Validation of Geant4 fragmentation for Heavy Ion Therapy

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International Conference on Monte Carlo Techniques for Medical Applications (MCMA2017), 15-18 October 2017, Napoli, Italy

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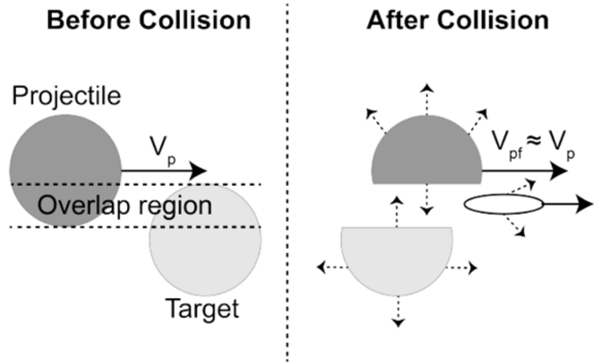
HIT mixed radiation field

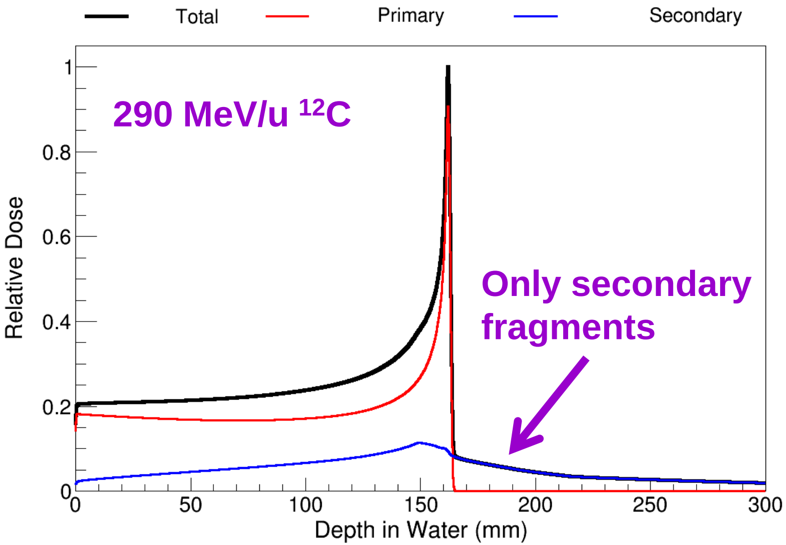
Reference:
Francis et al, PMB, 59 (2014) 7691

Contribution to the **dose**:

- 64% - ^{12}C ions via em interactions
- 36% - produced fragments and their secondaries
    - 14% - protons
    - 13% - alpha particles
    - 4.2 % - B ions
    - 1.7% - Li ions
    - 1.3% - Be ions

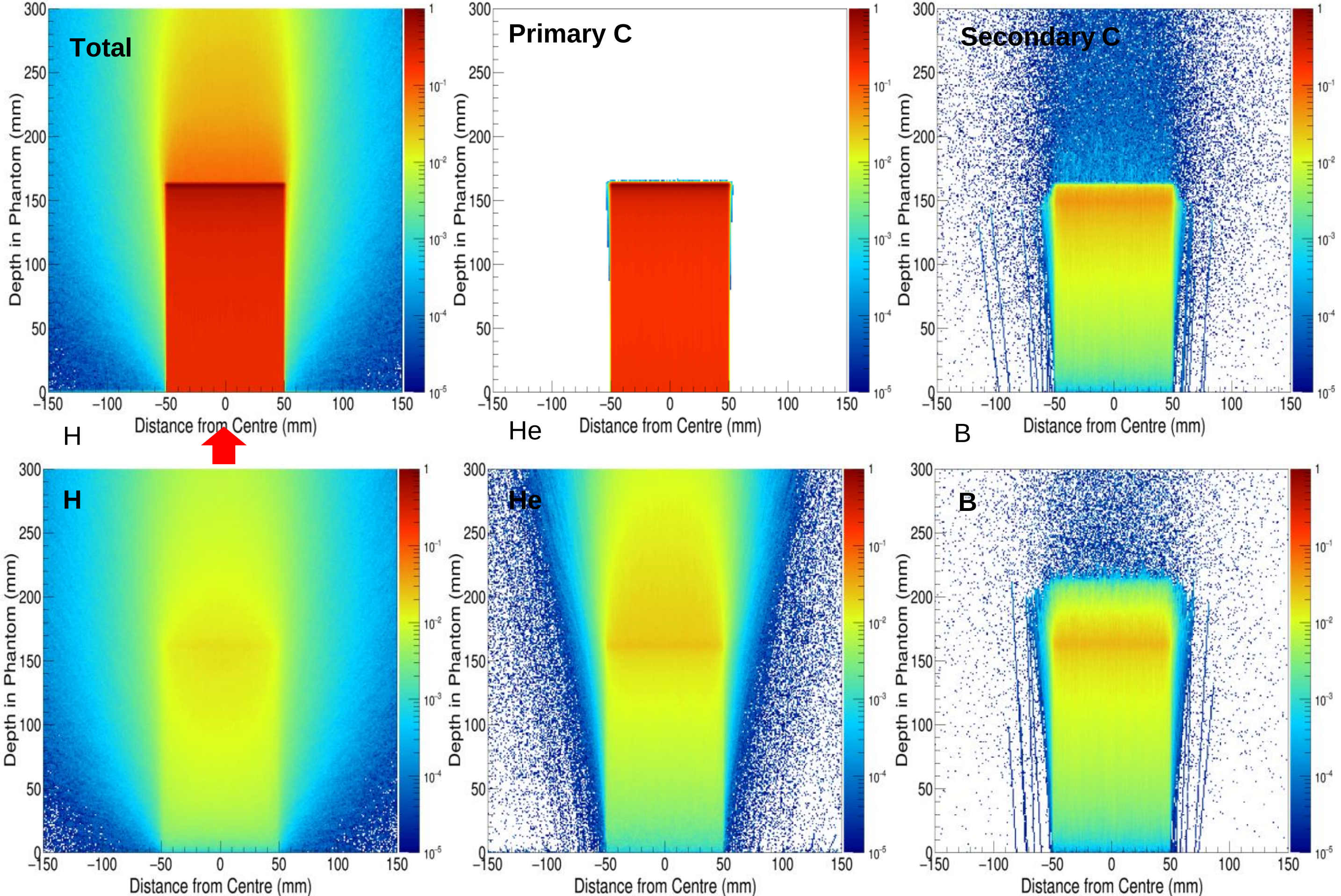


Creation of an excited product which will de-excite by emitting nucleons and smaller fragments (depicted by the dashed arrows).



