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A Cross-comparison of MARS and FLUKA Simulation Codes

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Abstract

A comparison of lateral attenuation of radiation field components predicted by FLUKA and MARS simulation codes in a simple heterogeneous cylinder is presented. Excellent agreement for neutral particle fluxes, corresponding energy spectra and energy deposition is obtained. Although some discrepancies are observed for charged hadrons, the comparison significantly increases the confidence in the FLUKA estimates of neutron and photon background around the CMS forward shielding and in numerous MARS applications.

1 Introduction

The two general-purpose Monte-Carlo codes FLUKA [1, 2] and MARS [3] are widely used in the high-energy physics, accelerator and radiation shielding communities. The design of the CMS radiation shielding system relies entirely on results of extensive Monte-Carlo simulations. The workhorse in these simulations has been the version [1] of the FLUKA code, which has been used to optimize or to cross-check all CMS shielding designs. Mitigation of beam-induced effects in the LHC machine and in the CMS detector, numerous applications at the Fermilab accelerators and collider detectors and in such new exciting projects as muon colliders and neutrino factories are heavily based on use of the MARS code [3, 4].

It is justified to ask how reliable these simulations are. It should be pointed out that the both codes – like most similar simulation codes – have undergone extensive benchmarking, i.e. comparison to experimental data in various conditions [4, 5]. FLUKA is extensively used in numerous applications at CERN. MARS is the only modern code which has been confronted with the real case of designing shielding for hadron collider experiments in operation at Fermilab. MARS uses for its low-energy neutron transport MCNP4 [6], which is generally regarded as the de-facto standard in low-energy neutron transport and certainly is the most carefully benchmarked of all neutron transport codes. Therefore a confrontation of another code with MCNP is the best approximation of a comparison with real experiment (but significantly easier to perform).

However, the radiation environments at accelerators are complicated and results from such benchmark experiments are not always unambiguous for all components of the radiation field. This is especially true for a neutron environment where an unfolding of the experimentally measured neutron spectrum is a very complicated task. In addition the codes, when applied to LHC, are extended into a domain where they cannot be fully tested because a truly LHC-like environment does not yet exist. Thus the simulations are really predictive and include a correspondingly large uncertainty.

To further validate the predictive power of the both codes in the most important and – at the same time – rather uncertain low-energy domain we have performed a cross-check between the two codes on a simple geometry which is representative of the forward shielding of CMS and has many features of other shielding situations, focusing on the physics not geometry.

It should be emphasized that a large number of different radiation simulation codes exist. In addition, various versions of the same code – or a code with the same name – can add some confusion. FLUKA results of this paper are obtained with the version [1] used for CMS radiation calculations. Since the latest official release of a complete users' manual [7], the code has undergone substantial revision and numerous additions and improvements [1, 8], which have made it adequate for LHC radiation calculations. Nevertheless, it should be pointed out that the version used in this study is not identical to the version used outside CMS [2]. Neither of these two versions should be confused with the FLUKA hadronic production models included in GEANT. Within CMS, the MARS situation might also appear rather confusing: the code mostly used for CMS calculations is the Protvino version [9] of the code. Some differences have been observed between this version and the Fermilab MARS [3], which is used in this comparison and for most MARS applications throughout the world.

2 Uncertainties in Radiation Estimates

The uncertainties of the radiation environment predictions arise from various sources and most of them are not easy to quantify. A very basic uncertainty is found already in the inelastic pp cross section at 7 TeV. To this adds the uncertainty in the structure of the events, i.e. the multiplicity and energy flow as a function of rapidity. These have been studied by using different event generators and a variation by about a factor of 1.3 was observed [10]. This uncertainty gives the minimum error bar that should be always added to all LHC radiation predictions. For instance for an inner pixel detector, where effects due to geometry and scattering are negligible, this can be expected to be the dominant uncertainty.

Elsewhere other effects are likely to be far more significant. Very important is the accuracy of the description of the geometry and the material composition. It is difficult to quantify this uncertainty, but experience has shown that already rather small changes, which easily go unnoticed, can change the result by a factor of 2 or even 3 when a shielding is designed to give an overall reduction by 3 orders of magnitude – like the CMS forward shielding. In the case of the CMS shielding the geometry description slowly becomes more realistic when detailed designs emerge and get implemented into the simulations. In general these tend to increase estimates because detailed design usually introduce more cracks. It seems justified to argue that while the estimates tend to increase the uncertainty due to geometry inaccuracies should correspondingly decrease. While this is most probably the case, it is just as difficult to quantify as the original uncertainty.

