Dose distribution and multiple Coulomb scattering for protons: intercomparison between various Monte Carlo codes

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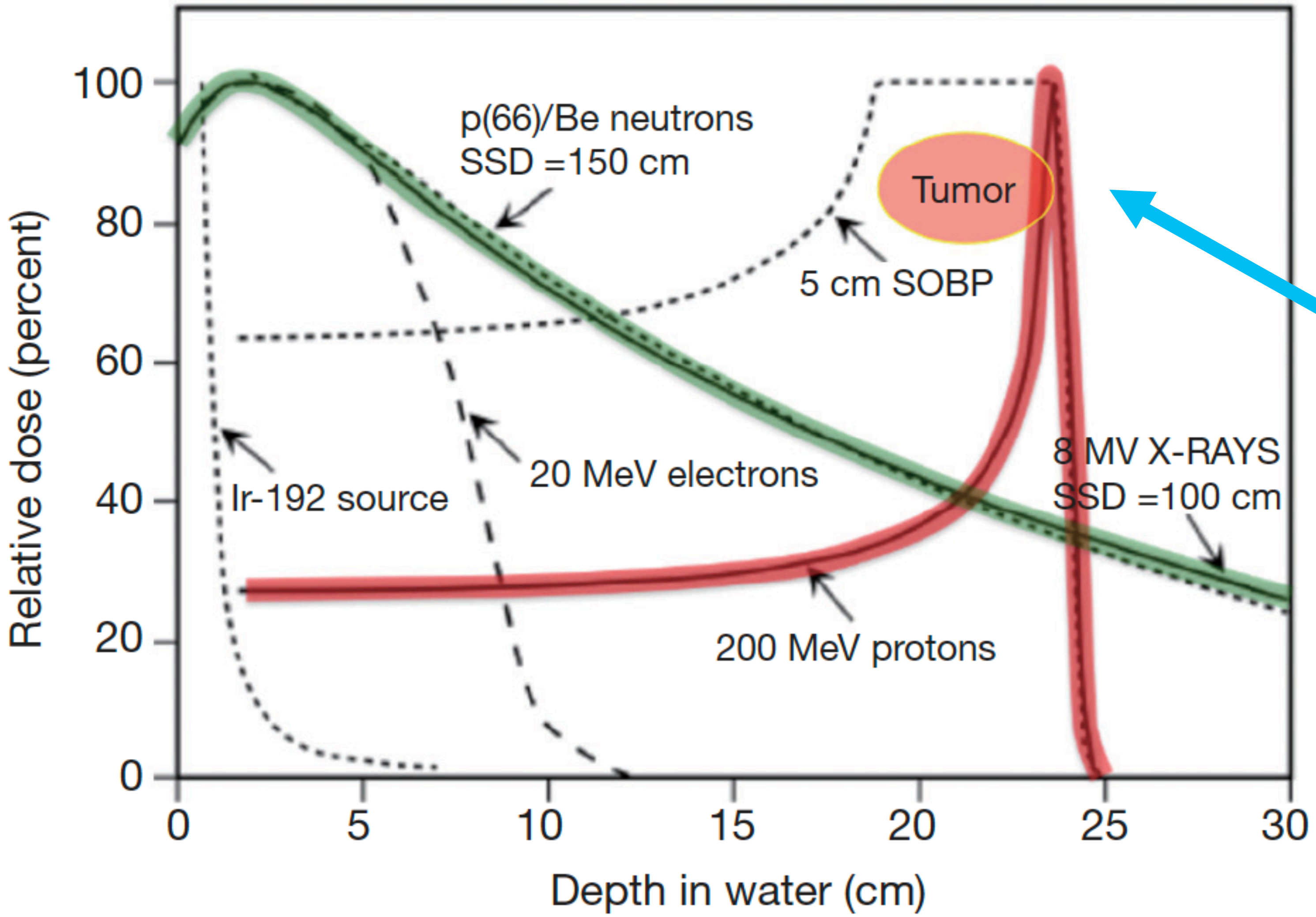
2nd WORKSHOP ELICSIR PROJECT, 9-10.03.2021

Overview

- Introduction
- Monte Carlo codes
- Interaction of protons with matter
- Results
- Future work

Introduction



BRAGG PEAK

H. Giap, D. Roda, F. Giap, Transl. Cancer Res. 4 (2015) E3–E15.

Introduction

- GOAL ➔ Comparison of **PENH**, **TOPAS** and **FLUKA codes** regarding the simulation of a monoenergetic proton pencil beam.

  - Simulation of interaction of protons with matter using Monte Carlo tecniques ➔ depth dose (Bragg peak), central-axis dose in water and angular distributions of protons after passing thin slabs of different materials.

  - Differences between **the physics ingredients** of the codes ➔ differences in the results?

  - Physics ingredients: theory of **Multiple Coulomb Scattering (MCS)** and treatment of **nuclear reactions**

  - Differences in the Monte Carlo procedure.

Monte Carlo codes

- Penh (Salvat 2013, Nucl. Instr. Meth. Phys. Res. B 316 (2013) 144). Versión 2014.
  - ✓ A mixed (class II) algorithm for Monte Carlo simulation of the transport of protons, and other heavy charged particles, in matter.
  - ✓ Emphasis on the electromagnetic interactions (elastic and inelastic collisions), simulated using strategies similar to those employed in the electron–photon code Penelope
- TOPAS (Perl et al., Med Phys. 2012; 39(11): 6818. Version 3.1.
  - ✓ Based in Geant4
  - ✓ Physics module ➔ g4em-standard opt4 as physics module.
  - ✓ In Geant4, electromagnetic (EM) interactions of the charged particles are grouped in the condensed history (CH) approach.
- FLUKA (Ferrari et al., , CERN Yellow report 2005-10 (2005) 1. Version 2011.
  - ✓ Single Coulomb scattering events are condensed in a multiple scattering algorithm.

