Simulation of the patient Quality Assurance on a CPO beam line

A Stankovskiy\textsuperscript{1}, S Kerhoas-Cavata\textsuperscript{1}, R Ferrand\textsuperscript{2}, C Nauraye\textsuperscript{2}

\textsuperscript{1} CEA/DSM/DAPNIA/SPhN, 91191 Gif-sur-Yvette, France
\textsuperscript{2} Institut Curie – Centre de protonthérapie d’Orsay Bât. 101 du Centre Universitaire d’Orsay, BP65-91402 Orsay, France

Alexey.Stankovskiy@cea.fr

Abstract. The Proton Therapy Center in Orsay (CPO) and CEA/DAPNIA launched the joint project on Monte Carlo modelling of a CPO beam line with the aim to achieve a prediction of dose distribution in all the calibration configurations (depth and the shape of the tumor) better than 2 \%. The calculation module is intended to be used for the absolute dosimetry of the clinical beam (patient Quality Assurance – QA), and in a second stage for predicting the dose distribution on a voxelized phantom constructed from the Computer Tomography (CT) patient’s data. The MCNPX code was used as a basic Monte Carlo simulation tool in this study. All the elements of a CPO beam line were modelled with sub-millimetric precision. To speed up the calculations of modulated dose profiles in water phantom, a routine simulating rotation of modulator wheel was created to save phase space of particle tracks crossing the modulator. The modelling of nuclear interactions, which contribute noticeably into the total absorbed dose in water phantom at the prescribed proton energy (average raw beam energy 201 MeV), was improved by means of creation and implementation of the two new evaluated proton-induced nuclear data files up to 200 MeV for \textsuperscript{1}H and \textsuperscript{16}O. Thus, the simulations of 3D dose profiles in water show excellent agreement with measured data allowing to move forward to the absolute dose calibrations.

1. Introduction

The Monte Carlo (MC) modelling of radiation transport might be the effective way to substitute the conventional tools for calculation the dose distribution inside a patient used for treatment planning in proton therapy. The latter usually is based on various parameterizations of measured proton dose distributions (so-called pencil-beam or broad-beam techniques) while the Monte Carlo simulation provides the accurate description of the almost all possible interactions of particles with matter. The disadvantage is still huge computational time making it difficult implementing in daily clinical routines.

The Proton Therapy Center in Orsay and CEA/DAPNIA launched the joint project on Monte Carlo modelling of a CPO beam line with the aim to achieve the targeted accuracy of the prediction of dose distribution in all the calibration configurations (depth and the shape of the tumor) better than 2 \%. The calculation module is intended to be used for the absolute dosimetry of the clinical beam (patient QA), and in a second stage for predicting the dose distribution on a voxelized phantom constructed from the CT patient’s data. Along with this ultimate goal, the Monte Carlo simulation tool could be helpful in better understanding of fundamental physical processes taking place in the beam delivery system and, probably, better configuration of beam line.

The project has 3 basic parts. First of all, the beam line has to be accurately modelled with respect to the dose delivered to water with targeted accuracy of Monte Carlo predictive power 1-2\% in the absolute dose values or 1-2 mm in range. This necessitated performing an extensive set of measurements of dose deposited in water. Second, the patient dependent elements (collimators, compensators) will be verified against another set of experimental data. Finally, the MC simulations will be performed in patient voxelized phantom constructed on the basis of CT data. This paper describes the first part of the project.
2. Methods

2.1. Beam line configuration

The general purpose Monte Carlo transport code MCNPX 2.5.0 [1] was chosen as the tool to perform simulations. The code, judging from its name (MCNP eXtended), is based on nuclear reactor transport code MCNP extended to the wider range of particles and energies far beyond the reactor ones. The brief description and basic features of MCNPX as applied to the simulation of proton therapy could be found in Refs. [2,3].

The CPO beam line simulated by Monte Carlo is schematically described in figure 1.

