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A Comparison of FLUKA Simulations with Measurements of Fluence and Dose in Calorimeter Structures

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Abstract

Measurements have been recently published of the spatial variation of hadron and low-energy neutron fluence and of absorbed dose in the cascades induced in iron and lead calorimeter structures irradiated by 200 and 24 GeV/c hadron beams. These experiments have been simulated using the FLUKA Monte-Carlo shower code which now includes the emission of nuclear de-excitation products and the transport of low-energy neutrons. In most cases the results agree with the measured data to better than 20%.

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1 Introduction

One of the many questions raised when designing detector systems for the new generation of hadron colliders such as the Large Hadron Collider (LHC) planned at CERN or the Superconducting Super-Collider (SSC) under construction at Waxahachie in Texas concerns the radiation damage by low-energy neutrons produced by spallation, evaporation and fission. Such neutrons may be particularly harmful to solid-state electronic devices or organic materials [1, 2]. In recent years three experiments were performed by a CERN, INFN-Milan, INFN-Turin and Carnegie-Mellon University collaboration, with the aim of providing data that could be used to predict neutron damage [3, 4, 5]. In these experiments, measurements were made of the radioactivity induced in certain elements: this can be related to the fluence of high-energy hadrons and low-energy neutrons. Radial and longitudinal distributions of activation have been measured in the following three situations:

1. An iron structure irradiated by a 200 GeV/c hadron beam (mainly protons) from the SPS accelerator at CERN [3].
2. The same iron structure irradiated by a 24 GeV/c proton beam from the CERN PS accelerator [4].
3. A lead structure irradiated by the same 200 GeV/c hadron beam as in the first experiment [5].

Distributions of absorbed dose were measured in the first two of these experiments using radiophotoluminescent (RPL) dosimeters.

These experiments were also intended to provide bench-marks for a number of Monte-Carlo programs which simulate the development of hadron-induced cascades and which now include the production and transport of low-energy neutrons [6, 7, 8, 9, 10]. This has been achieved by coupling a high-energy code with one of the elaborate neutron transport programs originally developed for nuclear reactor studies. Checks of these codes in simple geometries and beam conditions are necessary in order to have confidence in their predictions in the complex conditions of collider detectors. The FLUKA program [6, 11] used in these studies is well-established and has been widely used in studies of cascades induced by high-energy particles in matter. Recently a new version of the code has been developed [6, 12, 13, 14] which generates and transports the low-energy nucleons from the intranuclear cascade and evaporation phases of inelastic nuclear collisions in addition to simulating the high-energy particle cascade.

The activation detectors and dosimeters used in the experiments are summarized in Table 1. They were chosen as forming the simplest set to cover the widest possible energy range in the region of interest above 100 keV. In the first reports on the experiments [3, 4, 5], the measured activities were converted into nominal fluences in different energy ranges using "effective" cross-sections. However in the present study, the measured activities were

compared with those obtained by folding the calculated spectra with the relevant energy-dependent cross-sections. Both predicted and measured quantities are expressed in terms of the number of radioactive nuclei produced by one incident proton per mole of the parent atom. Comparison of predicted and measured doses have been made only for the first two experiments since dose measurements were not available for the lead irradiation.

Table 1: Summary of Activation and Dosimetry Techniques

Main contributing reaction	Sample size	Nominal energy range
$^{115}\text{In}(n,n')^{115m}\text{In}$	0.3 mm $\times$ 10 mm ϕ	0.8–15 MeV
$^{32}\text{S}(n,p)^{32}\text{P}$	6 mm $\times$ 23 mm ϕ	3–25 MeV
$^{27}\text{Al}(n,x)^{24}\text{Na}$	0.5 mm $\times$ 10–30 mm ϕ	6–25 MeV
$^{27}\text{Al}(h,x)^{18}\text{F}$	0.5 mm $\times$ 10–30 mm ϕ	> 35 MeV
Absorbed dose	6 mm $\times$ 1 mm ϕ	

In the following section the improved physical models used in the recent version of FLUKA are summarized. Section 3 gives a description of the geometrical modelling of the calorimeter structures used in the experiments, of the scoring procedures and of the cross-section data. Results and conclusions are presented in the final section.