Dose in the water phantom

290 MeV/u ^{12}C



Experimental Data

- Fragmentation study of a 400MeV/u ^{12}C pencil beam (FWHM 5mm) studied at GSI
- Bragg Curve, fragment yields, angular and energy distribution of fragments

IOP PUBLISHING PHYSICS IN MEDICINE AND BIOLOGY

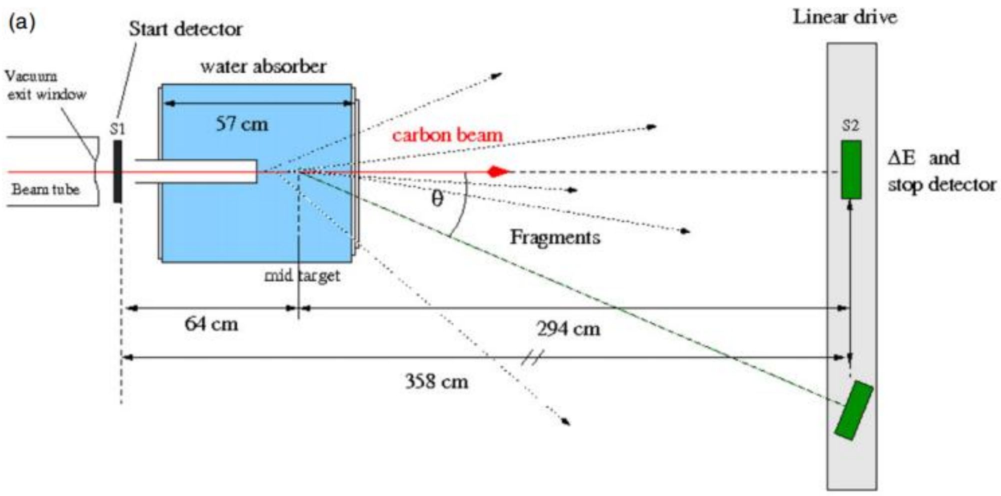
Phys. Med. Biol. 58 (2013) 8265–8279 doi:10.1088/0031-9155/58/23/8265

Experimental study of nuclear fragmentation of 200 and 400 MeV/*u* ^{12}C ions in water for applications in particle therapy

E Haettner, H Iwase[1], M Krämer, G Kraft and D Schardt

GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany

Experimental reference data



Sketch from PMB 58, (2013), 8265-8279

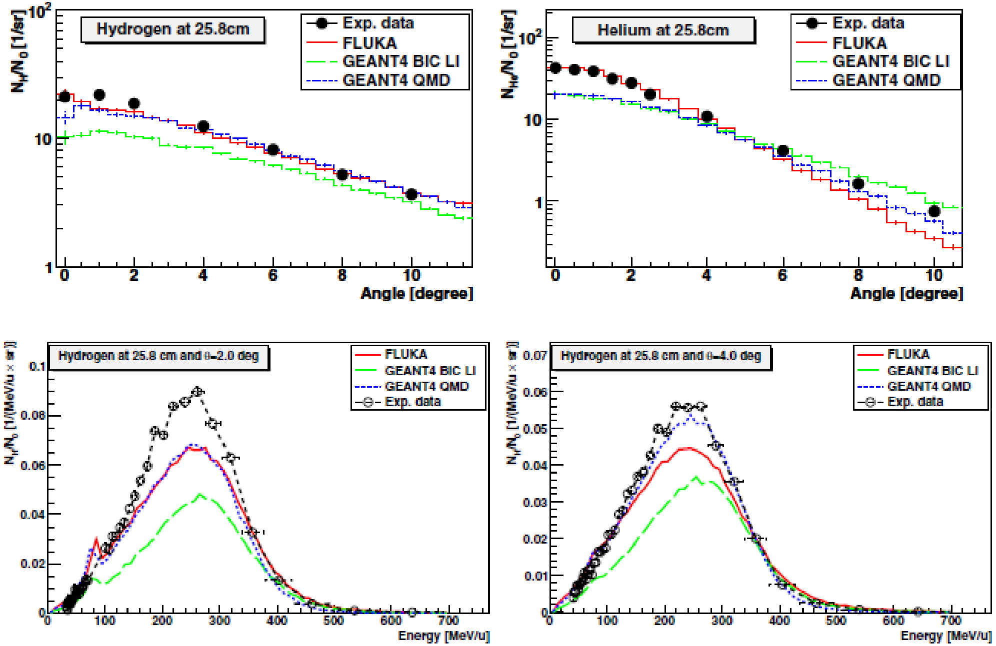
400 MeV/u ^{12}C beam incident upon a water phantom performed at GSI in Germany by Haettner et al. PMB 58 (2013) 8265-8279

The experiment was conducted using a variable thickness water
Phantom

Time of flight measurements for fragments were carried out
using a start detector and a second detector placed on a linear drive after the phantom

Previous Work

- Böhlen et al studied BIC and QMD in Geant4 v9.3 and FLUKA



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Phys. Med. Biol. 55 (2010) 5833–5847 doi:10.1088/0031-9155/55/19/014

Benchmarking nuclear models of FLUKA and GEANT4 for carbon ion therapy

T T Böhlen[1,2], F Cerutti[1], M Dosanjh[1], A Ferrari[1], I Gudowska[2], A Mairani[3] and J M Quesada[4]