Interaction of protons with matter

- Radiotheraphy protons (3-300 MeV) interacts with matter in three ways:

✓Multiple collisions with atomic electrons cause them to lose energy and eventually stop : **Stopping (Bethe-Bloch equation)**

✓Multiple collisions with atomic nuclei cause them to scatter by a few degrees : (Multiple Coulomb Scattering) ➔ Molière theory

✓Occasional hard scatter by nuclei or their constituents throw dose out to large distances from the beam ➔ **Nuclear interactions**

Interaction of protons with matter

- Around 20% of the protons in a radiotherapy beam suffer a hard scatter before stopping.
- Many physics problems (beam line design) → solved considering only **Stopping** and **MCS** → **primaries protons**
- For predicting dose distribution in a patient → needed to include **nuclear reactions** → **secondaries**
- **Then, dose in a medium can be calculated approximately well neglecting secondaries**

Interaction of protons with matter

▪ Dose calculation:

- *A simple example* ➔ an infinitesimal volumen (water) of frontal area **dA** and thickness **dz** exposed to **dN** monoenergetic protons of 160 MeV at normal incidence:

$$D = \left(\frac{\mathrm{d}N}{\mathrm{d}A}\right) \times \left(-\frac{1}{\rho}\frac{\mathrm{d}E}{\mathrm{d}z}\right) = \Phi \times \frac{S}{\rho}$$

$$\frac{S}{\rho} = 5.167 \frac{\mathrm{MeV}}{\mathrm{g/cm^2}}$$

$$\frac{S}{\rho} = -\frac{1}{\rho}\frac{dE}{dx} = \frac{4\pi N_A(z^2=1)}{m_e c^2}(\alpha\hbar c)^2 \frac{Z}{A}\frac{1}{\beta^2}\left[ln\left(\frac{2m_e c^2\beta^2}{I\,(1-\beta^2)}\right) - \beta^2\right] \frac{\mathrm{MeV}}{\mathrm{g/cm^2}}$$

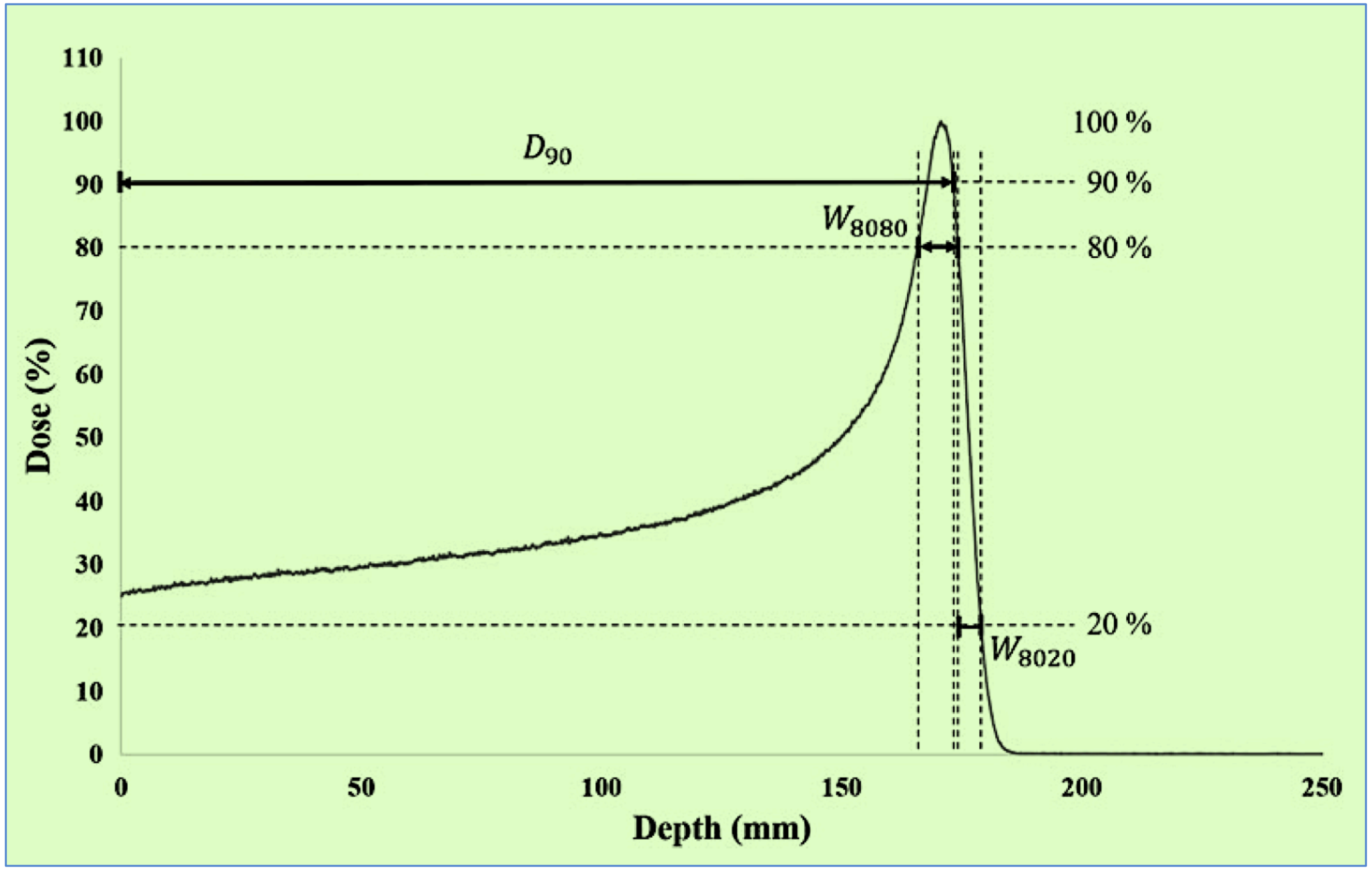
$$\mathrm{Range}\,(E_0) = \int_{E_0}^{\sim 0}\left(\frac{S}{\rho}\right)^{-1} dE \approx aE^b \,\frac{\mathrm{g}}{\mathrm{cm^2}} \qquad b \sim 2$$