2 Recent Developments of the FLUKA Code

The inelastic event generator of the earlier versions of FLUKA was based on the Dual Parton Model for incident particles having energies higher than 5 GeV [15, 16] and on a resonance production model for incident particles below this energy [17]. In both projectile energy ranges the emission of nucleons from intranuclear cascades and the excitation energy of the residual nucleus were sampled from empirical parametrizations of experimental data. Low-energy nucleons, heavy fragments and gamma rays from the excited residual nuclei were not generated. The transport threshold for hadrons and muons was set at 50 MeV.

The new version of FLUKA includes the production and transport of low-energy neutrons as well as many other modifications and additions to both the physical models and the code structure. Improvements to the inelastic event generator that are of relevance for the present calculations are:

1. New procedures for sampling the number of primary collisions inside the target nucleus and the number and spectra of nucleons emitted during the intranuclear cascade. As a result, the code reproduces correctly the experimentally observed multiplicities of the

particles which cause black, grey and shower tracks in nuclear emulsions, together with their mutual correlations, as well as the experimental energy and angular distributions of cascade nucleons [18].

2. A more detailed treatment of the nuclear well potential and Fermi motion.
3. A determination of nuclear excitation energy from energy conservation (taking into account the holes left in the nuclear well after the high-energy collision), including a detailed balance of the binding energies of the struck and resulting nuclei, rather than sampling it from parametrized formulae. In this way, excitation energy correlates correctly with the number of primary and secondary collisions of the incident hadron inside the nucleus. In this context, use has been made of recent nuclear data.
4. The incorporation of a nuclear evaporation model, accounting for the emission of neutrons, protons and heavy fragments from the excited residual nucleus. The nuclear evaporation model of FLUKA has been derived from the EVAP-5 module of the HERMES code system from KFA Jülich [7] (itself a version of the HETC code of the Oak Ridge National Laboratory). However, the treatment of pairing and shell effects has been improved and relativistic kinematics included.
5. A new generator for nucleon-induced interactions in the energy range 20-250 MeV, based on a detailed description of the intranuclear cascade, pre-equilibrium emission and evaporation [13].
6. A simple model to describe the production of de-excitation gamma rays after completion of particle evaporation.
7. A more accurate treatment of collisions with hydrogen nuclei.
8. The introduction of a proper treatment of antiparticle capture, based on the FLUKA resonance production model for $\bar{n}$, $\bar{p}$, and on the cascade pre-equilibrium model for π^- .

As a result of these improvements, FLUKA is now able to simulate inelastic nuclear collisions in detail, in an energy range extending from several TeV down to 20 MeV.

The most important change to the hadron transport module of FLUKA, has been the lowering of energy thresholds for particle transport. It is now possible to simulate neutron collisions and transport down to optionally defined region-dependent energy cut-offs which can be as low as thermal energies. Below 20 MeV this is accomplished by using a new multigroup neutron cross-section library [19], supplied by ENEA-Bologna, which is based on the JEF-1.1 cross-section compilation [20]. The low-energy neutron collision algorithm is similar to that used in the MORSE code [21]. The energy deposited by charged recoils and products from low-energy neutron reactions is estimated using kerma factors [19, 22]; however for collisions with hydrogen nuclei the recoiling protons are explicitly produced and transported in a kinematically correct manner. Updated stopping power data have been used.

The simulation of electron and photon interactions and transport, originally based on the EGS4 code [23], has been extensively improved. These changes have no relevance to the calculation of neutron fluence, but have an effect on the evaluation of energy deposition. In the simulation of electron and positron transport algorithms specifically developed for FLUKA [6] are now used; these are also used for charged hadrons and muons. The bremsstrahlung cross-sections have been taken from the most recently evaluated data [24, 25], corrected for the polarization effect [26] and, at high energies, for the Landau-Pomeranchuk-Migdal effect [27, 28]. Differences between electron and positron bremsstrahlung are taken into account and the proper angular distributions of emitted bremsstrahlung photons, as well as of the e^+ and e^- created by pair production, replace the original fixed angle approximations of EGS4. The photoelectric effect is described by a detailed algorithm which accounts for the separate probabilities of photon interactions with each atomic shell, the proper angular distribution of photoelectrons and the emission of both fluorescent photons and Auger electrons. The production of electron pairs and photons by high energy hadrons and muons is included.

