

# Validation of Geant4 fragmentation for Heavy Ion Therapy

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## Geant4 Users Workshop 2017, Wollongong

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# Carbon Therapy

## ► Conformal treatment

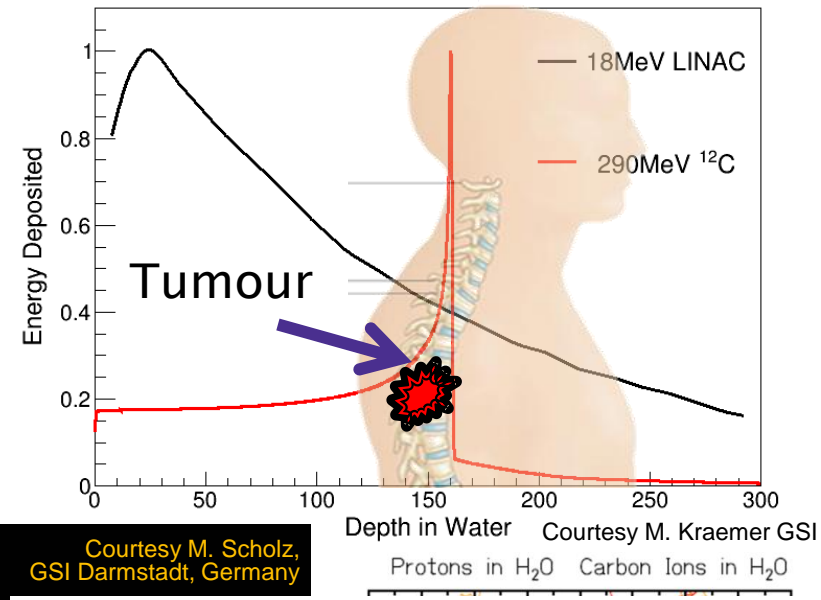
- Sparing Organs at Risk (eg. spinal chord) close to the target tumour

## ► High LET

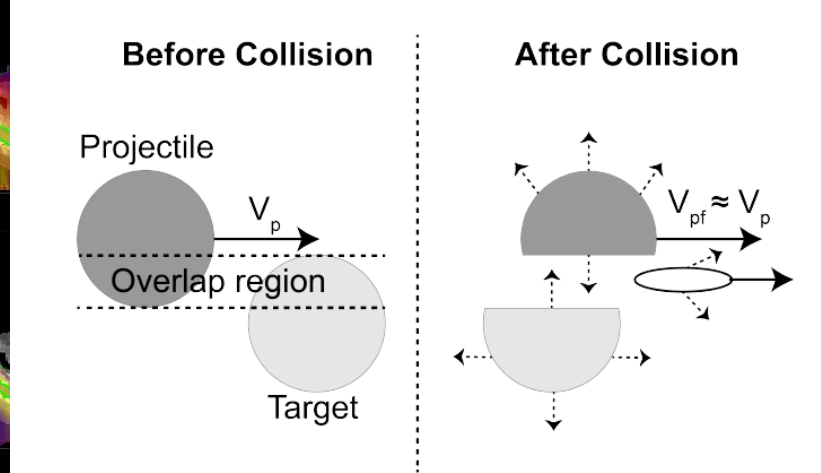
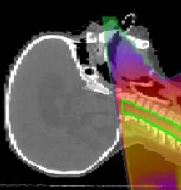
- Ideal for hypoxic/fast proliferating tumours

## ► Complex radiation field

- Fragmentation of primary beam produces diverse secondary field
- Vital to take into account for treatment planning