- A reasonable clinical dose rate is around 1 Gy/min ➔ proton radiotherapy currents are on the order of nA

Interaction of protons with matter

- **Stopping → definition of range:**

➢ From the Bragg peak:

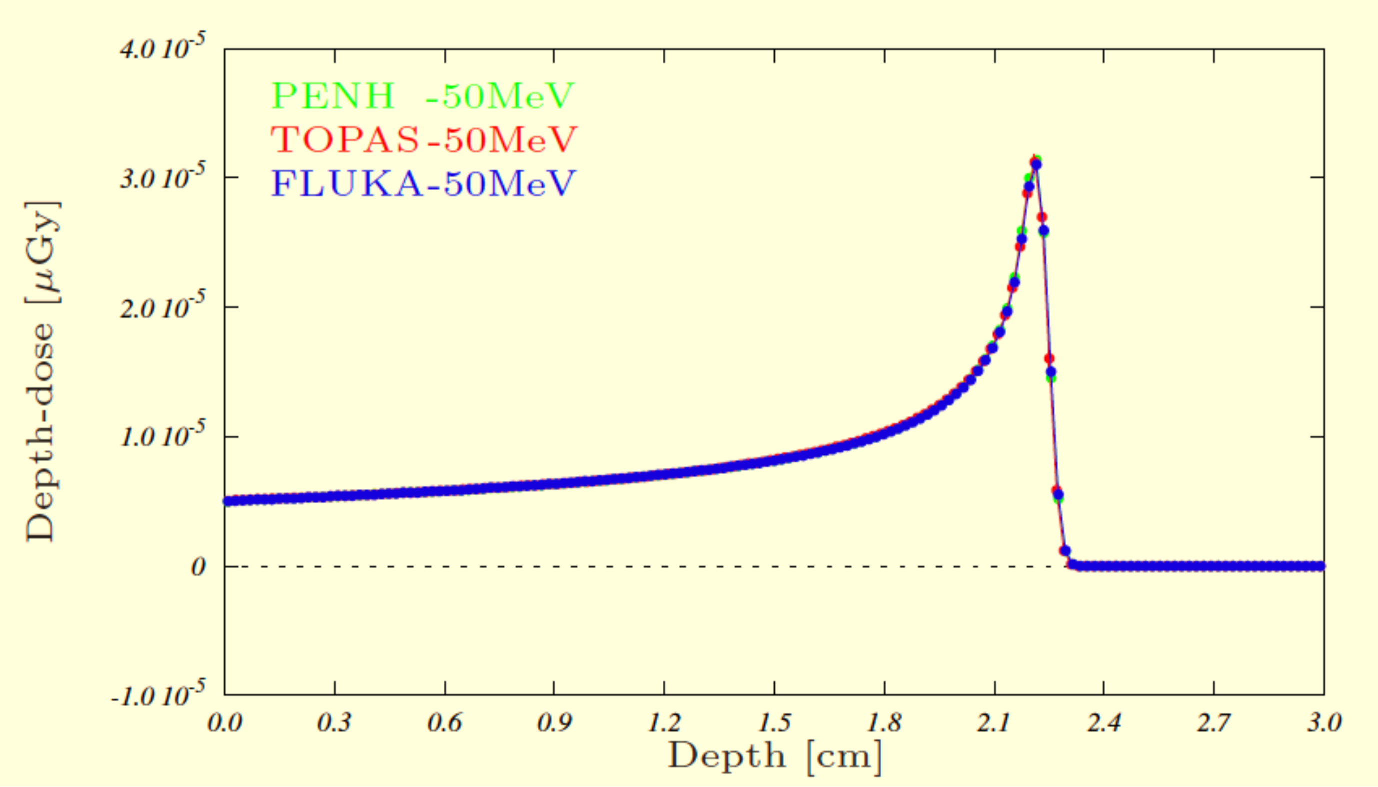


➢ Theoretical CSDA:

$$\rho\, R(T_{\rm i}) = \int_{T_{\rm f}}^{T_{\rm i}} \frac{{\rm d}T}{S/\rho(T)}$$

Interaction of protons with matter

- Comparison with theoretical range



ATOMIC DATA AND NUCLEAR DATA TABLES **27**, 147–339 (1982)

Part 1

PROTON RANGE–ENERGY TABLES, 1 keV–10 GeV

Energy Loss, Range, Path Length, Time-of-Flight, Straggling, Multiple Scattering, and Nuclear Interaction Probability

In Two Parts. Part 1. For 63 Compounds
Part 2. For Elements $1 \leqslant Z \leqslant 92$

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Kirtland Air Force Base, New Mexico

