Calculation of energy-deposition distributions of a $^{9}$C beam using the PHITS code

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Abstract. Carbon-9 beams represent one of the possible alternatives (presently under consideration and investigation) to conventional $^{12}$C beams for heavy-ion cancer treatment. Interest in this exotic isotope stems from the expected boost in biological effectiveness due to the $\beta$-delayed emission of two $\alpha$ particles and a proton that takes place at the ion stopping site. Experiments have been performed [1] to characterise $^{9}$C beams physically and models have been developed [2] to estimate quantitatively its biological effect.

In this work, we have used the PHITS code [3] to calculate energy-deposition and LET distributions for a $^{9}$C beam in water and we have compared the results with some published data [1]. Even though PHITS fails to reproduce some of the features of the distributions, its result is that decay gives a negligible contribution to the energy-deposition distributions, thus contradicting the previous interpretation of the measured data.

1. Introduction
Heavy-ion cancer therapy is nowadays a well-established tool for the treatment of certain types of tumours [4], thanks to its peculiar characteristics. The most popular choice for the beam by far is $^{12}$C, which is believed to strike the best compromise between high biological effectiveness in the tumour volume and low damage to the surrounding healthy tissue. However, attention has been paid to the possibility of using other beams: one of the most recent candidates is $^{9}$C, which could have a more favourable peak-plateau ratio with respect to conventional $^{12}$C beams; such expectations are based on the fact that $^{9}$C is a $\beta^+$ emitter, with a half-life of 126.5 ms, a
Q-value of about 16.5 MeV and the following decay scheme [5]:

\[ ^{8}\text{Be} + p \rightarrow ^{9}\text{B} \]

\[ ^{9}\text{C} \beta^{+} \rightarrow ^{9}\text{B} \]

\[ 2\alpha + p. \]

\[ ^{5}\text{Li} + \alpha \]

The half-life of $^{9}\text{C}$ is sufficiently long to hinder in-flight decay; once a projectile comes to a stop in the cancer region, however, its decay will generate three high-LET particles that could possibly boost the local biological effect and would remain mostly confined to the target volume due to their short ranges (in the µm–mm range). Experimental verification of these expectations is obviously necessary if one wants to implement $^{9}\text{C}$ beams in treatment-planning systems; moreover, accurate models for the eventual decay-related boost in biological effect must be developed; some work has already been performed in both directions [6, 7, 1, 2].

The purpose of the present work is to use the PHITS code [3] to calculate energy-deposition distributions for a $^{9}\text{C}$ beam traversing different thicknesses of water, compare with experimental data [1] and help with the physical interpretation of the latter. A more extensive account of the simulation strategy and of the results will be available in a coming paper [8].

2. Materials and methods
2.1. The PHITS code
The PHITS (Particle and Heavy-Ion Transport System) code [3] is a three-dimensional Monte Carlo code, designed with the purpose of simulating the transport of nuclei and other particles in complicated geometries and calculating fluxes, doses, energy-deposition distributions and many other observables. It is currently maintained by a cooperation among RIST (Research Organisation for Information Science and Technology, Japan), JAEA (Japan Atomic Energy Agency, Japan), KEK (High-Energy Accelerator Research Organisation, Japan) and Chalmers University of Technology (Sweden).

2.2. The experiment
The experiment we have simulated with PHITS is described in Li et al.'s paper [1] and it will only be briefly outlined here.

The experiment was performed at the Secondary Beam Line of HIMAC (Heavy Ion Medical Accelerator in Chiba, Chiba, Japan), where $^{9}\text{C}$ ions were produced as spallation products of the reaction between 430 MeV/n $^{12}\text{C}$ and a 40-mm-thick beryllium target. Beam characterisation [7] has revealed that, under optimal conditions, the resulting $^{9}\text{C}$ beam contains several contaminating fragments with broad energy distributions and that the $^{9}\text{C}$ component has a Gaussian momentum distribution, centred at 838.9 MeV/c/n and with a standard deviation of 26.1 MeV/c/n.

The purpose of the experiment [1] was to measure energy-deposition ($\Delta E$) distributions (i.e. number of events as a function of energy deposition in the detector) of the $^{9}\text{C}$ beam after traversal of different thicknesses of water; this was accomplished by means of a water column of adjustable thickness and a gas-flowing-type multi-wire parallel-plate proportional chamber, filled with P-10 gas, acting as an LET counter.
Figure 1. Measured energy-deposition distribution at a depth of 14.22 cm, together with the results of the transport simulations for 14.2, 14.4 and 14.6 cm. The calculated energy depositions have been converted to LET by dividing by the detector thickness.

3. Simulation
The purpose of the simulation was to calculate the $\Delta E$ distributions and identify their different components, in order to help with their physical interpretation. The strategy of the calculation was the following:

(i) transport $^9$C ions through the water column to their stopping point, neglecting $\beta$ decay, and tally their stopping density;

(ii) use the stopping density as a source for a second calculation, that simulates $^9$C decay and transport of the decay products.

