Accuracy of the EGSnrc code system

D. W. O. Rogers,
Carleton Laboratory for
Radiotherapy Physics,
Physics Dept,
Carleton University,
Ottawa

http://physics.carleton.ca/~drogers
ICCR Melbourne Australia May 9, 2013

Carleton
UNIVERSITY
Canada's Capital University

Accuracy and Limitations of EGSnrc

- Fano test
- real ion chambers
- k_Q calculations
- multiple scattering tests
- backscatter data for x-rays and megavoltage
- transmission test of extreme conditions
- brachytherapy spectra and dose rate constants

How accurately can we calculate ion chamber response? The Fano test

Fano's theorem

Under conditions of charged particle equilibrium the electron fluence in a medium is independent of the density.

Fano cavity chamber,

- full build up wall
- cavity either: gas of wall material or wall material
- perfect CPE => no attenuation or scattered photons

Carleton UNIVERSITY
Canada's Capital University

Fano test (cont)

Consider the case with cavity of wall material

$$(K_{col})_{\text{wall}} \overset{CPE}{=} D_{\text{wall}}$$

but since, by Fano's theorem the electron fluence is unchanged => $D_{\text{gas}} \overset{CPE}{=} D_{\text{wall}}$

and hence:

$$(K_{col})_{\text{wall}} = E\phi\left(\frac{\mu_{en}}{\rho}\right)_{\text{wall}} = D_{\text{gas}} = D'_{gas}K_{\text{wall}}$$

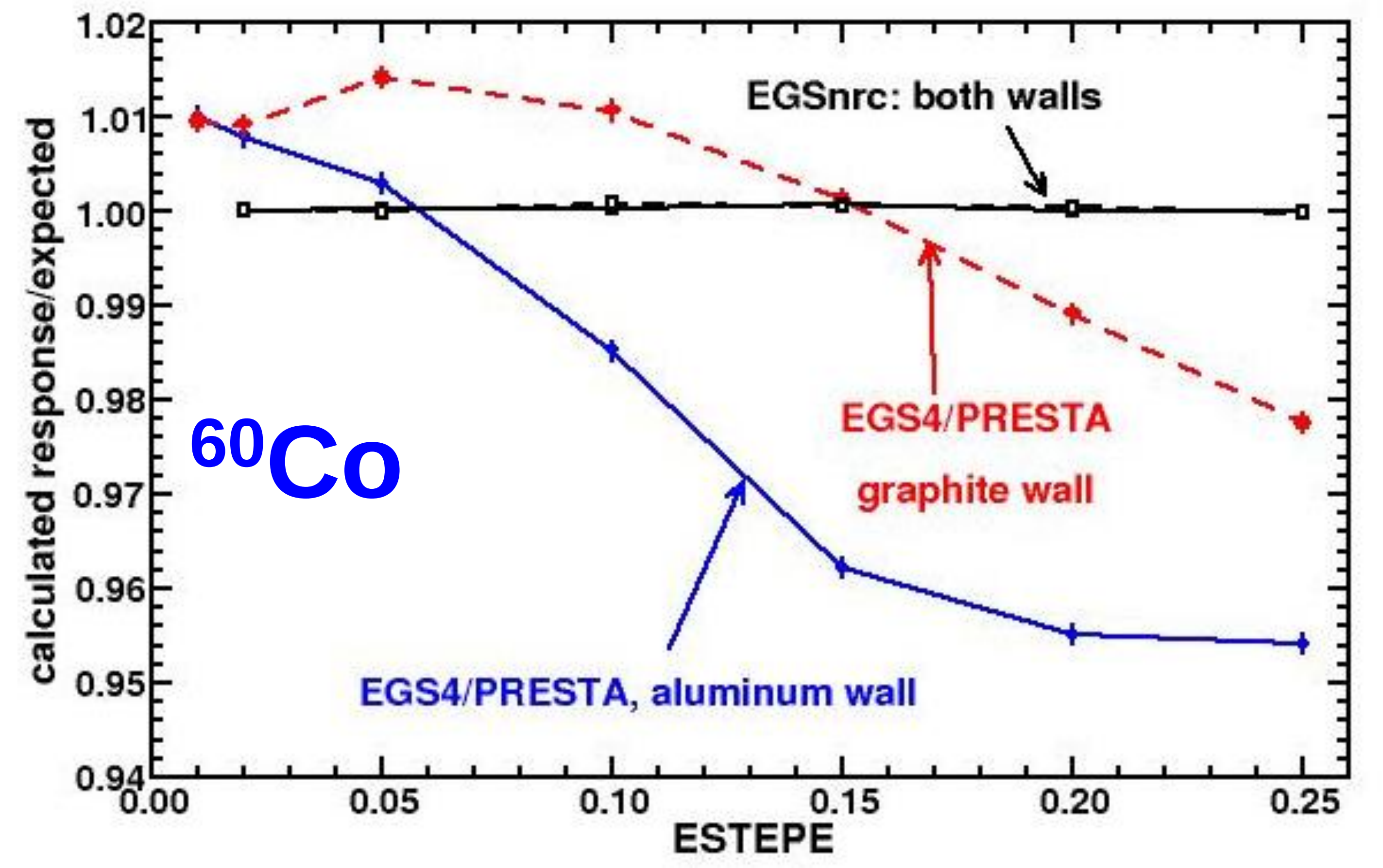
where D_{gas} is the dose to the gas without any attenuation and scatter (so there is CPE) and D'_{gas} is the dose calculated with attenuation and scatter and then corrected by the wall correction factor, i.e. K_{wall} (not another kerma!)

Fano test (cont)

-cover of EGSnrc manual

-against own cross sections

-ESTEPE is max fractional step size



This is the toughest test I know for any electron-photon Monte Carlo code

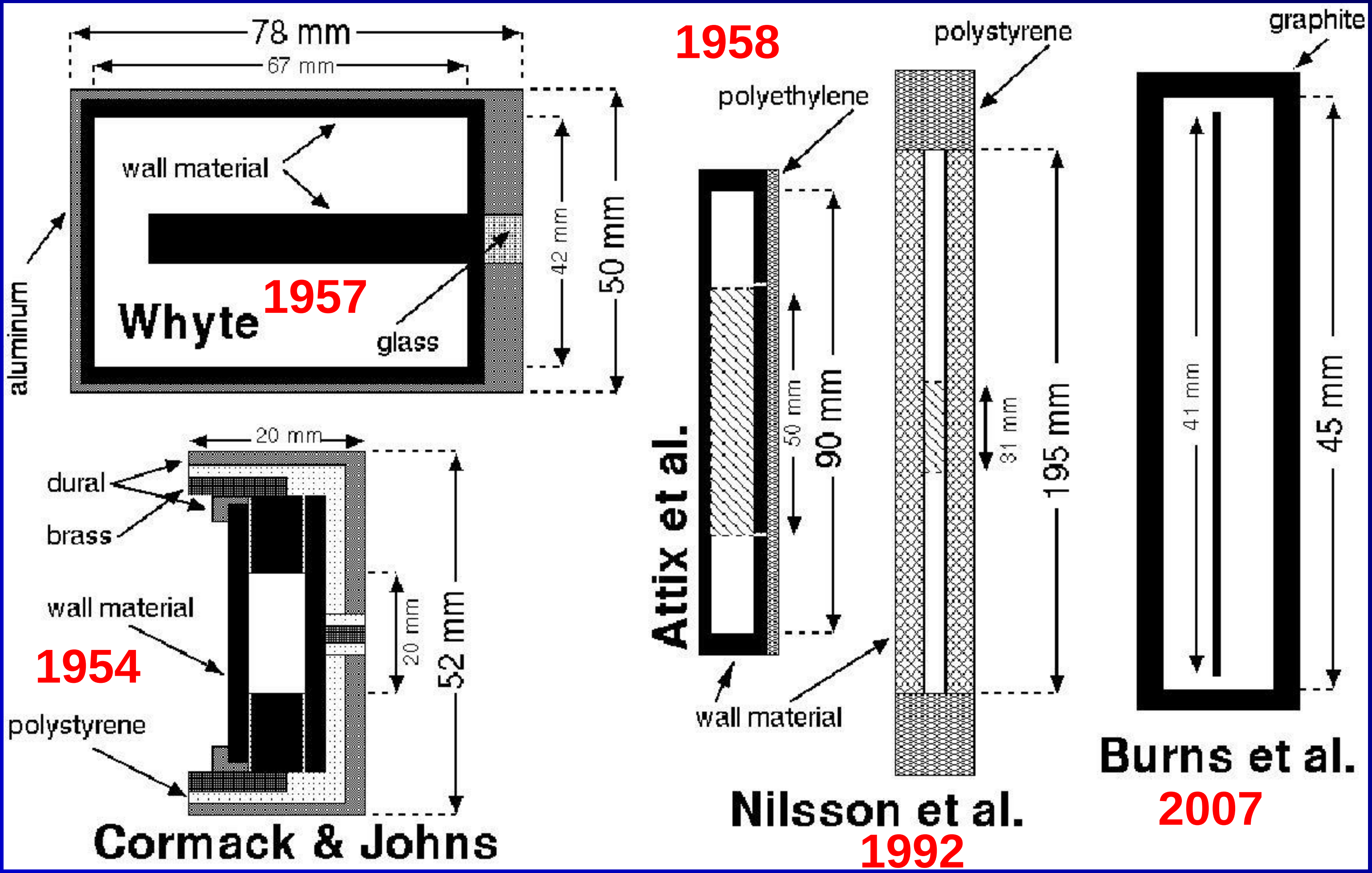
Fano test (cont)

- with lead walls, EGSnrc passes at 0.1 % level in ^{60}Co (La Russa, Med Phys 35(2008) 5629).
  - No parameter adjustment needed
- Sempau and Andreo (PMB, 51 (2006) 3533-3548) achieved similar accuracy with PENELOPE (used different version of Fano test) as did Yi et al (Med Phys 33 (2006) 1213)
  - both cases needed adjustment of parameters
- Poon et al (PMB 50 (2005) 681 - 694) showed that GEANT4 failed Fano test by as much as 39%.
  - now within 1% at expense of long CPU times (Sawakuchi, private communication)

Fano test (cont)

- the Fano test assesses accuracy against its own cross sections.
  - If cross sections are wrong, test can still be passed if mass energy absorption coefficients are calculated with same cross sections.
- real test is against measured ion chamber data.

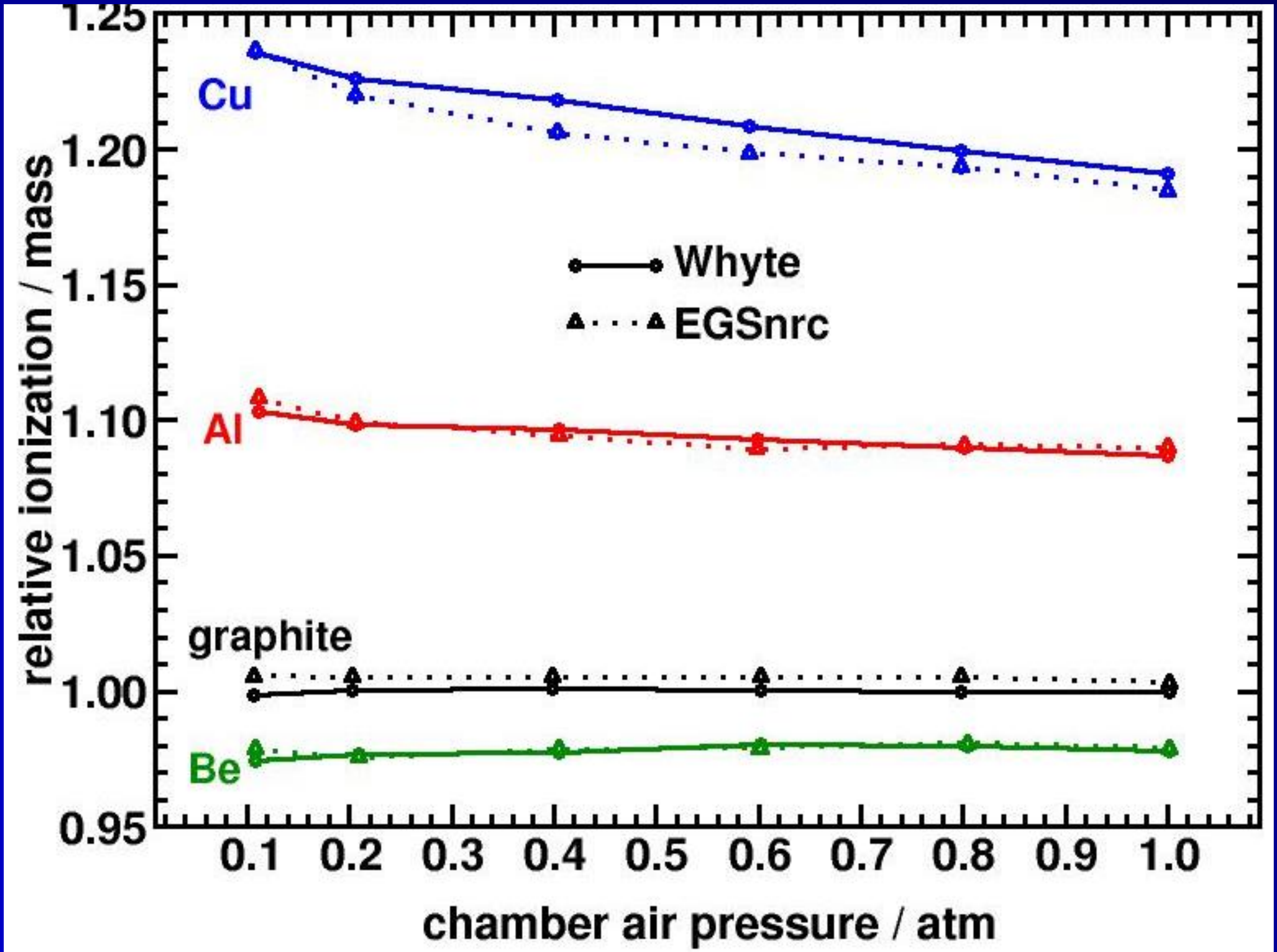
real chambers in ^{60}Co beams



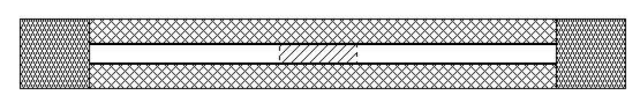
La Russa & Rogers Med Phys 35 (2008) 5629-5640

Whyte: variation of pressure/wall

- Co-60 beam
- data normalized only once
  - i.e. relative values are meaningful
  - depends on cross sections
- RMSD = 0.5%