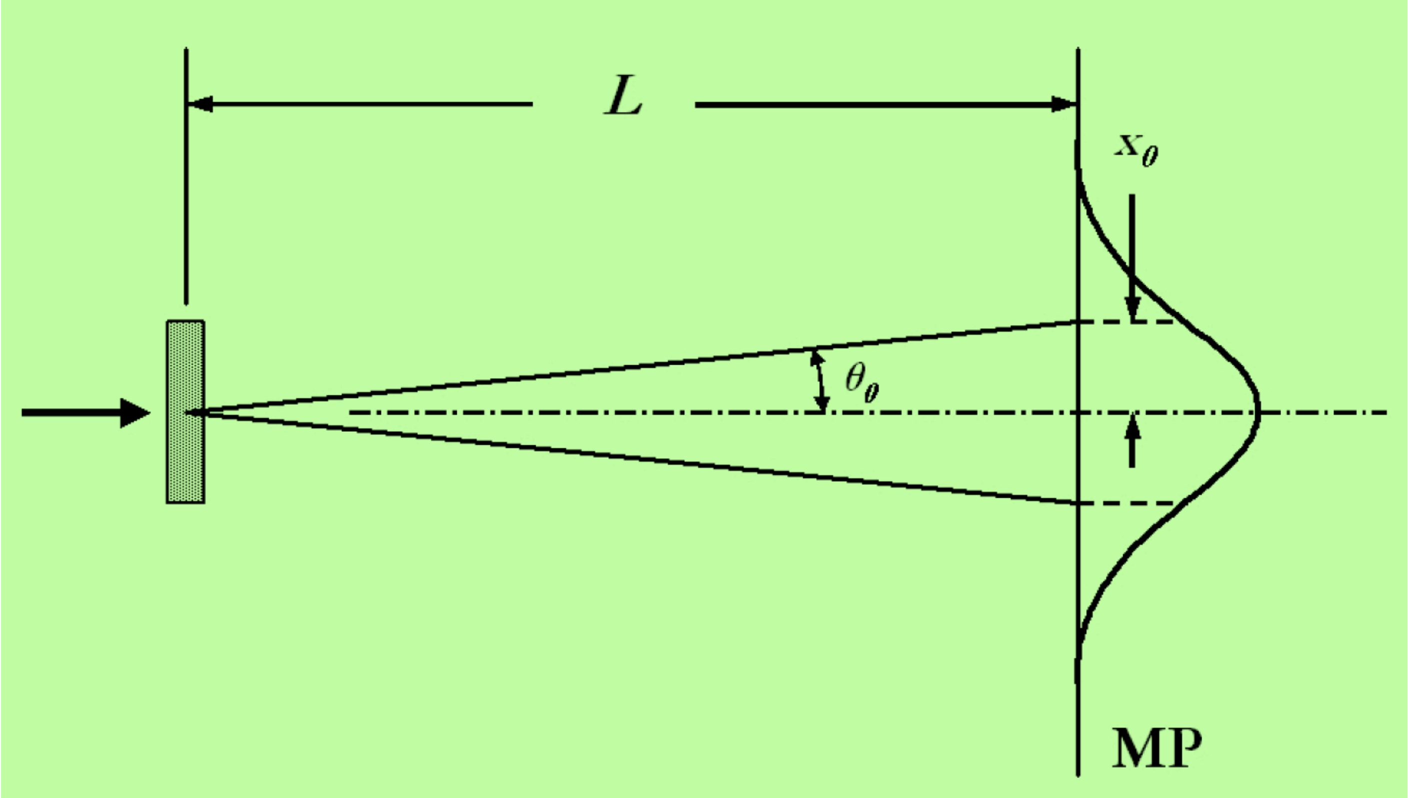
Proton energy [MeV]	Theoretical Range [cm]	PENH Range [cm]
50	2.25 ± 0.03	2.25 ± 0.05
100	7.79 ± 0.08	7.8 ± 0.1
150	15.92 ± 0.15	15.8 ± 0.1
200	26.2 ± 0.2	25.9 ± 0.1
250	38.3 ± 0.3	38.0 ± 0.1

Interaction of protons with matter

- **Multiple Coulomb scattering (MCS):**

✓Gaussian approximation ➔

$$f(\theta) = \frac{1}{2\pi\,\theta_0^2}\, e^{-\frac{1}{2}\left(\frac{\theta}{\theta_0}\right)^2}$$



Interactions of protons with matter

- Highland approach ➔ from the Molière theory. Hanson, an aditional correction.
- Experimental data: From Gottschalk et al.

Nuclear Instruments and Methods in Physics Research B74 (1993) 467–490
North-Holland

