BENCHMARKING OF THE MODELLING TOOLS WITHIN THE EURISOL DS PROJECT

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Abstract

The European Community decided to support the design study and R&D for a next generation ISOL radioactive ion beam facility in Europe named EURISOL. The envisaged increase of beam intensities, by several orders of magnitude compared to actual facilities, means a drastic increase of the radioactive inventory and corresponding radioprotection related issues. Benchmark calculations with the MCNPX and FLUKA codes on neutron, charged particle and residual nuclei production within the pre-defined EURISOL parameters (e.g., incident particle-energy, targets, structure materials, etc.), have been done. The extensive comparison of different model predictions with data allowed us to recommend the best physics model parameters within the above particle transport codes. The importance of these benchmarks is illustrated by sensitivity simulations using realistic target geometries.

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Introduction

The validation of the physics models implemented in the MCNPX [1] and FLUKA [2] codes, which will be the main Monte-Carlo tools used for the EURISOL Design Study (DS) [3], is very important in order to ensure the reliability of the results obtained for the RIB production target optimization, radioprotection and safety, and beam intensity calculations.

The neutron production by spallation reactions in different materials has to be well reproduced by simulation codes for both radioprotection purposes and the EURISOL primary target optimization. It is also an important ingredient for the beam intensity calculations in the double stage production targets. Scattered primary protons and secondary proton production will contribute to the energy deposition and radiation level around the targets and accelerator structures. Equally, it is important to take into account with a good precision the production of other light charged particles as deuterons, tritons, and helium particles being the important contributors to the gas production and damage rates in the target window or other structure materials.

In this paper we report the results obtained from the simulation of double differential cross sections of neutron and light charged particle production for various target materials as a function of incident proton energy. Model calculations are compared with existing experimental data. The importance of these benchmarks is illustrated by sensitivity simulations using realistic target geometries.

Benchmark calculations

The beam energy foreseen for the proton driver of EURISOL is about 1 GeV, consequently data around this energy have been selected for the benchmarks. Two major observables were examined, namely neutron and light charged particle production.

Both MCNPX [1] (Version 2.5.f) and FLUKA [2] (Version 2005.6) have been used for benchmark. The physics models used by FLUKA are fixed and cannot be changed by the user. In this case, a pre-equilibrium cascade model called PEANUT is coupled to an implementation of the RAL fission evaporation code, both with predefined input parameters [2].

The code MCNPX allows the user to choose between different intra-nuclear cascade and fission-evaporation model combinations among ISABEL, BERTINI and INCL4 for cascade and DRESNER (associated with RAL or ORNL fission models) and ABLA for deexcitation. The last possibility with MCNPX is to use the package CEM2k (cascade and deexcitation). For both ISABEL and BERTINI models, pre-equilibrium has been used. For microscopic cross section predictions the code MCNPX has been used without the particle transport [1].

Neutron double differential cross sections (thin targets)

Among a large number of combinations of incident proton energy, material and angles we could study, we have chosen to make calculations for 6 materials, namely Be, C, Fe, W, Pb, and U at the energy of 800 MeV for 5 angles (2.5°, 30°, 60°, 120°, and 150°). The data are taken from [4] using the EXFOR database [5].