![Figure 1: Composition of beam line (not to scale). Beam is entering from the left. The distance from the accelerator tube vacuum window (not shown) to water tank is about 7 m.](image)

This line uses passive scattering technique. The raw beam (pulses of 20 μs, produced at a frequency of 448 Hz), coming from the accelerator tube, first faces the rotating wheel which modulates the proton energy spectrum. Between the accelerator tube vacuum window and the modulator, two transmission ion chambers are situated to monitor beam parameters. After being cut by the first collimator with diameter 3 cm, the beam interacts with the range shifter (so-called “binary filter”) that consists of lexan and lead layers of various thicknesses. The patient-dependent range and flatness of the dose distribution are formed by the proper combination of these range shifting and pre-scattering layers. Another element of the double-scattering system, so-called “scatterer”, consists of the set of thin lead foils put together as it is shown in figure 1. Then beam enters the treatment room through a hole in the concrete shielding separating the treatment room from the accelerator beam line. After passing through a number of collimators and ion chambers, the beam is finally collimated and protons deposit their energy in water. In the clinical case, the patient-dependent collimators and compensators to cover the tumor shape are attached to the final aperture.

All the elements of a CPO beam line were modelled according to the technical data provided by manufacturer. The distance between the isocenter, which for the calculations was accepted to be an entrance face of water tank, and the accelerator tube vacuum window, is about 7 m. The dose to water was scored experimentally by IBA-Scanditronix-Wellhöfer CC13 chamber. In MCNPX, the dose was calculated in the cylindrical volumes of 0.13 cm³ positioned in a chain along beam axis (for depth profiles) and perpendicular to it (for lateral profiles).
2.2. Raw beam parameters

The raw beam spatial distributions in vertical and horizontal directions were measured experimentally and taken as beam parameters for Monte Carlo simulations. They are shown in figure 2. As it might be seen, the distributions are not symmetric and not completely Gaussian, however, the similar measurements by monitor chambers placed after each collimator show that beam acquires Gaussian shape.

![Figure 2](image-url)

**Figure 2.** Spatial beam profile measured close to vacuum window.

The mean energy of the beam is suggested by the accelerator manufacturer to be 201 MeV with the energy spread 0.5% that corresponds to full-width-at-half-maximum 1.005 MeV. These values have been also used as beam input parameters for Monte Carlo simulations.

The beam angular spread was measured experimentally and was found to be the Gaussian with FWHM $\Delta \theta = 4.4$ mrad. This value was also used as input parameter for MCNPX calculations.

3. Results and discussion

The starting point for simulations was the validation of the MCNPX code on relative dose distributions in water from unmodulated beam. Hereinafter, all relative depth dose distributions correspond to normalization to 100% at the peak value for unmodulated beam and at the middle of the plateau in case of SOBP, while lateral profiles are normalized to 100% at the beam axis. To find how adequately the physics inside the MCNPX reproduce the real dose distributions, all the beam-scattering devices, i.e. diffuser, binary filter, and, of course, modulator, were removed from the line so that the beam line was composed from collimators only, plus ion chambers. The comparison of measured and simulated “native” Bragg curves and the lateral dose profiles taken at the entrance of water tank are shown in figure 3.

Dose profiles were calculated using nuclear data tables for protons supplied with MCNPX (the study of capabilities to model nuclear interactions is presented below in Section 3.3). Figure 3,a reveals the good agreement between measured and calculated curves – in terms of range, the coincidence is within 1 mm while in the relative dose value the difference is less than 1%. Thus, the simulations reproduce the measured data within the values of experimental uncertainties. Figure 3, b shows the influence of beam angular spread to the lateral dose profile in water. The native profile is found to be very sensitive to that. Earlier measurements of the beam angular spread gave the value of 4.85 mrad of FWHM. The use of this value in MC simulation could not allow reproducing well the data measured recently, so, the angular spread was re-measured and found to be 4.4 mrad which resulted in the significant improvement of the simulated lateral profile shape. However, another source of uncertainty was found. The multi-wire ion chamber located close to beam entry point for simulations (figure 1), is made of 2 stainless steel layers 38$\mu$m-thick containing tungsten wires and gas. These two layers significantly modify the lateral profile, as it might be seen from figure 3,c.
Protons traveling through steel undergo multiple Coulomb scattering (MCS) which is known to have a simplified description in MCNPX, based on work of Rossi [4] adopting Molière theory. It overestimates angular deflections, especially for high-Z materials, and this overestimation was found here even for iron. However, the solution safe from the viewpoint of subsequent simulations of whole beam line was reduction of the thickness of these layers from 38 μm to 15 μm. MCS realization in MCNPX obviously needs improvement, however the use of present version of the code (2.5.0) does not necessarily lead to wrong description of dose distributions.

