepancy is generally within a factor of 2; for atoms whose production rate is between 1E-5 and 1E-3 atoms/proton the discrepancy is generally within a factor of 10; for lower values the discrepancy becomes higher.

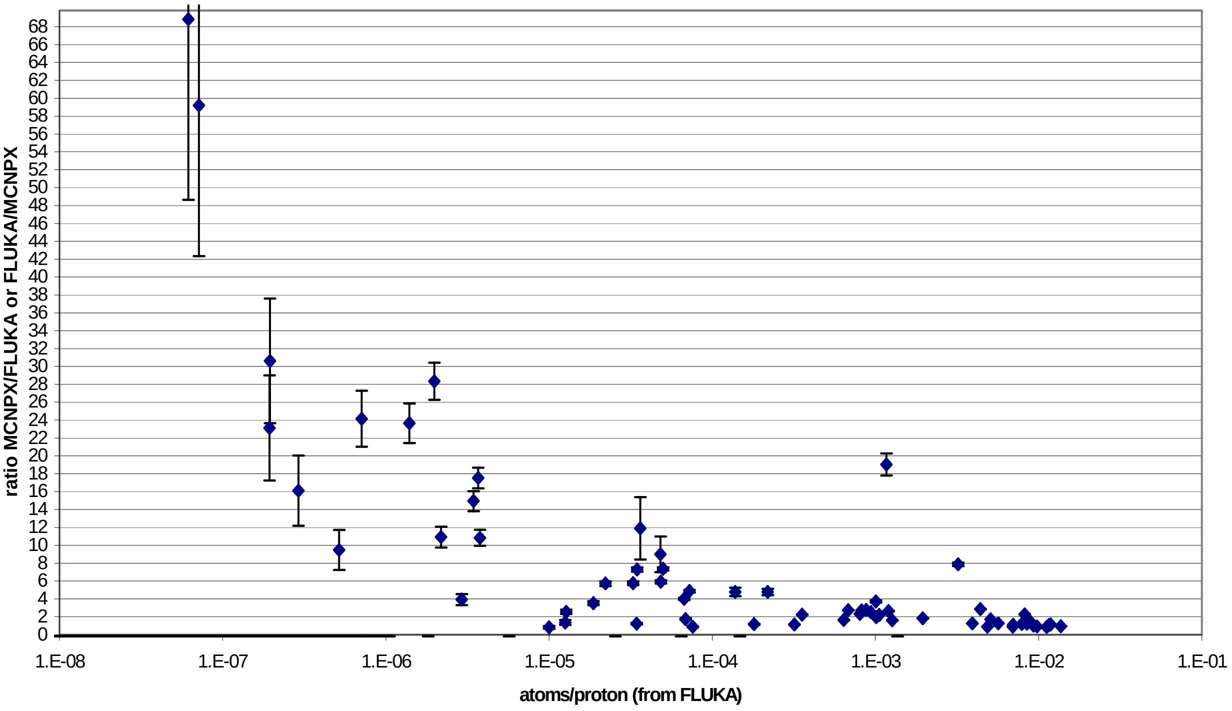

Figure 11. Ratio between the residual nuclei production calculated with MCNPX (CEM2k) and FLUKA versus the amount of production.

The biggest differences arise for the isotopes of Hydrogen and Helium where a difference of a factor of about 1700 is reached (see Table III). In this mass atomic range the use of the Bertini model in MCNPX produces results closer to those of FLUKA than the CEM2k model. The discrepancies between the results can be explained with the intrinsic differences in the models implemented by the two codes.

Table III. Comparison of Hydrogen and Helium production.

	FLUKA (atoms/proton)	MCNPX with CEM2k (atoms/proton)	MCNPX with Bertini (atoms/proton)	ratio CEM2k/FLUKA	ratio Bertini/FLUKA	ratio CEM2k/Bertini
Deuterium	1.47E-04	1.01E-02	1.79E-03	68	12	6
Tritium	6.45E-05	1.75E-03	4.24E-04	27	7	4
He3	2.63E-07	4.39E-04	7.25E-06	1671	28	61
He4	1.36E-03	3.80E-03	1.95E-03	3	1	2

In order to assess the impact of all these discrepancy on an integral value, the activity of the whole target has been calculated and compared. The activation due to the neutron flux under 20 MeV has not been included here. The evolution of residual nuclei calculated with SP-FISPACT is shown in Fig. 12 and in Table IV. The discrepancy is of a factor of 1.5 after 1 second of irradiation and it cancels out after 1 day of cooling time. At 100 years of cooling time, the discrepancy (a factor of 23) is almost entirely due to the difference in the tritium production.