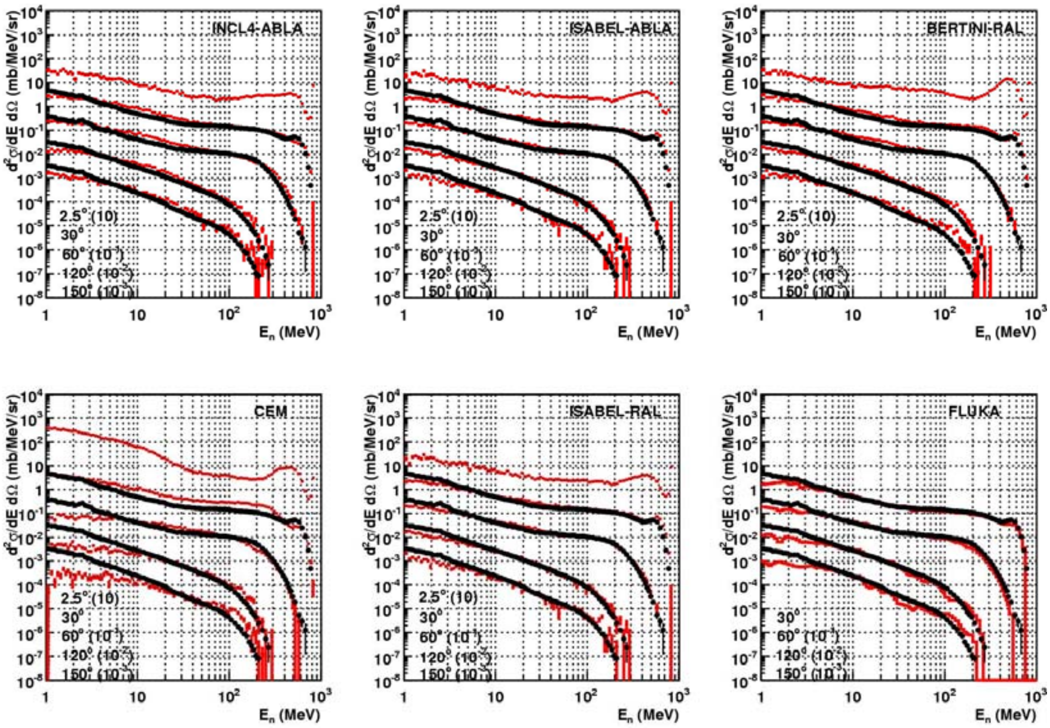

Figure 1 : Neutron double differential cross section in the case of the reaction Be(p,xn) at E_p=800 MeV. The experimental data are represented in black, and the results of different model predictions - in red.

Figures 1 and 2 show the neutron double differential cross section for light target nucleus as Be and heavy target nucleus as U correspondingly. Both FLUKA and MCNPX reproduce well the shape and magnitude of the double differential cross section spectra. Two distinct contributions are visible in the spectra: the evaporation neutrons between 1 and ~20 MeV are emitted isotropically, and cascade neutrons, being more forward peaked, with energies above ~20 MeV. We note that the results obtained are more accurate for heavy nuclei than for light nuclei, where some important discrepancies appear at low neutron energy, say, below 10 MeV. For MCNPX, five models combinations have been used: INCL4-ABLA, ISABEL-ABLA, BERTINI-RAL, ISABEL-RAL, and CEM2k as explicitly shown in Figures 1-2.

For a more quantitative comparison we have also plotted the ratio between model predictions and data (an example is given in Figure 3 for the emission angle of 30°). Taking into account the combined statistical and systematic error on data and simulation, the agreement is within a factor of 2 up to 600 MeV, except for the CEM2k model used within MCNPX. Above 600 MeV, and for forward angles in particular, around the quasi-elastic and quasi-inelastic peaks, the agreement is not so good whatever the code and models are used. We expect that this disagreement is less important for realistic target simulations, where the neutron energy and angular distributions will be influenced by the multiple scattering with the increasing target thickness.