The third source of uncertainty arises from the accuracy of the simulation code itself, i.e. given certain well defined conditions, how accurately can the code predict the radiation environment. This is exactly what benchmarking experiments try to test, but as discussed above they are confronted with uncertainties in the real geometry (like composition of concrete) and purely experimental uncertainties.

In this paper we try to estimate the importance of this third source of uncertainty by comparing the results of FLUKA and MARS in a simple well-defined geometry. The advantage of this, compared to an experiment, is that the other uncertainties discussed above can be completely removed. The obvious disadvantage is that both codes could be wrong the same way. The latter worry is diminished if two completely independent codes are used and this again suggest that a comparison of FLUKA with MARS is very reasonable since these two codes are based on different physical models, tracking algorithms and geometry description.

3 Simulation Geometry

The simulations are done in a simple end-stop geometry consisting of a central steel cylinder of 40 cm radius. This central cylinder was surrounded by 60 cm (R=40–100 cm) of shielding material (steel, concrete or magnetite concrete). Around this was a 10 cm thick layer of borated polyethylene followed by 10 cm of air before a 'black-hole'. The length of the complete cylinder was 200 cm. A pencil proton beam of 10 GeV/c, directed along the central axis, was hitting the upstream end of the cylinder.

This geometry was selected because it is rather representative of the forward shielding of CMS. It might be questioned if a 10 GeV energy is representative of LHC, which is a 7 TeV collider. The answer is *Yes*, because the shielding will be hit only by secondaries which even in the forward direction have energies far below the TeV range. The resulting cascades are always dominated by particles in the energy range below 10 GeV. A higher primary energy would mainly increase the longitudinal extent of the cascade, which is not subject of this study. In addition 10 GeV should be a good choice because it is just above the energy range of 2-5 GeV where hadron interaction models are known to have the largest uncertainties.

The composition of steel was (by weight): 0.1% C, 0.1% Si, 1% Ni, 0.2% Cu and 98.6% Fe. Density 7.87 g/cm^3.

The composition of concrete was (by weight): 0.6% H, 3% C, 50% O, 1% Na, 3% Al, 20% Si, 1% K, 20% Ca and 1.4% Fe. Density 2.35 g/cm^3.

The composition of magnetite concrete was (by weight): 0.35% H, 1.3% B, 35% O, 1.3% Na, 2% Al, 2% Si, 2.7% Ca and 55.35% Fe. Density 3.67 g/cm^3.

The composition of borated polyethylene (BPE) was (by weight): 11.6% H, 61.2% C, 5% B and 22.2% O. Density 0.93 g/cm^3.

Fig. 1 shows MARS-calculated isocontours of neutron and photon flux in a steel/magnetite concrete cylinder. At large radii, one sees a broad maximum at about z=75 cm. In the rest of the paper, the flux of particles was scored in the z-range from 50 cm to 100 cm in radial steps of 2 cm. Particle spectra were scored within the same z-boundaries inside of the polyethylene layer surrounding the cylinder (radial range 100–110 cm).