3 Details of the Simulations

3.1 Geometrical modelling of the experimental arrangement

The calorimeter structures consisted of rectangular absorber slabs of 5 cm thickness, separated by 7 mm slots in which thin aluminium plates supporting the activation detectors and dosimeters were placed. The transverse dimensions of the slabs were 30×30 cm in the experiments with iron and 50×50 cm in the experiment with lead. The thickness of the aluminium detector plates was 4 mm in the experiment with iron at 200 GeV/c and 0.5 mm in the other two. An aluminium detector plate was also placed in front of the first absorber slab in order to measure albedo effects. In the experiment with lead the material contained about 4% Sb in weight, but this value was not known with great accuracy. In order to assess the importance of the antimony component, two different simulations were performed, one with pure lead and one with 96% Pb and 4% Sb in weight. The three structures were modelled in Combinatorial Geometry [29, 21].

3.2 Incident beams

In the 24 GeV/c experiment the beam consisted entirely of protons, but in those with 200 GeV/c incident hadrons its composition was 2/3 protons and 1/3 positive pions. The beams were assumed to be monoenergetic and their projected distributions on the horizontal and vertical planes were assumed to be Gaussian with the width parameters determined in the experiments: for the 200 GeV/c irradiations the standard deviations of the projected horizontal and vertical beam profile distributions were 1.2 and 0.9 cm respectively; in the 24 GeV/c case they were both 0.13 cm. The beams were incident on the centre of the first

absorber slab in both the experiments with iron; in that with lead the beam axis was 10 cm off-centre in the horizontal mid-plane.

3.3 Simulation of particle transport

Calculations of induced radioactivity and dose were performed in separate computer runs. In both cases, a 20 MeV transport cut-off was applied to charged hadrons and muons, and 0.1 MeV to neutrons. Particles other than hadrons, irrelevant for activation, were followed only when calculating absorbed dose, the electromagnetic cascade contributing about 50-60% of the total energy deposition. The electron and positron cut-off was set at 1 MeV kinetic energy, and that of photons at 0.1 MeV. A maximum energy loss of 10% per step was imposed on the electron transport step length to ensure an accurate path-length correction in connection with multiple Coulomb scattering [6].

The calculations were performed on a personal VAX-station. In order to determine statistical errors of the estimated values, several runs were performed for each case. For the activation calculation a total of 1000, 6000 and 500 primary histories were simulated, corresponding to the three experiments; for the calculation of energy deposition in the two experiments with iron, 600 and 2000 histories were simulated respectively at 200 and 24 GeV/c.

3.4 Description of the scoring procedures

The radioactivity induced in each detector was computed as a function of slot number and radial position using the following procedure.

Neutrons and high-energy hadrons were scored when crossing a plate boundary in either direction at a detector position. To improve statistics, the scoring surface was taken to be an annulus centred on the beam axis and of radial width equal to the diameter of the particular detector. Inverse-cosine weighting was applied to the number of trajectories crossing the annulus in order to determine the fluence. Radionuclide production was estimated by folding the particle spectral fluence with energy-dependent activation cross-sections as discussed in the following section. A geometrical correction was applied to account for scoring in an annulus rather than in a detector of circular shape.

The dose absorbed in the RPL dosimeters was estimated from a radial binning of the energy deposited by all particles in the aluminium plates, the two materials having similar densities and stopping powers. The radial bin-size of the scoring annuli was 0.5 cm, smaller than the diameter of the capsules containing the RPL dosimeters. The bin whose centre most nearly corresponded with the centre of the dosimeter capsule was taken as representing the position at which dose was measured.

3.5 Reaction cross-section data

The production of ^{115m}In from ^{115}In was assumed to be due to neutrons only. Inelastic scattering on ^{115}In leading to a metastable state is physically possible with particles other than neutrons but it was not possible to find any cross-section data in the literature except for the photon inelastic scattering reaction [30]. However the cross-section is very small. The production of ^{32}P from ^{32}S was also assumed to be solely due to neutrons since the only other channels available to this charge-exchange reaction involve incident pions. With their low cross-section and relative paucity in the cascade compared to low-energy neutrons, they cannot be expected to contribute significantly to the ^{32}P activity.

Below 20 MeV, neutron cross-sections for the activation of indium, sulphur and aluminium were taken from the ENDF/B-VI Dosimetry File [31]. At higher energies, data for neutron-induced reactions are rare in the literature and are often incomplete or inconsistent. Cross-sections extrapolated up to 44 MeV by Greenwood [32] were adopted for the (n,n') reaction in indium and the (n, α) in aluminium. In all cases, the neutron cross-sections were assumed to be constant at energies above 50 MeV.