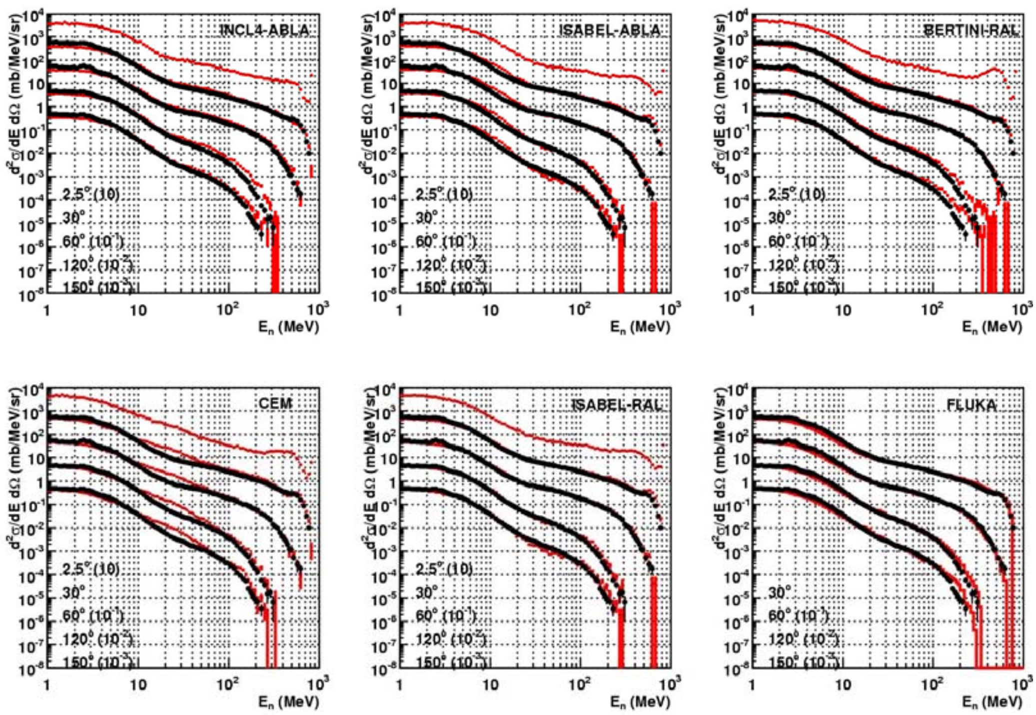

Figure 2 : Same as Fig. 1 but for the reaction U(p,xn) at E_p=800 MeV.

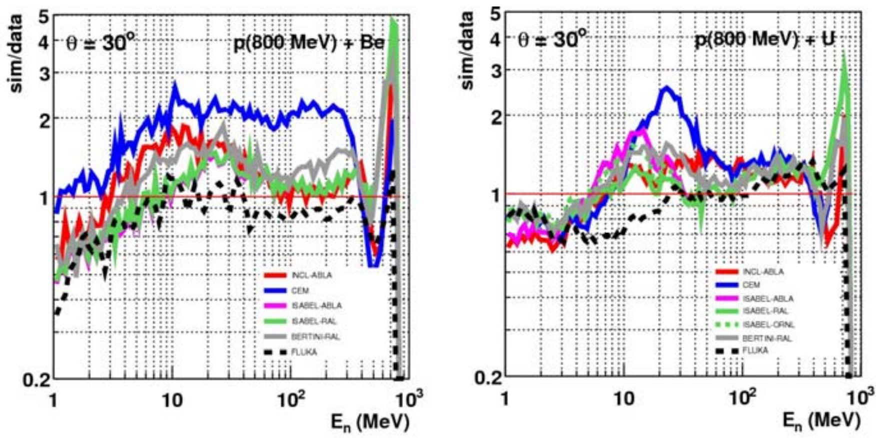

Figure 3 : Ratio between simulation and data for the Be(p,xn) reaction (on the left) and the U(p,xn) reaction (on the right) for the emission angle of 30°. Note that the thickness of the lines is larger than the resulting error from data and simulation.

Light charged particle production

Figure 4 shows the proton double differential production cross section obtained for thin carbon and niobium targets. Data are taken from [6]. Results obtained by simulation are rather good for FLUKA and MCNPX used with ISABEL, INCL4 and CEM2k models. On the other hand, some important discrepancies are seen at forward angles and high secondary proton energies.

In the case of production of helium (Figure 5) also huge differences between models have be seen: except for CEM2k there is no ^{4}He particles emitted above ~50 MeV at all, and the shape of the distribution is not reproduced correctly. It has to be stressed separately that only CEM2k is able to emit high energy alphas, while the other intranuclear cascade models (like ISABEL, INCL4, Bertini inside MCNPX and PEANUT inside FLUKA) are unable to emit energetic composites (clusters).Data are taken from [7].