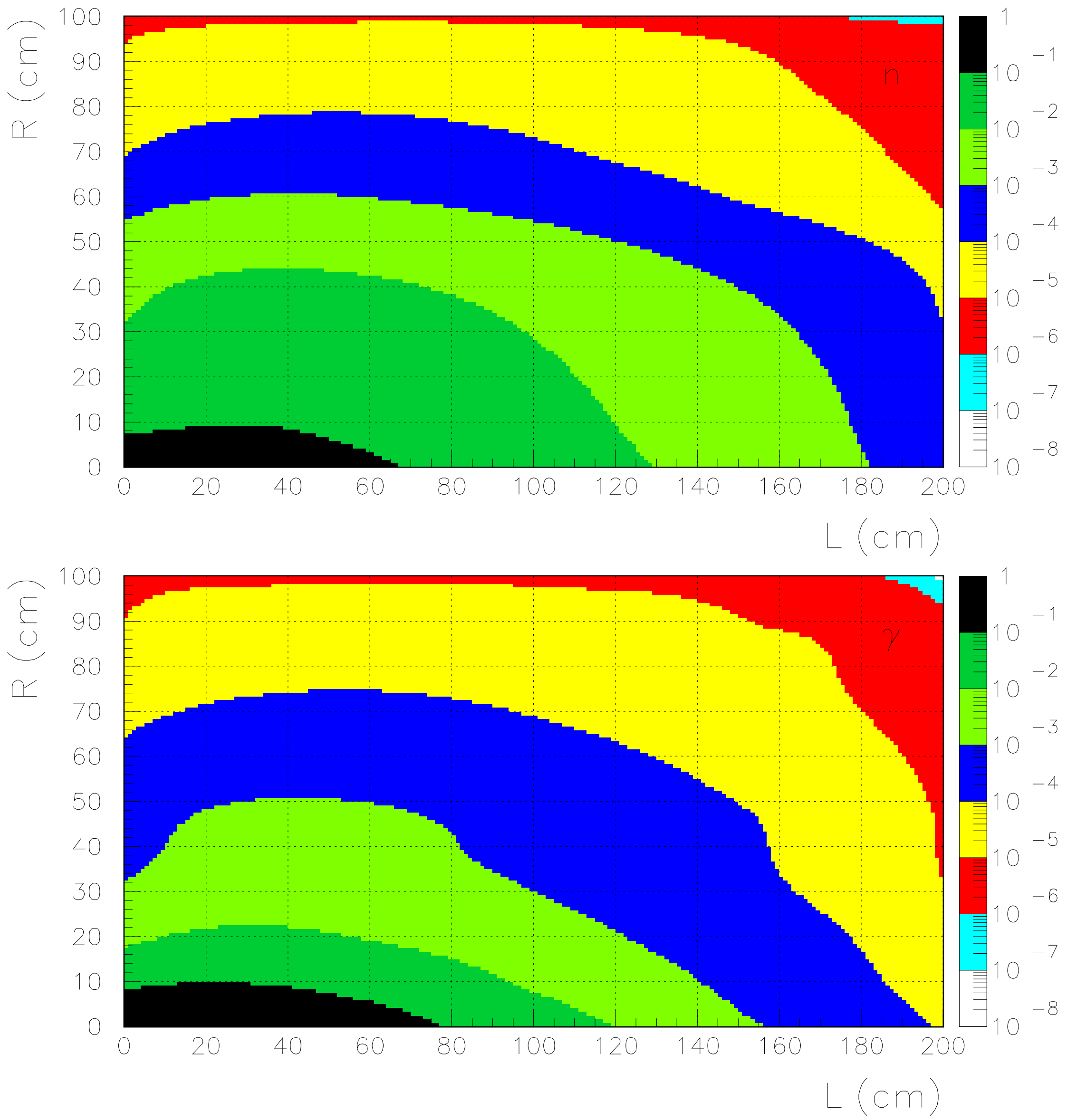

Figure 1: Neutron and photon isofluxes (cm^{-2} per 1 proton) in a steel/magnetite concrete cylinder.

4 Results

Figs. 2-4 show the radial attenuation of flux and energy deposition in the three different cylinder compositions.

We can observe excellent agreement for neutrons, photons and energy deposition, but some disagreement for charged hadrons. For photons it should be remarked that the FLUKA transport threshold was set to 30 keV while that in MARS was 100 keV. An analysis of the FLUKA spectrum (in the BPE) shows that 12% of the photons are below 100 keV. Taking this effect into account further decreases the already small discrepancy.

The agreement in the energy deposition is remarkable. In fact our initial comparisons showed significant disagreement in the BPE layers around the full-steel cylinder. It was then realized that most of the energy deposited in the BPE is due to the Li and α recoils from the thermal neutron capture on ^{10}B. The perfect agreement was obtained by implementing in MARS an accurate treatment of these fragments generated in MCNP.