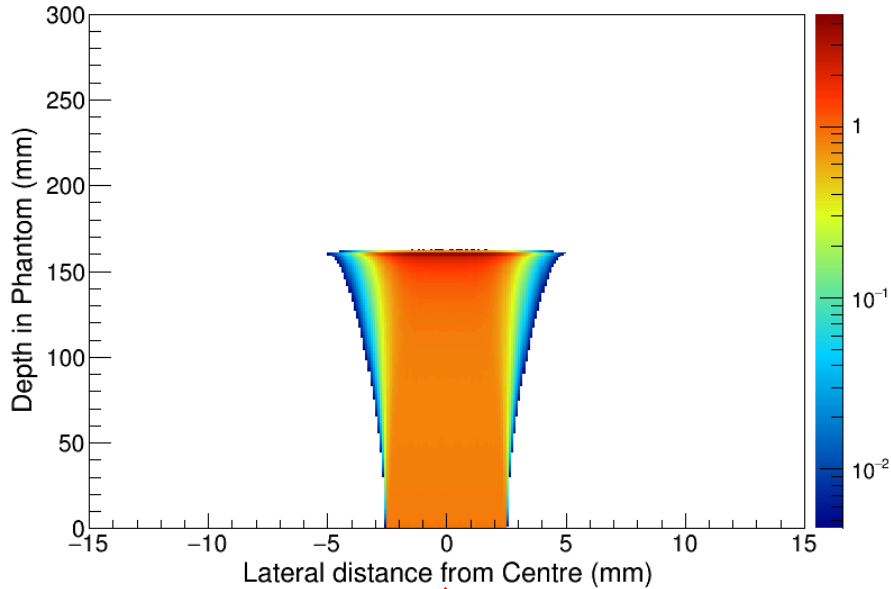



**Photon**  
Courtesy M. Scholz,  
GSI Darmstadt, Germany



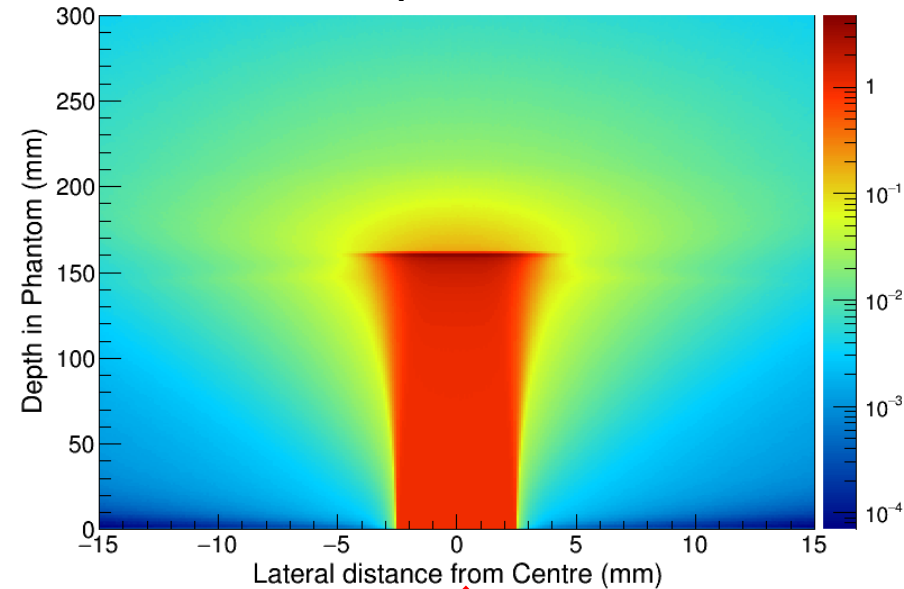
# Energy Deposition in the water phantom


## Energy Deposition by incident $^{12}\text{C}$ ions



  $^{12}\text{C}$  ion beam

## Total Energy Deposition



  $^{12}\text{C}$  ion beam



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### Validation of Geant4 fragmentation for Heavy Ion Therapy



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# Experimental Data

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

IOP PUBLISHING

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PHYSICS IN MEDICINE AND BIOLOGY

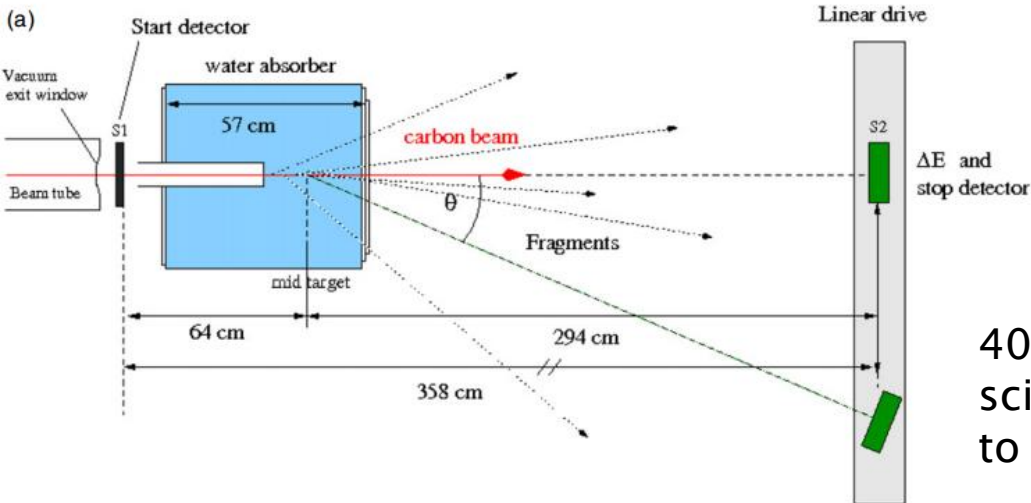
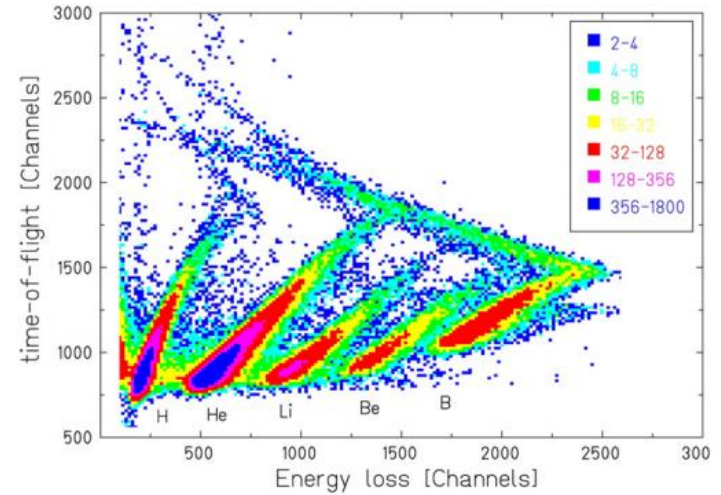
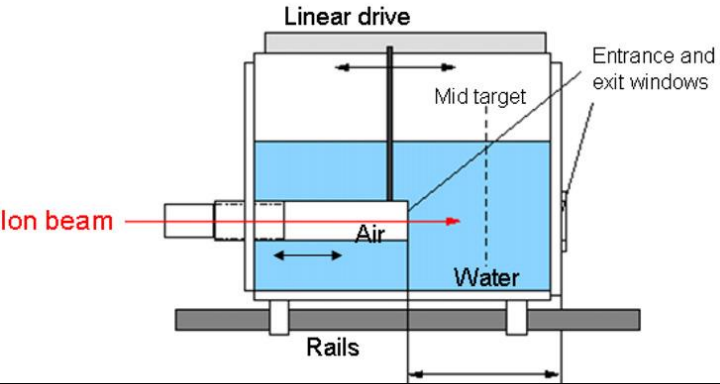
[doi:10.1088/0031-9155/58/23/8265](https://doi.org/10.1088/0031-9155/58/23/8265)

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

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GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany