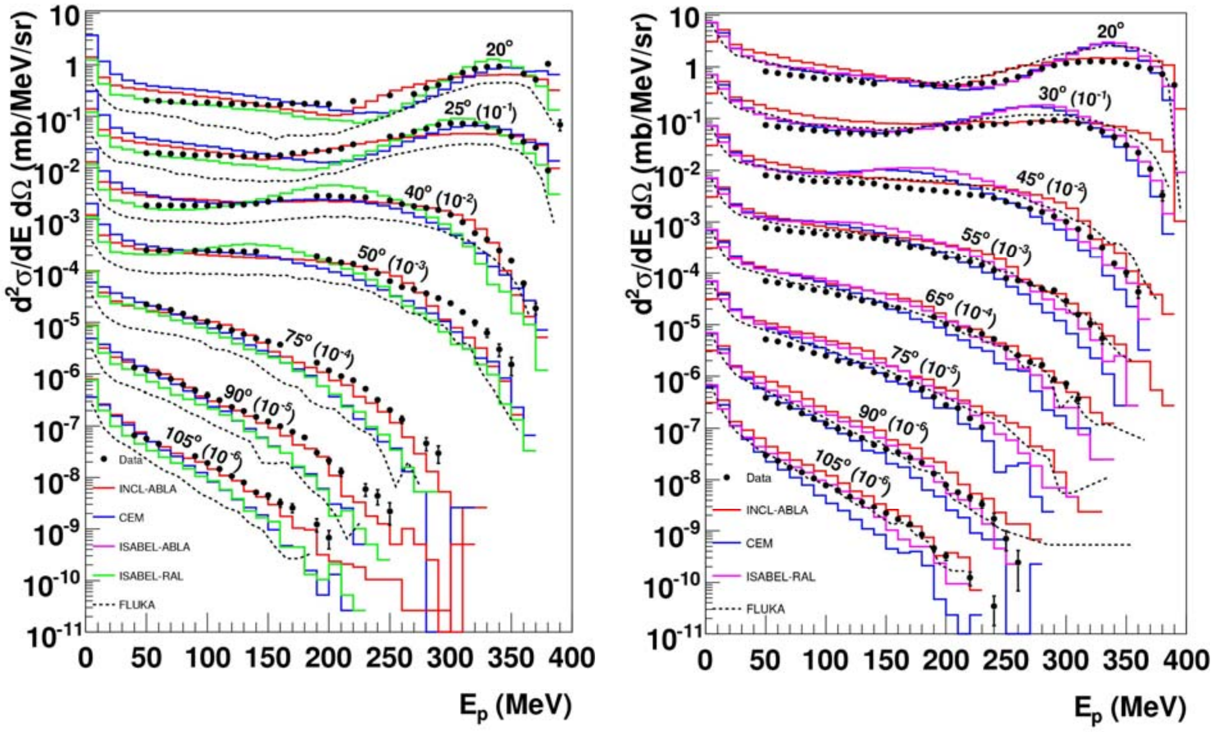

Figure 4 : Double differential cross section for proton production from 392 MeV incident protons interacting with carbon (on the left) and niobium (on the right) targets.