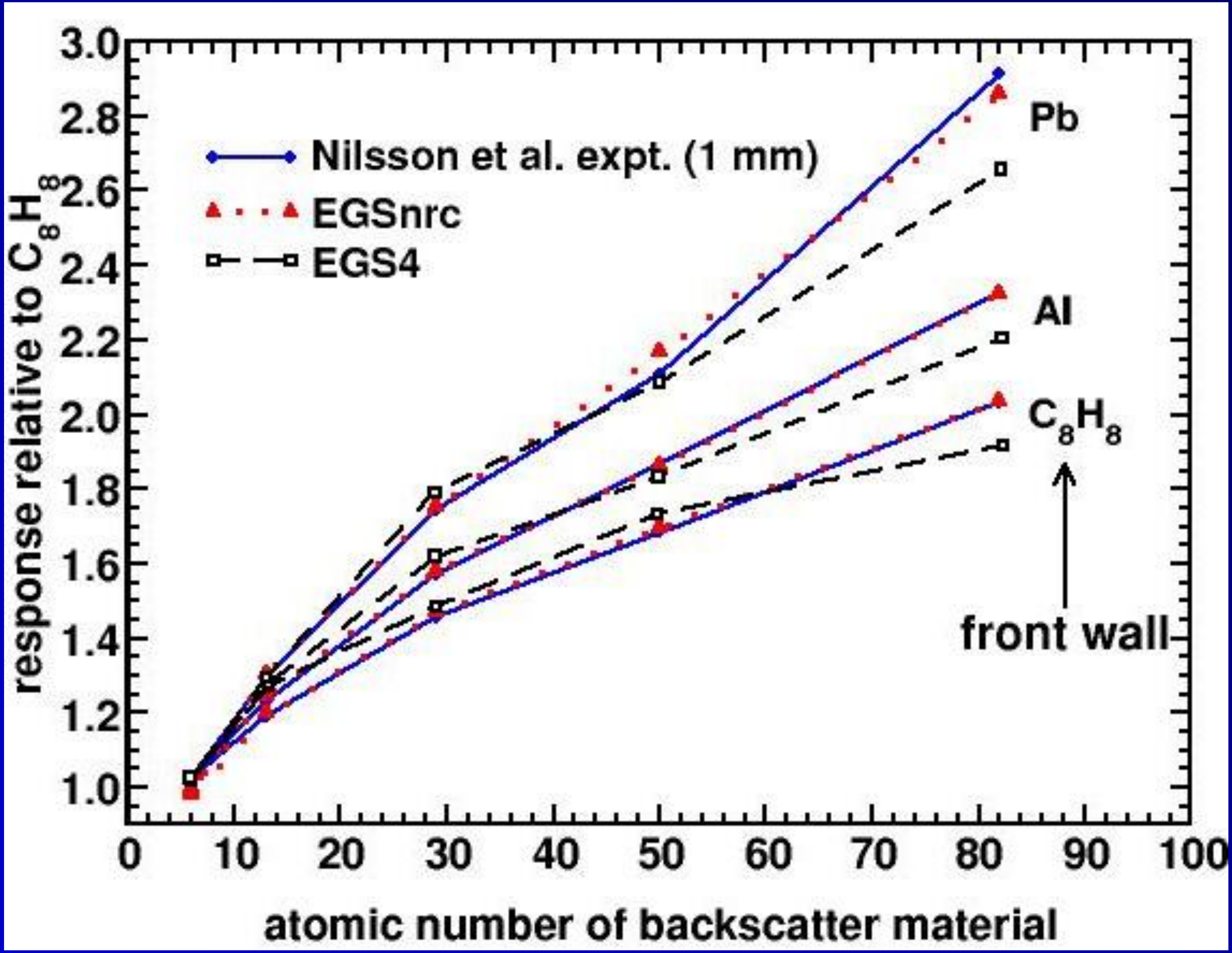


Med Phys 35 (2008) 5629-5640



Nilsson et al: wall variations

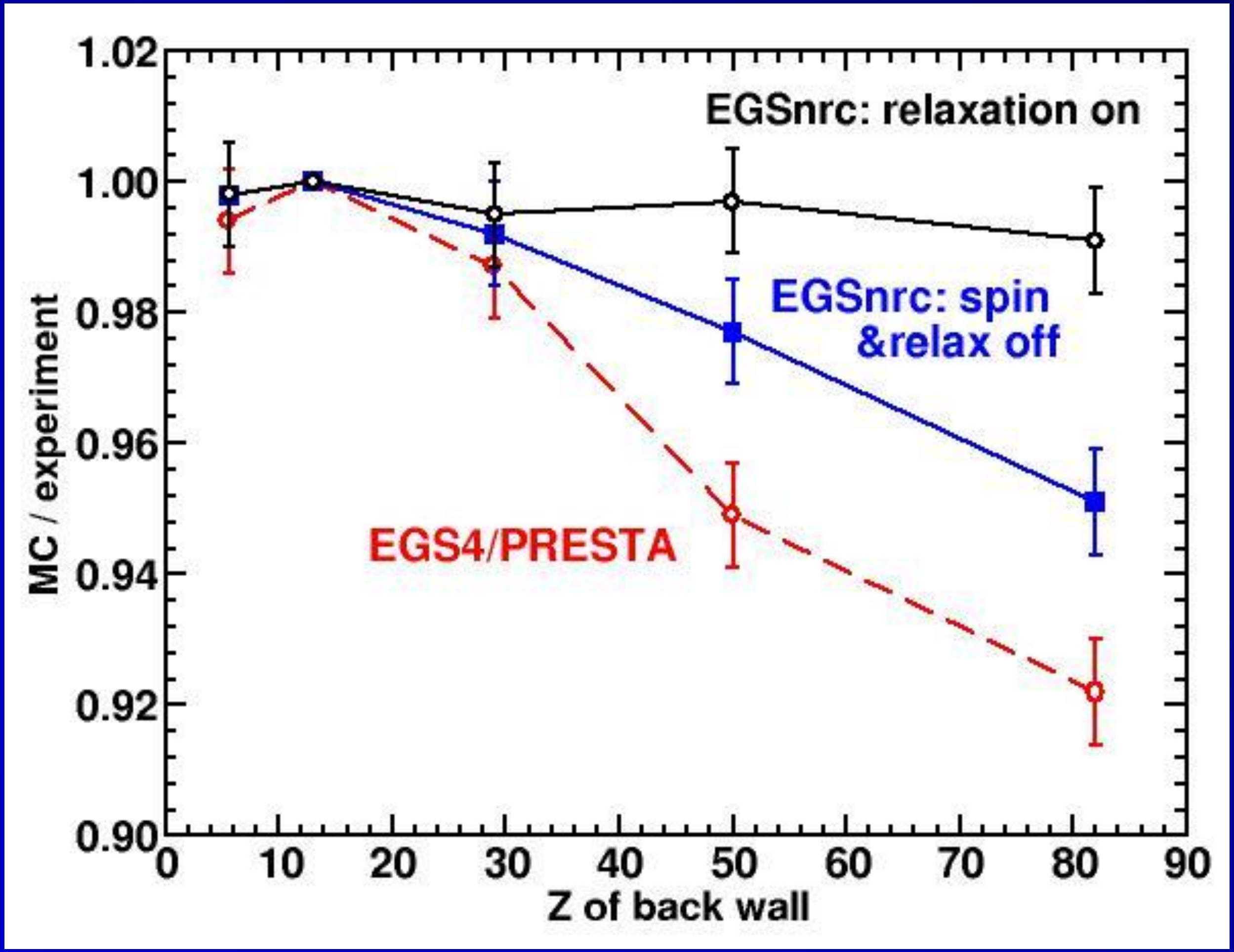
- ^{60}Co
- normalized to polystyrene chamber
- RMSD=1.4% (EGSnrc/expt)
- depends on cross-sections



Med Phys 35 (2008) 5629-5640

What affects the calculation?

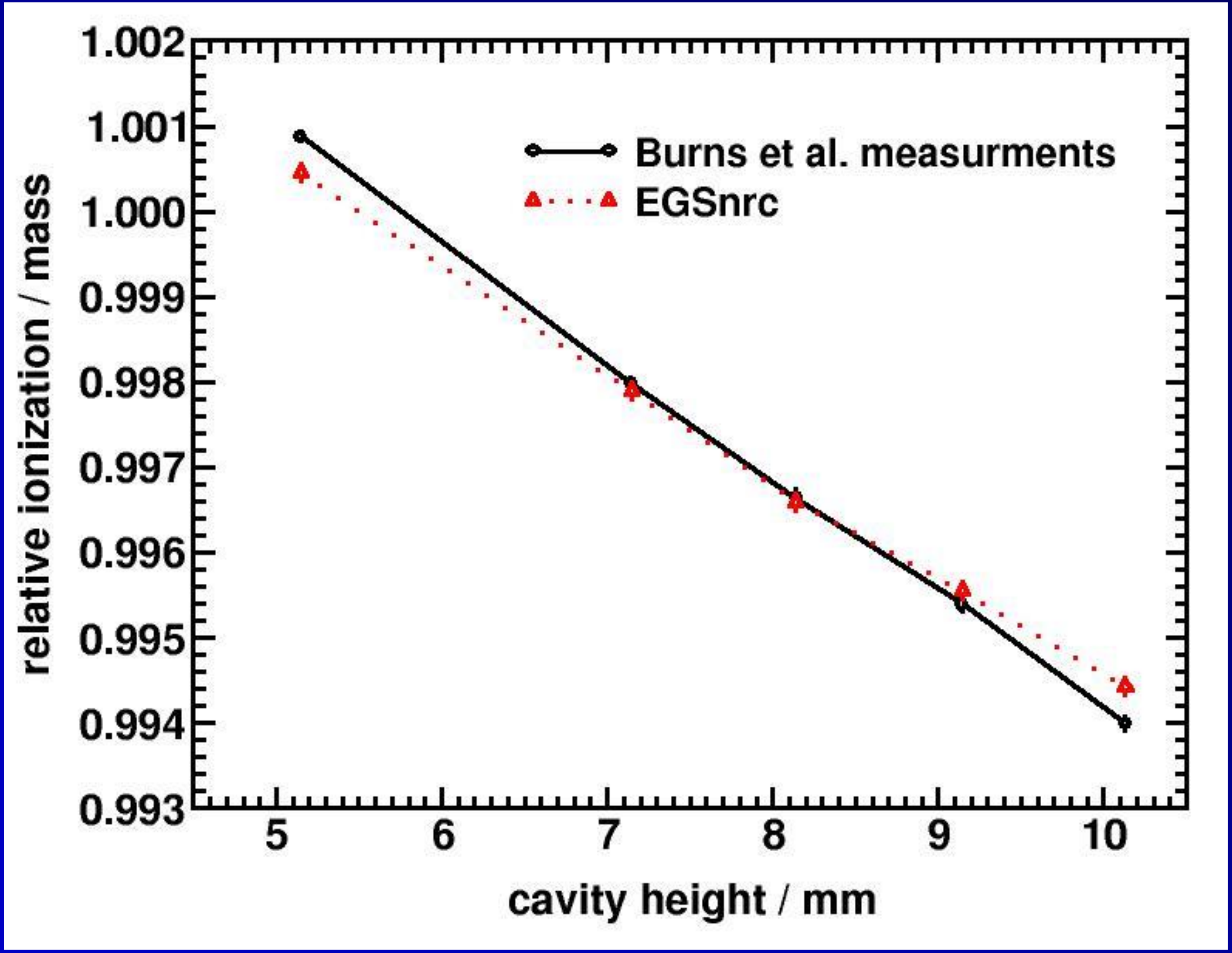
against measured data



Kawrakow & Rogers, MC2000, p135 based on data of Nilsson et al, Med Phys 19(1992)1413

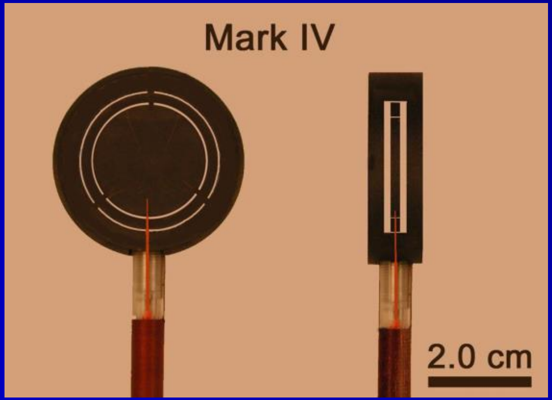
Burns: variation of graphite chamber

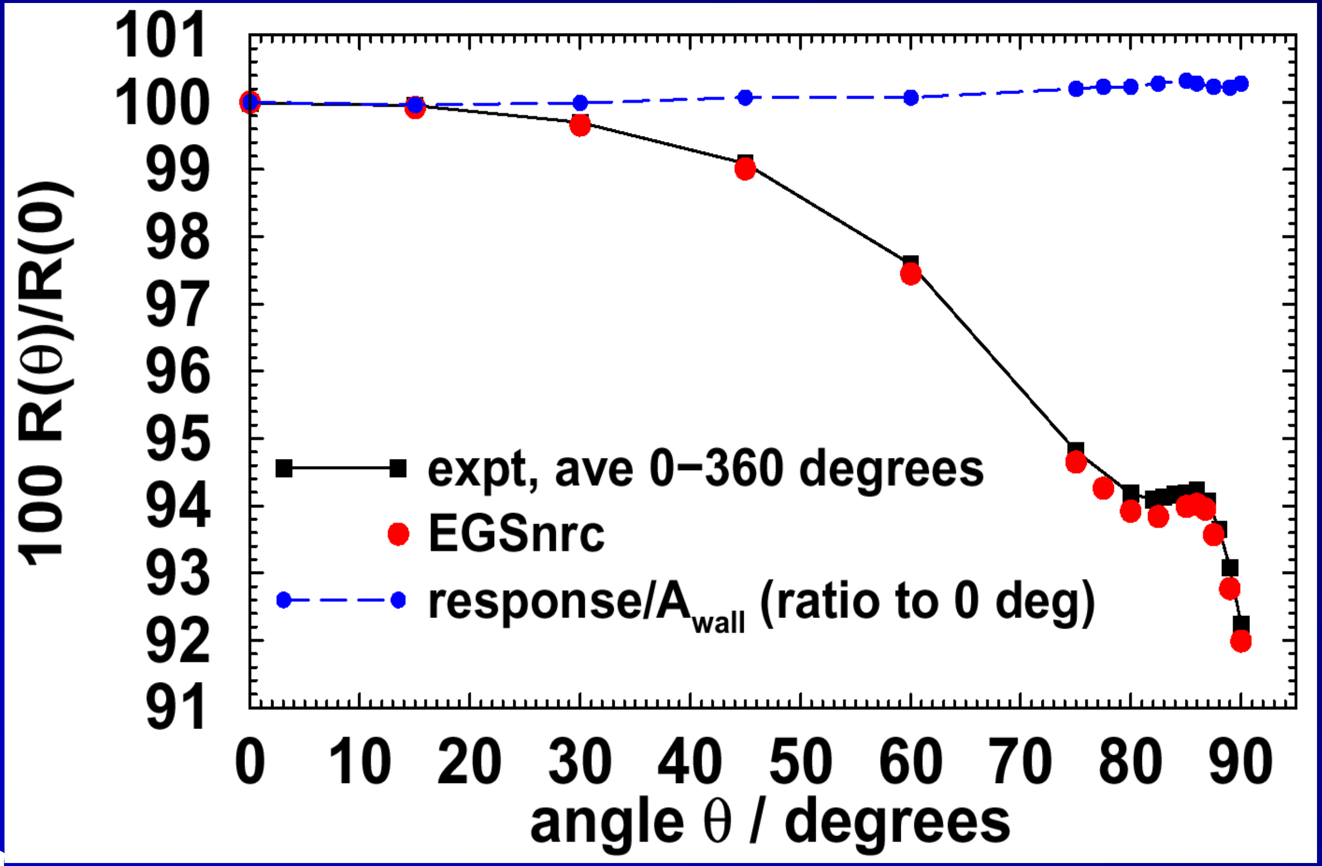
- ^{60}Co
- RMSD = 0.03%
- (0.7% overall variation)



La Russa Med Phys 35 (2008) 5629-5640

Response vs angle of pancake chamber





R/A_{wall} should be constant.

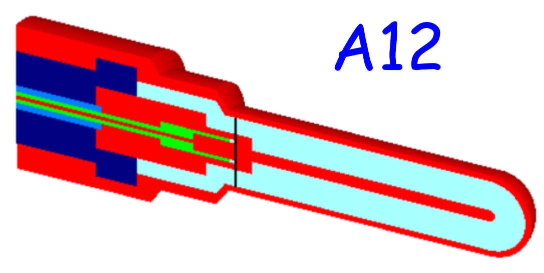
It is, within 0.3% despite 8% variation.

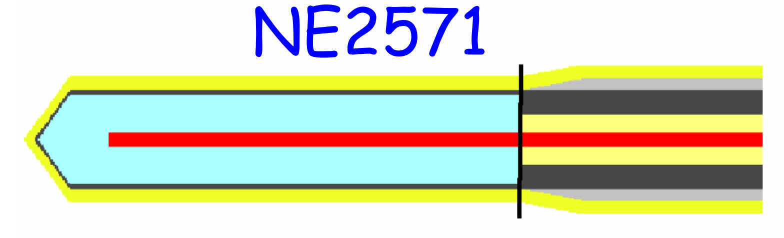
(residual 0.3% is a K_{an} effect)

McCaffrey et al PMB 49(2004) 2491

ab initio Monte Carlo calculations of k_Q for clinical ion chambers

- Fano test is usually for simple `in air' ion chambers
- real interest is `in-phantom'
- egs_chamber code of Wulff et al (Med Phys 35 (2008) 1328)
  - very efficient: correlated sampling
  - handles complex realistic geometries





Calculating k_Q (protocol clinical dosimetry)

- definitions:

$$k_Q = \frac{N_{D,w}^{Q}}{N_{D,w}^{Co}}$$

$$D_{\mathrm{gas}} = \frac{Q \left(\frac{W}{e}\right)_{\mathrm{air}}}{m_{\mathrm{air}}}$$

$$N_{D,w} = \frac{D_{\mathrm{w}}}{Q} = \frac{D_w}{D_{\mathrm{gas}} \frac{m_{\mathrm{air}}}{\left(\frac{W}{e}\right)_{\mathrm{air}}}}$$

assume (W/e) is independent of beam quality

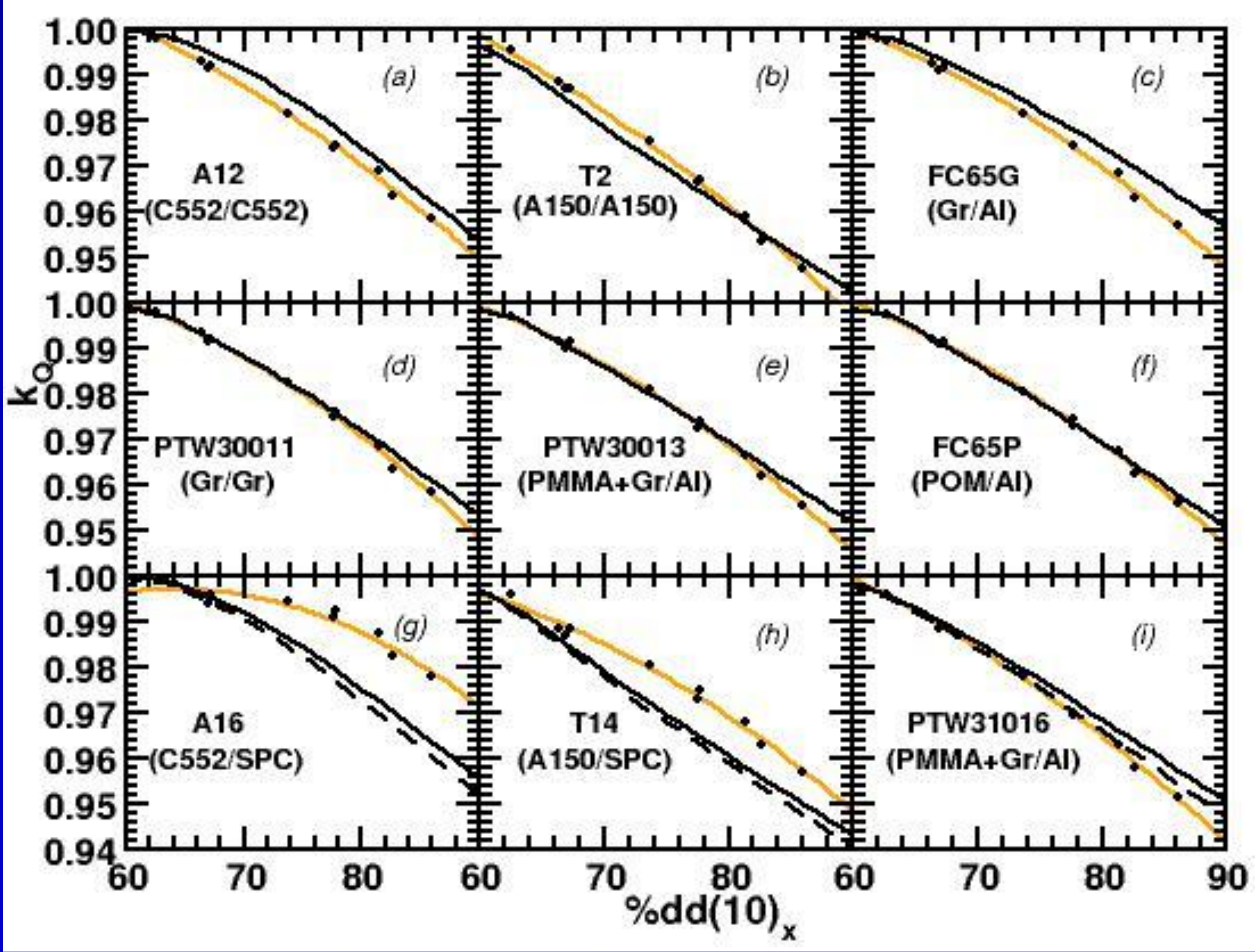
$$k_Q = \frac{N_{D,w}^{Q}}{N_{D,w}^{Co}} = \frac{\frac{D_w^Q}{D_{\mathrm{gas}}^Q}}{\frac{D_w^{Co}}{D_{\mathrm{gas}}^{Co}}} = \left(\frac{D_w}{D_{\mathrm{gas}}}\right)_{Co}^{Q}$$