Activation by protons and charged pions was taken into account for the production of ^{24}Na and ^{18}F from ^{27}Al . Cross-section data for the proton-induced $^{27}\text{Al}(p,3pn)^{24}\text{Na}$ reaction were taken from Hitz and Ramsey [33] for the energy range from 40 to 100 MeV, from Tobailem *et al.* [34] from 100 to 220 MeV and from Baker *et al.* [35] at 28 GeV and above. For the deep spallation reaction $^{27}\text{Al}(h,x)^{18}\text{F}$ the neutron cross-section was assumed to be equal to that of the reaction induced by high energy protons, taken from the same sources. The production of ^{24}Na and ^{18}F from ^{27}Al by π^+ and π^- was estimated using data from Dropesky *et al.* [36].

Cross-section uncertainties could be in principle an important source of inaccuracy in the present comparisons. However, trials with different cross-section values for energies higher than 20 MeV indicated only a very small sensitivity of the calculated reaction rates on high-energy data. This can be explained by most of the activity being due to low-energy neutrons, by far the dominant component of the hadronic cascade.

For the calculations of activity, a linear energy interpolation was used between the cross-sections of the original data files.

4 Results and Conclusions

Selected comparisons between the activities or dose calculated in the FLUKA Monte-Carlo simulations and those measured at different depths in the cascades are given in Figures 1–5. Each Figure shows the radial distribution for one of the five detector systems selected from the three experiments. For the sake of clarity in the Figures comparisons are only given at four depths: at or near the front of the structure, before cascade maximum, at or near

cascade maximum and past cascade maximum where the so-called "equilibrium" cascade should have developed. A complete set of comparisons is given in [37].

All the results are normalized to one incident hadron. The experimental data are represented by discrete symbols and the results from the simulations by solid-line histograms. It should be noted that each horizontal line segment of the histogram represents the calculated value at the centre of the segment; this centre corresponds to the radial position of the measurement.

In order to avoid superposition of the distributions in the Figures, the values at different depths have been multiplied by the indicated factors before plotting. Statistical errors in the calculations (the standard error of the mean obtained from at least five separate computer simulations) are shown by vertical bars whenever they exceed 5%.

Concerning the third experiment, the ^{115m}In activities were finally calculated by including the nominal 4% content of antimony in the lead of the calorimeter structure. The results so obtained were found to be closer to the experimental values than those with pure lead (40% average overestimation instead of 60%). This shows the sensitivity of low-energy neutron transport to the presence of small amounts of impurities. The calculated activities of the detectors with higher thresholds are practically identical in the two cases.

Recent analysis has shown that the experimental data published in [3, 4, 5], need to be modified in two important ways. The first concerns the assay of ^{32}P where a new calibration has been made of the Geiger-Müller counting system. From this it was found that all measured ^{32}P activities must be multiplied by 1.61. The second modification concerns the dose as measured by the RPL dosimeters which were calibrated in terms of exposure in air. The Monte-Carlo simulations predict the absorbed dose in aluminium. Since the dosimeters were calibrated using photons from a ^{137}Cs source this means that the apparent doses measured in the experiments have to be reduced by the factor 0.84.

The ratio of the activity or dose determined from the Monte-Carlo simulations to the measured value was examined as a function of radial and longitudinal position for each detector technique and experiment. For a given detector technique used in a particular experiment, there is in general no discernable variation of this ratio either with radial position or with longitudinal depth in the cascade. The means of these individual ratios at different depths and radii, weighted according to the errors of the experiment and the statistical errors of the simulations, and the standard errors on these means were calculated on a geometric basis. Generally the means are based on between 50 and 150 measurements for a given technique in a given experiment. The values of these means and standard errors are given in Table 2 for each detector system in each experiment as well as for each detector technique averaged over the three experiments and for each experiment averaged over each technique used.