**Figure 3.** Relative depth dose profile (a), sensitivity of lateral dose profile to the beam angular spread (b) and to the thickness of stainless steel layer of multi-wire monitor chamber (c).

3.1. **On the speedup of the calculations**

The MCNPX code has capability to transport all types of particles (except for recoil nuclei with A>4) through the matter. With the aim of possible application of the MC calculation tool in daily clinical routine, at least from the viewpoint of fast calculation of the spatial dose distribution, it is expedient to find a way how to reduce the computational time at the same cost, i.e. by means of software rather than hardware improvement. MCNPX has a variety of possibilities to do that, mostly applying variance reduction technique. The additional set of tests with unmodulated beam was performed with the purpose of reduction the computational time. It was found that applying variance reduction...
technique and suppressing the transport of neutrons, photons and electrons, it is possible to produce the dose distributions (both depth and lateral) 15 times faster than in the base case (when all possible particles are transported without any variance reduction) without losing the quality of results (i.e. the agreement with experimental data in the range, modulation width, and lateral penumbra is within 1 mm).

However, such problems as calculation of dose delivered by neutrons (or photons and electrons) outside the irradiated volume, as well as estimation of output factors for beam calibration, will obviously require tracking all particles. It should be noted here, that the typical statistical uncertainties were within 1%, thus the differences of dose curves from that of the base case are well below these uncertainties.

3.2. Modulated beam
As it was mentioned above, the CPO beam line is of passive scattering type, the rotating aluminum wheel along with binary filter consisting of lead and lexan layers are used to provide flat dose distribution covering the tumor at desired depth. The simulation of modulated beam, in general, represents certain difficulties when using MCNPX since the code does not treat time-dependent geometry changes. However, for the modelling of CPO beam line geometry set-up, it was easily avoided. The idea behind that was to create phase space files just after modulator. The wheel shown in figure 4 consists of three “rings” with sectors of various thicknesses. It was described within sub-millimeters in terms of MCNPX combinatorial geometry, and the routine realizing “quasi-time-dependent” simulation was created to save information on particles crossing modulator after each rotation step. This routine performs automatic transformation of the modulator geometry according to the value of rotation angle, launches the MCNPX simulation in single processor mode (parallel calculation mode was found to be ineffective since time to send/receive subtasks from master to slave processors is comparable with typical simulation time on single processor for each angular step) and adds particle track information to surface-source write (SSW) file. It was found that to have smooth particle distributions (for each particle type the energy, position, direction and momentum were scored) the angular step of rotation 0.5 degree is enough. Three surface-source read (SSR) files containing phase space for each modulation ring were created.

Figure 4. Aluminum modulator wheel and its realization in MCNPX simulations (cross section plane perpendicular to beam axis).
The use of these three distributions as new particle sources allowed to reduce significantly (up to a factor of 100) the computation time. Moreover, the actual number of particle tracks (limited by the available disk storage capacity, at present about 4 millions tracks are stored in each file) might be increased in subsequent simulation to ensure the better quality of results. Each starting particle track is repeated with new random number seed. The recycling factor is ranged from 2 (for unmodulated depth profiles) to several hundreds (for lateral profiles).

Typical computing time to obtain SOBP of the quality better than 2% for dose and 1 mm for range and modulation width is about 15 min to simulate $10^7$ particle histories originated from the phase space right after modulator. The cluster of nine 2 GHz processors running under Linux was used to perform calculations for this study. This seems to be acceptable from the viewpoint of further integration of Monte Carlo dose calculation into the treatment planning.

3.3. Nuclear interactions

Despite the main mechanism for protons to loose their energy along flight path is electromagnetic interaction, they may also undergo nuclear interactions. Typically the secondary particles, originated from nuclear non-elastic interactions of protons with materials along the beam line, contribute insignificantly to the total dose delivered to water. The exception is secondary protons whose contribution might be as high as 10-15% to the energy deposited proximal to single Bragg peak and in the case of SOBP, they in addition influence the flatness and may undergo another nuclear interactions [5]. Other particles generated in nuclear interactions (deuterons, tritons, $^3$He and alphas) are contributing less than 2%. Neutrons, electrons and photons deposit their energy far outside the irradiated volume while their contribution to dose to water is approximately 0.1%.