9 different "classes" of detectors

black: TG51
gold: fit

labels: (wall/ electrode)

Note large effects of high-Z electrodes



Carleton UNIVERSITY
Canada's Capital University

Uncertainties on calculated k_Q

- EGSnrc is accurate to 0.1 % against its own cross sections

- what are effects of cross section uncertainties?
  - are they correlated or not?
    - probably correlated for megavoltage photons

- what is uncertainty on $(W/e)_{air}$ being constant?
  - TRS-398 says 0.5% but evidence for any value is very thin

Carleton UNIVERSITY
Canada's Capital University

Cross section uncertainties on k_Q

standard error propagation, assuming uncorrelated

$$u_{k_Q} = \left[\sum_{i=1}^{n} \left(\frac{\partial k_Q}{\partial x_i} \right)^2 u^2(x_i) \right]^{\frac{1}{2}}$$

where $u(x_i)$ is the uncertainty on cross section x_i

Approximate $\boxed{\left(\frac{\partial k_Q}{\partial x_i} \right) = \frac{\Delta k_Q}{\Delta x_i}}$

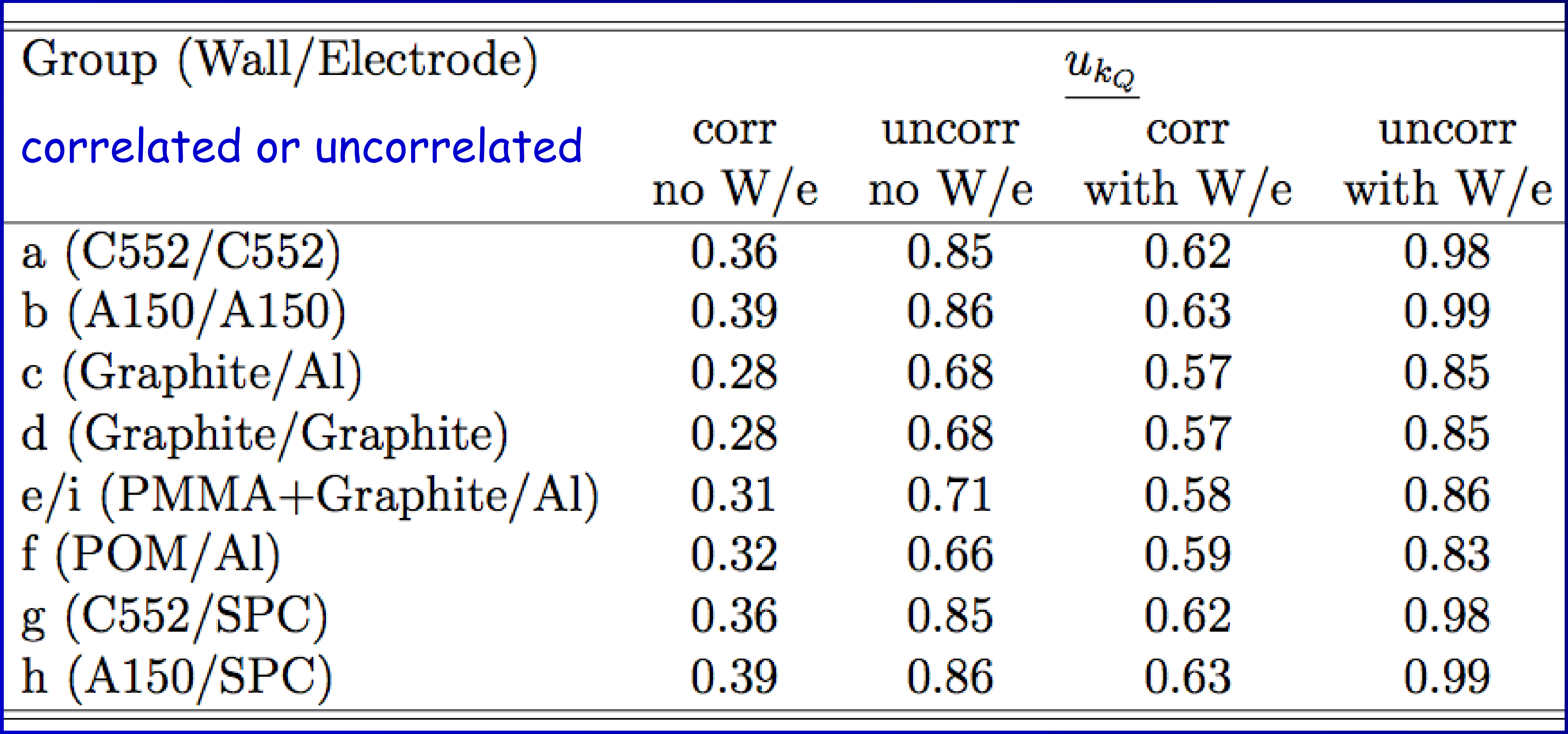
where Δk_Q is change in k_Q when i-th cross section is changed by Δx_i .

Calculate Δk_Q for Δx_i corresponding to $u(x_i)$.

$$\boxed{u_{kQ} = \left[\sum_{i=1}^{n} (\Delta k_Q)_i^2 \right]^{\frac{1}{2}}}$$

Carleton UNIVERSITY
Canada's Capital University

Uncertainties on k_Q for all chambers



Group (Wall/Electrode) correlated or uncorrelated	u_{k_Q} corr no W/e	 uncorr no W/e	 corr with W/e	 uncorr with W/e
a (C552/C552)	0.36	0.85	0.62	0.98
b (A150/A150)	0.39	0.86	0.63	0.99
c (Graphite/Al)	0.28	0.68	0.57	0.85
d (Graphite/Graphite)	0.28	0.68	0.57	0.85
e/i (PMMA+Graphite/Al)	0.31	0.71	0.58	0.86
f (POM/Al)	0.32	0.66	0.59	0.83
g (C552/SPC)	0.36	0.85	0.62	0.98
h (A150/SPC)	0.39	0.86	0.63	0.99

worst case: 0.39% 0.86% 0.63% 0.99%

Muir & Rogers Med Phys 37 (2010) 5939

Experimental measurements of k_Q

- many measurements done, but most papers measure one or two types of chambers
- McEwen measured k_Q for 27 different types against the Canadian primary standards of absorbed dose using ---->

  (Med. Phys. 37 (2010) 2179)

$$k_Q = \frac{N_{D,w}^{Q}}{N_{D,w}^{Co}}$$

- for "well-behaved" chambers

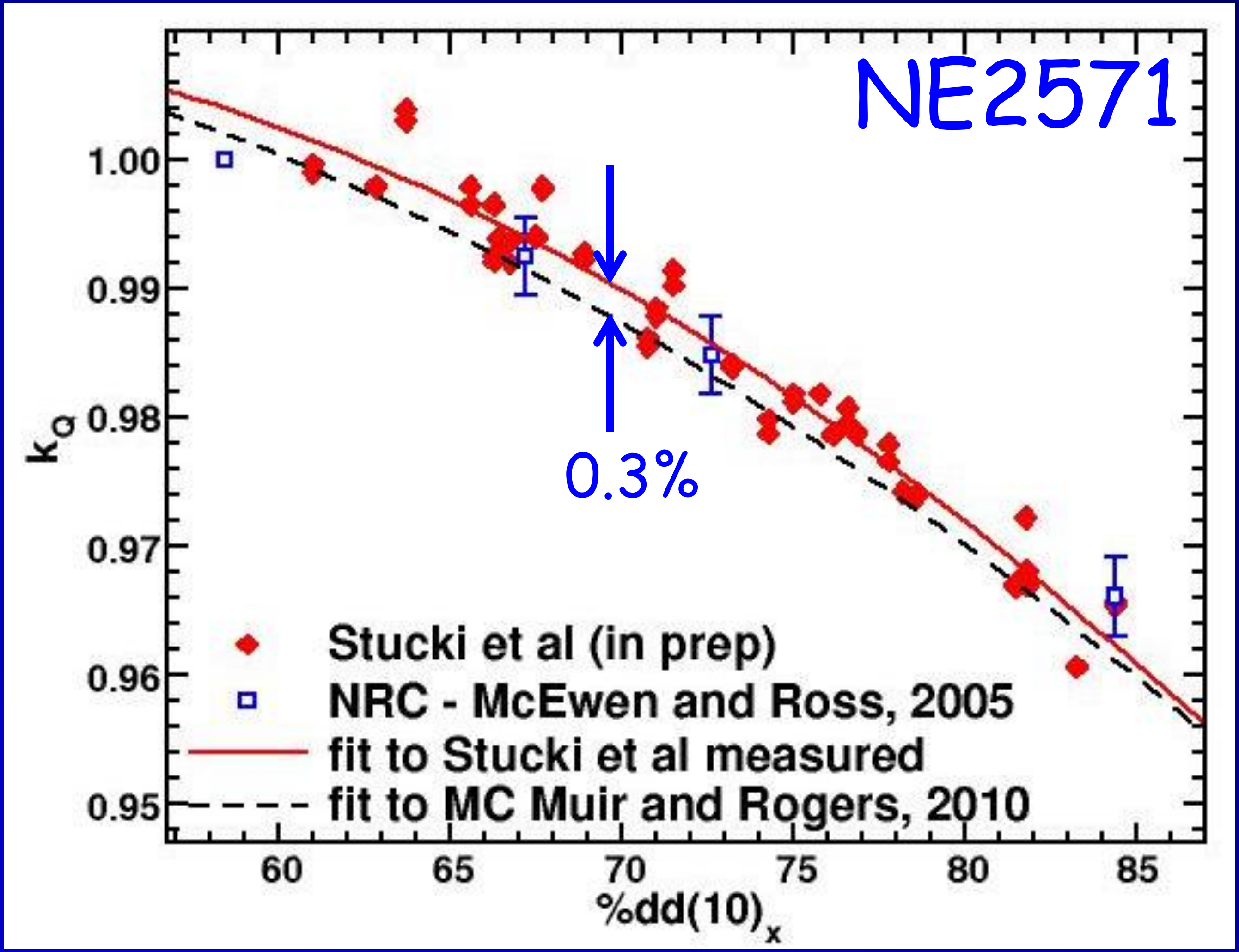
  measurement uncertainty on k_Q was 0.30%
- agreement with TG—51 values is excellent,

  typically 0.5% or better for "well-behaved"

Carleton UNIVERSITY
Canada's Capital University

Consistency of measured k_Q

diamonds are from standards labs (Stucki et al, to be published)



Muir et al Med Phys 38 (2011) 4600

How well do calculations and measurements agree?

$$\Delta_i = \frac{k_{Q,i}(calculated) - k_{Q,i}(measured)}{k_{Q,i}(measured)} \times 100\%$$