# Experimental Method



40x40mm<sup>2</sup> plastic scintillator coupled to Hamamatsu PMT

# Simulation Setup (1)

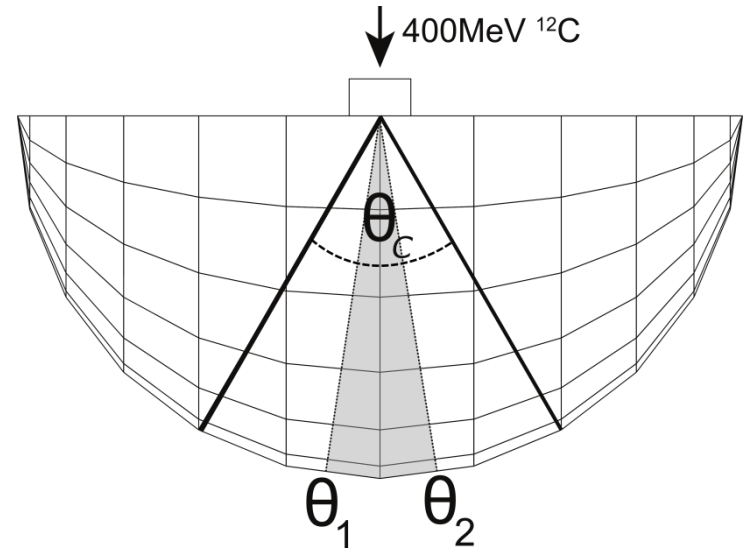
## ▶ Geant4 10.2p2

- BIC, QMD, QMD-F and INCL
- EM Std Opt3

(QMD-F (frag) changes the interaction criterion and only changes the fragment yield)

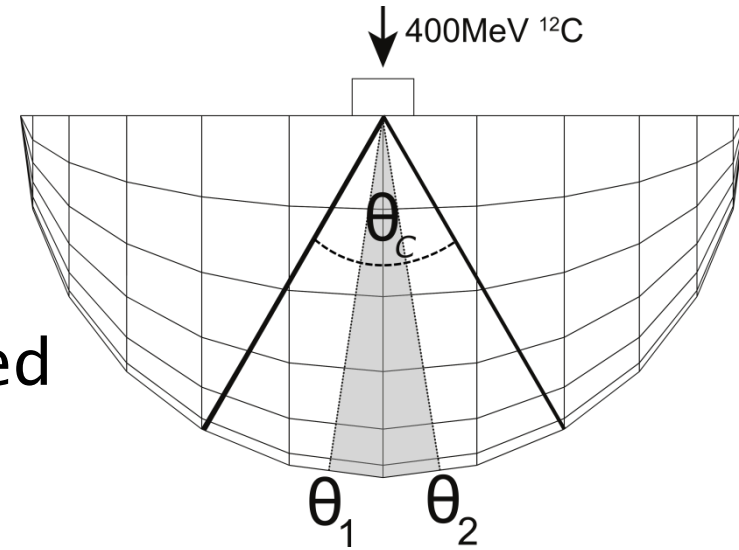
## ▶ Fragment yields, angular and energy distributions measured

400MeV/u  $^{12}\text{C}$  pencil beam is fired onto a variable thickness of water and fragments with  $Z=1-5$  are recorded in a 2.94m radius hemisphere



# Simulation Setup (2)

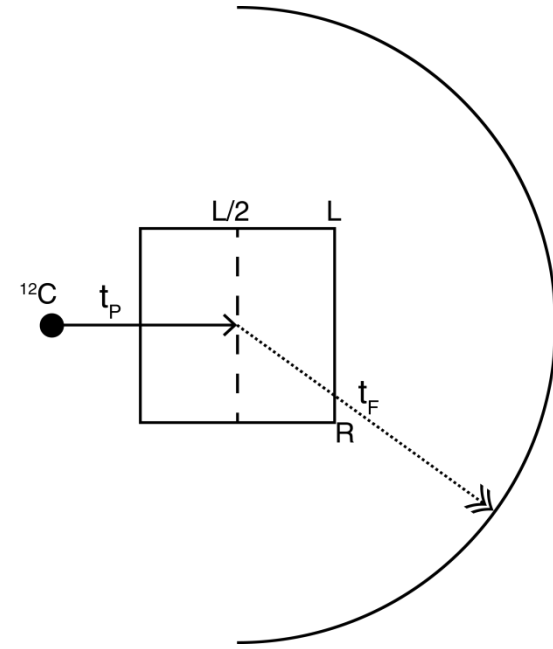
- ▶ **Total fragment yields** were calculated within a  $10^\circ$  cone ( $\theta_C = 10^\circ$ ) for different water thicknesses
- ▶ **Angular distributions** were recorded within  $0.4^\circ$  spans ( $\theta_2 - \theta_1 = 0.4^\circ$ )





# Simulation Setup (3)

- ▶ **Energy distributions** were measured based on the time to reach the collection hemisphere
- ▶ Assumptions made:
  - All fragments are created at the centre of the phantom
  - Recorded fragments are due to the only most abundant isotope ( $^1\text{H}$ ,  $^4\text{He}$ ,  $^7\text{Li}$ ,  $^9\text{Be}$ ,  $^{11}\text{B}$ )

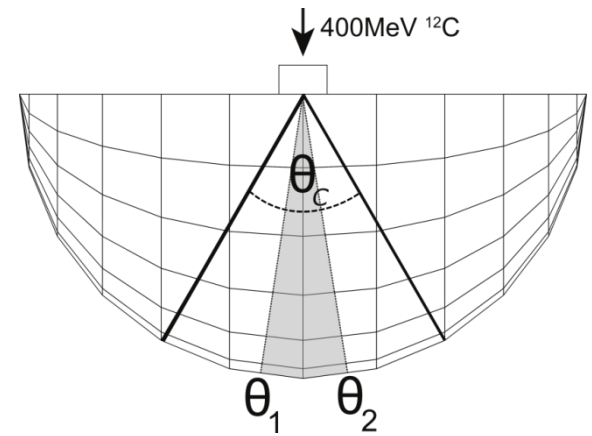


$$KE_F = \left( \frac{1}{\sqrt{1 - \beta^2}} - 1 \right) m_0 c^2$$

$$\beta = \frac{R}{ct_F}$$

# Ranking Models

- ▶ To quantify how well each model performs they were ranked using a combination of:
  - $\langle PE \rangle$  the mean percentage error
  - $X^2$  (analogous to Chi2 value except no p-value is calculated)