In general, of great importance is to carefully account for nuclear interactions (both elastic and non-elastic) which take place close to and inside in the irradiated volume, i.e. water tank in our case. MCNPX has two options of treatment the nuclear interactions: to invoke various physics models (up to 8 combinations of intranuclear cascade/preequilibrium/evaporation models) or to sample them according to nuclear data tables read in from corresponding files. In case the data table for particular isotope is not present or the energy range of data does not span the energies characteristic to the problem, the code uses model calculations. Strictly speaking, especially for the energies characteristic to proton therapy (up to ~ 200 – 250 MeV) the data files provide more precise description of nuclear interactions than inherent in MCNPX models for 2 reasons: the proton induced data are evaluated from the external model calculations and experimental data, and, secondly, the quality of preequilibrium and evaporation models in MCNPX which dominate at these energies remains questionable.

However, the data files, in general, have upper energy limit of 150 MeV which is not enough to cover our problem. The comparative analysis of the quality of the data and models for two most important isotopes – hydrogen-1 and oxygen-16 which almost compose the water was performed. It revealed that, especially for $p^+\,^1$H interactions, proton elastic scattering cross sections contained in LA150H library [6] and calculated by MCNPX physics models have strange behavior and large discrepancies between each other. This resulted in creation of two new evaluated data files for $p^+\,^1$H and $p^+\,^{16}$O interactions up to 200 MeV. The description of these new files will be reported at [7].

Figure 5 shows the depth dose distributions calculated with different model/data options and experimentally measured. The difference between red curve, which corresponds to the use of new evaluated data for $^1$H and $^{16}$O, and green curve representing the case of LA150H library, is small enough, but the value of least squared deviation factor is less for the curve corresponding to new evaluated data (up to 5%). In the same time, due to the large underestimation of proton elastic scattering cross section on hydrogen below 150 MeV, the MCNPX model option significantly underestimates the shape of the curve (blue curve in figure 5). In case of SOBP the difference between model calculations and calculations with the use of evaluated data files is more pronounced, than in case of single non-modulated Bragg curve, due to accumulation of this discrepancy when summing up the doses deposited by protons at each angular position of modulator wheel.
There was found no dependence of distal fall-off edge of the SOBP and lateral dose profile from the model/data choice. The SOBP was simulated with accuracy below the experimental uncertainties, i.e. within prescribed value of 1 mm.

![Graph showing depth dose distribution for modulated beam calculated with model option, LA150H library, and new data files.](image)

**Figure 5.** Depth dose distribution for modulated beam calculated with model option, LA150H library, and new data files.

3.4. **Lateral profiles**

As a rule, to score lateral dose profiles the longer computing time with increased statistics is necessary to ensure the statistical uncertainty being comparable with experimental one. Typically, obtaining 3D dose distribution requires \(~10^9\) particles starting from the modulator phase space to be followed. This value corresponds to \(~20\) millions particles contributing to the dose to water. The average computing time is about 1 day on nine 2 GHz processors cluster. The simulated dose profiles taken at different depth in water are shown in figure 6.

![Graphs showing lateral dose profiles taken at different depth in water: at the entrance of water tank (a) and at middle of SOBP plateau (b).](image)

**Figure 6.** Lateral dose profiles taken at different depth in water: at the entrance of water tank (a) and at middle of SOBP plateau (b).
As it is seen from figure 6, the difference between measured and simulated data is within prescribed value of 2% in shoulders and lateral penumbra. Thus, the MC simulation ensures the required quality of 3D dose distribution representation.

4. Conclusions
Monte Carlo simulation for CPO treatment head geometry has been achieved using MCNPX 2.5.0 code. The validation done with reference data revealed good agreement within 1-2 mm in range, modulation width, distal and lateral penumbra for all sets of data (more than 40 depth and lateral dose distributions for modulated and unmodulated beam were simulated). The novel approach to simulate time-dependent geometry with MCNPX was proposed. The use of new evaluated proton-induced nuclear data files up to 200 MeV for hydrogen-1 and oxygen-16 allowed to improve the predictive power of MCNPX dose calculations. The validation phase manifested the applicability of MCNPX for carrying out MC simulations of a CPO beam line allowing to launch a new campaign of measurements and simulations related to absolute dosimetry in terms of output factors.

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