$$\chi^2/df = \frac{1}{f}\sum_{i=1}^{f} \frac{\Delta_i^2}{s_m^2 + s_c^2}$$

For 26 chambers in common,

- $\chi^2/df < 0.65$ for all chambers at 1 energy

- $\chi^2/df < 1$ for all chambers vs energy except 1

Suggests, if anything, uncertainties are too large

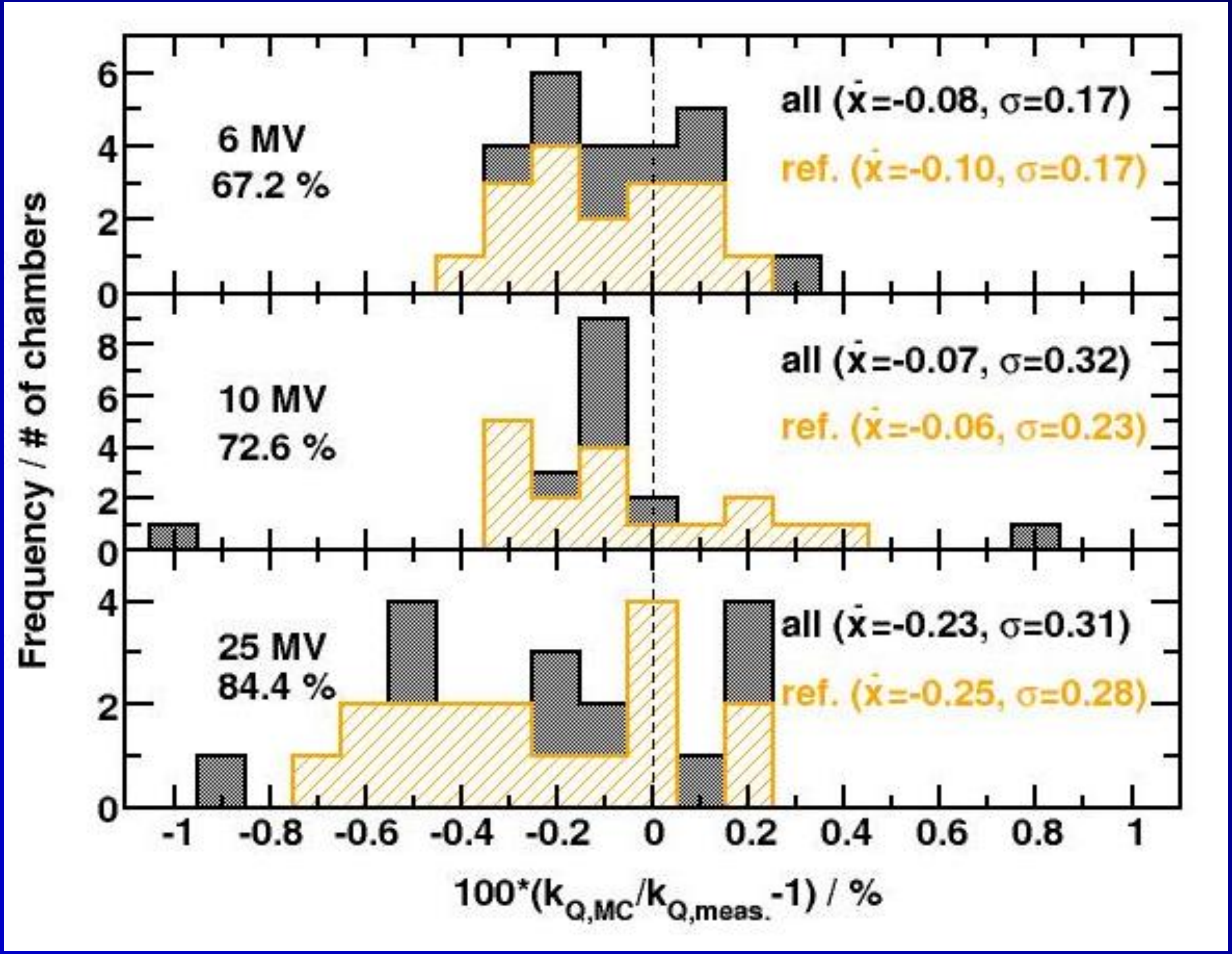
http://www.physics.carleton.ca/clrp/kQ

Measured vs calculated k_Q

26 chambers in common

shaded part is less precise chambers

remarkable agreement

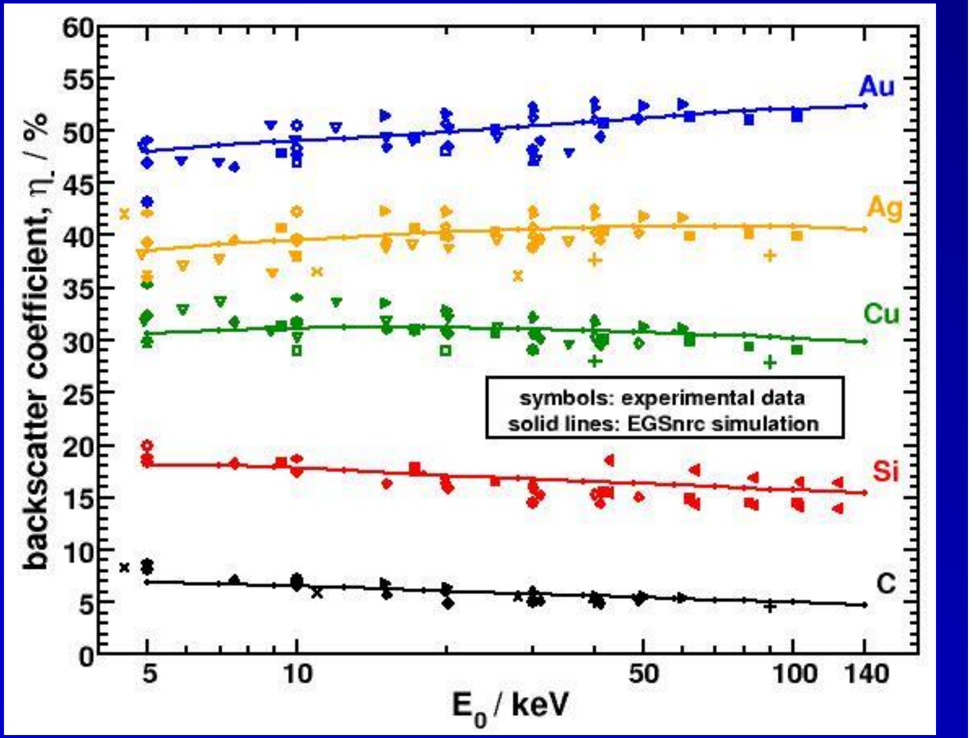


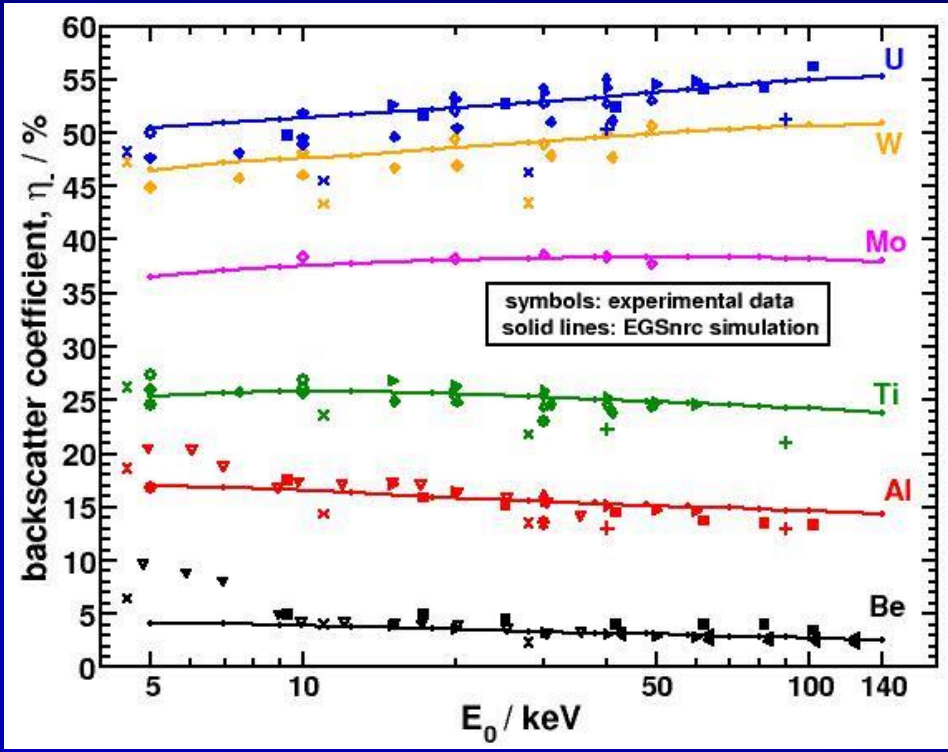
Carleton UNIVERSITY
Canada's Capital University

Backscatter coefficients

- e^- backscatter is the most difficult physical quantity for Monte Carlo to calculate
  - unfortunately it is also hard to measure accurately
- it is defined as the number of e- reflected from a surface per incident e- (above a low energy cutoff, about 50 eV to exclude secondary electron emission from the surface)

Backscatter - a tough test: kilovolts

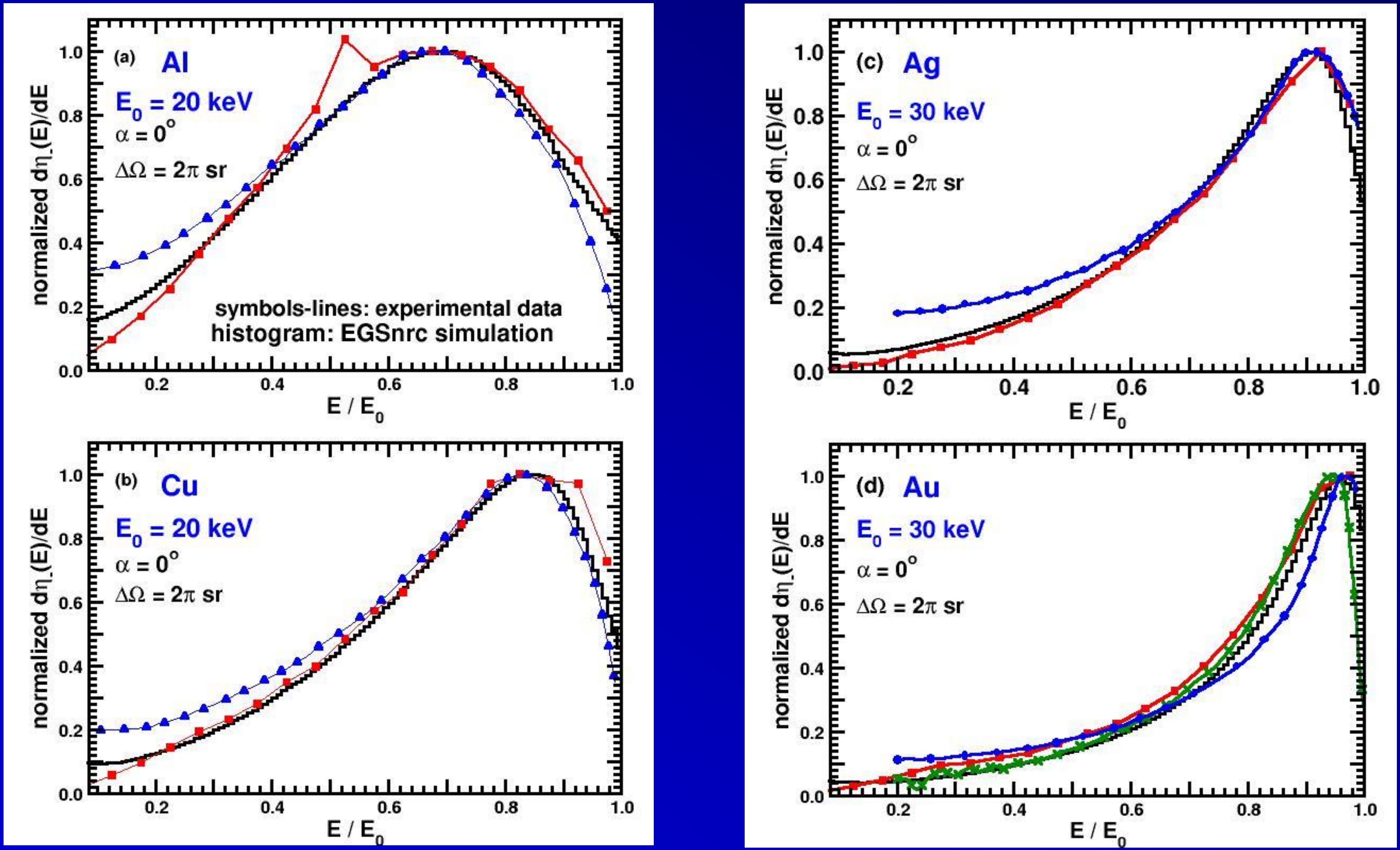




experimental data scatter about calculated values

Ali & Rogers PMB 53(2008) 1527-1543

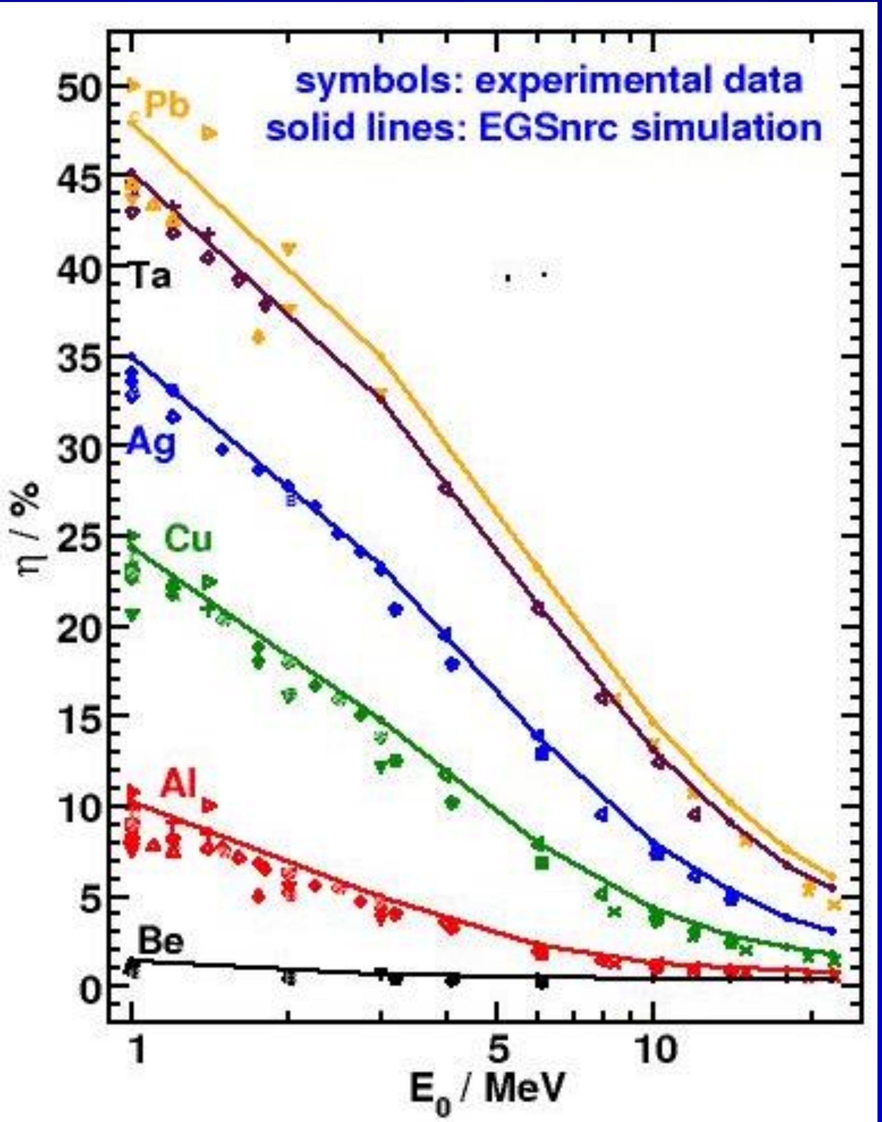
Backscatter - spectra

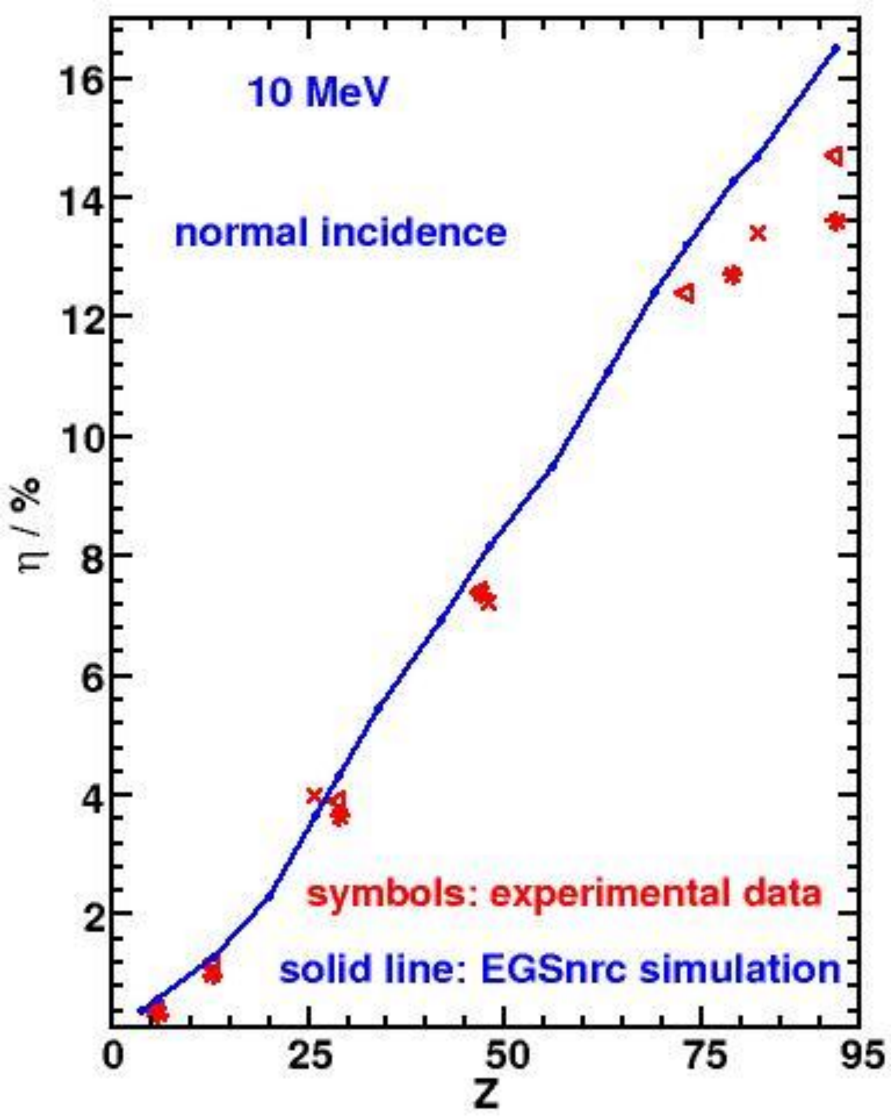


Ali & Rogers J Phys D: App Phys 41 (2008)055505

Backscatter: megavolts

Ali et al, in preparation





Accuracy of multiple scattering

Multiple scattering is a dominant physical effect for e-

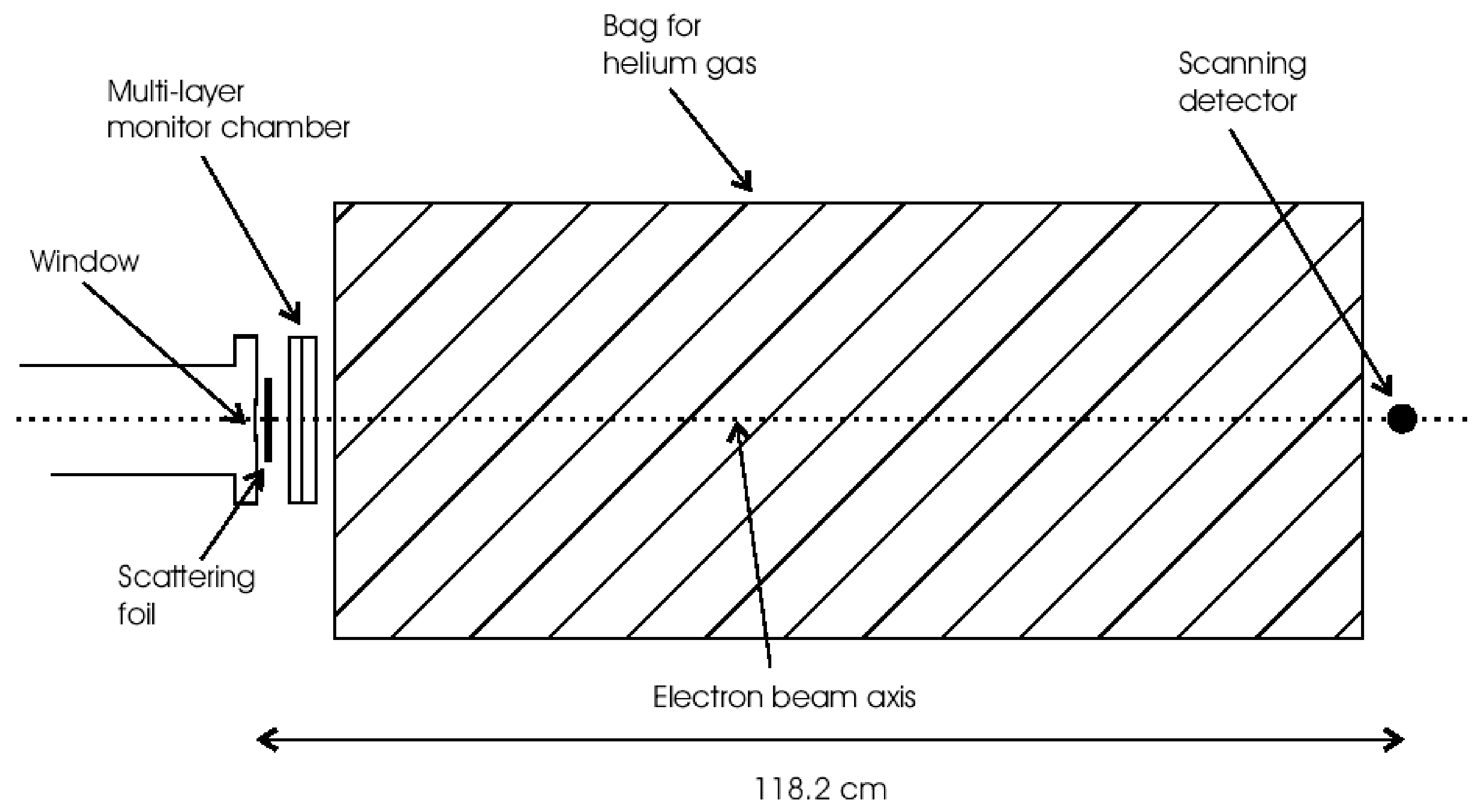
EGSnrc uses a multiple scattering theory developed by Kawrakow (NIMB 134 (1998) 325-336)

It has the advantage of seamlessly converting into a single scattering theory for very short steps.