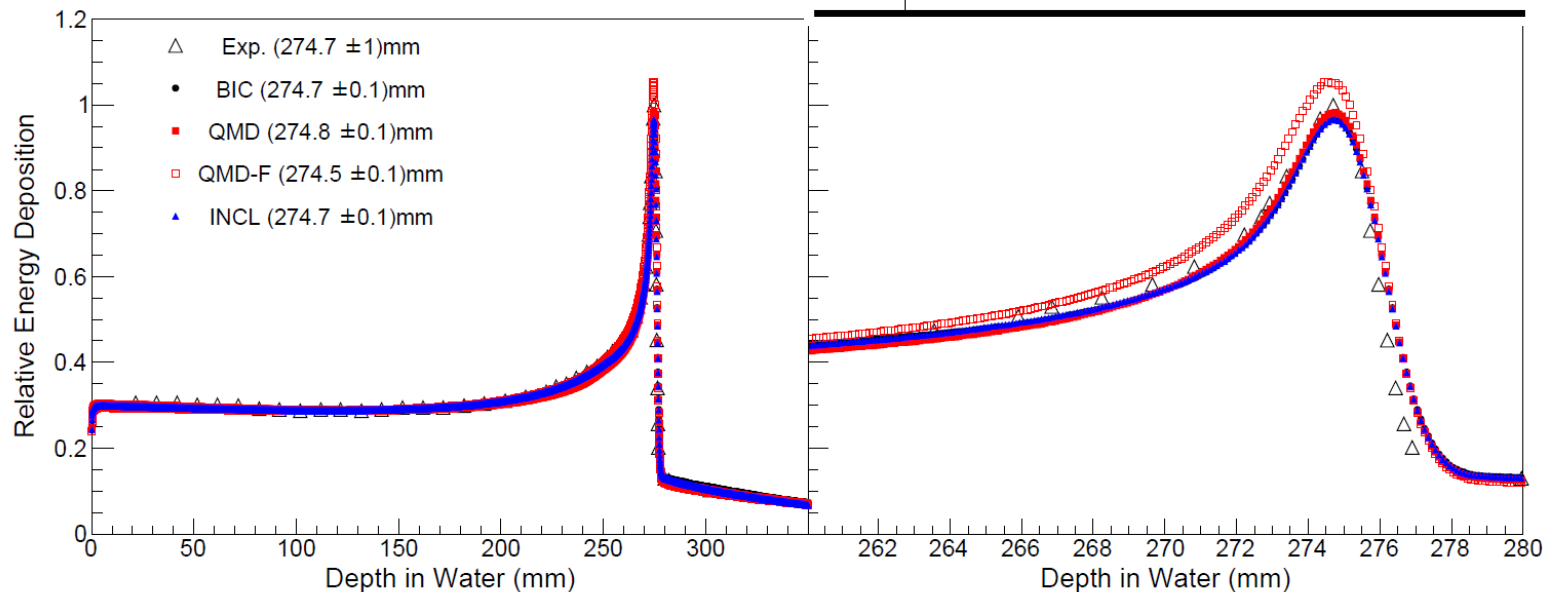
$$\langle PE \rangle = \frac{100}{n} \left( \sum_{i=1}^n \left| \frac{Sim_i - Exp_i}{Exp_i} \right| \right)$$

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

# Results

# Bragg Peak

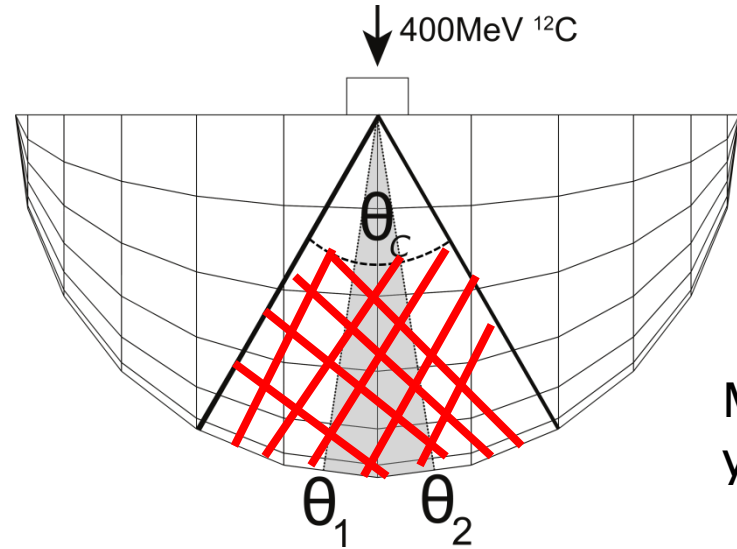
- ▶ All four models tested agreed well with experimental measurements
- ▶ BIC and INCL performed slightly better QMD