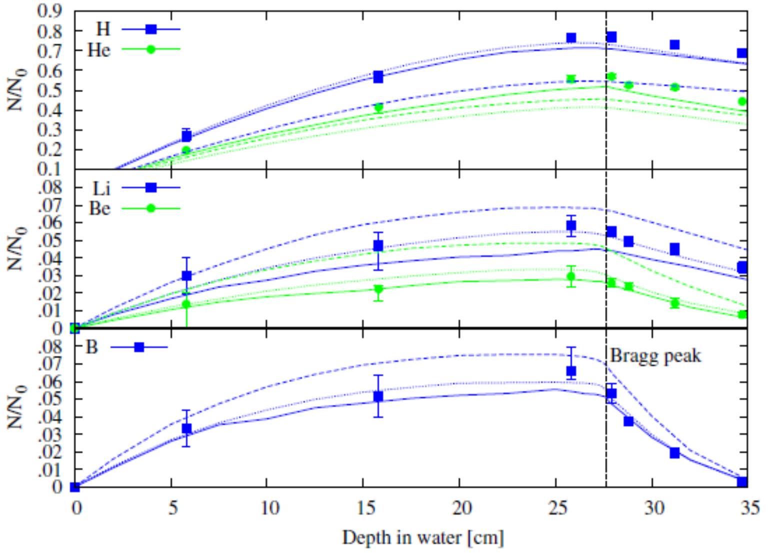
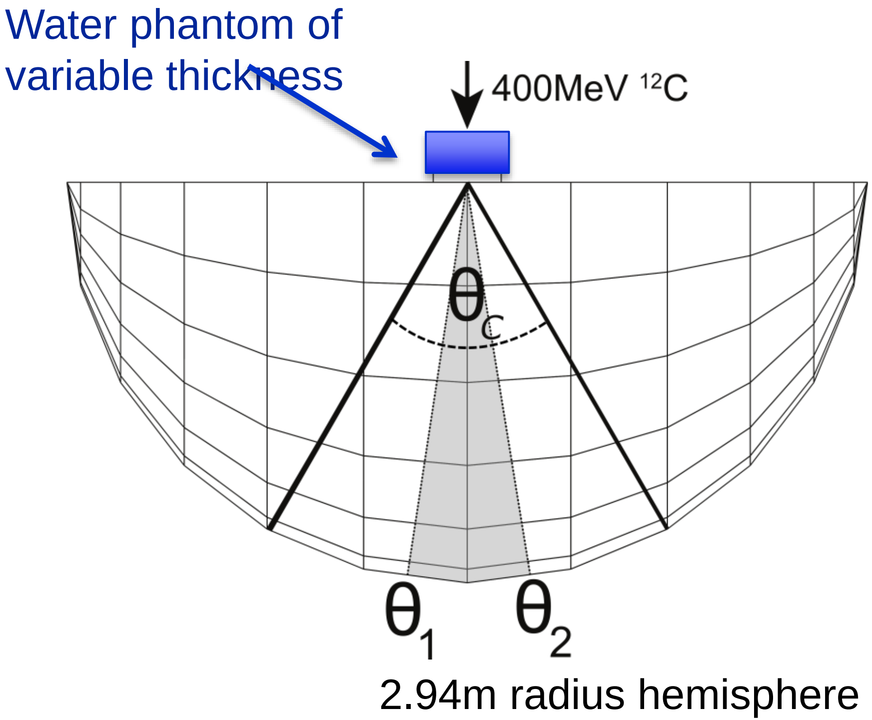


Figure 5. Fragment build-up curves in water of a 400 MeV/u carbon beam as a fraction of primary carbon ions N/N_0. Experimental data are shown as points (Haettner *et al* 2006). Simulations done for FLUKA (solid) and for GEANT4 using the BIC LI (dashed) and the G4QMD (dotted) model are displayed as lines. The dashed vertical line indicates the position of the Bragg peak.

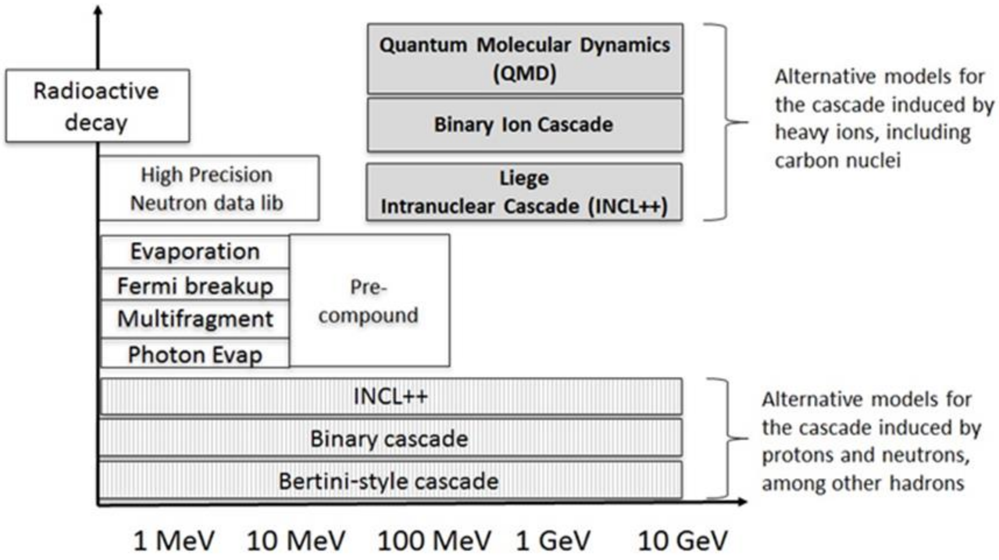
Project Summary

- Quantify the accuracy of different fragmentation models in Geant4 benchmarked for a 400MeV/u ^{12}C beam
  - Fragment yields
  - Angular distributions
  - Kinetic energy distributions

  of fragments with Z=1-5
- Geant4 10.2.patch2
- EMStandardOption3



Geant4 ion cascade models



Partial Geant4 hadronic physics inventory
Of interest for carbon ion therapy

- BIC
  - interaction between a projectile and a single nucleon of the target nucleus interacting in the overlap region as Gaussian wave function
- QMD and QMD-Frag
  - all nucleons of the target and projectile, each with their own wave function; greater computation times than BIC
- INCL
  - nucleons as a free Fermi gas in a static potential well.
  - Targets and projectiles with $A \leq 18$.

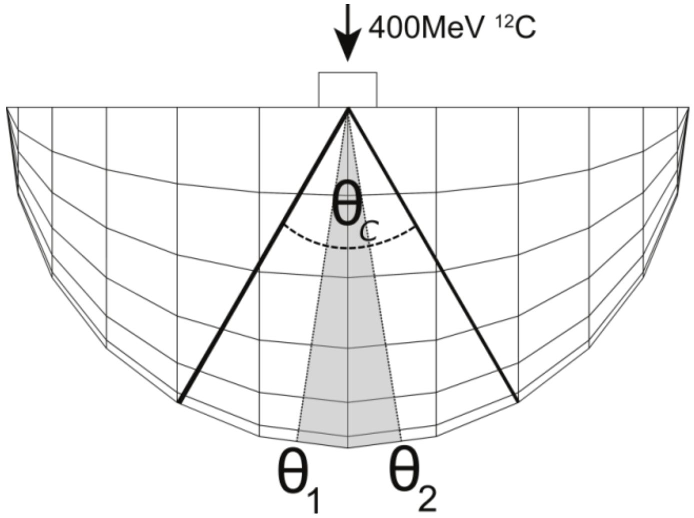
Ranking Models

- To quantify how well each model performs:
  - <PE> : mean percentage difference

$$\langle PE \rangle = \frac{100}{n}\left(\sum_{i=1}^{n}\left|\frac{Sim_i - Exp_i}{Exp_i}\right|\right)$$

