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Calorimetric Calculation of Electron Energy Deposition in Extended Media

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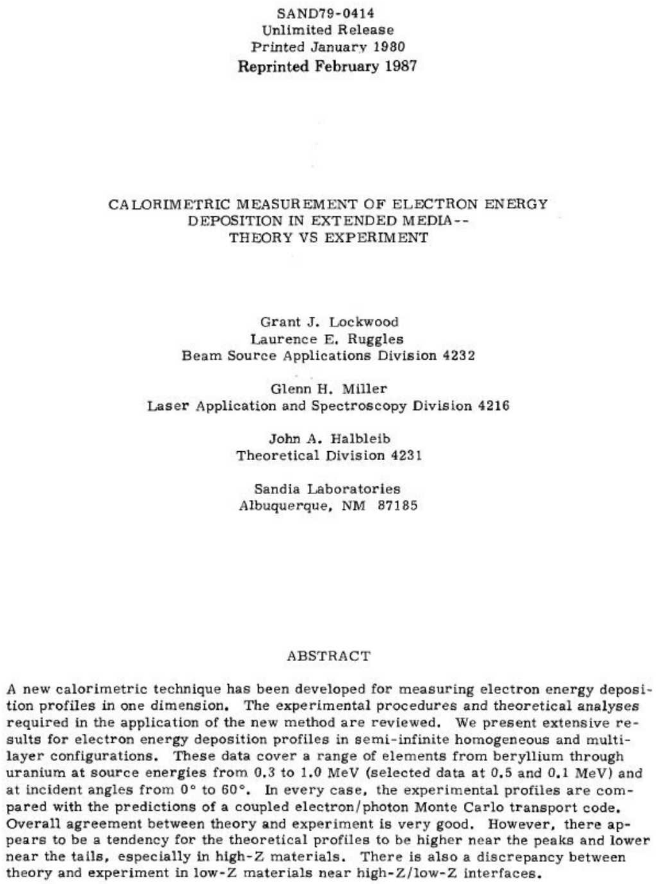
Lockwood Energy Deposition Experiment

- Developed new calorimetric technique for measuring electron deposition profiles in 1-D slabs.
- Covered low- to high-Z materials such as Be, C, Al, Fe, Cu, Mo, Ta, U, for both single- and multi-layer geometries.
- Experiments for 0.05 – 1 MeV electron beams, 0-60° angles.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CALORIMETRIC MEASUREMENT OF ELECTRON ENERGY DEPOSITION IN EXTENDED MEDIA-- THEORY VS EXPERIMENT

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ABSTRACT

A new calorimetric technique has been developed for measuring electron energy deposition profiles in one dimension. The experimental procedures and theoretical analyses required in the application of the new method are reviewed. We present extensive results for electron energy deposition profiles in semi-infinite homogeneous and multilayer configurations. These data cover a range of elements from beryllium through uranium at source energies from 0.3 to 1.0 MeV (selected data at 0.5 and 0.1 MeV) and at incident angles from 0° to 60°. In every case, the experimental profiles are compared with the predictions of a coupled electron/photon Monte Carlo transport code. Overall agreement between theory and experiment is very good. However, there appears to be a tendency for the theoretical profiles to be higher near the peaks and lower near the tails, especially in high-Z materials. There is also a discrepancy between theory and experiment in low-Z materials near high-Z/low-Z interfaces.

G. J. Lockwood, et. al. “Calorimetric measurement of electron energy deposition in extended media- theory vs experiment.” Technical Report SAND79-0414, SNL, 1987.

Lockwood Energy Deposition Experiment

- Experimental results used for ITS code validation in 1970s/80s, just right before ITS move to enhanced ionization/relaxation models.
- Electron x-sections and sampling distribution based on DATAPAC-4 and LIBRARY TAPE 2 of ETRAN.
- Theoretical results were more accurate at higher energies.

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Lockwood Energy Deposition Experiment