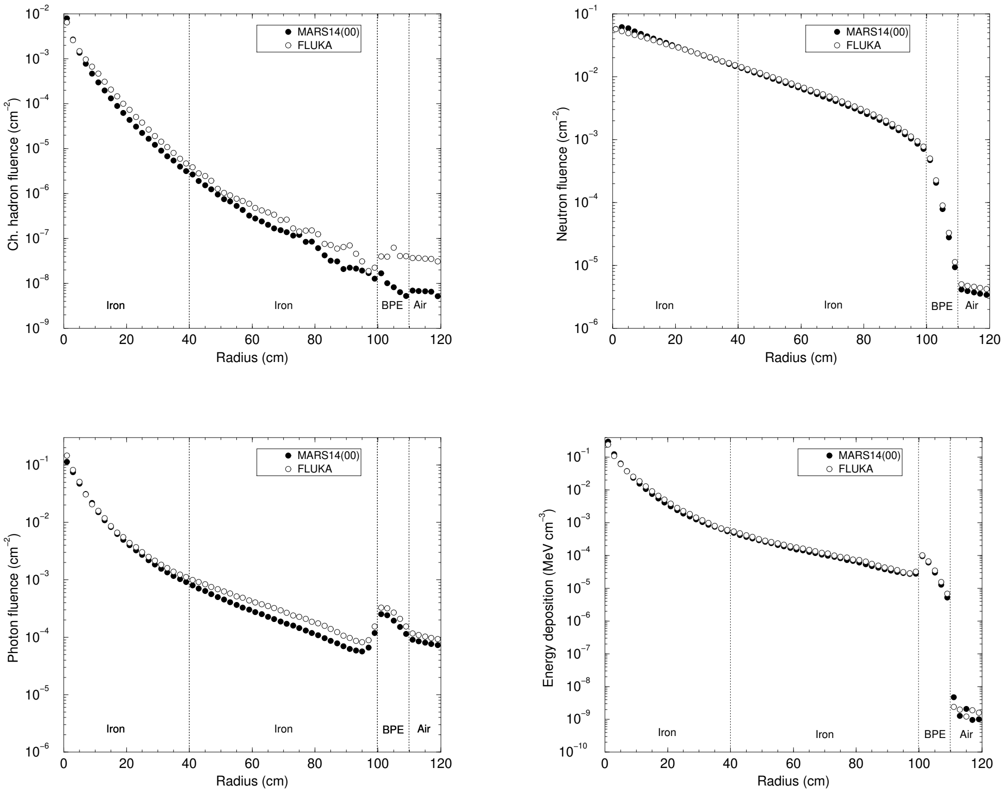

Figure 2: Radial dependence of charged hadron, neutron and photon fluxes and of energy deposition in a pure steel cylinder covered by a borated polyethylene layer.

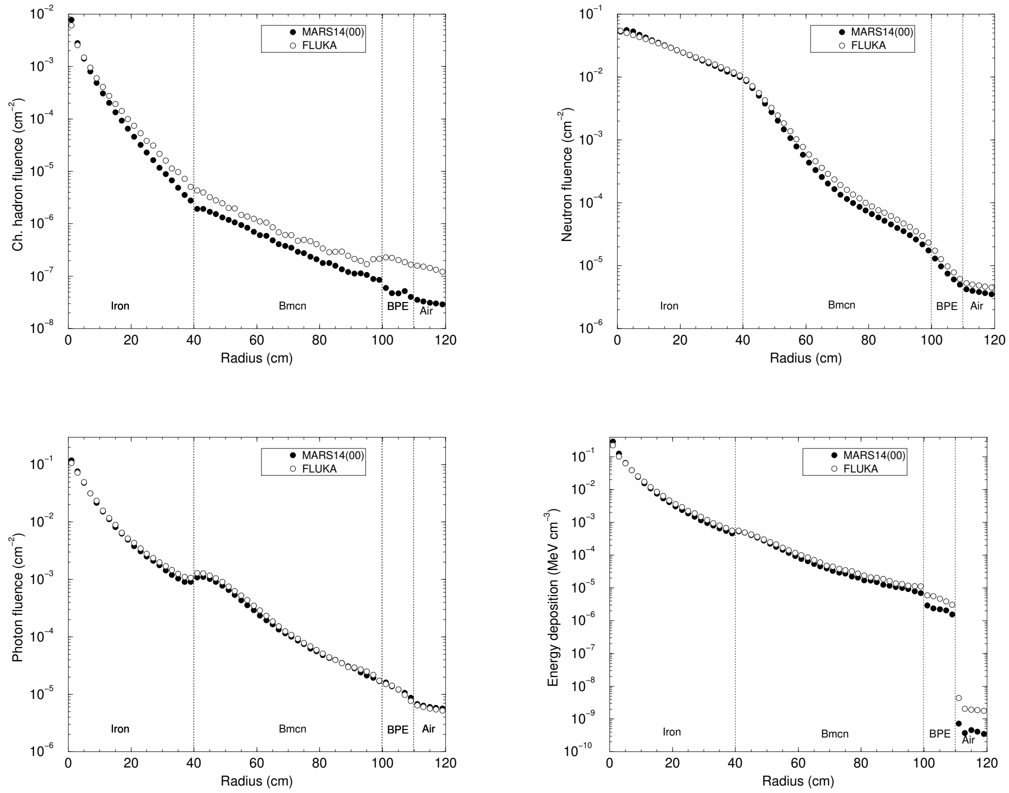

Figure 3: Radial dependence of charged hadron, neutron and photon fluxes and of energy deposition in a steel/magnetite concrete cylinder covered by a borated polyethylene layer.