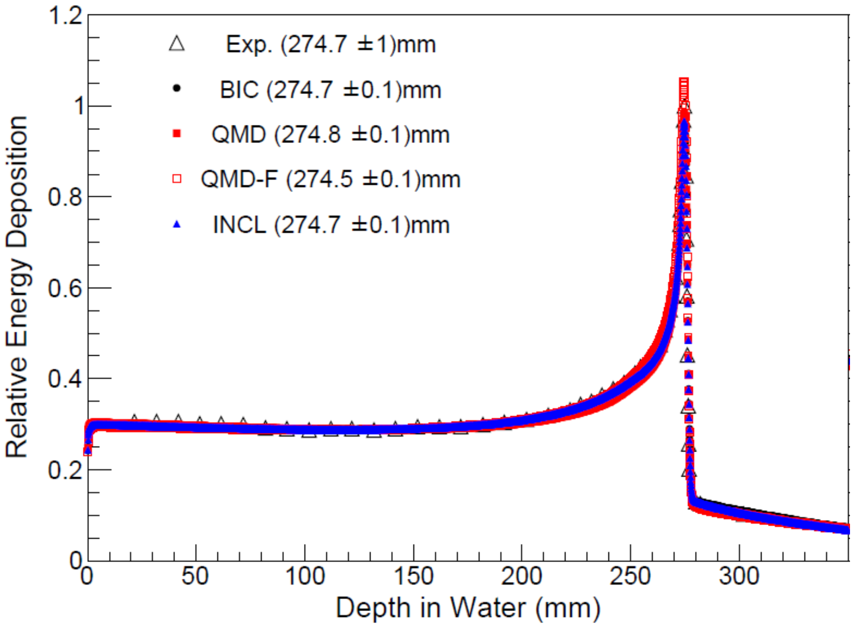
  - X²

$$X^2 = \sum_{i=1}^{n}\frac{(Sim_i - Exp_i)^2}{Exp_i}$$

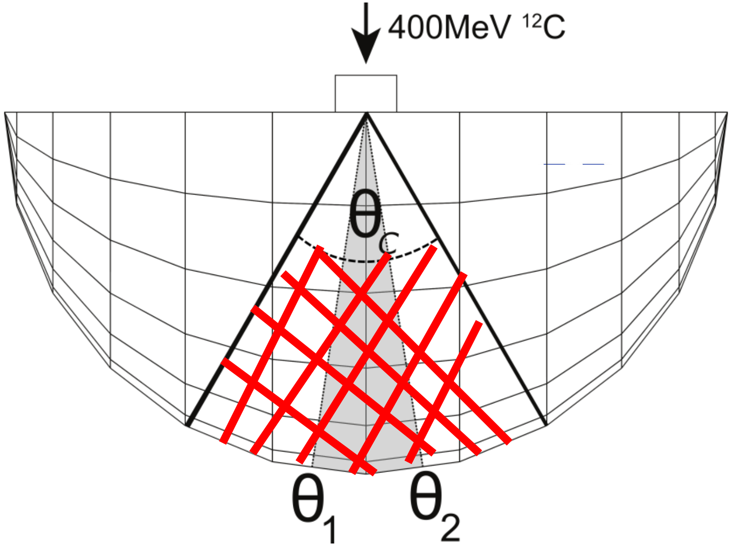


Results: Bragg Peak

- Good agreement with experimental measurements
- QMD-F provides best agreement

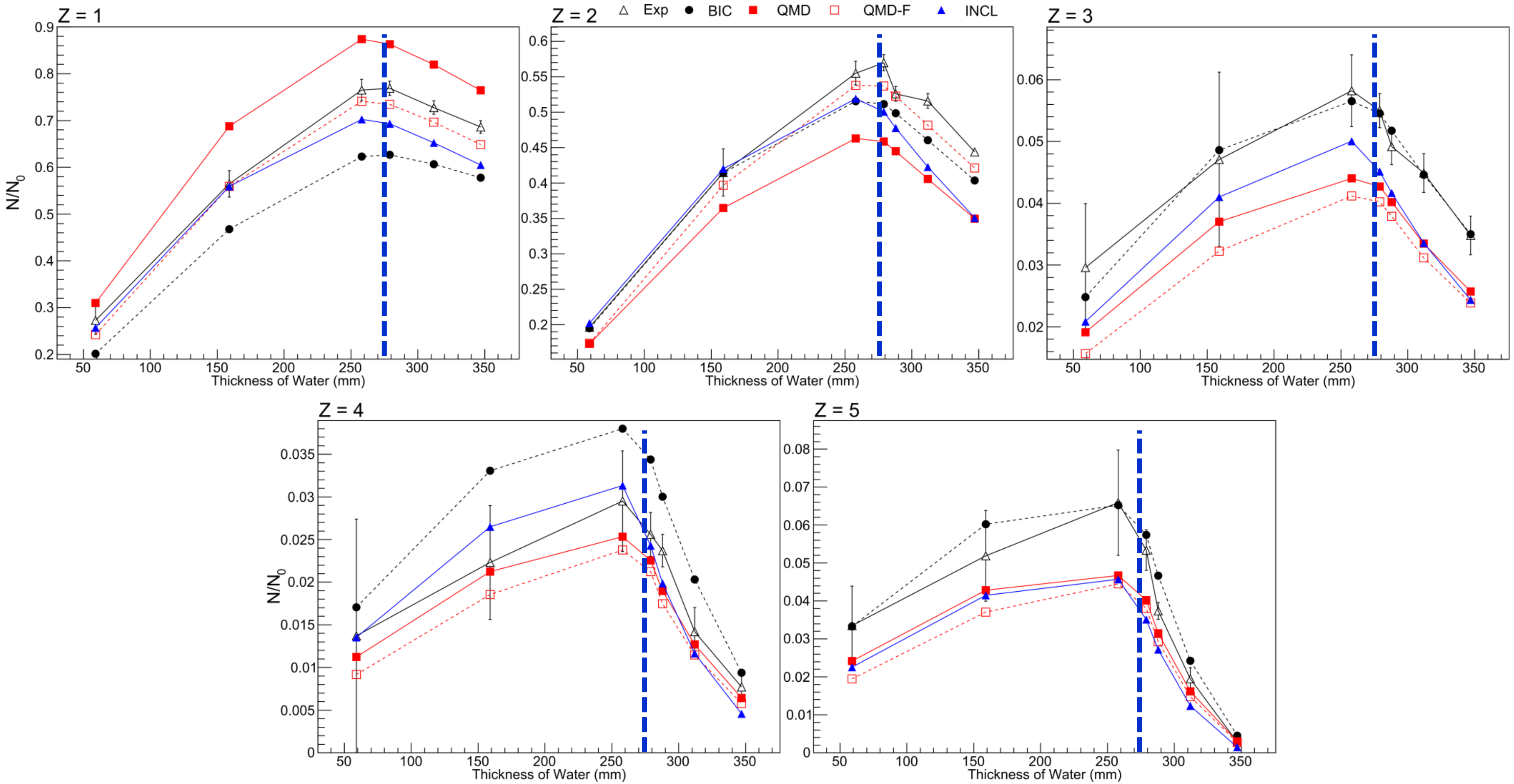


	BIC	QMD	QMD-F	INCL
X^2	53.098	54.335	46.720	52.021



Fragment Yields

Measuring Fragment yield in 10° cone (θ_C)