Inspecting Table 2 it will be seen that in general the 24 GeV/c Monte-Carlo predictions are about 20–30% higher than the measurements whereas the averages for the other two experiments are very close to unity suggesting a possible proton normalization error in the

Table 2: Ratios of the results from FLUKA simulations to the measured data, averaged over detector positions, for the different measurement techniques and experiments

Detector system	200 GeV/c Fe	24 GeV/c Fe	200 GeV/c Pb	Mean over experiments
$^{115}\text{In}(n,n')^{115m}\text{In}$	0.91 ± 0.02	1.20 ± 0.05	1.34 ± 0.09	1.12 ± 0.03
$^{32}\text{S}(n,p)^{32}\text{P}$	0.96 ± 0.03	1.35 ± 0.05	0.70 ± 0.02	0.85 ± 0.03
$^{27}\text{Al}(n,x)^{24}\text{Na}$	0.85 ± 0.02	1.03 ± 0.02	0.63 ± 0.01	0.82 ± 0.01
$^{27}\text{Al}(h,x)^{18}\text{F}$	1.30 ± 0.04	1.32 ± 0.05	1.04 ± 0.03	1.17 ± 0.03
Mean over detectors	0.92 ± 0.02	1.14 ± 0.02	0.76 ± 0.02	0.91 ± 0.01
RPL dosimeters	0.91 ± 0.06	0.93 ± 0.07	—	0.92 ± 0.05

experiment. Averages over experiments for the different activation detector techniques differ from unity by less than 25% and the average for all detectors over all techniques is only 9% too low. There is also no difference between the means calculated for the activation detectors and the means calculated for dose. This level of agreement is in most cases better than that found in previously reported comparisons with the first experiment, made with other Monte-Carlo programs [38, 39].

These results still do not take into account possible systematic errors in the experimental data and in the cross-sections used. These latter must certainly exceed several percent. Non-random errors in the experimental data may arise from several sources: imperfect beam alignment, beam composition, monitoring of the beam intensity, factors affecting counter efficiency *etc.*. The overall uncertainty on the measurements is difficult to assess with certainty, but it has been estimated in the reports on the experiments to be not less than 20–30%.

In the case of the irradiation of the calorimeter of an LHC or SSC detector, the scale of the spatial variation of the fluence of the incident hadrons is larger than that of the radial variation of the hadron cascade inside the calorimeter. It is of interest, therefore, to compare the predicted and measured variation with depth in the cascade of the radially integrated isotope production and dose. These comparisons are illustrated in Figures 6–10, which show that the differences indicated in Table 2 are valid over all depths of the cascade.

It can thus be concluded that the level of accuracy that can be obtained from FLUKA concerning the spatial distribution of hadron fluence, including low-energy neutron fluence, and the spatial distribution of energy deposition in cascades induced by high-energy hadrons is close to the best level that can be tested by this kind of experiment.

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Figure 1: Comparison of the calculated and measured production of ^{115m}In from ^{115}In as a function of radial distance off-axis at different depths in an iron structure irradiated by 200 GeV/c hadrons.

Figure 2: Comparison of the calculated and measured production of ^{32}P from ^{32}S as a function of radial distance off-axis at different depths in a lead structure irradiated by 200 GeV/c hadrons.

Figure 3: Comparison of the calculated and measured production of ^{24}Na from ^{27}Al as a function of radial distance off-axis at different depths in an iron structure irradiated by 24 GeV/c protons.

Figure 4: Comparison of the calculated and measured production of ^{18}F from ^{27}Al as a function of radial distance off-axis at different depths in a lead structure irradiated by 200 GeV/c hadrons.

Figure 5: Comparison of the calculated and measured absorbed dose as a function of radial distance off-axis at different depths in an iron structure irradiated by 200 GeV/c hadrons.

Figure 6: Comparison of the calculated and measured variation of the radially integrated production of ^{115m}In from ^{115}In as a function of depth in iron and lead structures irradiated by 200 GeV/c and 24 GeV/c hadrons.

Figure 7: Comparison of the calculated and measured variation of the radially integrated production of ^{32}P from ^{32}S as a function of depth in iron and lead structures irradiated by 200 GeV/c and 24 GeV/c hadrons.

Figure 8: Comparison of the calculated and measured variation of the radially integrated production of ^{24}Na from ^{27}Al as a function of depth in iron and lead structures irradiated by 200 GeV/c and 24 GeV/c hadrons.

Figure 9: Comparison of the calculated and measured variation of the radially integrated production of ^{18}F from ^{27}Al as a function of depth in iron and lead structures irradiated by 200 GeV/c and 24 GeV/c hadrons.

Figure 10: Comparison of the calculated and measured variation of radially integrated dose as a function of depth in iron structures irradiated by 200 GeV/c and 24 GeV/c hadrons.