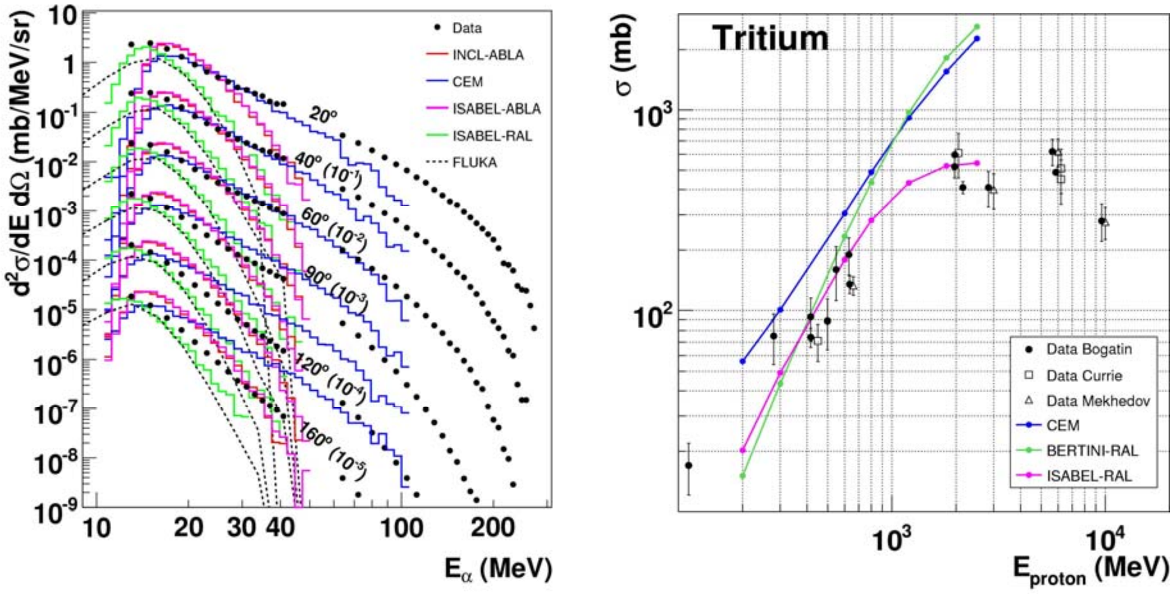

Figure 5 : (on the left) helium double differential cross section production in the case of the reaction Ag(p,^{4}He) at Ep=300 MeV (left); (on the right) tritium production cross section in a thin lead target as a function of proton incident energy.

Some various data on tritium production cross sections have been compiled [8][9][10][11] for the natural lead target, and are compared (see Figure 5) to the results given by MCNPX code using model combinations only which result in non zero triton emission. The ISABEL-ABLA and INCL4-ABLA models combination are then excluded, and only CEM2k, BERTINI-RAL and ISABEL-RAL can be used for this particular observable. The first and the second model combinations seem to overestimate the data, only ISABEL-RAL is showing the saturation visible in the data occurring around 1-2 GeV incident proton energy.

Residues production

Comparison of fission yields from thick targets between MCNPX models and ISOLDE data [12] has also been performed. ISOLDE experiment at CERN collected data of yields and release of noble-gas isotopes from UCx/graphite and ThCx/graphite targets. Proton beams of 1.0 and 1.4 GeV were used. Figure 6 presents the in-target production yield of Krypton isotopes for CEM2k, INCL4-ABLA, ISABEL-ABLA and ISABEL-RAL models with 1.4 GeV protons impinged on the uranium carbide target. Note that in these simulations all secondary reactions, including low energy neutrons, are taken into account. In brief, we can see that only the combinations using ABLA fission-evaporation model are able to reproduce the shape of the mass distribution. The CEM2k and ISABEL-RAL models predict too broad distribution and therefore overestimating the production of isotopes on the neutron rich side in particular. Similar conclusions are drawn also for the isotopic distribution of Xe (J.C. David et al., “Megapie: Residue yields and radioactivity predictions with different models in MCNPX”, Topic 3 of this SATIF-8 meeting).