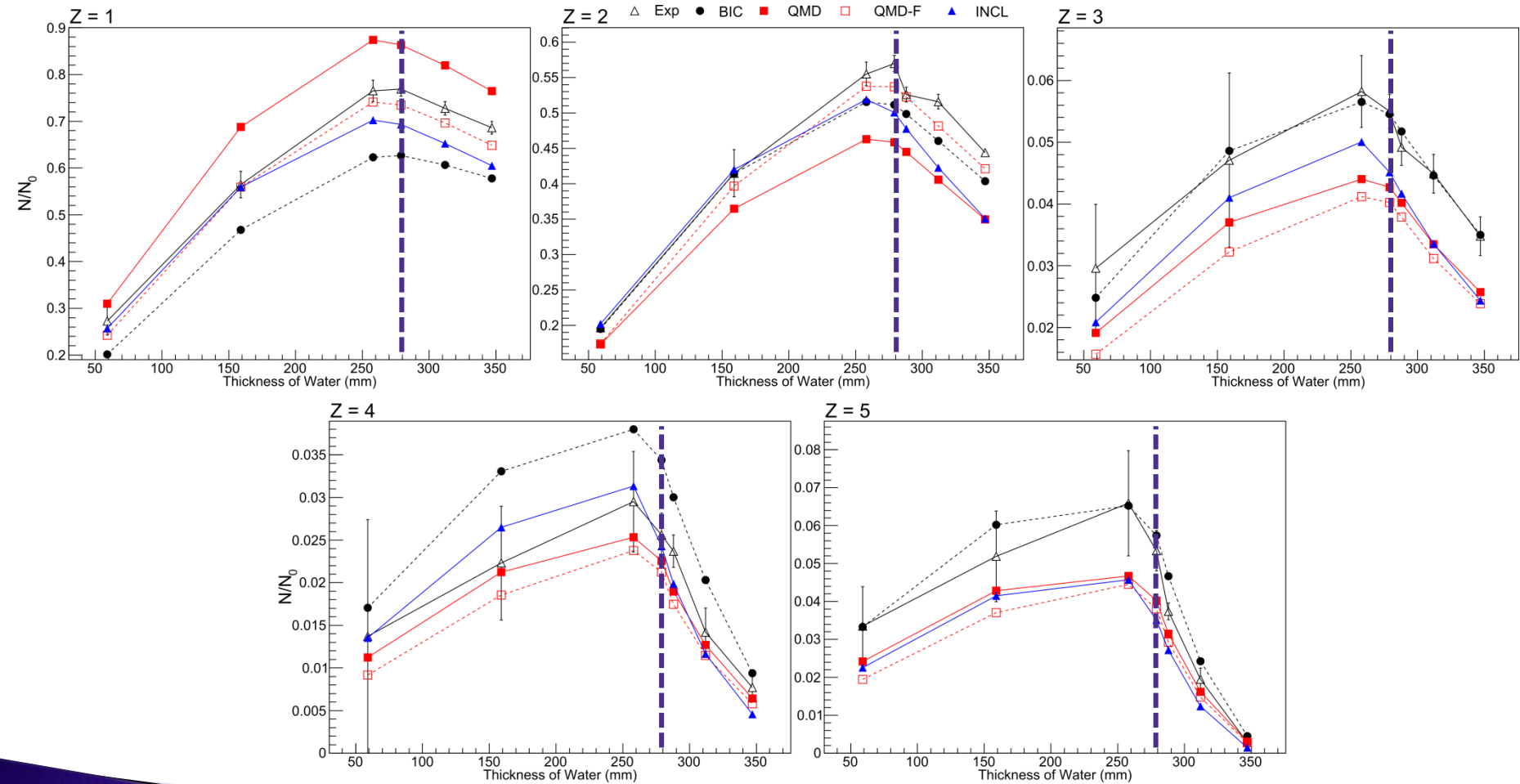


# Fragment Yields

Version 10.2p2

Measuring Fragment  
yield in  $10^\circ$  cone ( $\theta_C$ )





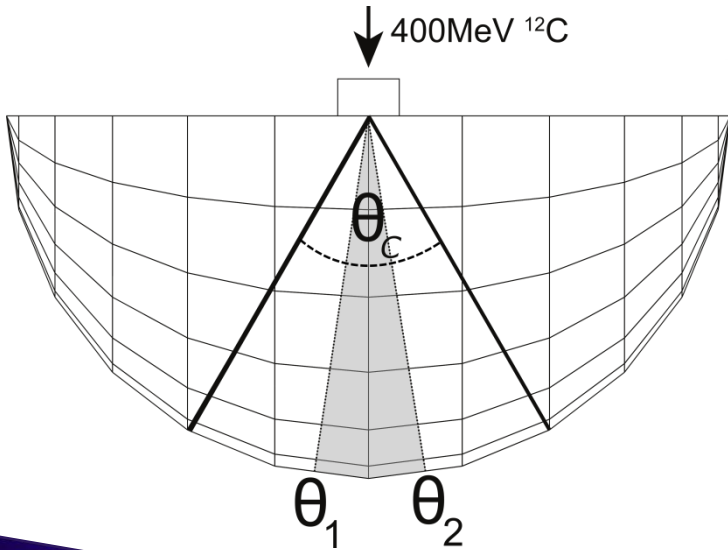
# Summary of Fragment yields

- ▶ Models agreed ~5–35% with exp
- ▶ QMD–F performed best for lighter fragments
- ▶ Larger Z exp results for infield were characterised by larger errors due to primary  $^{12}\text{C}$  masking events
  - Comparison more important for out-of-field

Mean %Error

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

# Angular Distribution



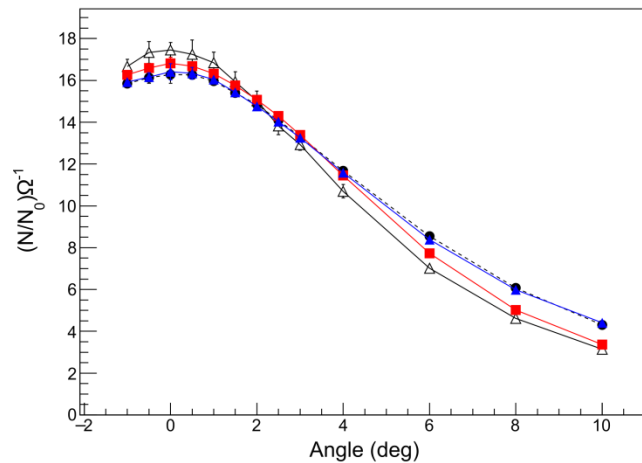
Angular Distributions are normalised to the total experiment counts