The energy spectra of neutrons and photons inside of the borated polyethylene layer are shown in Fig. 5. An almost perfect agreement can be observed for neutrons. A remark should be made on the absolute scaling of the spectra: these are plotted as $d\phi/d(\log(E))$. If the bin is narrow so that the flux does not significantly vary within the bin the exact choice of the energy bin limits is not important. This condition is fulfilled for all others, but not the thermal bin. The energy limits of the thermal group in FLUKA are 10^{-11}–4.14×10^{-7} MeV while the corresponding limits in MARS are 2.15×10^{-9}–2.15×10^{-7} MeV. However, at room temperature there are no neutrons far below the thermal energy of 2.5×10^{-8} MeV. Therefore the lower limit of the FLUKA group artificially increases the d(log(E)) term. If only the flux (ϕ) in the lowest energy bin is considered FLUKA and MARS agree. In order to reproduce this agreement also in Fig. 5 the lower limit of the thermal FLUKA group has been set to 4.14×10^{-9} MeV, giving d(log(E))=2 both in FLUKA and in MARS.

Also in the photon spectra good general agreement can be observed for the steel and steel/concrete cases. In particular the discrete peaks corresponding to the 480 keV capture gamma from ^{10}B and the 2.2 MeV gamma from hydrogen are predicted with equal intensities by both codes. These peaks are particularly pronounced

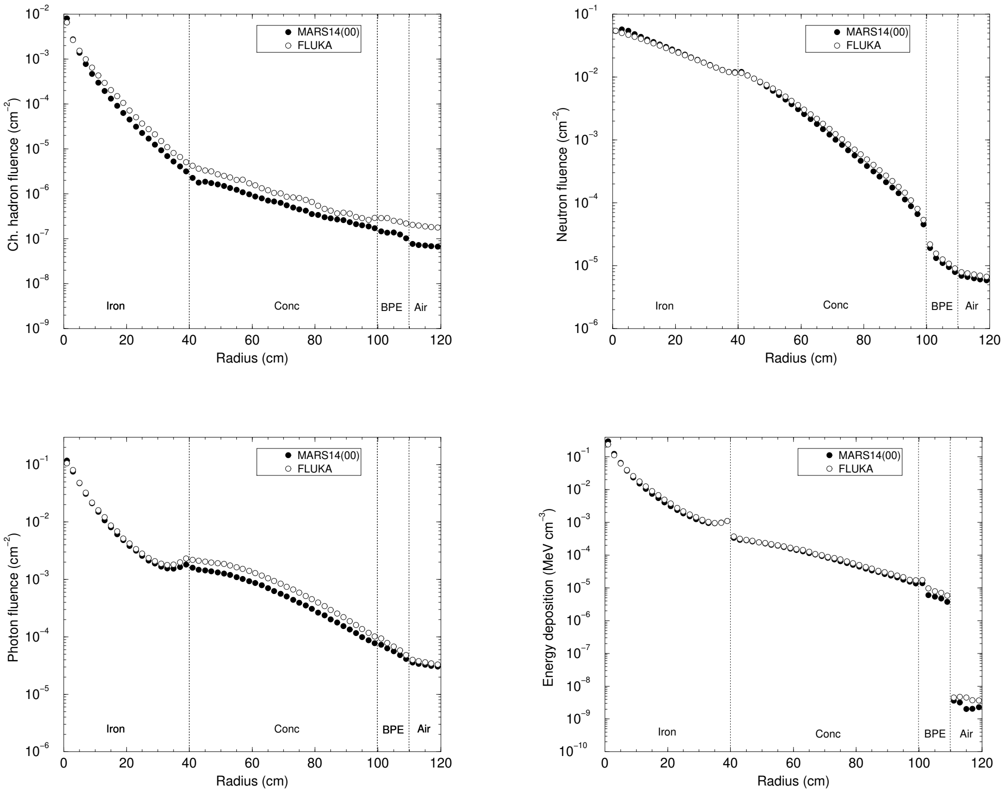

Figure 4: Radial dependence of charged hadron, neutron and photon fluxes and of energy deposition in a steel/concrete cylinder covered by a borated polyethylene layer.