NIM B
Beam Interactions with Materials & Atoms

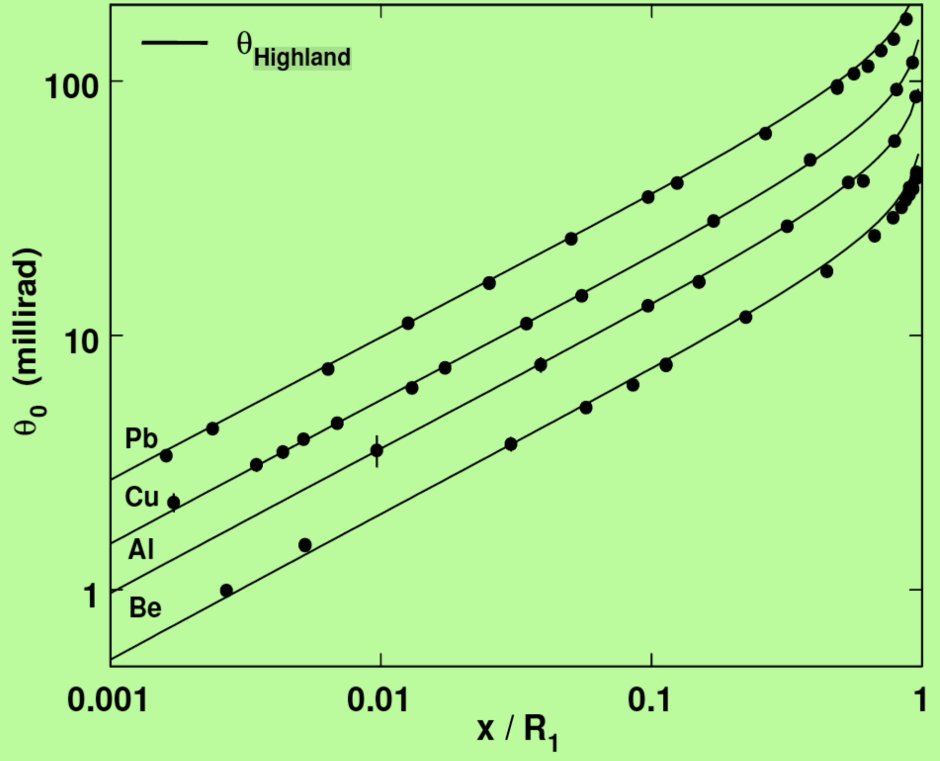
Multiple Coulomb scattering of 160 MeV protons

B. Gottschalk, A.M. Koehler, R.J. Schneider, J.M. Sisterson and M.S. Wagner
Harvard Cyclotron Laboratory, 44 Oxford St., Cambridge, MA 02138, USA

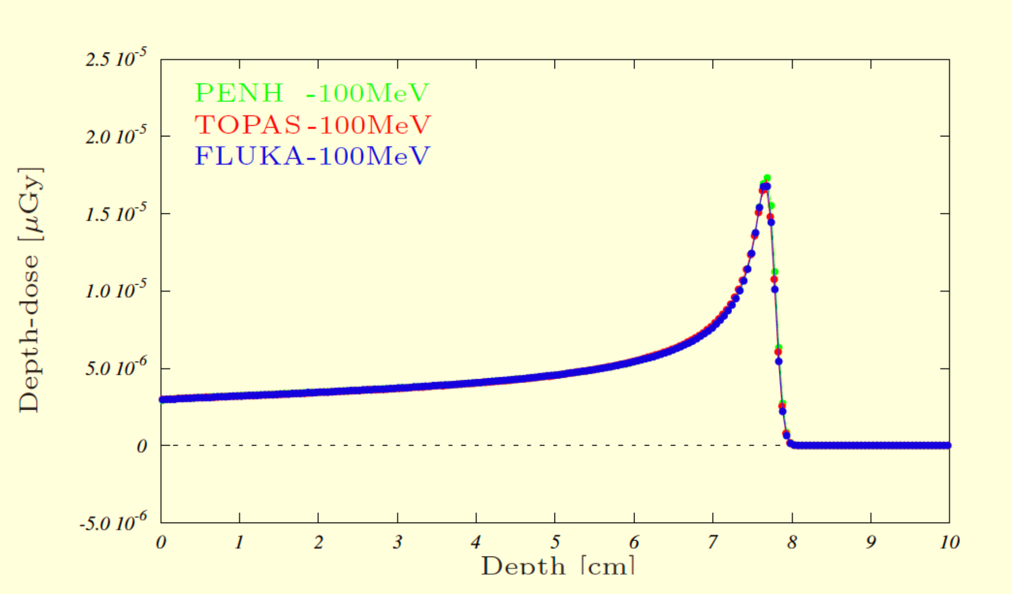
Received 25 September 1992 and in revised form 1 December 1992

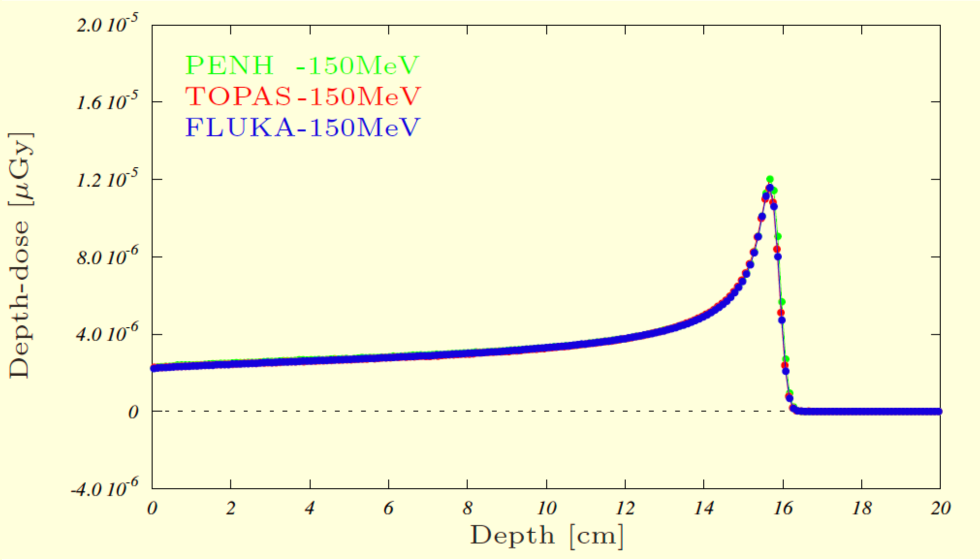
We have measured multiple Coulomb scattering of 158.6 MeV protons in fourteen materials from beryllium to uranium including brass and several plastics. Targets ranged from thin (negligible energy loss) to very thick (greater than the mean proton range). The angular distribution was measured by means of a single diode dosimeter scanned typically over two decades of dose falloff. Each data set was fitted with a Molière scattering distribution (using Bethe's tables) to extract a characteristic angle θ_M as well as a Gaussian distribution to extract a characteristic angle θ_0. As expected in the small angle region, the Gaussian fits about as well as the Molière shape.