Experimental errors of H and He fragments are ~5%,
for heavier fragments they increase to ~20%, before the BP and ~10% After BP

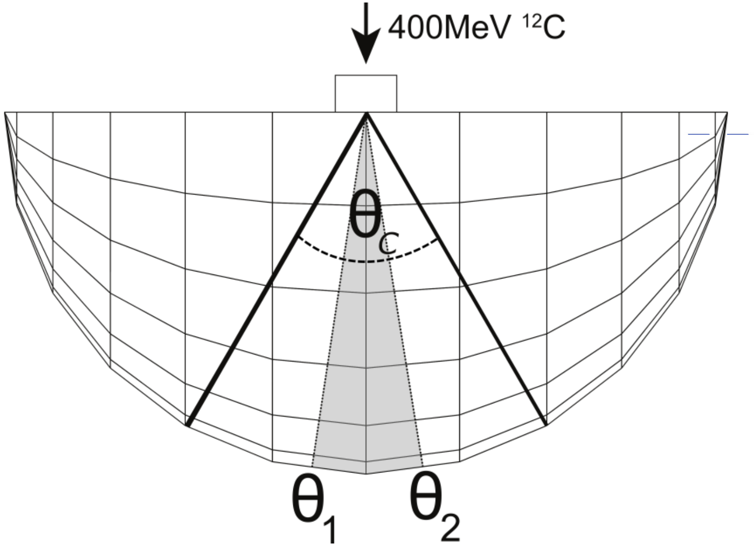
Results: Fragment yields

- Models agree ~5-35% with exp
- QMD-F performed best for lighter fragments

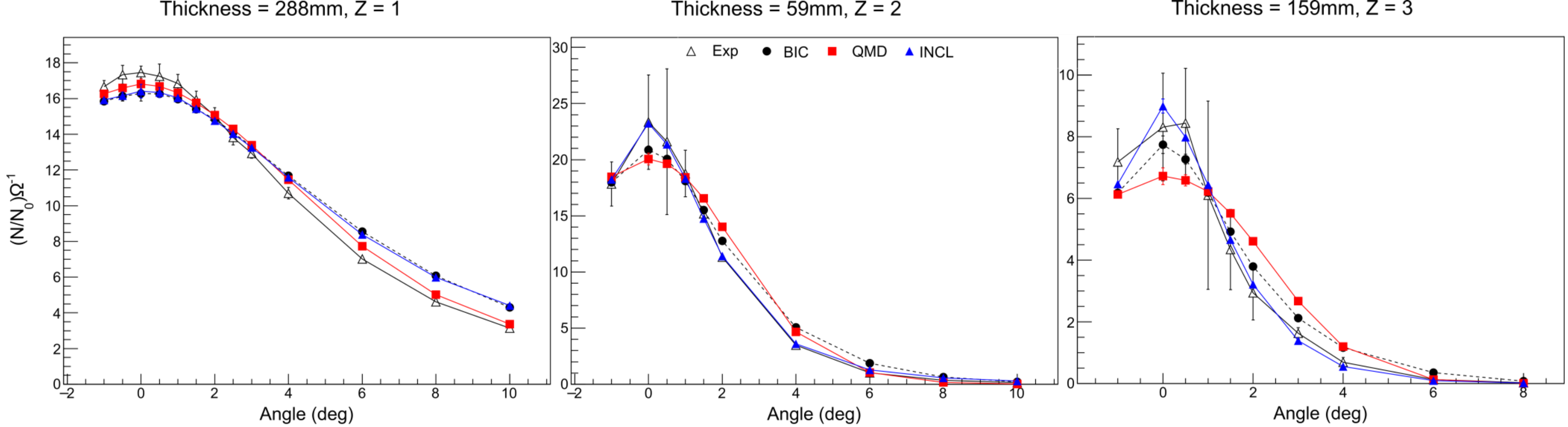
Mean %Difference

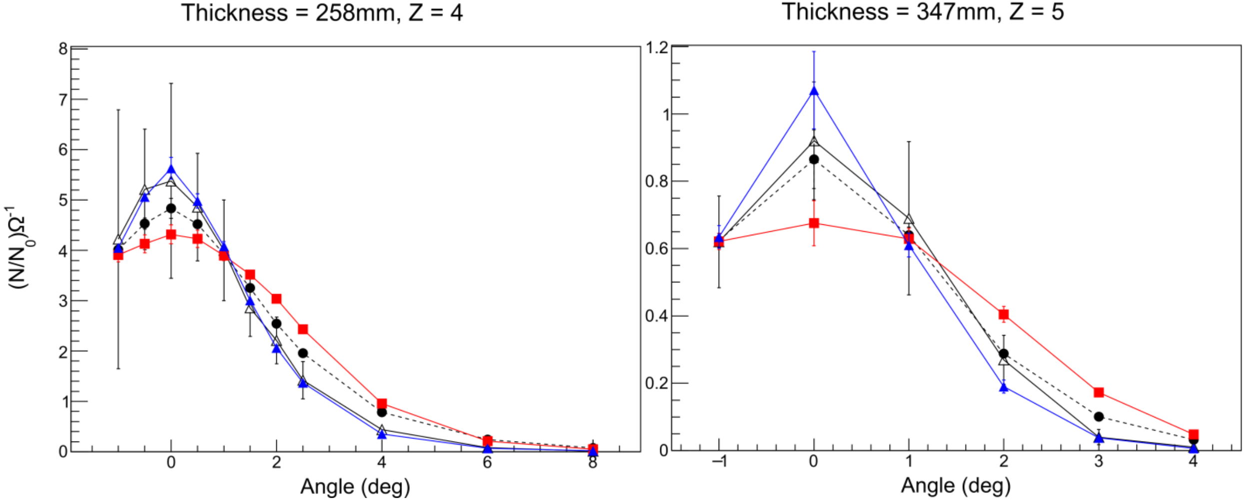
Z	BIC	QMD	QMD-F	INCL
1	19 ± 2	14 ± 2	5 ± 2	8 ± 2
2	6 ± 1	17 ± 1	5 ± 1	10 ± 1
3	4 ± 7	25 ± 7	31 ± 7	21 ± 7
4	32 ± 10	14 ± 10	22 ± 10	15 ± 10
5	19 ± 8	20 ± 8	26 ± 8	33 ± 8