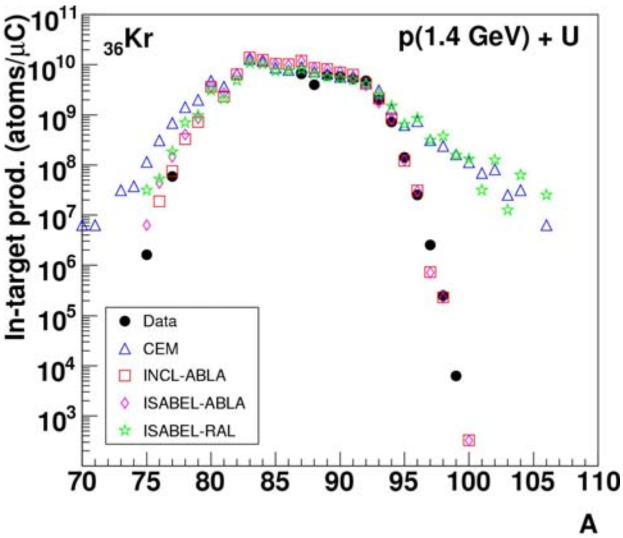

Figure 6 : Mass distribution of Krypton isotopes given by different models within MCNPX and compared to ISOLDE data (right).

Realistic target calculations

The first simulation of the EURISOL 4 MW power target for the radioprotection purposes has been done using the MCNPX code. A view of the geometry implemented in MCNPX is shown in Figure 7. In brief, this is a two-stage target, in which the power of the primary incident proton beam is dissipated in the liquid Hg (target-converter), whereas the resultant neutron flux is used to induce fissions in the secondary uranium carbide target (production target), which in principle should not be overheated by the primary beam. The target-converter (liquid Hg) is of 16 cm diameter and of the stopping length (~45 cm long). The mercury is surrounded by 8 production targets that contain the fission material (uranium or thorium carbide tablets), which will be heating to ~2000°C in order to increase the effusion-diffusion process (extraction efficiency) of the fission products. Extracted fission products are driven to a single or multiple ion sources by 8 beam tubes. The entire target assembly is maintained by a stainless steel structure isolated electrically and surrounded by a moderator (thick graphite layers). The incident beam is 1 GeV protons (up to 4 mA beam intensity) with a Gaussian profile.

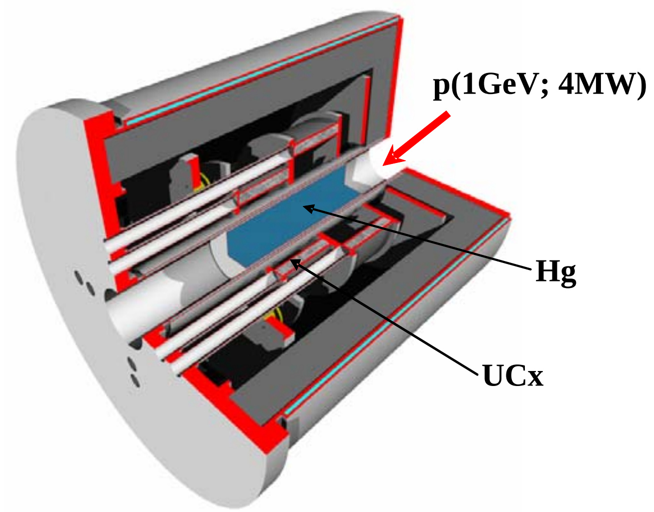

Figure 7 : Schematic view of the "realistic" EURISOL 4 MW power target geometry implemented in MCNPX.

Using the target geometry presented in Figure 7 we calculated the spallation residues charge and mass distributions in the mercury target using ISABEL-ABLA, INCL4-ABLA and CEM2k model combinations. The results are shown in Figure 8, where important discrepancies are observed among different model predictions. Note that these differences will accumulate with the irradiation time of the target, and will give increased difference in production yield.