Recently there have been some high quality measurements done by my ex-colleagues at NRC to test the theory as implemented in EGSnrc

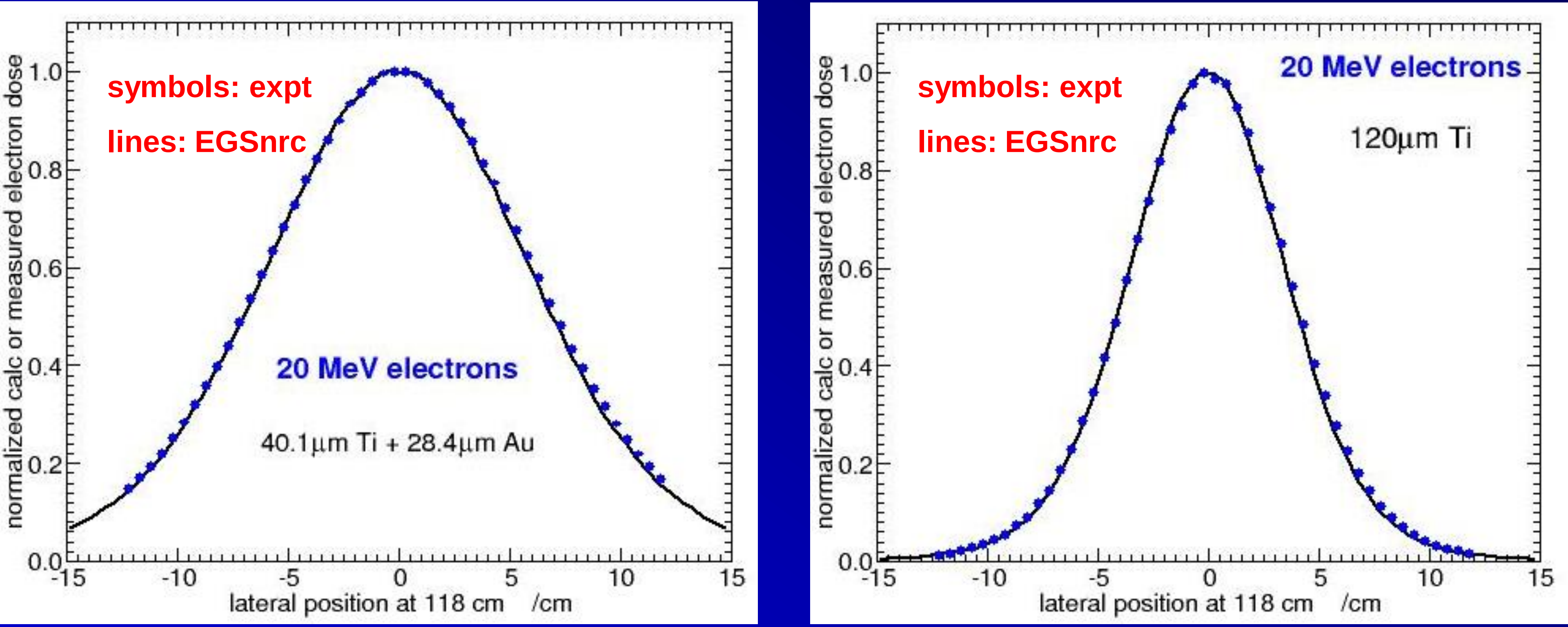
Ross et al, Med Phys 35 (2008)4121 - 4131

NRC experimental setup



Med Phys 35 (2008)4121 - 4131

NRC's results



Note the experiment is slightly wider than calculations

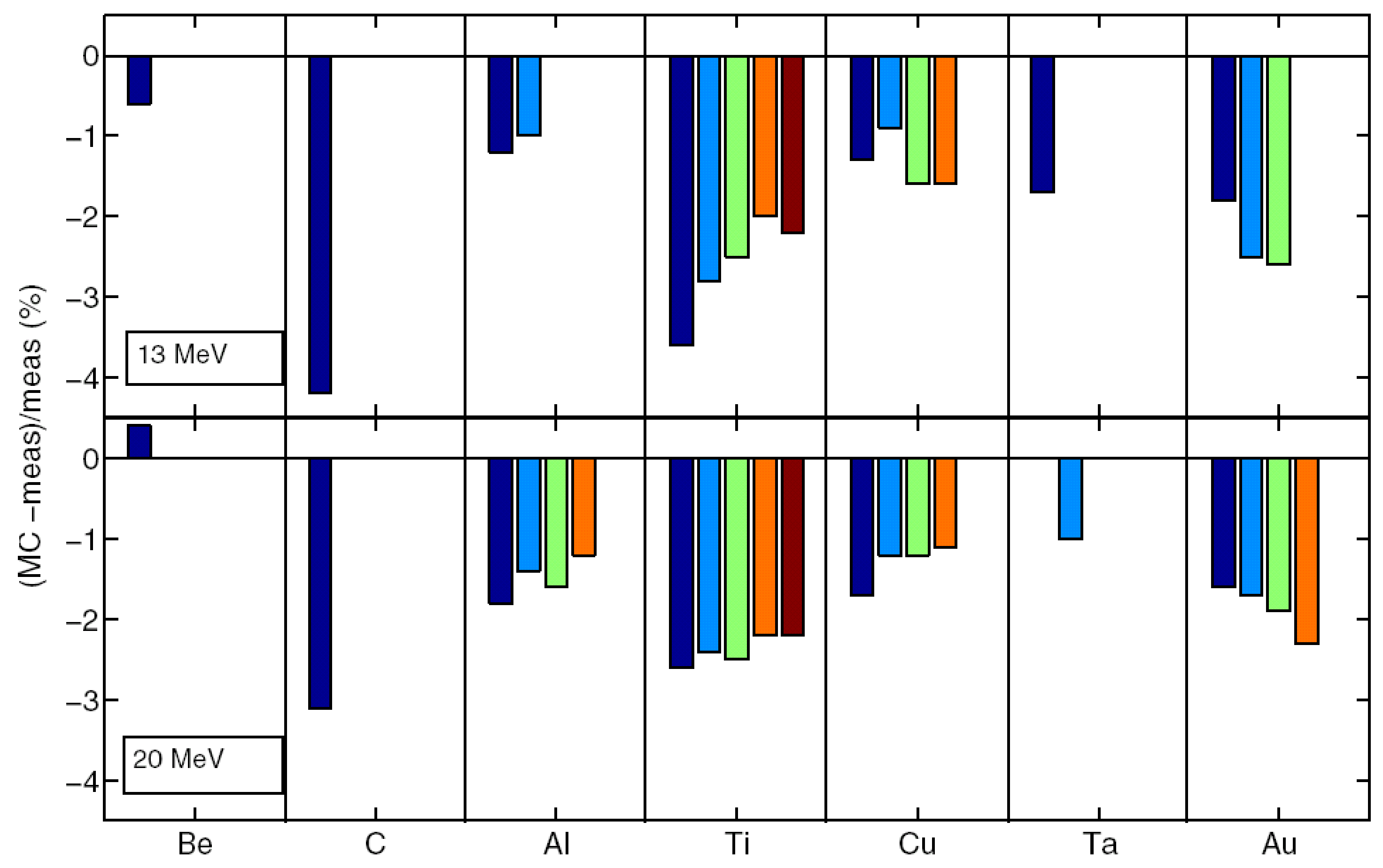
Thanks to Malcolm McEwen for the raw data

Med Phys 35 (2008) 4121 - 4131

NRC's results for $\theta_{1/e}$ widths

Experimental uncertainty

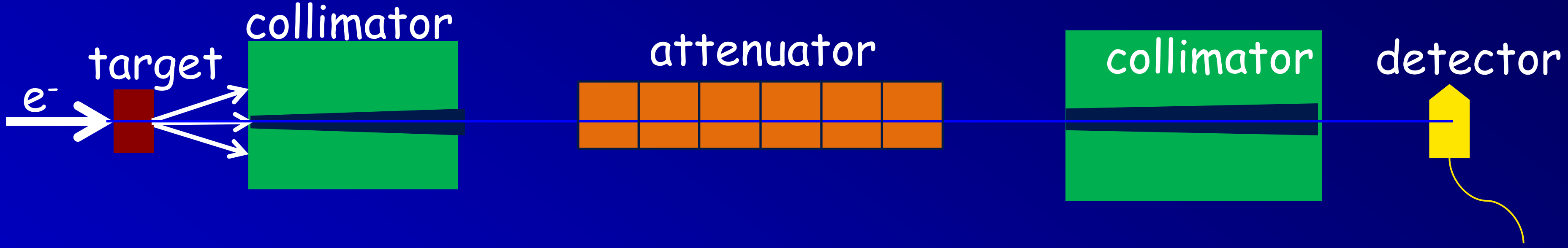
about 1 %.



each bar is a measurement with a different thickness foil

Ross et al Med Phys 35 (2008) 4121 - 4131

Transmission analysis



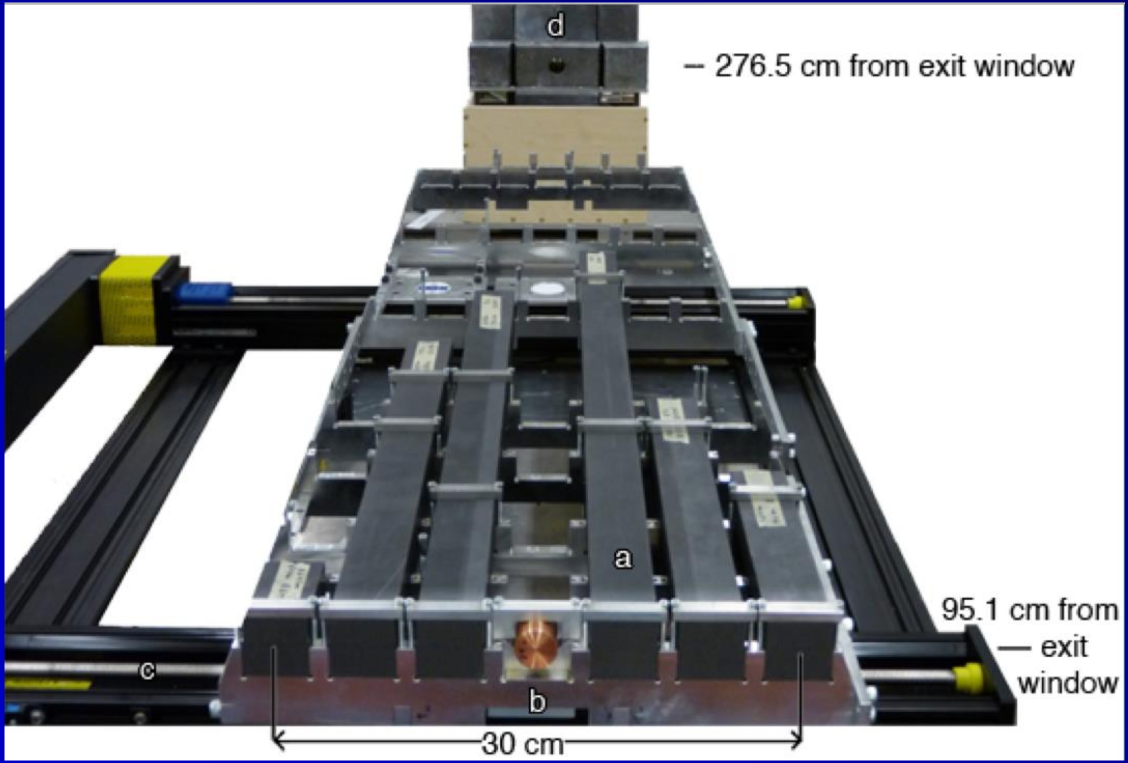
$$T(d, x_i) = \frac{M(d, x_i)}{M(d, 0)}$$

Goal of project was accurate determination of brem spectra from linac beams. Also provides a very stringent benchmark.

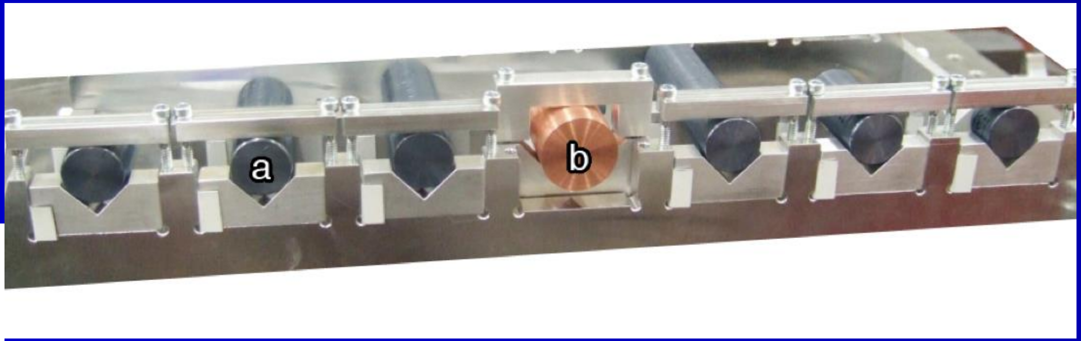
Ali et al Med. Phys. 39 (2012) 5990

Carleton UNIVERSITY
Canada's Capital University

Attenuator rack



graphite



lead

Uncertainty budget on $T(d,x_i)$

- 10 MV much worse since low energy limit of machine
- take into account
  - short term drifts < 0.15% P_{pol} < 0.15%
  - leakage < 0.1% P_{ion} < 0.03%
  - Monitor stability 0.1%
  - attenuator thickness <0.15% & non-uniformity< 0.1%
  - incident e- beam:
    - -mean energy varied 0.01 to 0.5%
    - -radial spread 0.15%, divergence 0.1%
- total without e- beam's u: < 0.35% (<0.55% 10 MV)
- total with e- beam's u: <0.64% (<0.88 % 10 MV)

e- beam's u only relevant for benchmark vs EGSnrc, not for clinical measurements

A problem

- the calculated transmission was wrong by up to 7% compared to the 0.64% experimental measurements.

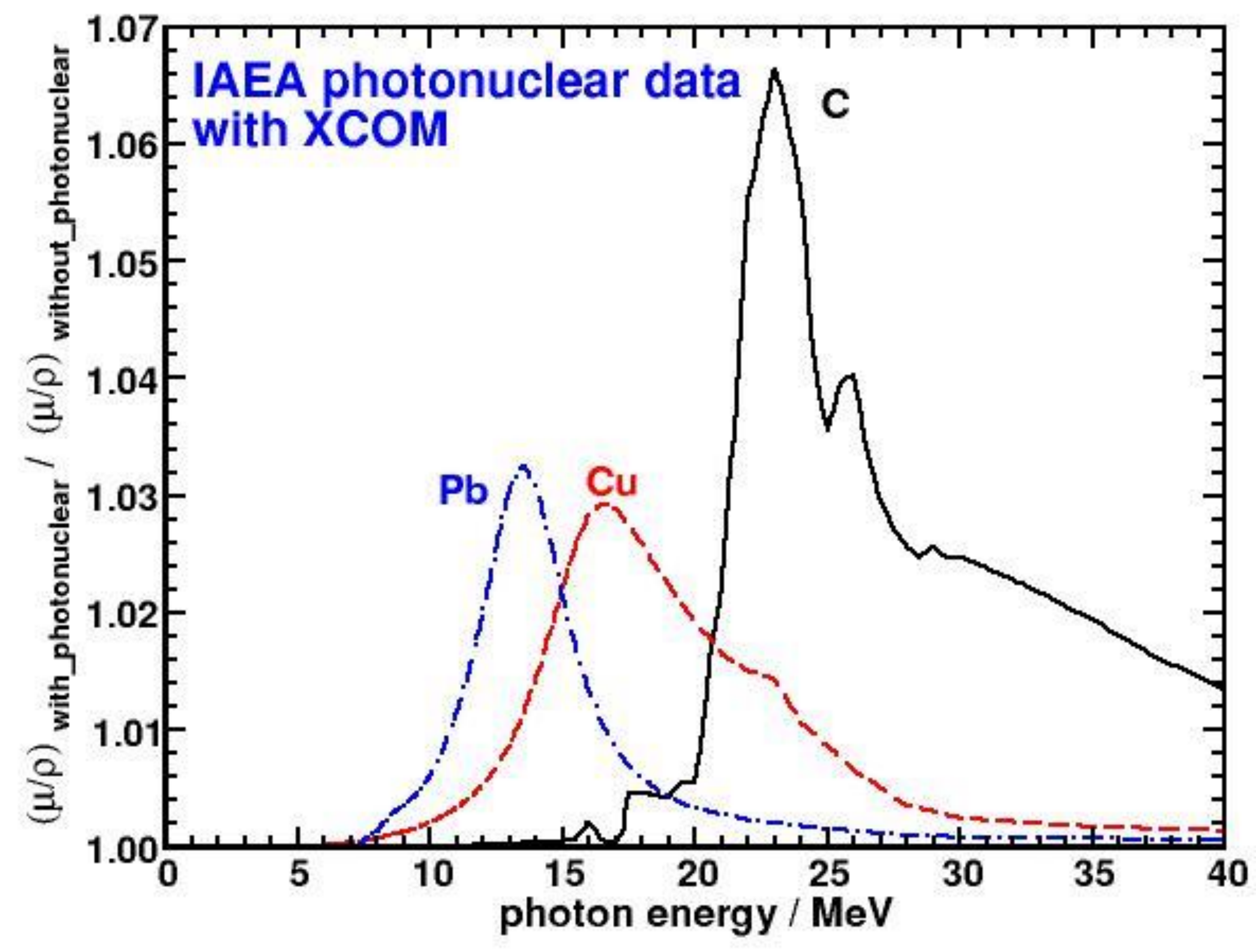
- attenuation by a factor of 100 is very sensitive to errors in cross section.
  - consider a monoenergetic case
    - $T=0.01 \Rightarrow e^{-\mu x}= 0.01$ but say μ should be 1.01μ

    and hence $T = e^{-1.01\mu x} = (e^{-\mu x})^{1.01} = 0.095$

    i.e. a 1% error causes a 5% change in T
- what about photonuclear interactions?