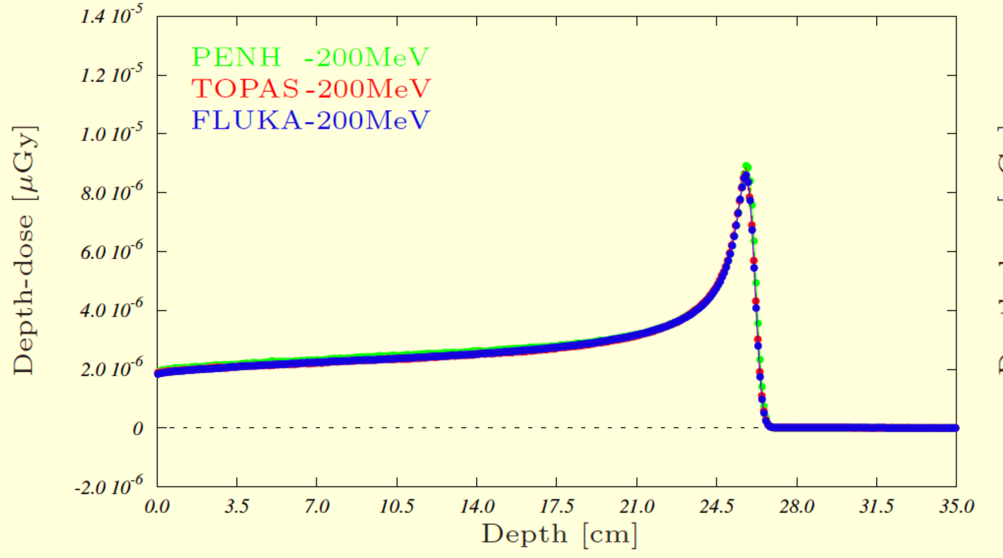
The θ_M values were compared with Molière's predicted value $(\chi_c\sqrt{B}/\sqrt{2})$ including Fano's correction for scattering by atomic electrons and using Molière's formalism to account for energy loss and/or compound targets or mixtures. The distribution of the deviation from theory for 115 independent measurements is approximately normal, with a mean value $-0.5\pm0.4\%$ and an rms spread of 5%.