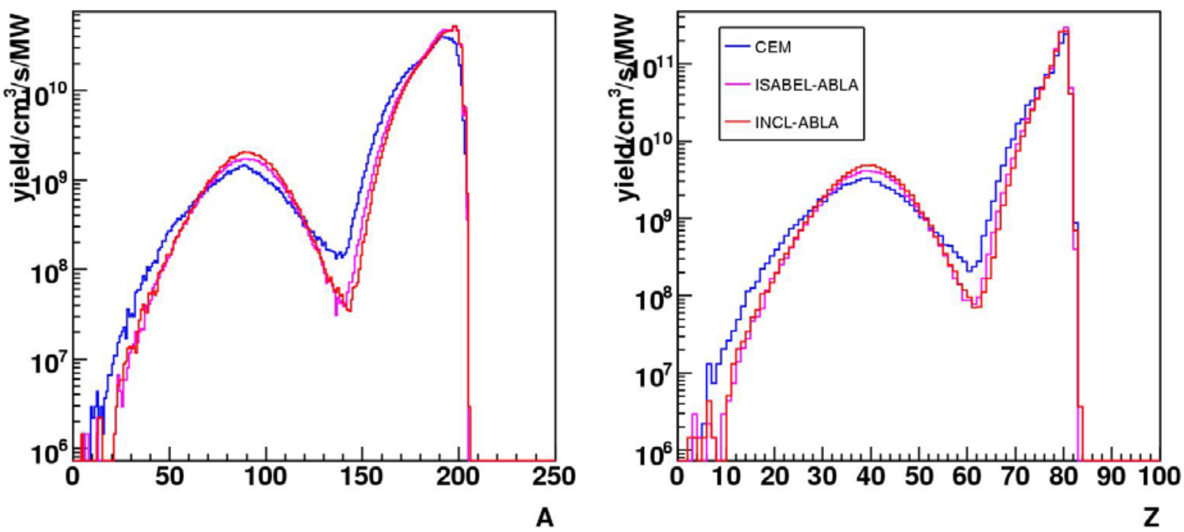

Figure 8 : Mass (left) and charge (right) distributions of spallation residues in thick mercury target interacting with 1 GeV protons. The following model combinations were used: ISABEL-ABLA (magenta), INCL4-ABLA (red) and CEM2k (blue).

A more detailed examination of the mass distribution for a particular isotope, for example Krypton isotope mass distribution as presented in Figure 9, confirms, as already earlier in this work, that CEM2k gives too broad distributions.

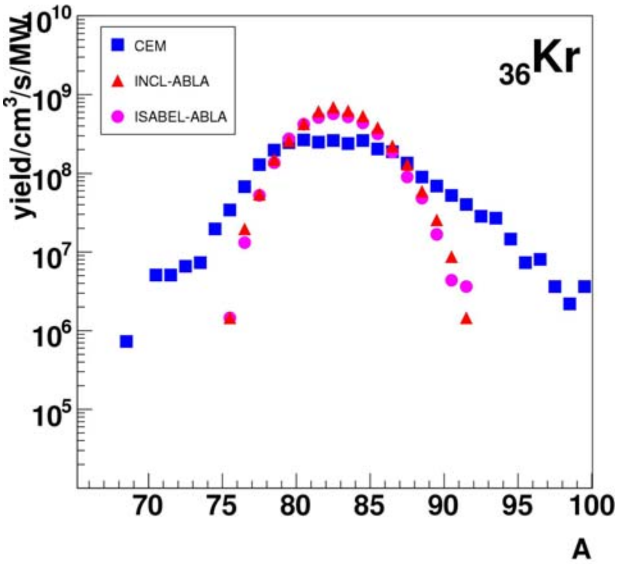

Figure 9 : Same as Fig. 8 but for mass distribution of Krypton isotopes.

The activation calculation of the mercury was done with the CINDER transmutation code [13] for a continuous irradiation time of 40 years with the proton beam intensity of 2.28 mA, representing an average load of the installation. The results are summarized in Figure 10 and Table 1. The calculation has been done with three models (INCL4-ABLA, ISABEL-ABLA and CEM2k) resulting in three different distributions of spallation residues and gas production in target.