We then summed up corresponding $\Delta E$ distributions in the two calculation steps; the resulting distributions are not the same as one would obtain by considering transport and decay in one step. This procedure is justified by the consideration that the half-life of $^9$C (126.5 ms) is much longer than the typical detector dead time; thus, any energy deposition in the detector due to decay will trigger the data-acquisition system separately and will be registered as an additional event.

4. Results
The experimental $\Delta E$ distribution at a depth of 14.22 cm is shown in figure 1, together with the results of the transport simulations at 14.2, 14.4 and 14.6 cm. The calculated energy depositions have been converted to LET by dividing by the detector thickness.

The distributions can be schematically divided in three parts:

(i) below $\sim 10$ keV/µm one can observe low-energy-deposition events, caused by deep spallation of the primary $^9$C projectiles;
(ii) between $\sim 10$ and 20 keV/$\mu$m the experimental distribution shows a flat peak which is absent in the calculated distributions;

(iii) above $\sim 20$ keV/$\mu$m there is the broad primary peak, due to events in which the $^9$C ions did not lose charge in nuclear reactions and managed to hit the detector.

The physical interpretation of the events in regions (i) and (iii) is very straightforward and has been given above; the events in region (ii) require some discussion. It is claimed in Li et al’s work [1] that the flat peak is due to decay products from $^9$C; however, even if this is consistent with the results in figure 1 (that do not take decay into account), we will show in the next section that this interpretation is probably wrong.

The PHITS code appears to be able to reproduce the overall features of the energy-deposition distribution quite accurately. The calculated distribution at 14.4 cm seems to fit the experimental primary peak best; the simulated depth is slightly larger than the experimental one; this is probably due to an underestimation of the reaction cross section in PHITS — or, rather, in the model it uses [9, 10, 11] — which has already been observed for other systems [12, 13].

### 4.1. Decay

Figure 2 shows the contributions of $^9$C transport and decay to the total $\Delta E$ distribution, for a simulated depth of 14.4 cm. We remind the reader that the measured $\Delta E$ distribution should be compared with the sum of the transport and the decay distributions (see section 3). It is apparent that the contribution of decay is several orders of magnitude smaller than the contribution of transport; it is therefore unlikely that the flat peak in region (ii) can be ascribed to decay, as it is claimed by Li et al [1].

However, one might wonder what the peak in region (ii) really is, and why PHITS cannot reproduce it. One plausible explanation is that the peak is due to events where the leading fragment is a boron fragment; this is supported by figure 3, where the calculated LET distribution (i.e. number of particles entering the detector as a function of their nominal LET) at 14.4 cm...
Figure 3. Calculated energy-deposition and LET distributions at 14.4 cm. An artificially boosted boron peak is superimposed for illustration purposes (see text).

| Energy (MeV/n) | \( \sigma_B \) (mb) |
|----------------|-----------------|
| 113.0          | 231             |
| 168.0          | 232             |
| 175.0          | 225             |
| 241.0          | 210             |
| 670.0          | 215             |

Table 1. Cross sections for the production of boron fragments from \(^{12}\text{C}\) in water. The energy for the calculated cross section is equal to the central energy of the \(^{9}\text{C}\) beam; the measurements were performed by Golovchenko et al [14, 15, for 113, 168, 175 and 241 MeV/n] and Schall et al [16, for 670 MeV/n].

is superimposed on the \( \Delta E \) distribution. The LET distribution shows clear peaks for carbon, boron and beryllium ions, whereas the \( \Delta E \) distribution does not because of energy straggling; as a rule of thumb, the \( \Delta E \) distribution can be thought as being derived from the LET distribution by “blurring” the peaks.

It can be seen that the boron peak of the LET distribution lies approximately in region (ii); if the calculated peak height were underestimated (if e.g. the boron yield in nuclear reactions were underestimated), the missing peak in the calculated \( \Delta E \) distribution would then be explained.

There is in fact evidence that PHITS underestimates boron yields for light systems. Table 1 shows cross sections for the production of boron fragments from \(^{12}\text{C}\) in water; measured data for a number of energies are presented, together with the result of a PHITS calculation for 329.5 MeV/n \(^{12}\text{C}\), which is the central energy of the \(^{9}\text{C}\) beam. The PHITS result, as can be seen, underestimates the measurements by a factor of 2.5–3. This trend has been observed for a number of light systems and is currently object of investigation.
If one makes the hypothesis that the boron yields from $^9$C are underestimated by a similar factor, one can renormalise "by hand" the boron peak in the LET distribution and obtain the result shown as a dotted line in figure 3, which seems to suggest that this would most likely compensate for the missing peak in the $\Delta E$ distribution.

5. Conclusions
We have used the PHITS code to calculate energy-deposition distributions for a $^9$C beam in water and compared with the results of an experiment [1]. The simulation indicated that the $^9$C-decay contribution to the energy-deposition distributions is negligible, thereby contradicting the previous interpretation of the experimental data. PHITS failed to reproduce the boron fragment peak in the energy-deposition distribution; similar behaviour has already been observed for other light systems.

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