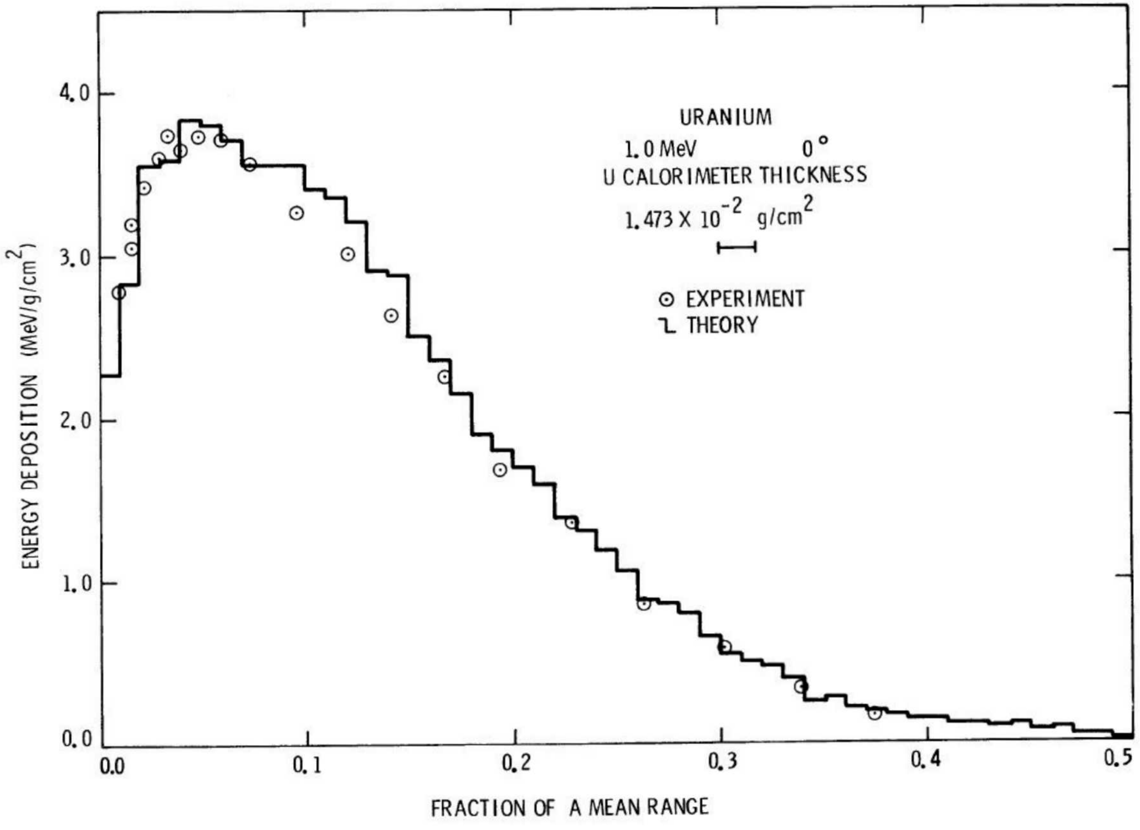
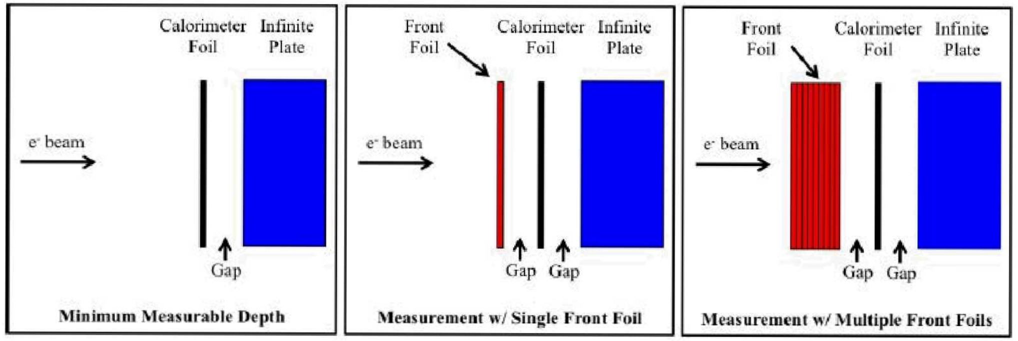


Figure V. H. 1. Comparison of Experimental and Theoretical Energy Deposition Profiles in Semi-Infinite Uranium for 1.0-MeV Electrons Incident at an Angle of 0°



D. A. Dixon & H. G. III Huges, “A Complete Reporting of MCNP6 Validation Results for Electron Energy Deposition in Single-Layer Extended Media for Source Energies <= 1-MeV.” Technical Report LA-UR-16-22749, LANL, 2016.

G. J. Lockwood, et. al. “Calorimetric measurement of electron energy deposition in extended media- theory vs experiment.” Technical Report SAND79-0414, SNL, 1987.

Lockwood Energy Deposition Experiment

Table V. H. 1

Electron Energy Deposition in Uranium[1,2,3]

Experimental Results
1.0 MeV, 0°

FMR	J
0.010	2.77
0.016	3.05
0.017	3.20
0.023	3.43
0.029	3.59
0.034	3.75
0.040	3.65
0.049	3.72
0.061	3.69
0.074	3.56
0.096	3.26
0.120	3.00
0.142	2.63
0.167	2.25
0.194	1.68
0.228	1.36
0.264	0.85
0.303	0.58
0.338	0.32
0.374	0.15

Total Deposition = 0.584 MeV

Theoretical Results
1.0 MeV, 0°

FMR	J	FMR	J
0.01	2.27	0.26	1.06
0.02	2.83	0.27	0.87
0.03	3.55	0.28	0.85
0.04	3.58	0.29	0.79
0.05	3.83	0.30	0.65
0.06	3.79	0.31	0.54
0.07	3.71	0.32	0.49
0.08	3.56	0.33	0.47
0.09	3.56	0.34	0.39
0.10	3.56	0.35	0.26
0.11	3.41	0.36	0.28
0.12	3.34	0.37	0.22
0.13	3.20	0.38	0.19
0.14	2.91	0.39	0.17
0.15	2.87	0.40	0.15
0.16	2.50	0.41	0.14
0.17*	2.36	0.42	0.12
0.18	2.14	0.43	0.12
0.19	1.90	0.44	0.10
0.20	1.81	0.45	0.12
0.21	1.61	0.46	0.08
0.22	1.59	0.47	0.09
0.23	1.38	0.48	0.05
0.24	1.30	0.49	0.05
0.25	1.18	0.50	0.03

Total Deposition = 0.615 MeV ±1%

1. FMR is fraction of a mean range.
2. J is energy deposited in $MeV/g/cm^2$.
3. Estimated experimental uncertainty is 1.4%.