Angular Distribution



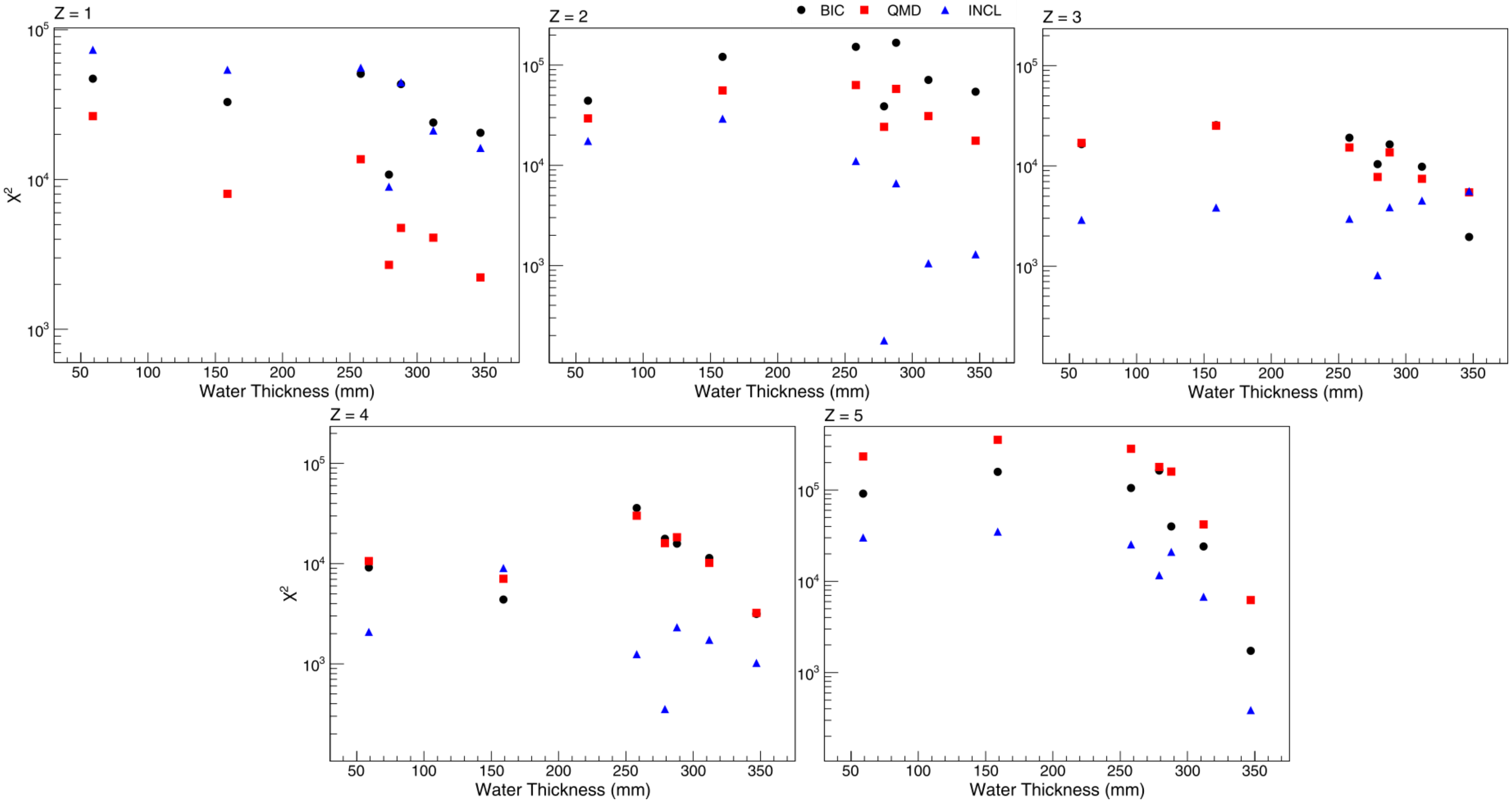
In total 32 distributions compared





Be and B have many angles with an error of more than 40%

X^2 values



Results: Angular Distribution

- INCL performs significantly better than the other models, particularly for higher Z
- QMD performs best for protons
- BIC and QMD produce broader distributions

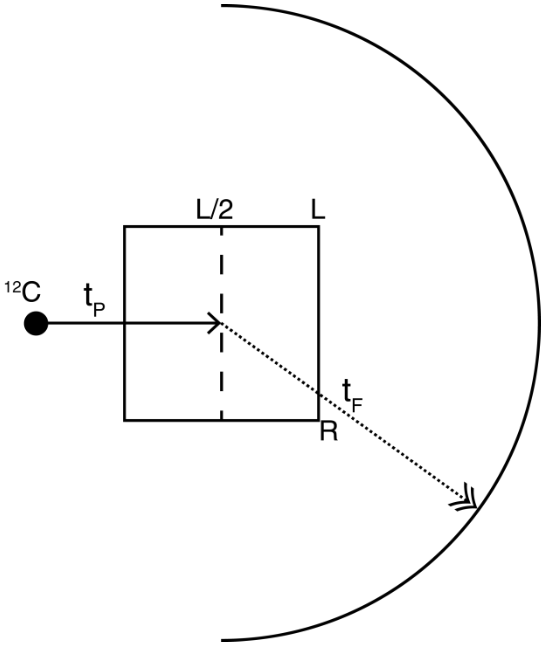
Mean %Difference

Z	BIC	QMD	INCL
1	14 ± 4	7 ± 4	15 ± 4
2	24 ± 2	16 ± 2	7 ± 2
3	29 ± 8	26 ± 8	16 ± 8
4	47 ± 14	42 ± 14	18 ± 14
5	132 ± 12	135 ± 12	28 ± 13