In total 32 distributions compared

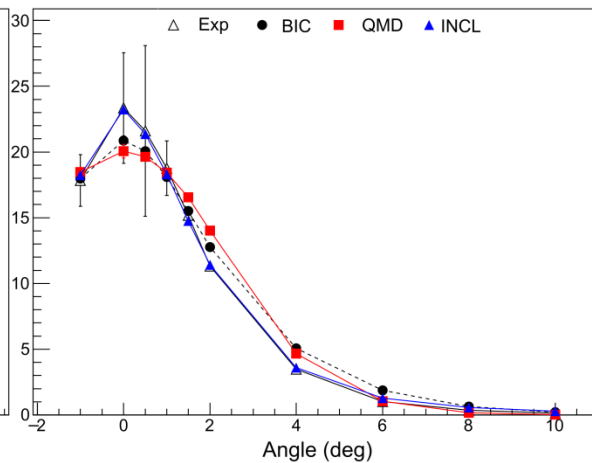
Version 10.2p2



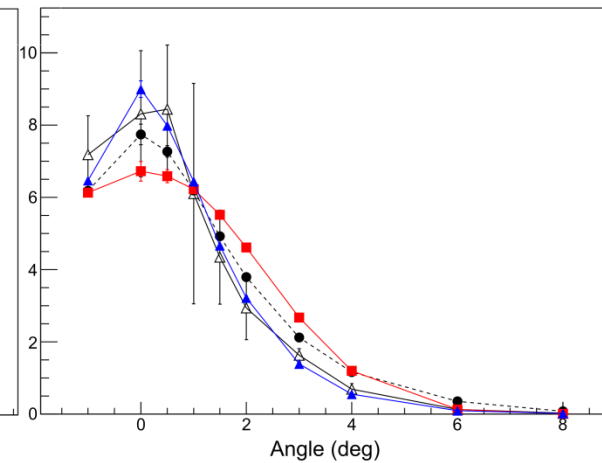
Thickness = 288mm, Z = 1



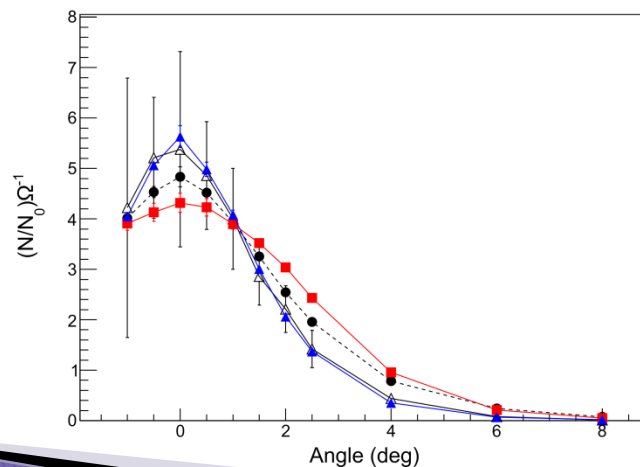
Thickness = 59mm, Z = 2



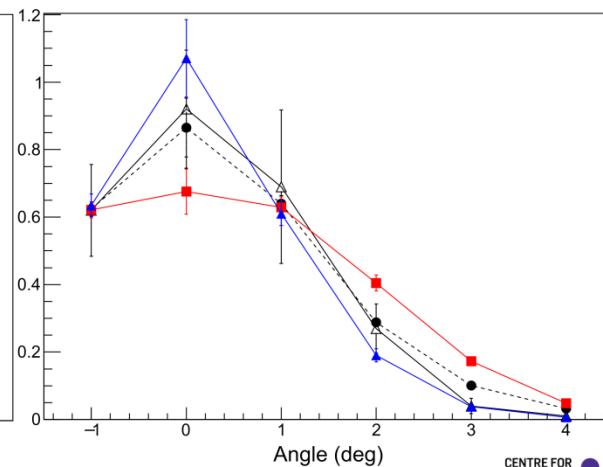
Thickness = 159mm, Z = 3



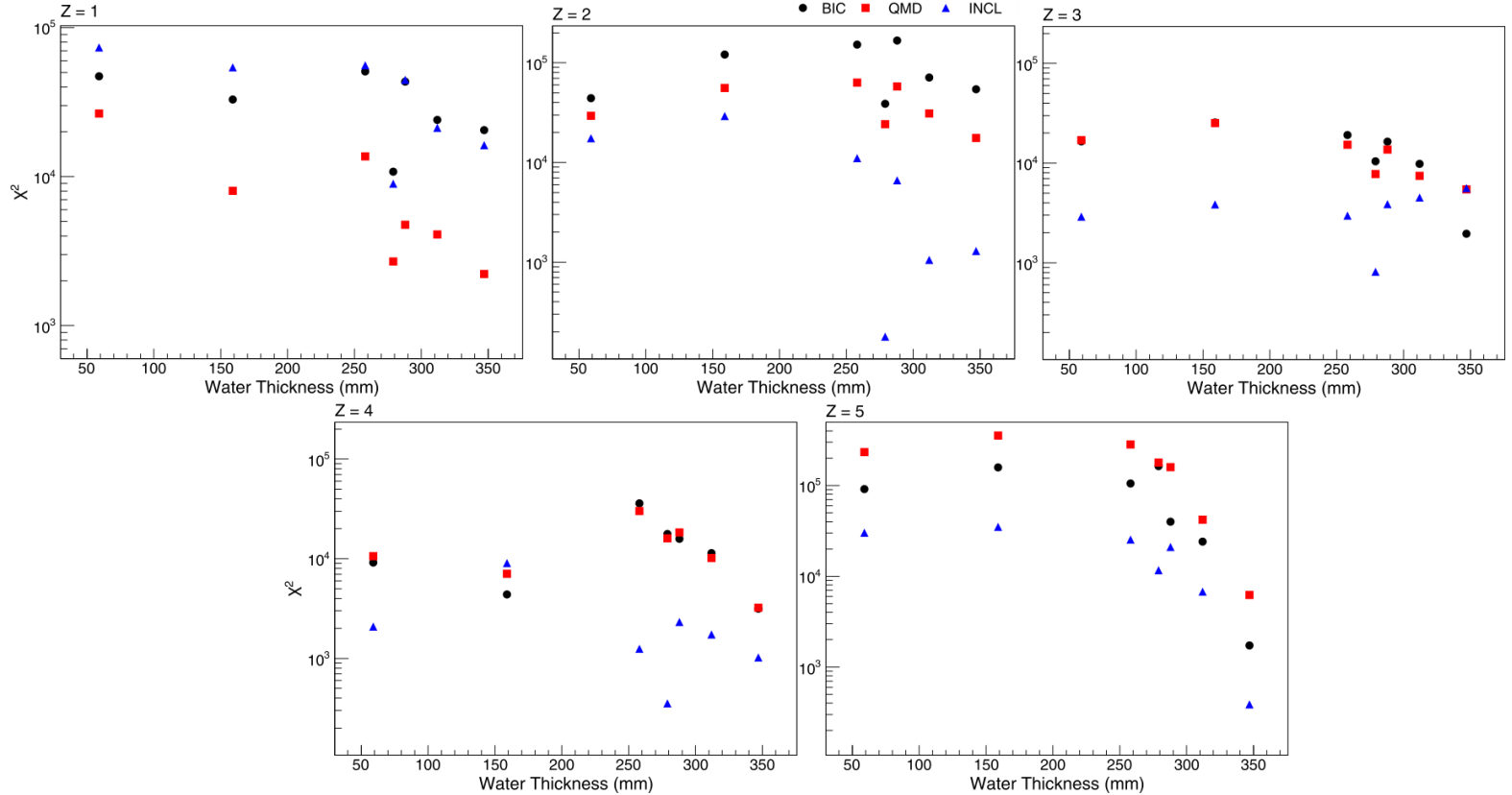
Thickness = 258mm, Z = 4



Thickness = 347mm, Z = 5