photonuclear cross sections

(γ,n) + (γ,p)



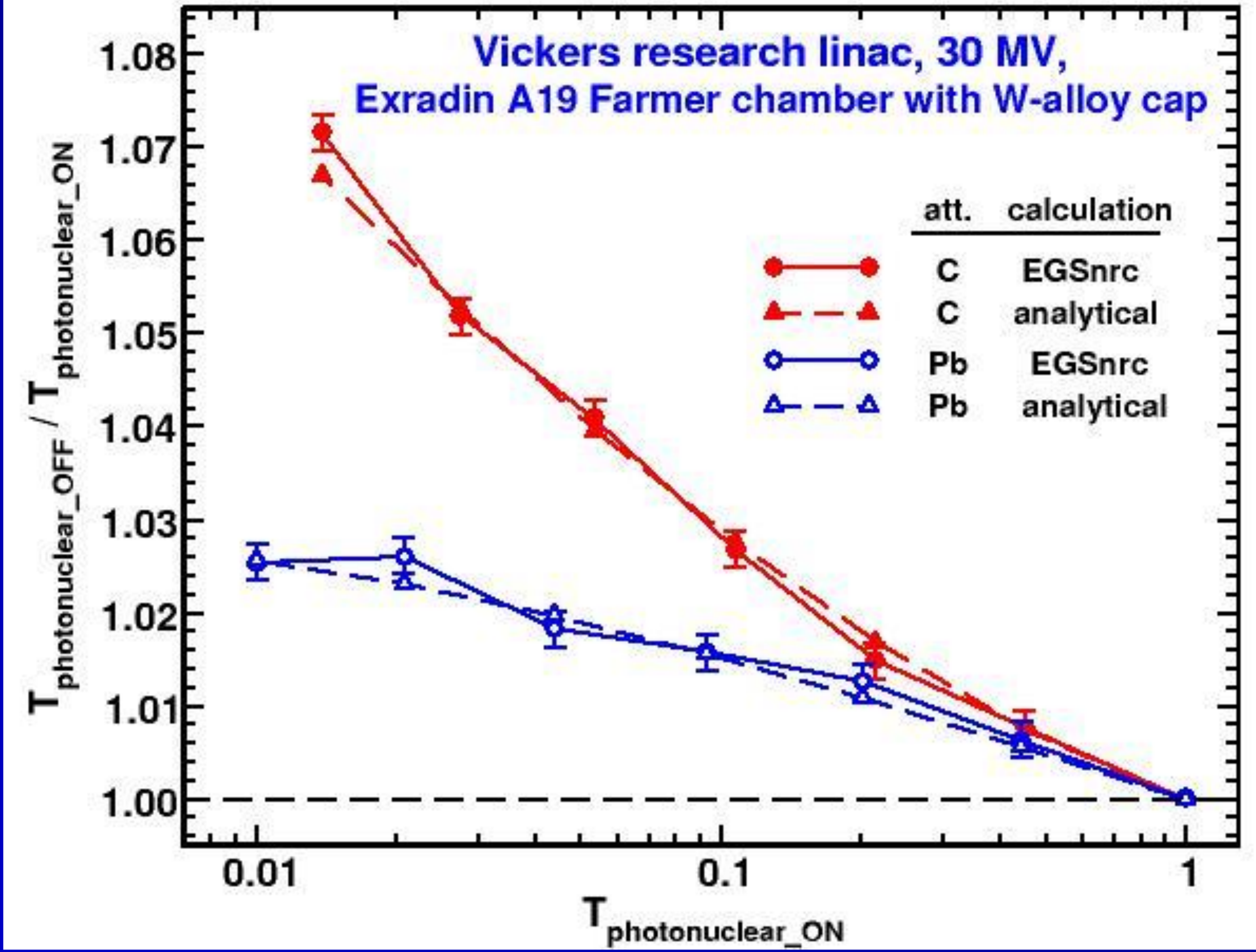
from E Ali
PhD thesis

Carleton UNIVERSITY
Canada's Capital University

Effects of photonuclear interactions

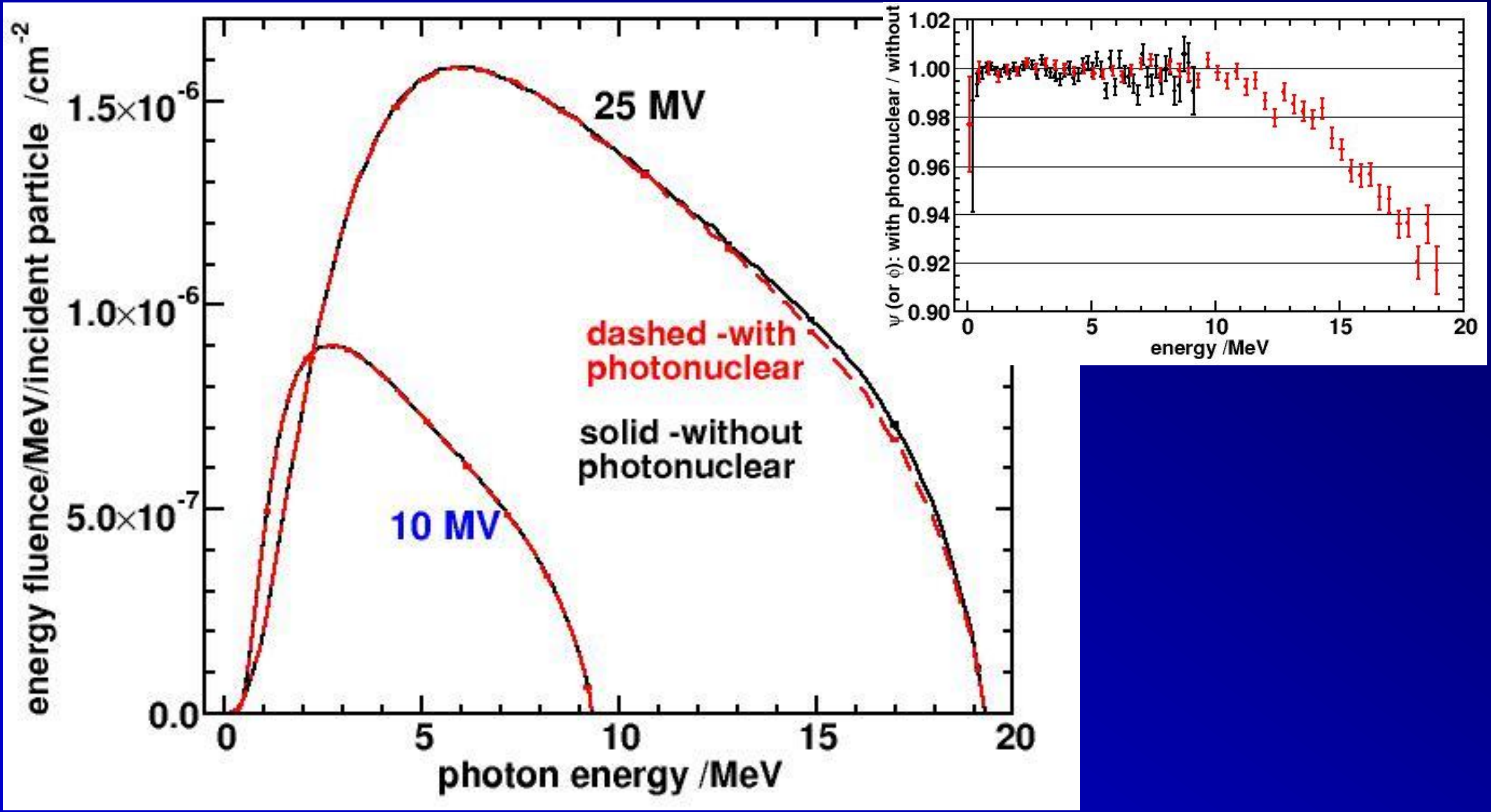
Ali added photonuclear attenuation (no energy deposition) into EGSnrc

case shown is worst case since high energy



analytic vs Monte Carlo as check on implementation

Aside: photonuclear effects on a clinical spectrum



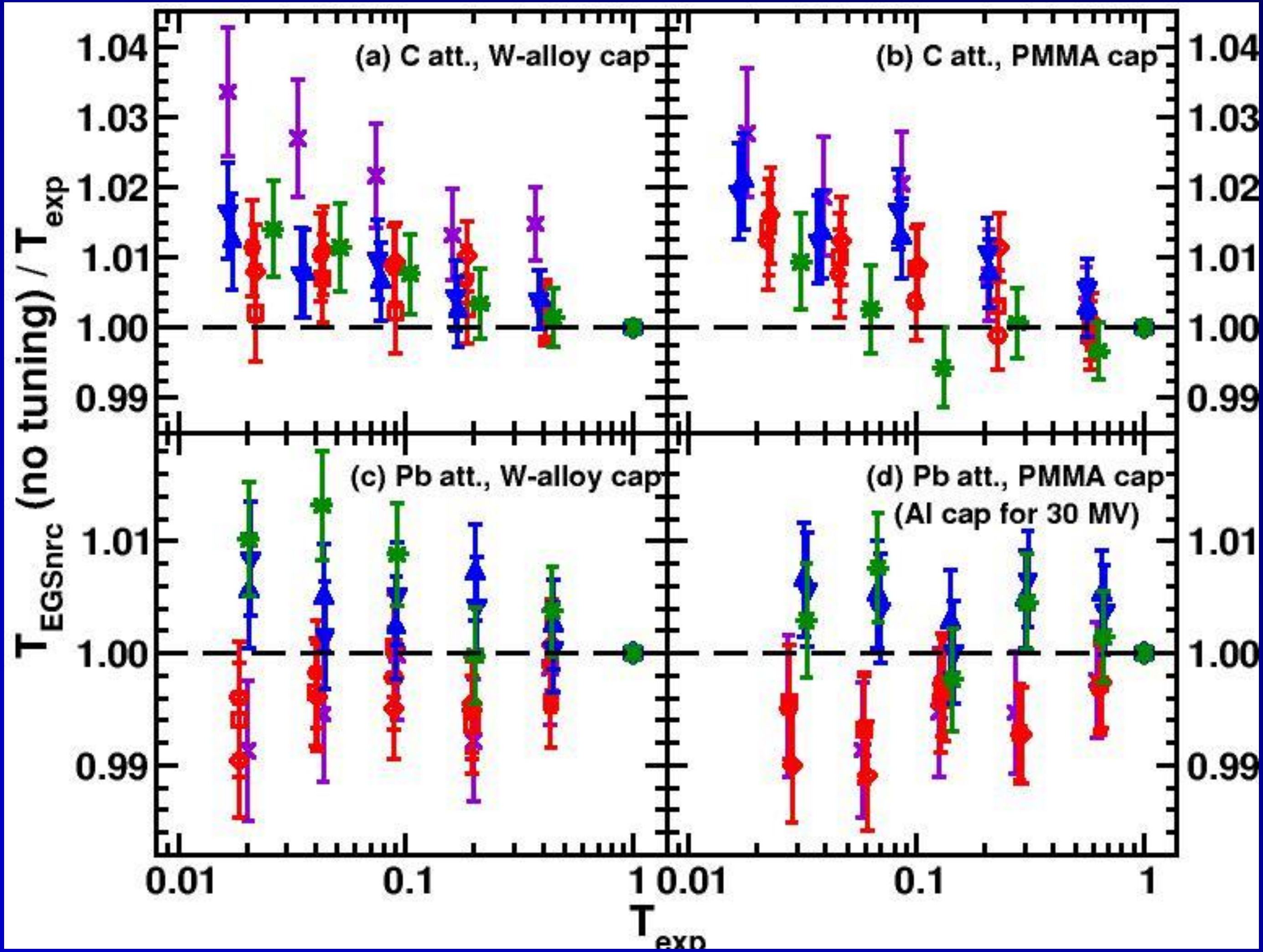
from E Ali (unpublished)

Carleton UNIVERSITY
Canada's Capital University

Direct comparisons of transmission data

Symbols → different target/energy combinations. x is 10 MV/Al

0.4% cross section change can explain all discrepancies within uncertainties.

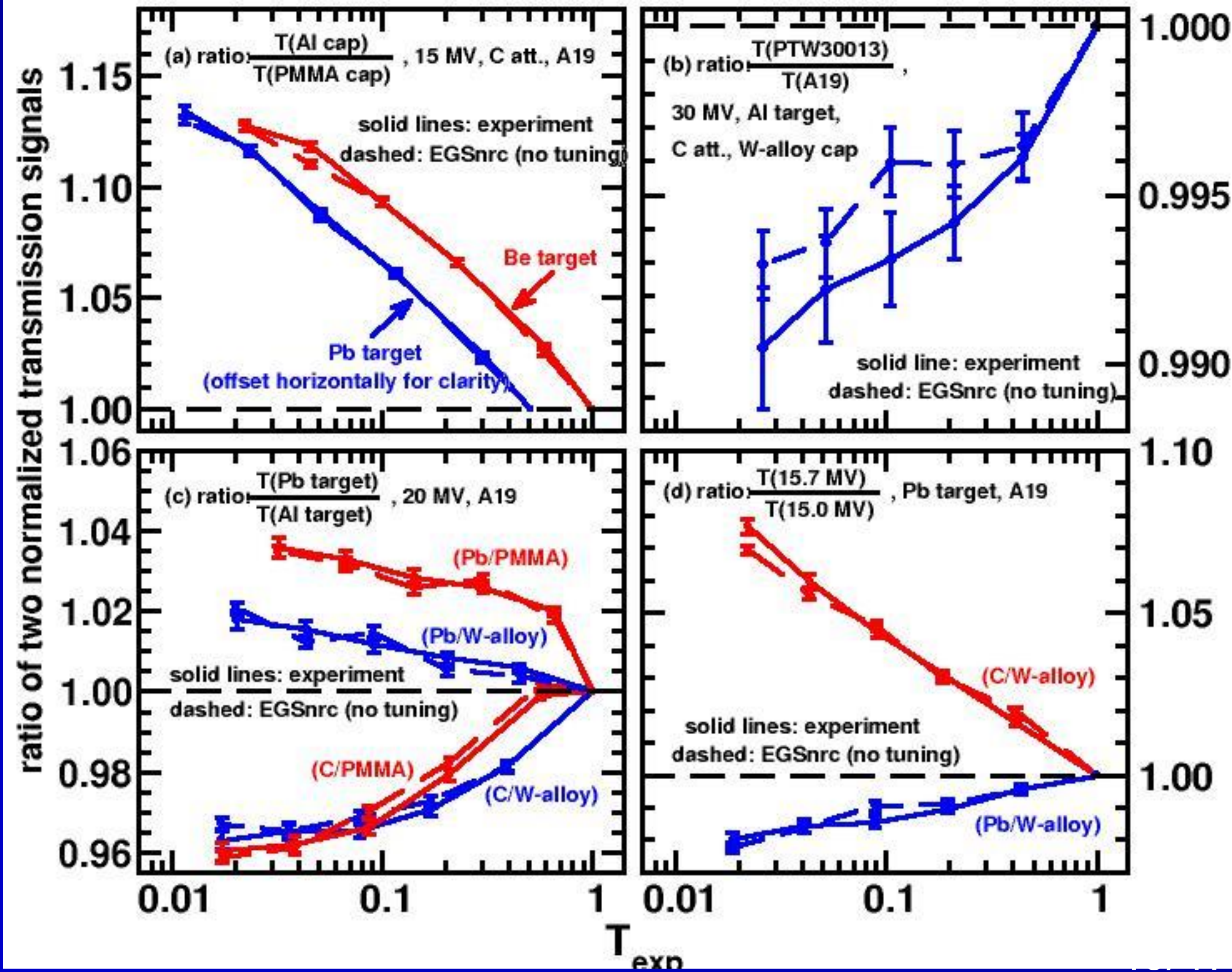


Do data tie down uncertainties on Xsections?

Calculation vs measurement
(ratios of T different targets,detectors,attenuators)

remarkable agreement

uncertainties from photon cross sections drop out of ratios (same in both)



Carleton UNIVERSITY
Canada's Capital University

Transmission: a very tough benchmark for Monte Carlo codes

- these data are a very stringent test of any MC code system
  - had to re-engineer XCOM cross sections
  - add photonuclear attenuation
  - use KM brem angular sampling rather than "simple" option in EGSnrc
- there is a report with all the data required to do a detailed comparison with Geant4, PENELOPE, MCNP.