Kinetic energy distributions

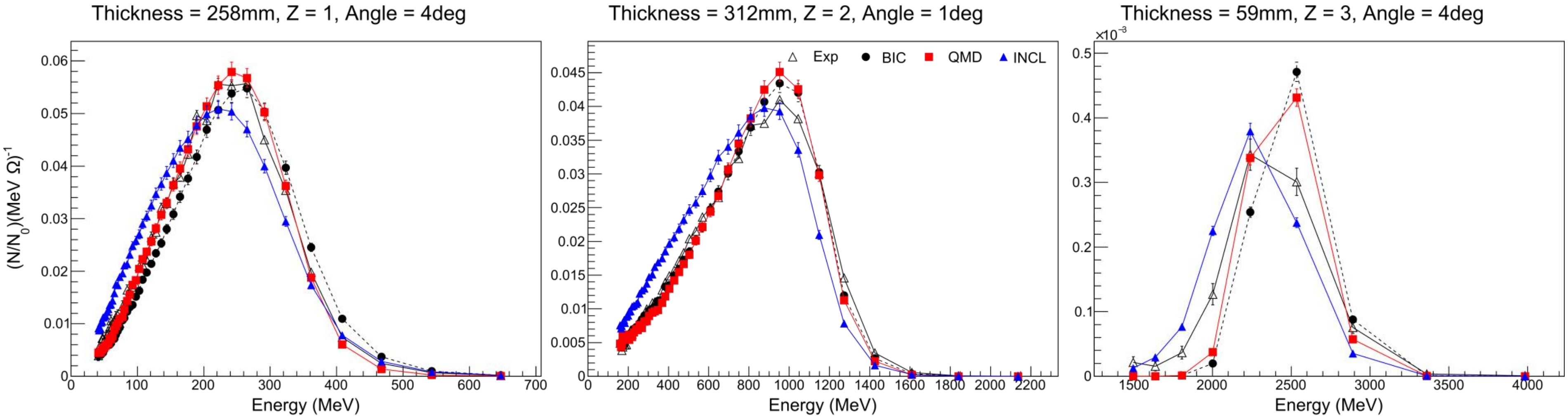
- Energy distributions calculated based on the time to reach the collection hemisphere
  - Same method adopted in the experimental measurements

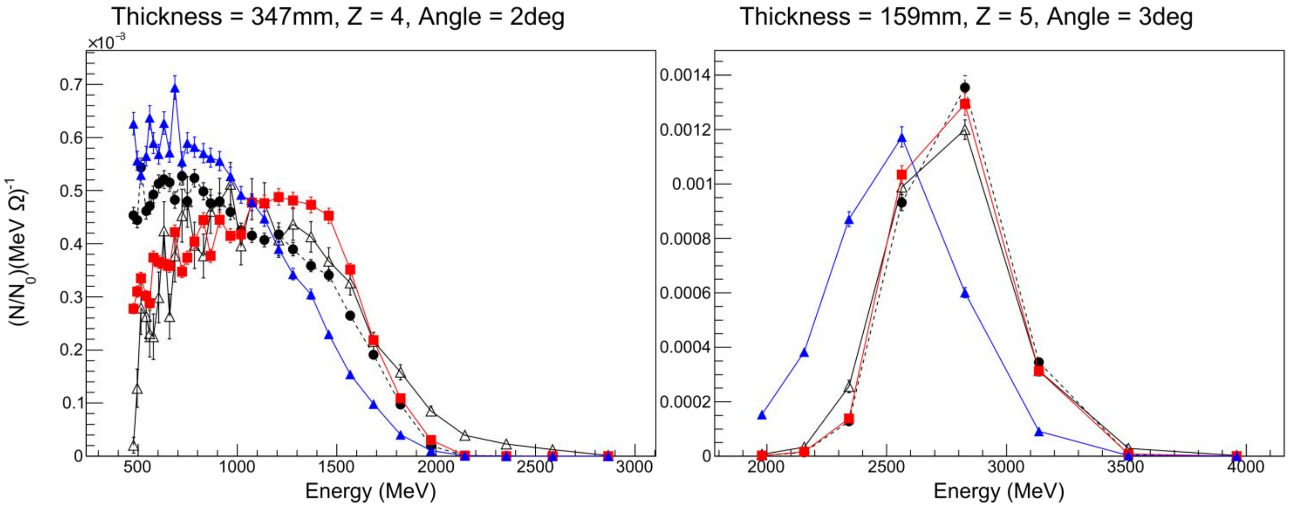
- Assumptions :
  - All fragments are created at the centre of the phantom
  - Recorded fragments are due to the only most abundant isotope (^{1}H, ^{4}He, ^{7}Li, ^{9}Be, ^{11}B)