# $\chi^2$ values



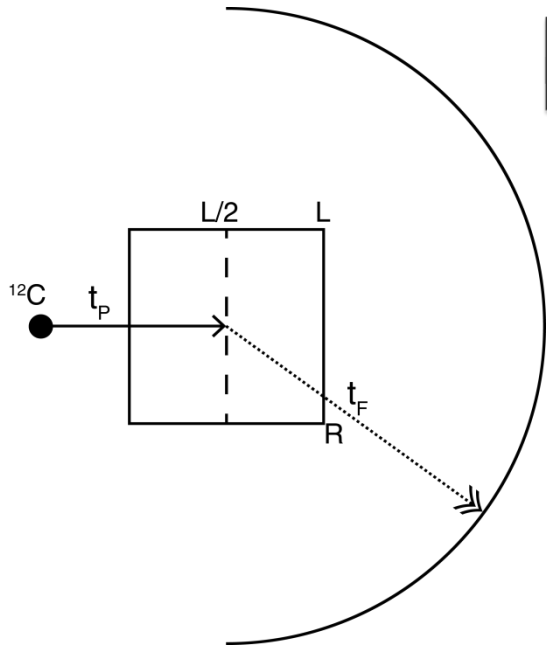
# Angular Distribution Summary

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

Mean %Error

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

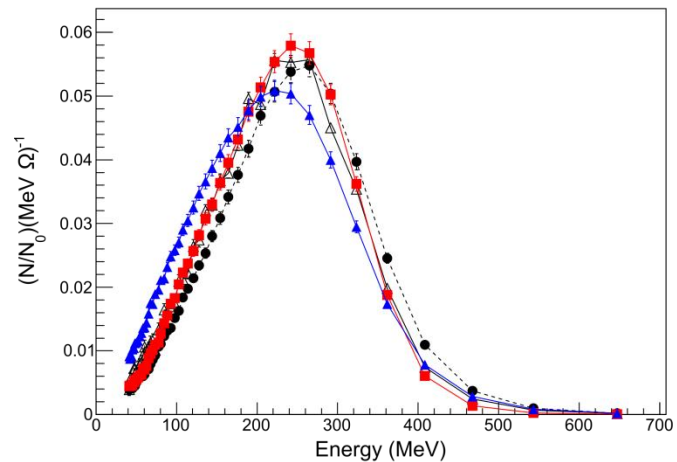
# Energy Distribution



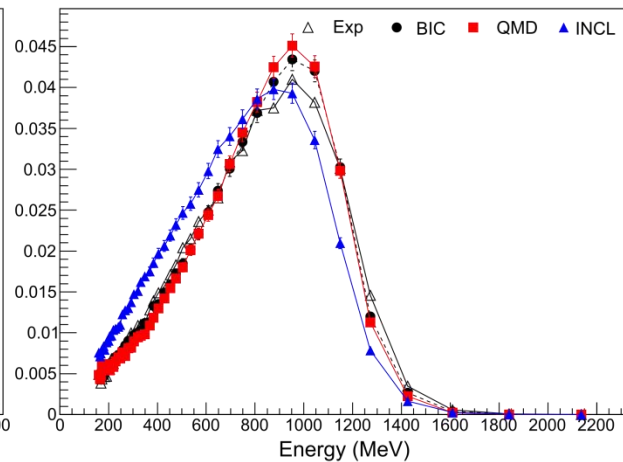
Energy Distributions are normalised to the total experiment counts  
In total 159 distributions compared