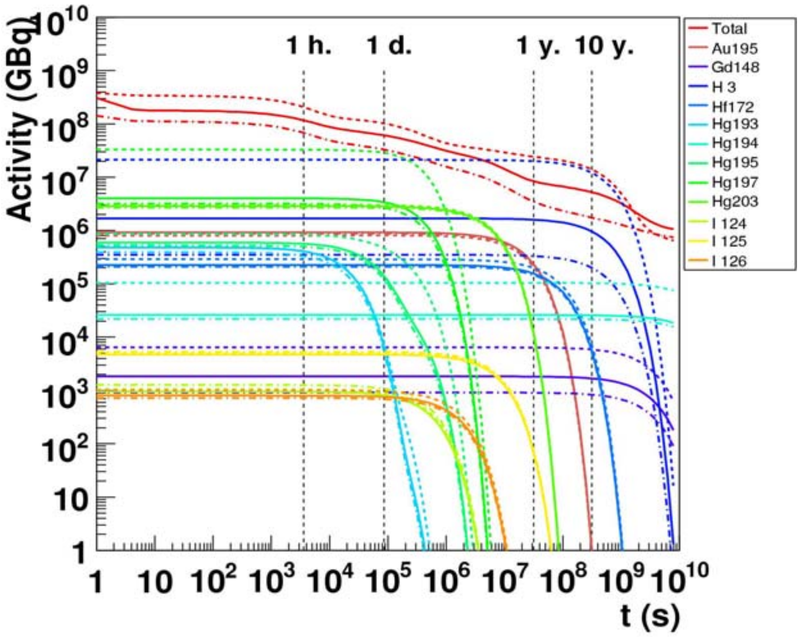

Figure 10 : Radioactivity estimates as a function of cooling time using ISABEL-ABLA (solid line), CEM2k (dashed line) and INCL4-ABLA (dashed-dotted line) models.

As one could expect, we can see that the different microscopic models are giving significant differences in isotope radioactivity, particularly for the important α emitter as ^{148}Gd (see Table 1), and also for tritium gas emission (see Figure 10) between 1 and 10 years of the decay time.

	1 year after irradiation			10 years after irradiation		
	ISABEL-ABLA	CEM2k	INCL4-ABLA	ISABEL-ABLA	CEM2k	INCL4-ABLA
Total activity	8.410^6	$2.4\ 10^7$	$3.5\ 10^6$	$5.2\ 10^6$	$1.4\ 10^7$	$1.7\ 10^6$
^{195}Au	$2.4\ 10^5$	2.110^5	$2.2\ 10^5$	1.8	1.6	1.7
^{148}Gd	1.810^3	$6.4\ 10^3$	$9.0\ 10^2$	1.710^3	5.910^3	$8.3\ 10^2$
^{3}H	$1.6\ 10^6$	$2.0\ 10^7$	$3.3\ 10^5$	9.610^5	$1.2\ 10^7$	$2.0\ 10^5$
^{172}Hf	1.610^5	2.010^5	$1.5\ 10^5$	5.610^3	7.110^3	$5.2\ 10^3$
^{194}Hg	2.610^4	1.010^5	$2.2\ 10^4$	2.610^4	1.010^5	$2.2\ 10^4$

Table 1: Activity (in GBq) contribution due to a few important isotopes for radioprotection in the irradiated mercury target as a function of ISABEL-ABLA, CEM2k and INCL4-ABLA models within MCNPX.

Conclusions

We have benchmarked the MCNPX and FLUKA codes to predict the production of neutrons, protons, tritons and alphas from incident protons on thin targets of different materials in the energy range around 1 GeV. Comparison of the model predictions with experimental data shows a good agreement of codes for neutron production. For secondary proton production FLUKA have difficulties to reproduce the energy-angle distributions for light targets. As long as production of alphas is concerned, only CEM2k within MCNPX gives reasonable results. The tritium production seems to be overestimated by CEM2k and BERTINI-RAL models above 1-2 GeV but well reproduced by ISABEL-RAL, i.e. the energy where the saturation of tritium production is observed experimentally.

Finally, the simulation done with MCNPX using realistic target geometry proves the importance of benchmark calculations and suggests a careful selection of adequate model combinations for different observables. It seems that up to know there is no a “unique” model combination able to reproduce all observables at the same time with desired precision.

References

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