$$KE_F = \left(\frac{1}{\sqrt{1-\beta^2}} - 1\right) m_0 c^2$$

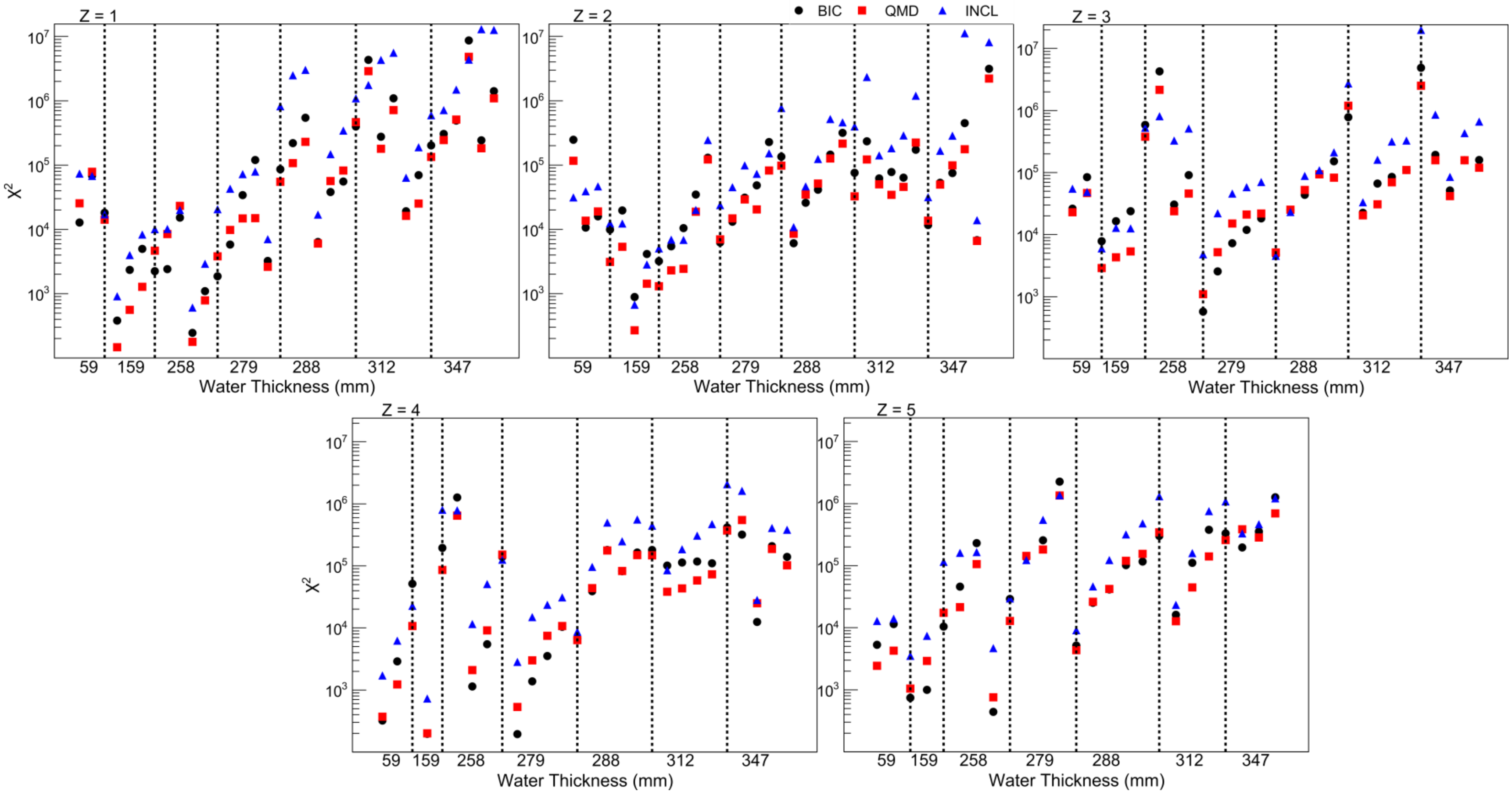
$$\beta = \frac{R}{c t_F}$$





Exp errors up to ~20%

X^2 values


Z = 1
Z = 2
Z = 3
Z = 4
Z = 5
BIC
QMD
INCL
X^2
10^3
10^4
10^5
10^6
10^7
59
159
258
279
288
312
347
Water Thickness (mm)

Results: Energy Distributions

- BIC and QMD perform similar to one another with INCL performing noticeably more poor
- INCL commonly produces lower energy distributions
- Possible energy miscalibration of experiment may contribute to poorer agreement
  - Measurements done over two session
  - Calculated kinetic energy of the ^{12}C ion beam shifts from lower to higher energies
  - Results improving only for INCL by ~10%

Mean %Error

Z	BIC	QMD	INCL
1	26 ± 6	22 ± 6	46 ± 6
2	30 ± 7	33 ± 7	73 ± 7
3	41 ± 8	42 ± 8	93 ± 8
4	61 ± 9	52 ± 9	116 ± 9
5	221 ± 11	194 ± 10	398 ± 10

Comparison of execution times

- Comparison of execution times of 10^5 primary particles for each model
- Intel Xeon E5-2650v3 @2.30GHz
- QMD/QMD-F is considerably more computationally intensive
- BIC and INCL have similar execution times

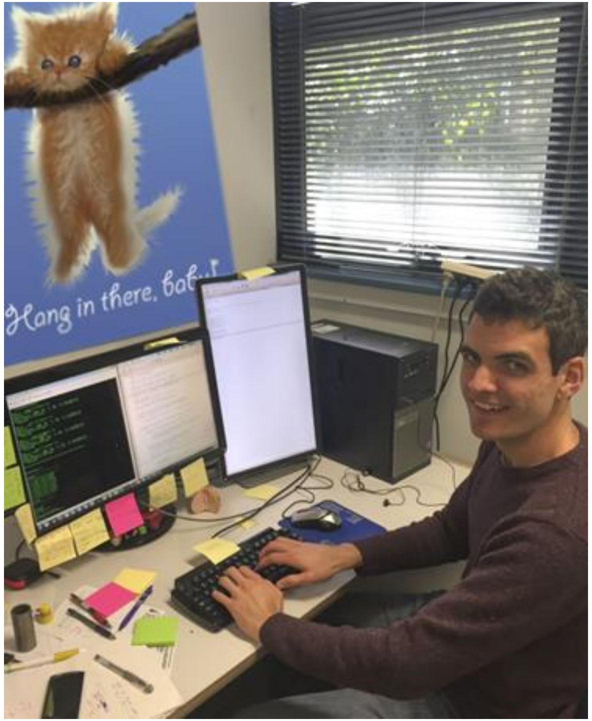
Thickness	BIC (seconds)	QMD/BIC	QMD-F/BIC	INCL/BIC
59	97.5 ± 3.3	10.83 ± 0.45	7.73 ± 0.29	0.79 ± 0.05
159	569 ± 18.2	5.40 ± 0.18	3.94 ± 0.14	0.97 ± 0.03
258	1382.9 ± 90.7	3.67 ± 0.25	2.85 ± 0.24	1.04 ± 0.06
279	1643.4 ± 57.9	3.41 ± 0.15	2.46 ± 0.31	1.03 ± 0.12
288	1765 ± 63.6	3.29 ± 0.13	2.11 ± 0.22	1.01 ± 0.10
312	1979.1 ± 73.9	3.16 ± 0.13	2.26 ± 0.13	1.03 ± 0.05
347	2380.3 ± 47.6	2.86 ± 0.06	2.17 ± 0.08	1.00 ± 0.04

Summary

- Fragment data from a 400MeV/u ^{12}C beam in water was used to benchmark Geant4 using version 10.2p2
- Fragment yield values agreed within ~5-35% of experimental values
  - QMD-F best for H and He, BIC/QMD for heavier fragments
- Angular Distributions agreed ~7-30% for INCL, which performed much better than BIC and QMD
- Energy distributions agreed noticeably poorer (possible experimental calibration error)
  - BIC and QMD performed similar for angular and energy distributions (both treat interaction as Gaussian wave functions)
  - INCL produced lower energies
- In general the agreement deteriorates with larger fragments
- Computation times showed QMD considerably more intensive, BIC and INCL are similar

Conclusions

- Which model for Geant4 fragmentation?
  - Maybe QMD/ QMD-F
  - Repeat simulation with all alternative models and see the range of variation of the results
- The test will be part of the regression testing of Geant4 performed at SLAC and CERN
- As next developments, include
  - INCL-ABLA
  - Abrasion-Ablation model of Wilson
- There is the need of systematic validation against sets of exp data
  - Of different research groups
  - With different detectors
  - With increased experimental accuracy



PhD student David Bolst, Centre For Medical Radiation Physics, University of Wollongong

Nuclear Inst. and Methods in Physics Research, A 869 (2017) 68–75

Contents lists available at ScienceDirect

Nuclear Inst. and Methods in Physics Research, A

journal homepage: www.elsevier.com/locate/nima

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