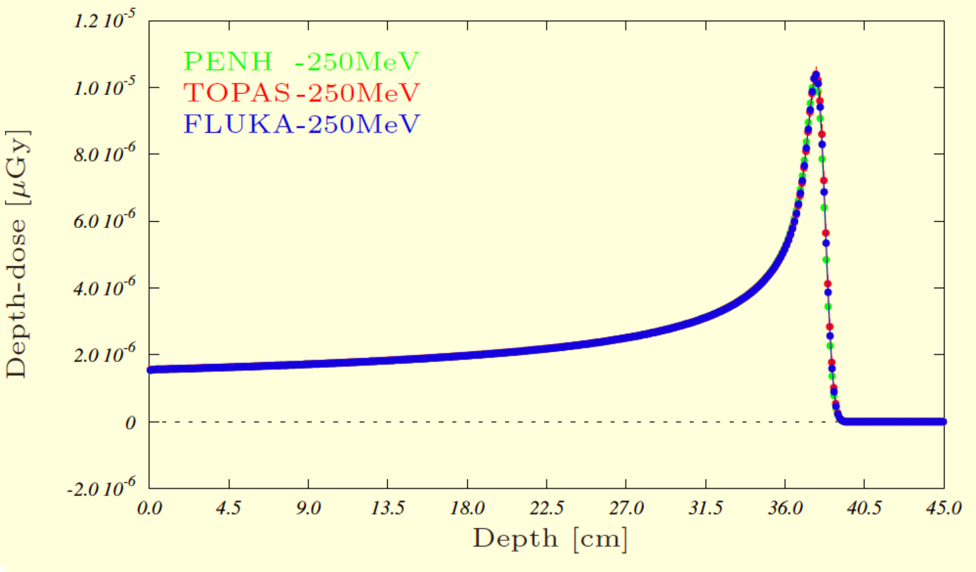


Results: Bragg peak in water

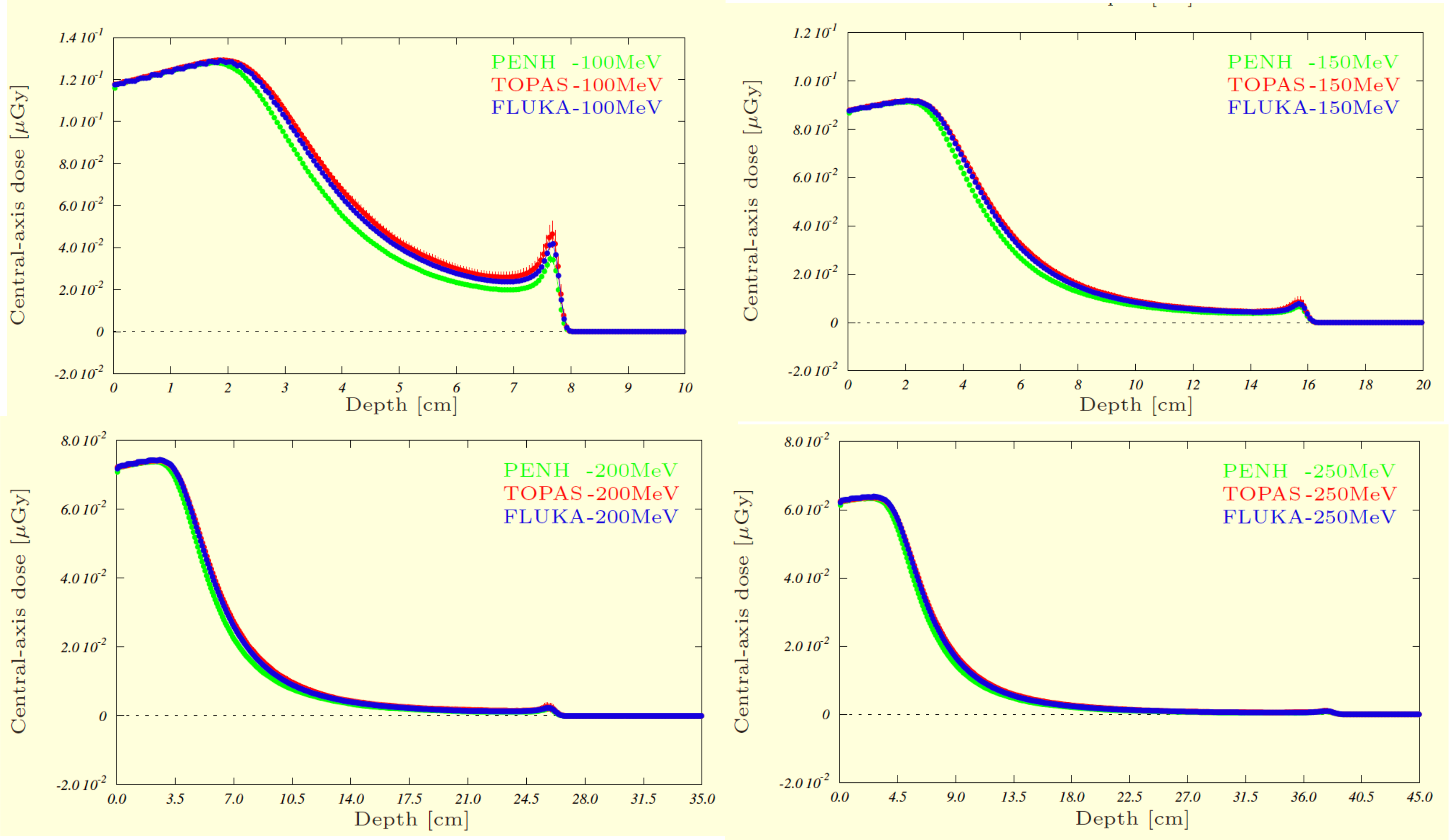




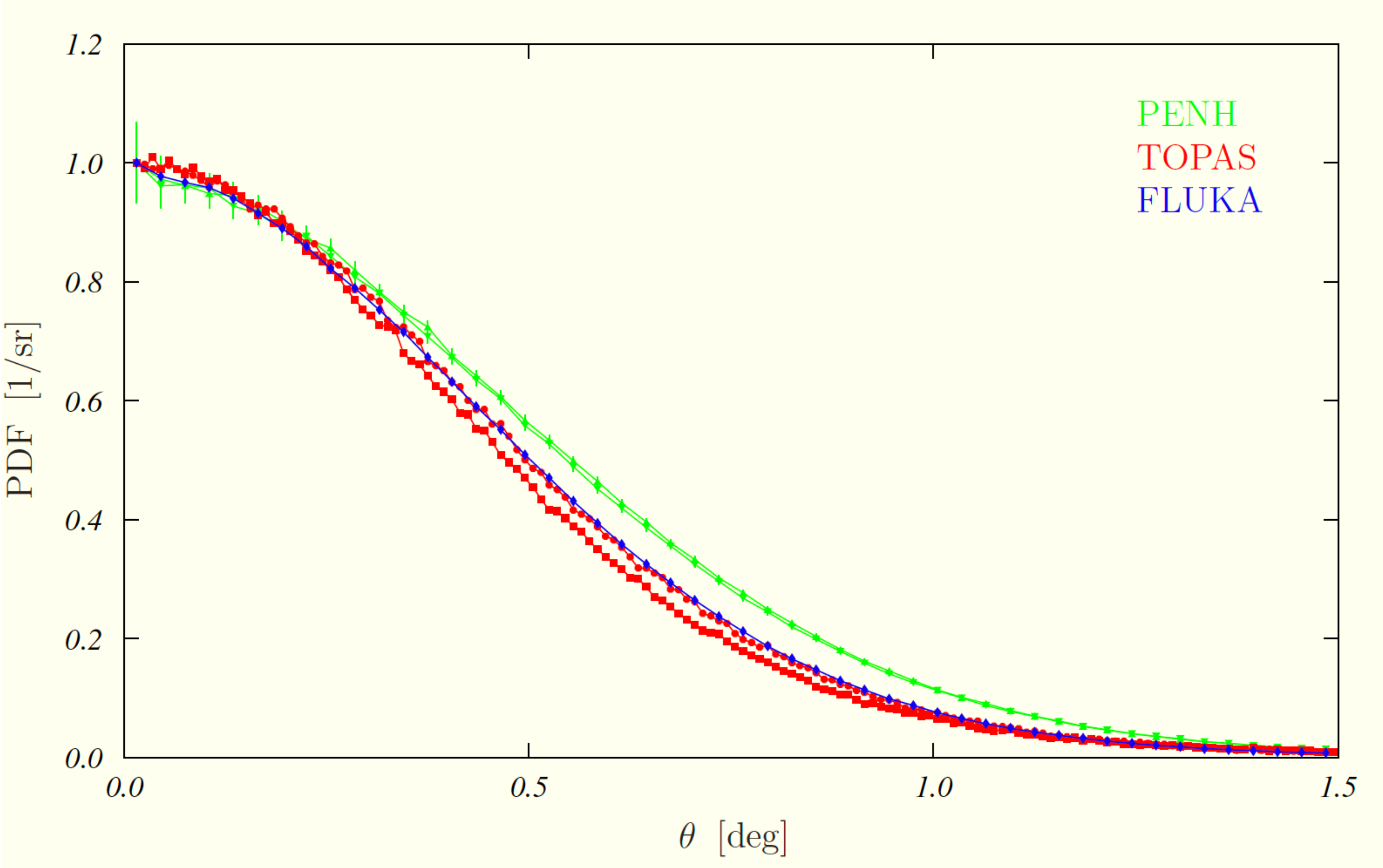




Results: Central-axis dose



Results: angular distribution

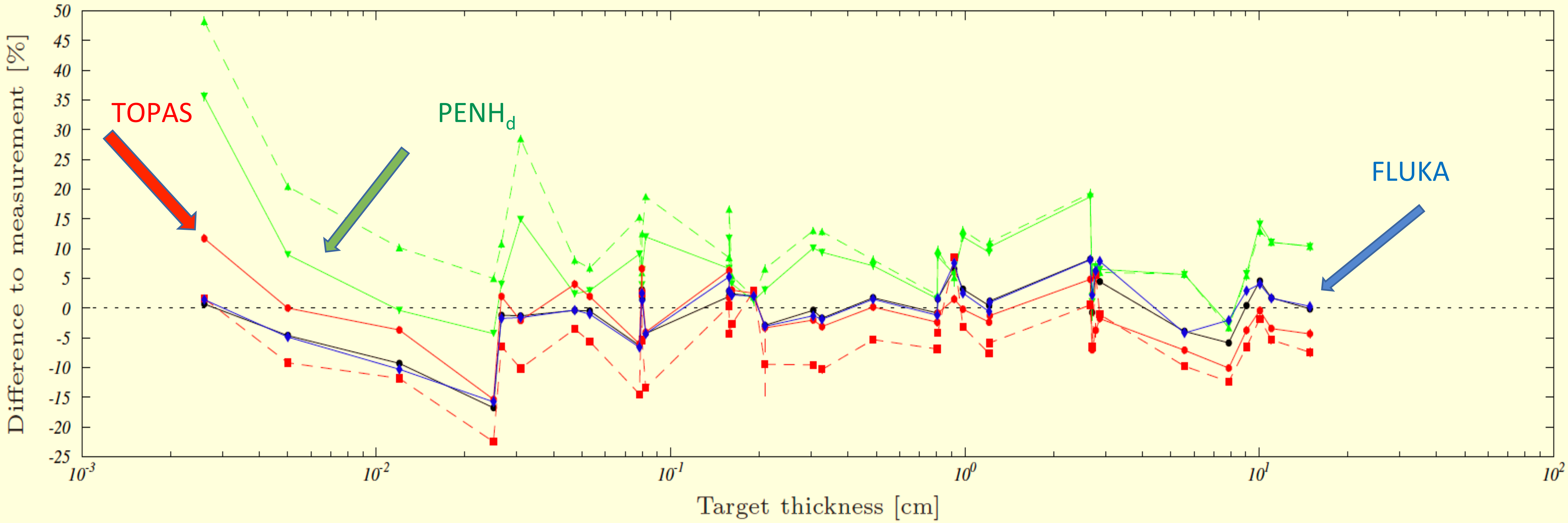


Lucite: 1.2075 cm

E= 158.6 MeV

	θ_0 [mrad]
$\mathrm{PENH_m}$	8.35(5)
$\mathrm{PENH_d}$	8.29(5)
TOPAS (opt3)	7.00(4)
TOPAS (opt4)	7.34(5)
FLUKA	7.51(1)
Exp. (Gottshalk)	7.579
Theo. (Hanson)	7.610

Results: angular distribution



Conclusions and perspectives

- Good intercomparison between the codes, but it is needed to include properly the effect of nuclear reactions ➔ calculations with the new versión of PENH (Version 2020).
- Recently, new experimental data from West German Proton Therapy Centre Essen (WPE) (N. Verbeek et al.)
- Aluminum, brass and lucite (PMMA) scatterers of clinically relevant 20 thicknesses were irradiated with protons at 100, 160 and 220 MeV.
- Goal ➔ to develop an experimental method to measure MCS angles at a proton therapy facility.
- The existing data set is extended for therapeutically relevant materials and energies and compared to TOPAS v3.2p1 (Geant4), PENH 2020, RayStation Monte Carlo, as well as the analytical models RayStation Pencil Beam Algorithm and the Molière/Fano/Hanson variant of the Molière theory.
- The Monte Carlo and analytical algorithms studied reproduce MCS data within the required accuracy for clinical applications.

References

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- F. Salvat, Nucl. Instr. Meth. Phy. Res. B 316 (2013) 144.
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- J. Perl et al., Med. Phys. 39 (2012) 6818.
- A. Ferrari et al., CERN Yellow report 2005-10 (2005) 1. Version 2011.
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- N. Verbeek et al., (submitted).

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THANK YOU FOR YOUR ATTENTION-
QUESTIONS?