Brachytherapy benchmarks

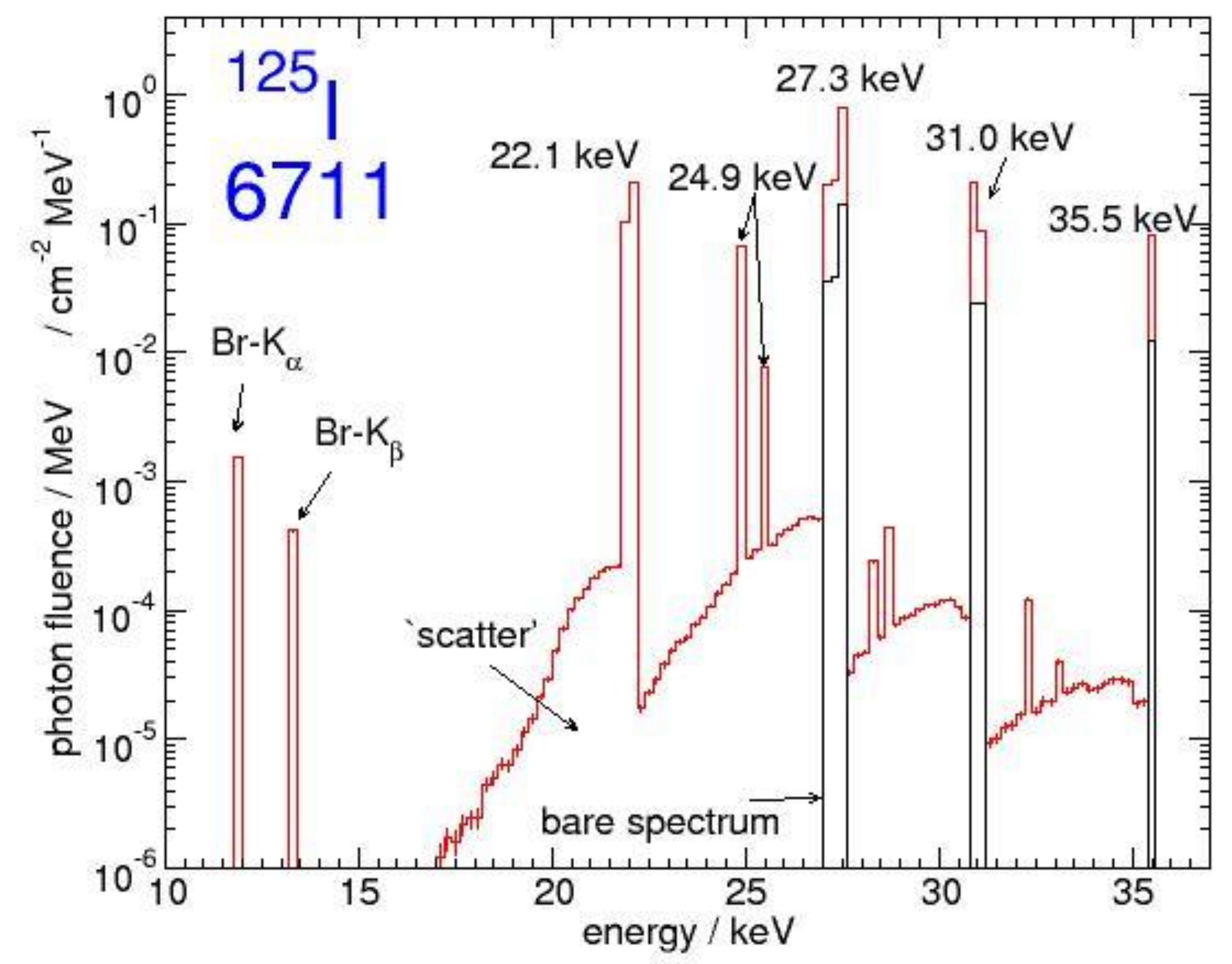
- Monte Carlo plays an essential role in brachytherapy dosimetry
  - calculates TG-43 parameters such as g(r), F(r,θ), Λ (dose rate constant)

- very hard to confirm these calculations with much accuracy as experiments have large uncertainties (5%).

- there have been teams measure spectra from multiple seeds with reasonable consistency

Carleton
UNIVERSITY
Canada's Capital University

^{125}I spectra (calculated)



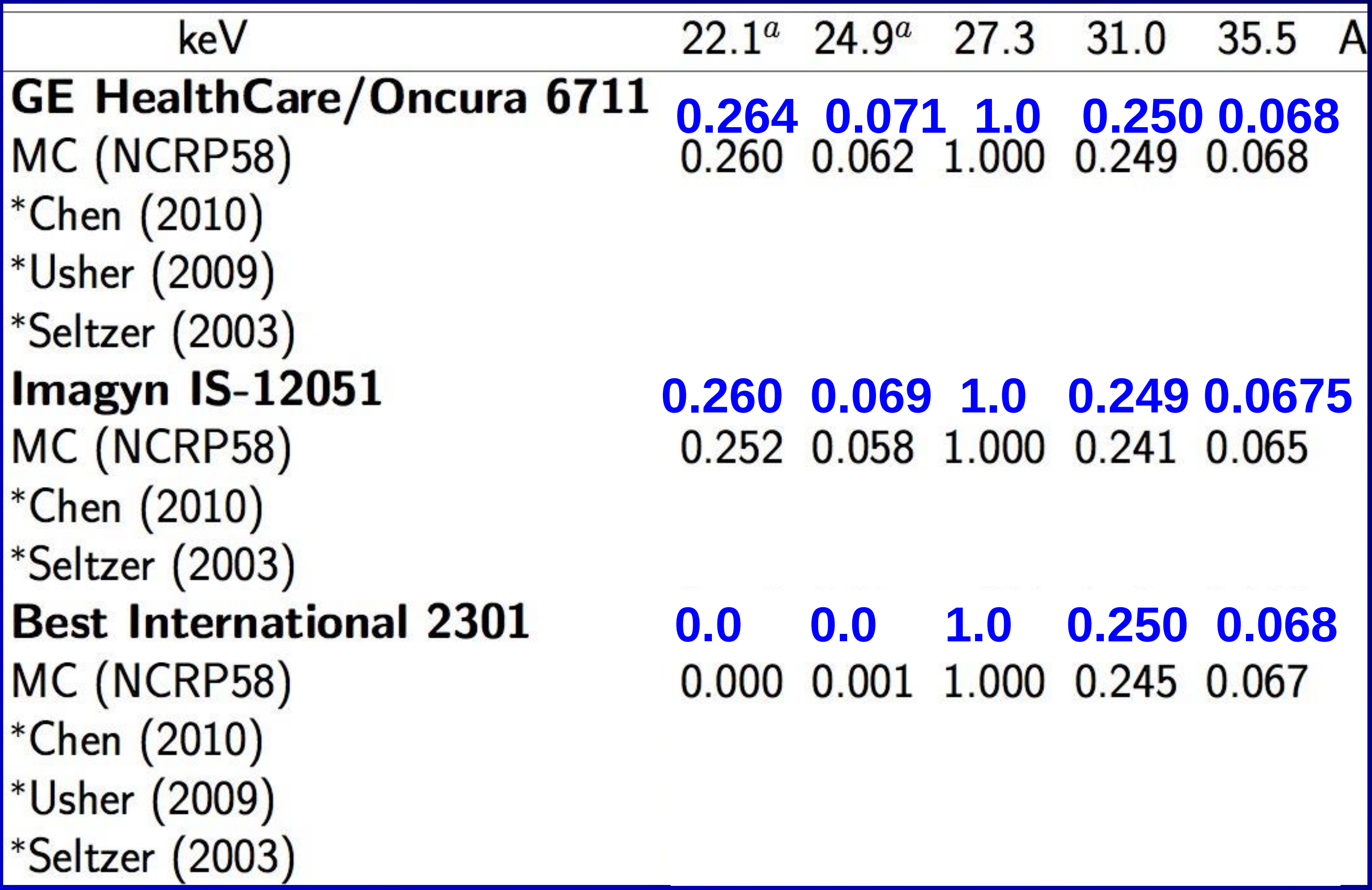
based on Rodriguez Med Phys 40(2013) 011713

Calculated vs measured branching ratios

Agreement

about same as variations in expt.

Same for 20 seeds total



keV	22.1^a	24.9^a	27.3	31.0	35.5	A
GE HealthCare/Oncura 6711	**0.264**	**0.071**	**1.0**	**0.250**	**0.068**	
MC (NCRP58)	0.260	0.062	1.000	0.249	0.068	
*Chen (2010)						
*Usher (2009)						
*Seltzer (2003)						
Imagyn IS-12051	**0.260**	**0.069**	**1.0**	**0.249**	**0.0675**	
MC (NCRP58)	0.252	0.058	1.000	0.241	0.065	
*Chen (2010)						
*Seltzer (2003)						
Best International 2301	**0.0**	**0.0**	**1.0**	**0.250**	**0.068**	
MC (NCRP58)	0.000	0.001	1.000	0.245	0.067	
*Chen (2010)						
*Usher (2009)						
*Seltzer (2003)						

Rodriguez and Rogers Med Phys 40(2013) 011713

What about measured vs calculated dose rate constants?

- TG-43 and its updates recommend averaging calculated and measured values of Λ
- this is because there is a systematic difference between them of 4.6% for ^{125}I as published.
- Problems:
  - intrinsic energy dependence of the TLDs used in the measurements was not properly accounted for (an 8.2% effect relative to ^{60}Co)
  - relative absorbed dose energy dependence of the different sizes of TLD chips used needed to be accounted for (a 2.7% effect)
- properly accounting for these, average difference for 22 measurements for 17 seeds drops to 0.8%

Carleton
UNIVERSITY
Canada's Capital University

Conclusions

- The EGSnrc code system is capable of accurately simulating a wide variety of experimental benchmarks

- By testing any computer code system we constantly are forced to make improvements
  - e.g. adding photonuclear attenuation and reworking the use of the XCOM cross sections

Thank you for your attention ☺

- much of the work was done by students and colleagues
  - Elsayed Ali, Bryan Muir, Dan La Russa, Manuel Rodriguez and Rowan Thomson at Carleton University
  - the k_Q experiments were in conjunction with NRC's Malcolm McEwen
  - EGSnrc and BEAMnrc systems have been developed and maintained by colleagues at NRC over the years
    - Iwan Kawrakow, Ernesto Mainegra-Hing, Blake Walters, Frederic Tessier

-work supported by a Vanier Scholarship, and NSERC CGS, OGSSTs, the CRC program, an NSERC DG, CFI and OIT

Carleton UNIVERSITY
Canada's Capital University

brem yield from thick targets

Faddegon et al Med Phys 17 (1990) 773 and

Med Phys 18 (1991) 727

measured brem yield as a function of energy and angle for many different target materials and compared their results to EGS4 calculations.

Typical experimental uncertainty: 5%

Faddegon et al Med Phys 35(2008) 4308 compared same measured data to 3 Monte Carlo codes:

EGSnrc, GEANT4 and PENELOPE

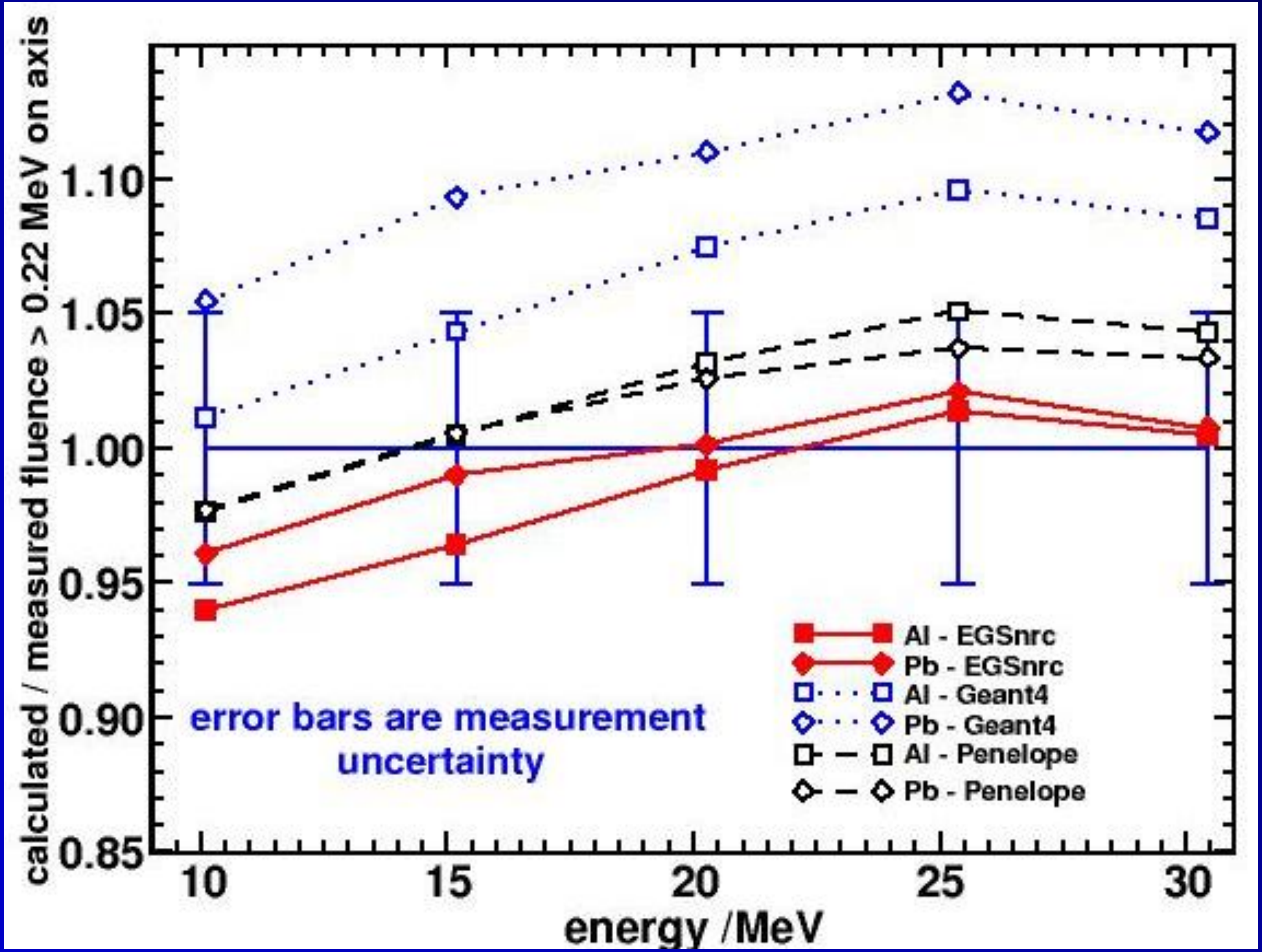
brem total yield vs incident energy

thick targets

5% uncertainty on measurements

photons

> 220 keV



Faddegon et al Med Phys 35 (2008) 4308

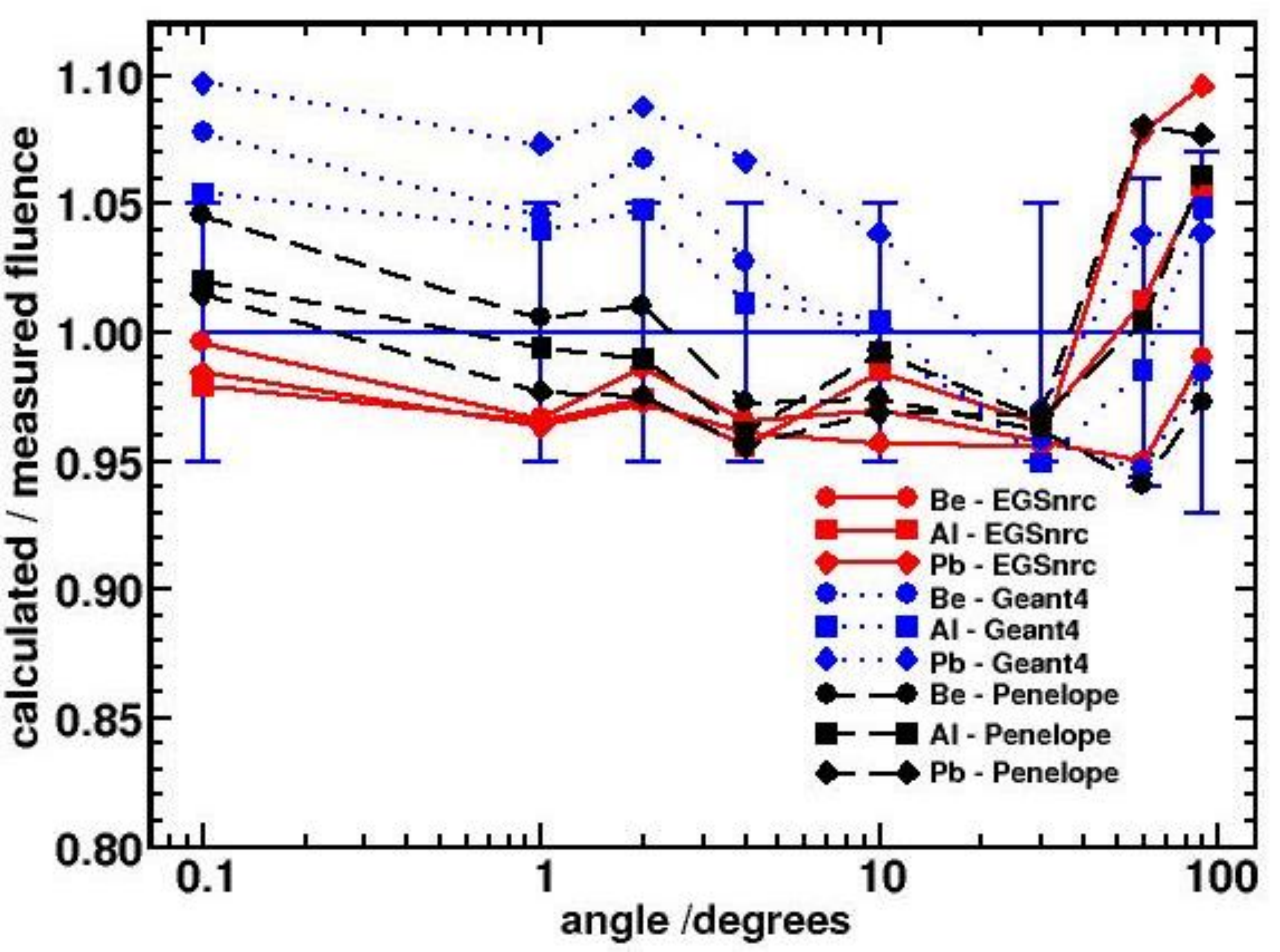
brem yield vs angle at 15 MV

thick targets

photons

> 145 keV

Note: yield at 90° is very small



Med Phys 35 (2008) 4308

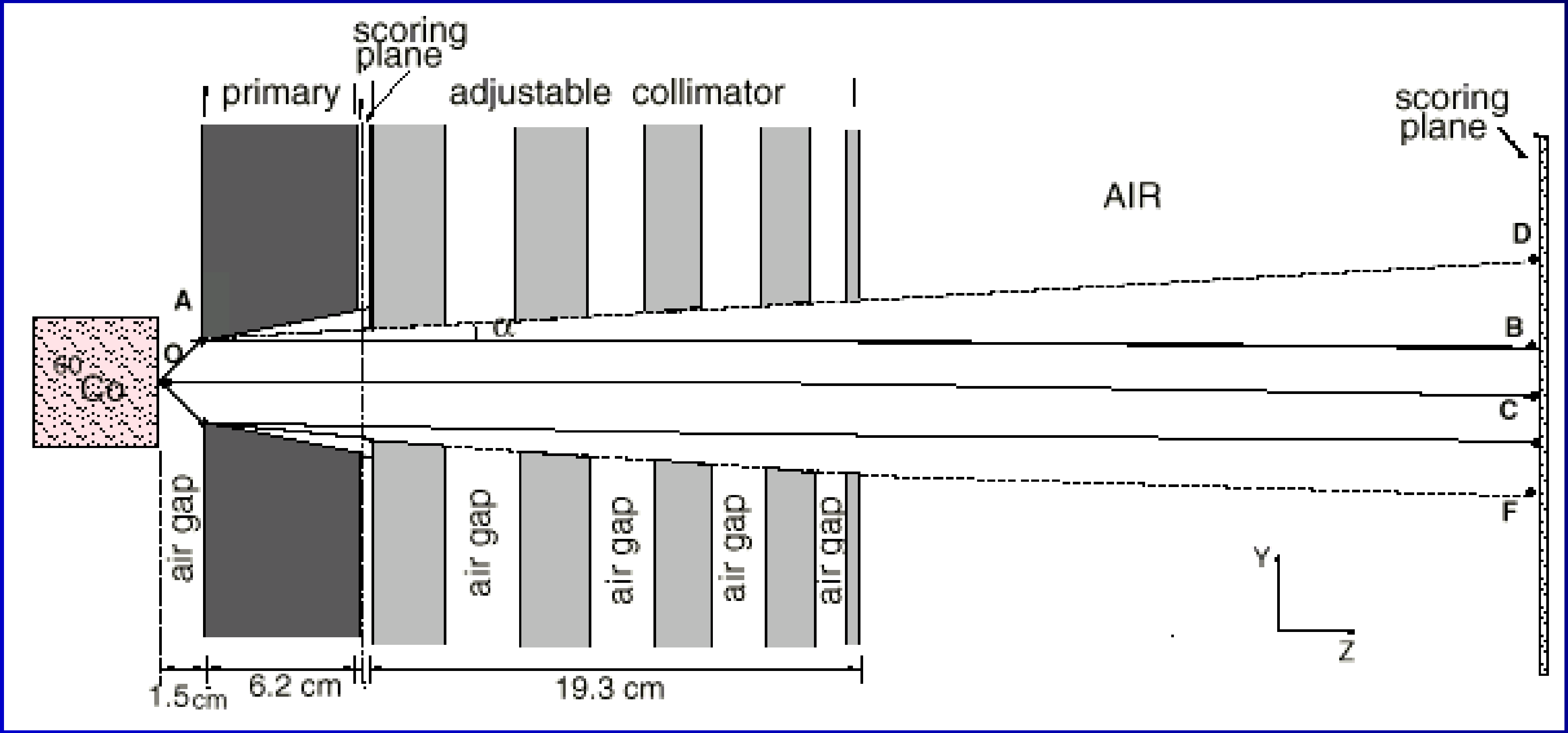
^{60}Co therapy unit

Issued
June 17,
1988

Carleton
UNIVERSITY
Canada's Capital University

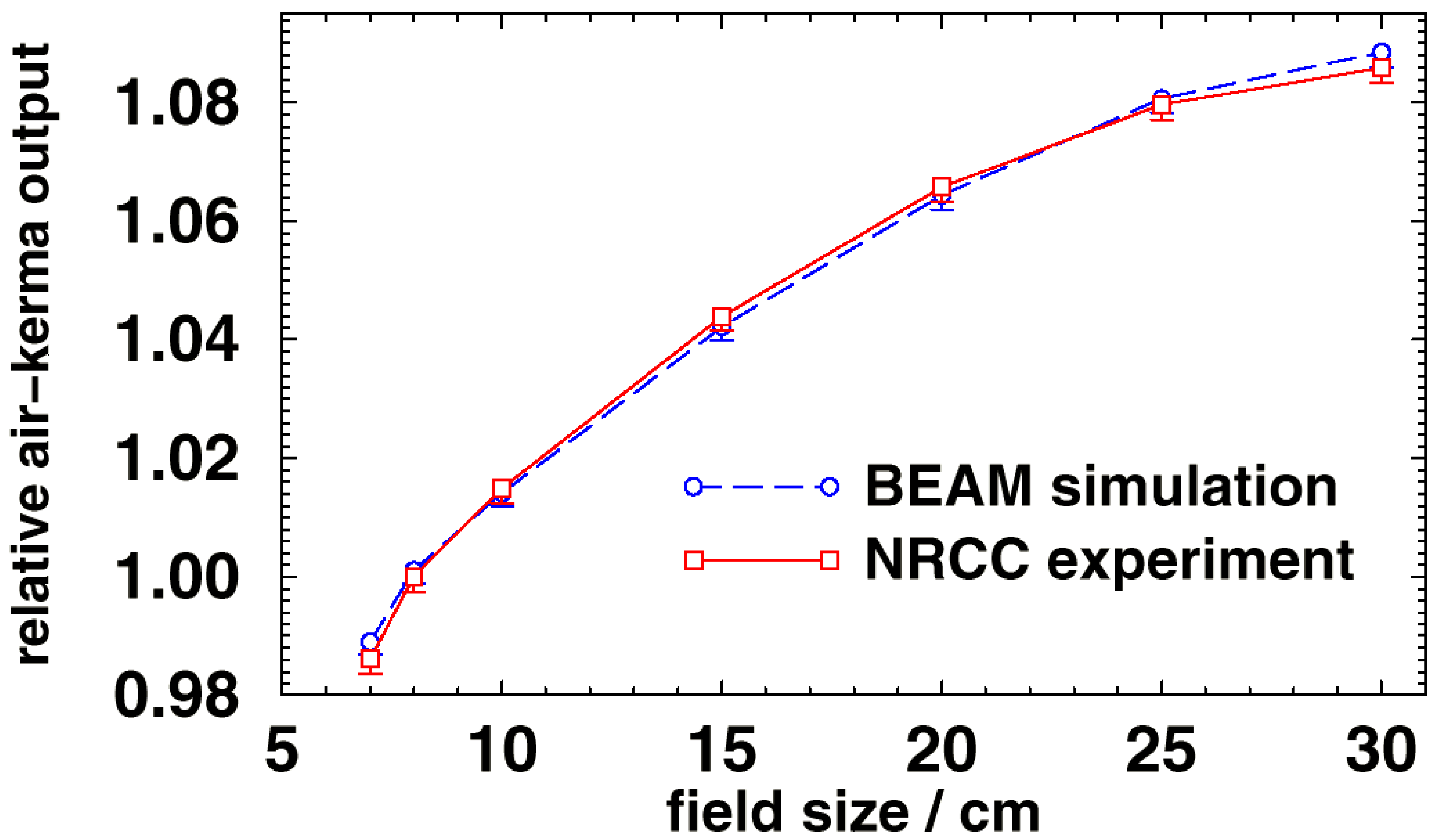
Thanks to
Jerry Battista

Simulating an Eldorado6



Mora et al Med Phys 26(1999) 2494

Output variation vs expt

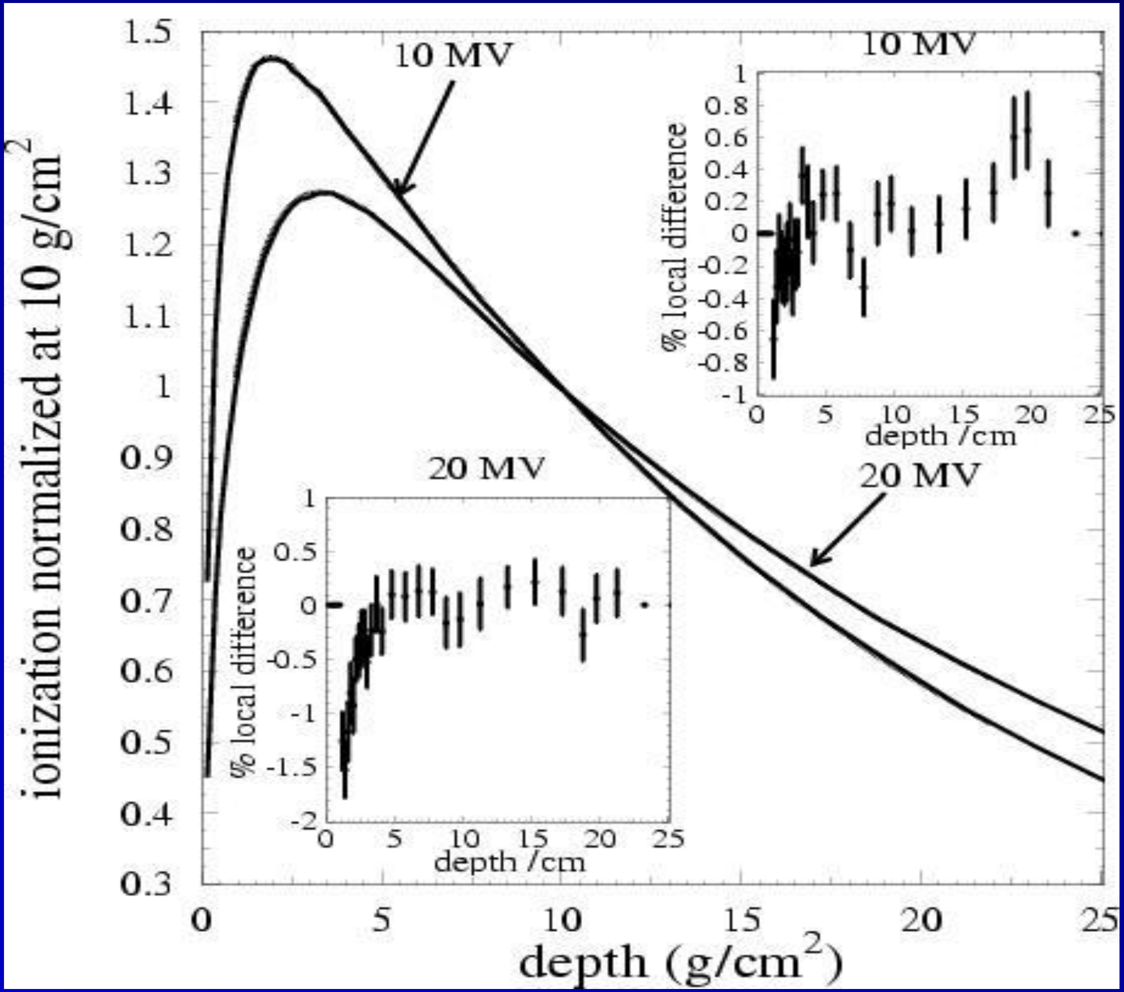


Med Phys 26(1999) 2494

10 & 20 MV beams from NRC linac

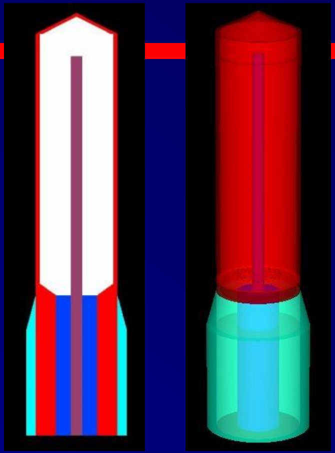
NRC research accelerator, everything is known about it, including incident electron beam energy. Ion chamber measurements.

A systematic problem near surface

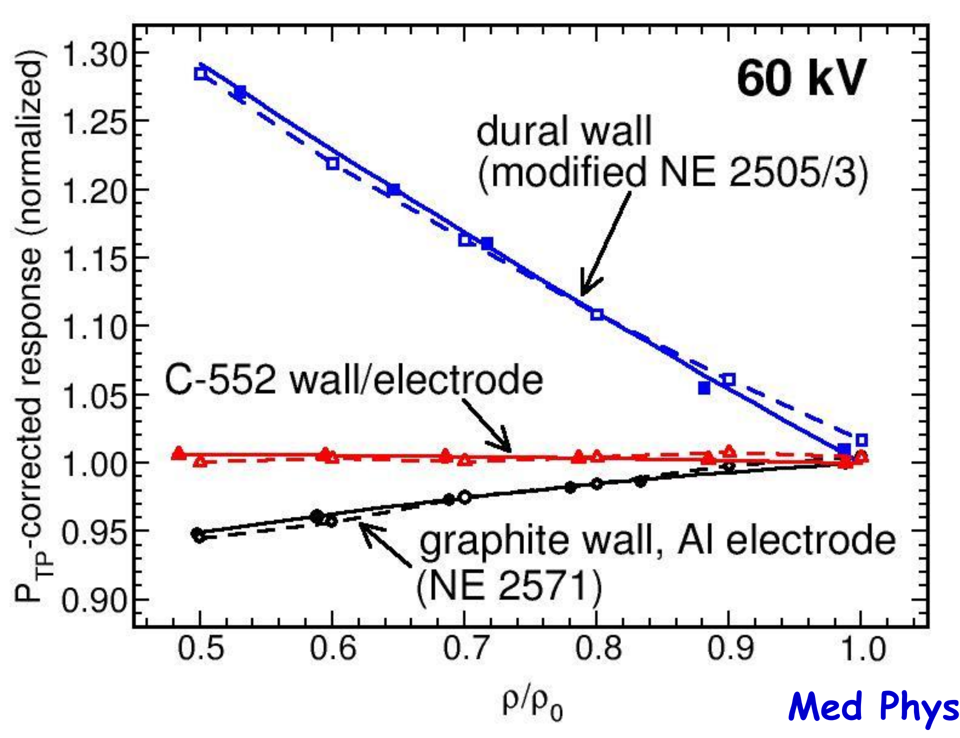


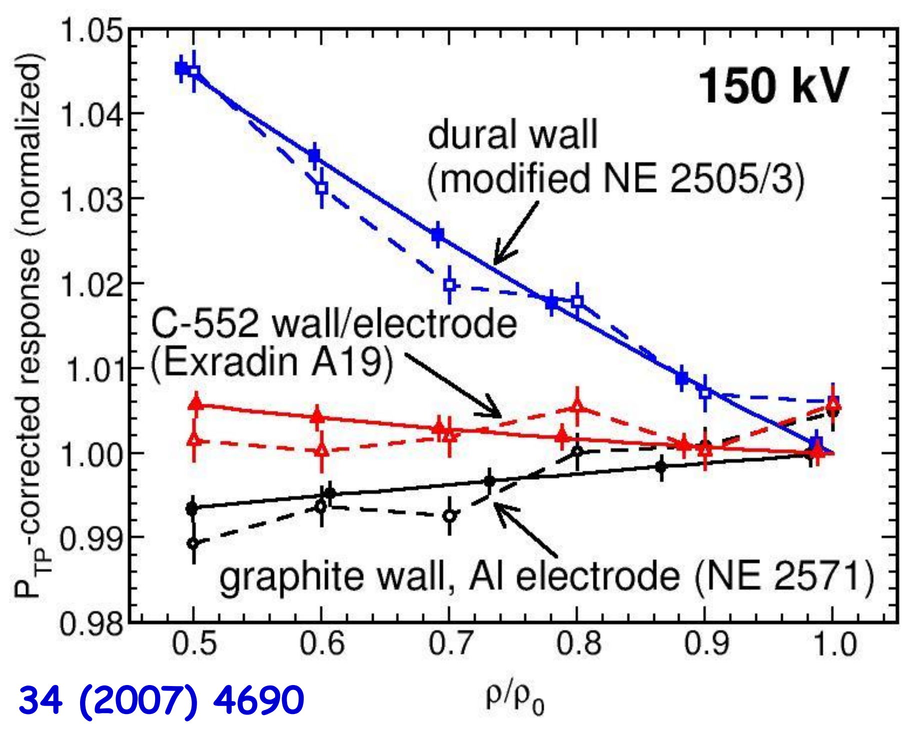
Sheikh-Bagheri et al Med Phys 27(2000) 2256-2266

LaRussa et al: variation of pressure x-ray beams



- experiment = solid line
- EGSnrc = dashed line
- Calculated results generally within 0.5%.





Med Phys 34 (2007) 4690