in the case of the pure steel cylinder where the BPE has a more important role in attenuating neutrons. A rather strange discrepancy is, however, seen in the photon spectrum for the steel/magnetite concrete case. The magnetite concrete is essentially a mixture of steel and normal concrete, thus it is surprising to find a significant difference in the mixture while there is good agreement in both individual components (steel and concrete). The only difference is that in pure steel there are essentially no thermal neutrons whereas there are some within the magnetite concrete. Thus, only in the magnetite concrete the steel is exposed to a thermal neutron flux. However, there are no capture photons in ^{56}Fe which could explain the step between 1 and 2 MeV, which is seen in the MARS spectrum. In addition the boron content should suppress much of thermal captures of iron in the magnetite concrete. At the moment we have found no explanation for the discrepancy.

The discrepancies observed in Figs. 2-4 for charged hadrons make one expect some discrepancies also in the corresponding spectra. In the present simulations the statistics for charged particles other than protons is so poor that a comparison is impossible. The proton spectra shown in Fig. 6 indeed reflect some puzzling discrep-

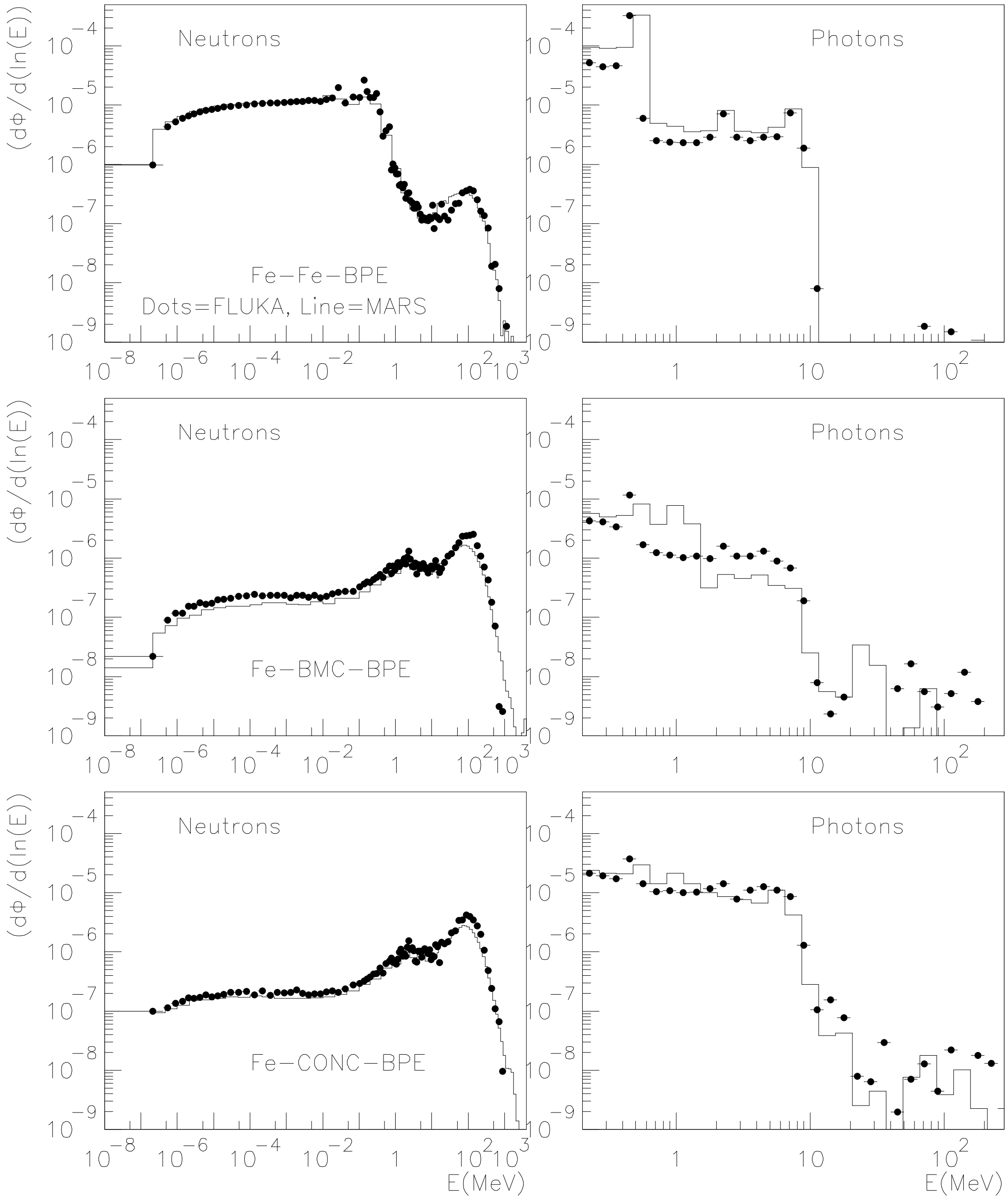

Figure 5: Energy spectra of neutrons and photons in the borated polyethylene layer around the cylinder.

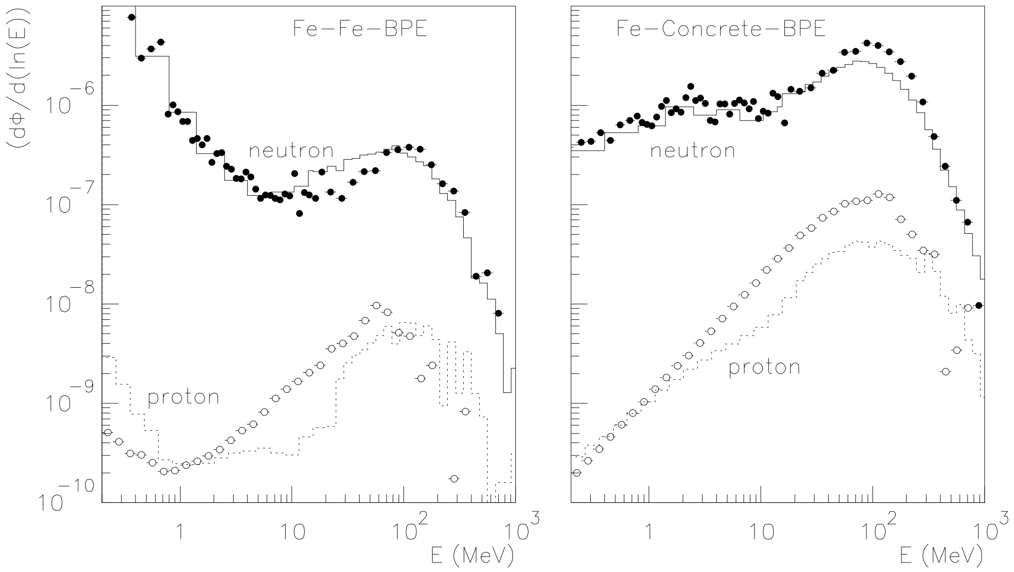

Figure 6: Energy spectra of neutrons and protons above 200 keV in the BPE layer around the cylinder. The symbols correspond to FLUKA results and the lines to MARS.