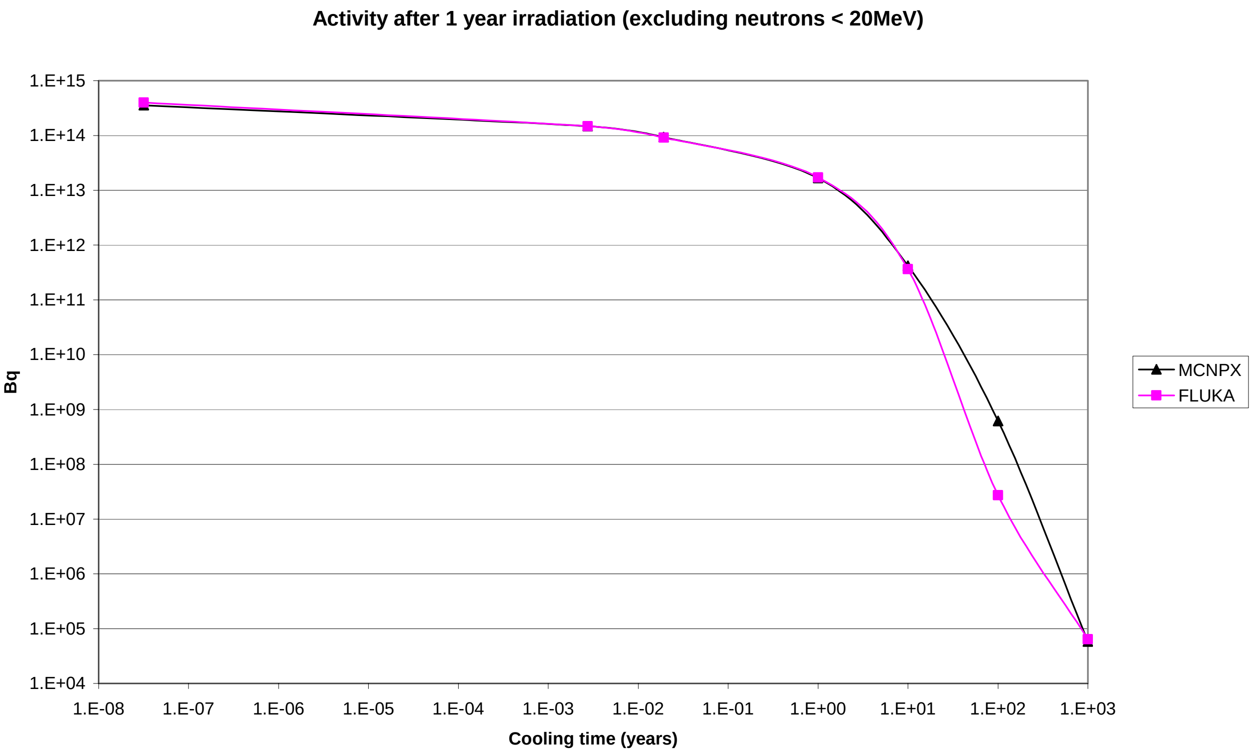

Figure 12. Activity after 1 year irradiation versus cooling time.

Table IV. Activity excluding the residual nuclei produced by low energy neutrons (MCNPX: E<20 MeV; FLUKA: E<19.6 MeV).

		MCNPX-CEM2k	**FLUKA**	
		Bq	**Bq**	**discrepancy**
IRRADIATION TIME	1 Sec	4.55E+10	6.71E+10	**+47%**
	1 Hour	7.00E+13	9.38E+13	**+34%**
	1 Year	3.57E+14	4.01E+14	**+12%**
COOLING TIME (after 1 year irradiation)	1 Sec	3.57E+14	4.01E+14	**+12%**
	1 Day	1.48E+14	1.48E+14	**0%**
	7 Days	9.32E+13	9.19E+13	**-1%**
	365 Days	1.67E+13	1.72E+13	**+3%**
	10 Years	4.18E+11	3.63E+11	**-13%**
	100 Years	6.17E+08	2.73E+07	**-96%**
	1000 Years	5.81E+04	6.38E+04	**+10%**

As far as the decay heat is concerned, after 1 year of irradiation and excluding the nuclides produced by low energy neutrons, FLUKA provides a value of 47 W and MCNPX of 38 W i.e. a discrepancy of a factor of 1.25.

Considering also the contribution to the decay heat and to the activation due to the neutrons with energy <20 MeV, which is treated by means of data libraries, some of the above mentioned discrepancies might have a lower value.

4 CONCLUSIONS

The comparison of the results obtained with MCNPX and FLUKA for a 140 MeV proton beam shows an excellent agreement in the shielding calculations (where the neutron emission and transport is involved), while appreciable differences arise in those of residual nuclei (where all reaction channels are considered). In particular, MCNPX has a higher production rate for the H and He isotopes. The impact of all these differences on integral values such as the overall activity (excluding neutrons <20 MeV) is contained, except when tritium becomes relevant.

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