Version 10.2p2

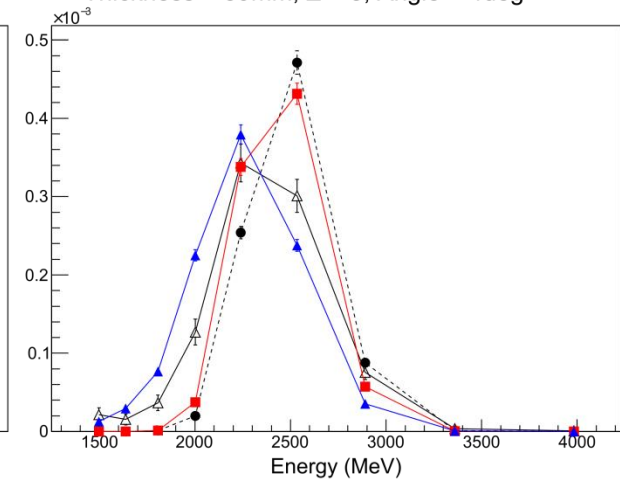
Thickness = 258mm, Z = 1, Angle = 4deg



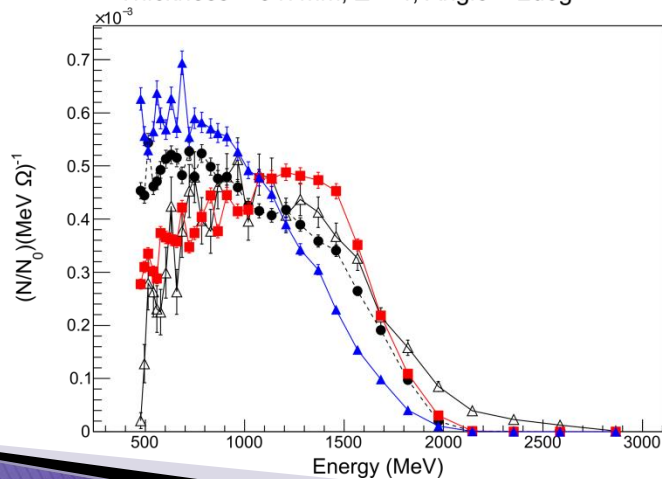
Thickness = 312mm, Z = 2, Angle = 1deg



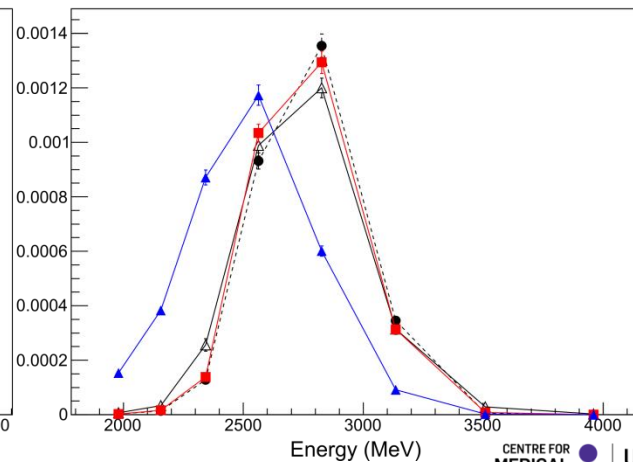
Thickness = 59mm, Z = 3, Angle = 4deg



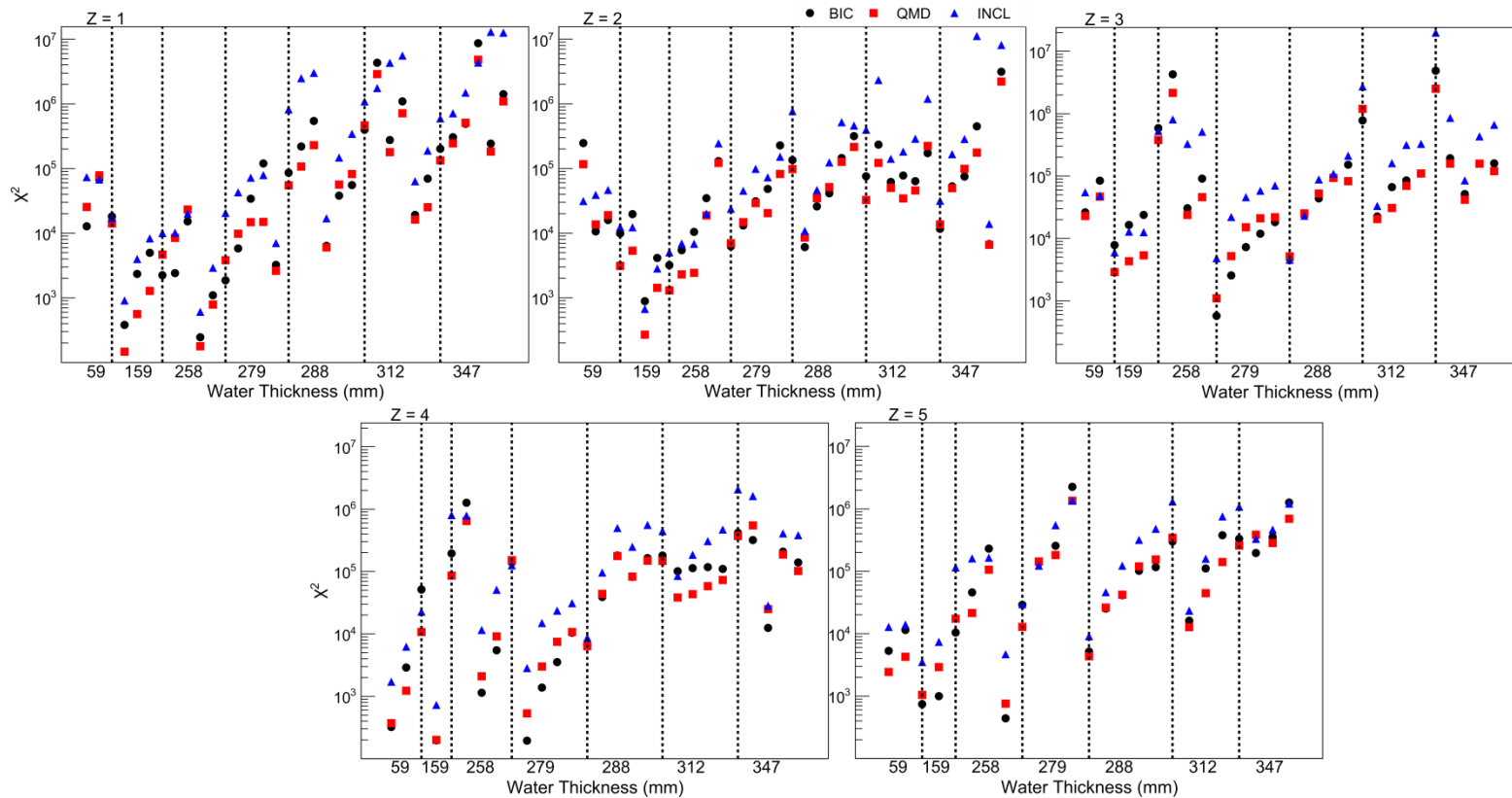
Thickness = 347mm, Z = 4, Angle = 2deg



Thickness = 159mm, Z = 5, Angle = 3deg



# $\chi^2$ values



# Energy Distribution Summary

- ▶ 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 be contribute to poor agreement
  - Measurements done over two session one calibration shifted from  $(358 \pm 23)\text{MeV/u}$  to  $(402 \pm 26)\text{MeV/u}$

Mean %Error

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

# Comparison of Runtime

- ▶ Compared runtimes of  $10^5$  primary particles for each model using an Intel Xeon E5-2650v3 @2.30GHz
- ▶ QMD/QMD-F was a considerably more computationally intensive for thinner targets
- ▶ BIC and INCL had similar runtimes apart from thinner targets

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



# Summary

- ▶ Fragment data from a 400MeV/u  $^{12}\text{C}$  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 ~5–35% for INCL, which performed much better than BIC and QMD in versions
- ▶ **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
- ▶ **Computation times** showed QMD considerably more intensive, BIC and INCL were similar

# Thank you