ancies. At high energies the variations in neighboring bins suggest that statistics is getting lost and firm conclusions cannot be drawn from the present results where statistical errors for spectra have not been evaluated. At lowest energies statistics appears good, but this could be just apparent. Below few MeV the proton range is very short and thus a single proton stopping within the region where the spectrum is scored can give a correlated contribution into all bins. Thus, again, an assessment of statistical errors would be needed to draw firm conclusion about the discrepancy below few MeV.

However, there can be little doubt about the statistical significance of the discrepancy between few MeV and few hundred MeV. A discrepancy in proton spectra up to a factor of 3 to 4 in some bins, given a good agreement for neutrons in the same energy region, is quite puzzling. In the polyethylene layer neutrons and protons dominate the hadron flux. Thus it seems that in FLUKA (n,p) reactions are much more frequent than in MARS at energies above about 10 MeV. Since the neutron flux is far higher than the proton flux a discrepancy in cross sections or average energy transfers might already explain the difference without significantly influencing the neutron spectrum. It is to be remarked that both FLUKA and MARS change from a dedicated neutron transport model to their native high-energy code at 20 MeV. It seems obvious that the discrepancies originate from the low energy end of these high-energy codes. Another possible explanation could be a difference in the dE/dx computation of protons at low energies. Both alternatives should be investigated in more detail.

5 Conclusions

We have compared lateral particle fluxes and spectra from MARS and FLUKA in a simple heterogeneous cylinder geometry. Three different material compositions of the cylinder were compared. The common feature in all cases was an iron core and a borated polyethylene layer around the cylinder. We observe almost perfect agreement of FLUKA and MARS for energy-integrated neutron and photon fluxes as well as for energy deposition within the cylinder as a function of radius. The agreement for charged hadrons is not as perfect, but here the rather poor simulation statistics might play some role, although it is unlikely that it could alone explain the discrepancy. Whereas there is generally good or even excellent agreement in the neutron and photon energy spectra, the discrepancies in the charged spectra cannot be overlooked and will require further investigation.

Despite some discrepancies were observed it can be concluded that the codes agree almost perfectly for the most important quantities for CMS shielding design, i.e. lateral neutron and photon leakage. Since the agreement in the corresponding energy spectra is also impressive, these studies provide significantly increased confidence in the accuracy of FLUKA estimates of the radiation environment around CMS and in numerous MARS applications.

References

[1] P. Aarnio it et al, CERN/TIS-RP/93-10. A. Fassò *et al*, *Proc. IV Int. Conf. on Calorimetry in High Energy Physics*, La Biodola, Sept 20-25, 1993, Ed. A. Menzione and A. Scribano, World Scientific, p. 493 (1993). A. Fassò *at al*, *Proc. Specialists' Meeting on Shielding Aspects of Accelerators, Targets and Irradiation Facilities*, Arlington, Texas, April 28-29, 1994. NEA/OECD doc., p. 287 (1995).

[2] A. Fassø, A. Ferrari, J. Ranft, P.R. Sala, "New developments in FLUKA modelling hadronic and EM interactions", *Proc. 3rd Workshop on Simulating Accelerator Radiation Environments*, KEK, Tsukuba, Japan, 7-9 May 1997, Ed. H. Hirayama, KEK Proceedings 97-5, p. 32-43. A. Ferrari, and P.R. Sala, "The Physics of High Energy Reactions", *Proc. the Workshop on Nuclear Reaction Data and Nuclear Reactors Physics, Design and Safety*, International Centre

for Theoretical Physics, Miramare-Trieste, Italy, 15 April-17 May 1996, edited by A. Gandini and G. Reffo, World Scientific, p. 424 (1998).

[3] N. V. Mokhov, "The MARS Code System User Guide, Version 13(95)", Fermilab-FN-628 (1995); N. V. Mokhov et al., Fermilab-Conf-98/379 (1998); LANL Report LA-UR-98-5716 (1998); *nucl-th/9812038 v2 16 Dec 1998*; http://www-ap.fnal.gov/MARS/.

[4] N. V. Mokhov, "MARS Code Developments, Benchmarking and Applications", in *Proc. of ICRS-9 International Conference on Radiation Shielding*, Tsukuba, Ibaraki, Japan, October 17-22, 1999, *Journal of Nuclear Science and Technology*, Suppl. 1, pp. 167-171 (March 2000); also Fermilab-Conf-00/066 (2000).

[5] A. Fasso *et al*, Nucl. Instr. and Meth. **A332**, 459 (1993).
C.Birattari *et al*, Nucl. Instr. and Meth. **A338**, 534 (1994).

[6] Briesmeister, J. F., editor, "MCNP - A General Monte Carlo N-Particle Transport Code", Version 4A. Pub. LA–12625–M, LANL (1993).

[7] P. A. Aarnio *et al*, CERN TIS-RP/168 (1986) and CERN TIS-RP/190 (1987).

[8] P. Aarnio and M. Huhtinen, *Proc. MC93, Int. Conf. on Monte Carlo Simulation in High Energy and Nuclear Physics,* p 1, ed. P. Dragowitsch, S. Linn and M. Burbank, World Scientific (1994).

[9] I. Azhgirey, I. Kurochkin and V. Talanov, "Development of MARS Code Package for Radiation Problems: Solution of Electro-Nuclear Installations Design", *Proc. of the XV Conf. on Charged Particles Accelerators*, Protvino, October 1996.

[10] M. Huhtinen and C. Seez, CERN CMS TN95-133 (1995).