*Estimated one-sigma statistical uncertainty exceeds 4% at larger FMR.

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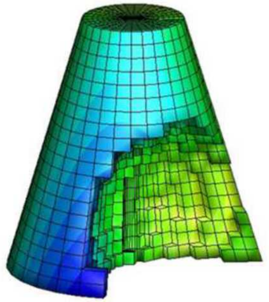
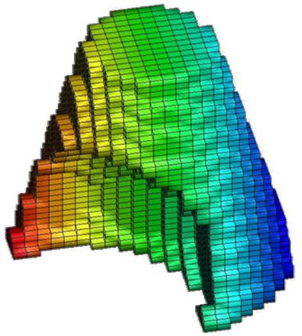
ITS Today

- Currently a set of 1D (TIGER), 2D (CYLTRAN), and 3D (ACCPET) Monte Carlo coupled electron/photon radiation transport codes.
- Continuous energy and multigroup cross sections.
  - XGEN: Continuous, works in the range of 1 keV to 1 GeV, can work below 1keV with LLNL data, materials are implicitly numbered in input order.
  - CEPXS: Multigroup, works in the range of 1keV to 1 Gev, LLNL data cannot be used, can be used for adjoint kerma calculations, materials are implicitly numbered in input order.
- Flexible 3D geometry allowing combinatorial geometry, CAD import and CAD libraries, and facetted formats either separately or together.

ITS Today – 1D Slab Geometry

- Geometry input
  - For a given layer normal to the z-direction: material number, number of subzones, thickness (cm).
  - Subzones are automatic uniform-thickness division of a layer.
  - Voids are not allowed.
- Minimal input required
  - Geometry and cross section files.
  - Default tallies for energy and charge deposition in output.
  - Integral forward and backward escape currents in output.
- Source specification
  - Default is monodirectional pencil electron beam centered at z=0.





MCNP Input

```
c ================================ CELL CARDS ================================
c
100 0                -10    imp:p,e=0 $ Graveyard
200 0                -20 10 imp:p,e=1 $ Vacuum for electron source
300 1000 -1.85       -21 20 imp:p,e=1 $ Be foil
400 0                -30 21 imp:p,e=1 $ 0.1 cm vacuum gap
500 1000 -1.85       -32 30 imp:p,e=1 $ Be calorimeter
600 0                -40 32 imp:p,e=1 $ 0.1 cm vacuum gap
700 1000 -1.85       -41 40 imp:p,e=1 $ Infinite Be plate
999 0                 41    imp:p,e=0 $ Graveyard

c =============================== SURFACE CARDS ===============================
c
10 px -2.000000000  $ Front of vacuum
20 px -0.105989189  $ Front of Be foil
21 px -0.101316486  $ Back of Be foil
30 px -0.001316486  $ Front of Be calorimeter
31 px  0            $ Plane to tally energy deposition in Be
32 px  0.001316486  $ Back of Be calorimeter
40 px  0.101316486  $ Front of infinite Be plate
41 px  1.101316486  $ Back of infinite Be plate

                    ---- -----
```

```
c ================================ DATA CARDS ================================
c
c --------------------------->>> Physics Options <<<---------------------------
mode p e
nps  1e6
area 1 1 1 1 1 1 1 1
vol j 1.894010811 0.004672703 0.1 0.002632972 0.1 1 j
cut:p j 1e-3
cut:e j 1e-3
c
c ---------------------------->>> Material Data <<<----------------------------
c
c Beryllium, density = 1.85 g/cc
m1000  4000 -1.000000 $ Be
c
c ---------------------------->>> Source Data <<<----------------------------
c
sdef par=e erg=1.033 x=-1 ext=0 dir=1 vec=1 0 0
c
c ------------------------->>> Tally Specifications <<<------------------------
c
c fc2 Energy deposition in Be calorimeter (MeV/g/cm^2)
c f2:p 31
c fm2 1 1000 -5 -6
c
fc6 Energy deposition in Be calorimeter (MeV/g/cm^2)
+f6 500
```

ITS Input

```
echo 1
title
 Calorimetric measurement of electron energy deposition in Be
*
********************************************************************************
* Run Length                                                                   *
********************************************************************************
*
*dump
*restart
histories-per-batch 1e3
batches 1e3
*
********************************************************************************
* File Names                                                                   *
********************************************************************************
*
file-names
* restart-file
*  'FMR_002.14'
* dump-file
*  'FMR_002.10'
xsection-file
 'xgen_be.11'
intermediate-file
 'FMR_002.12'
```

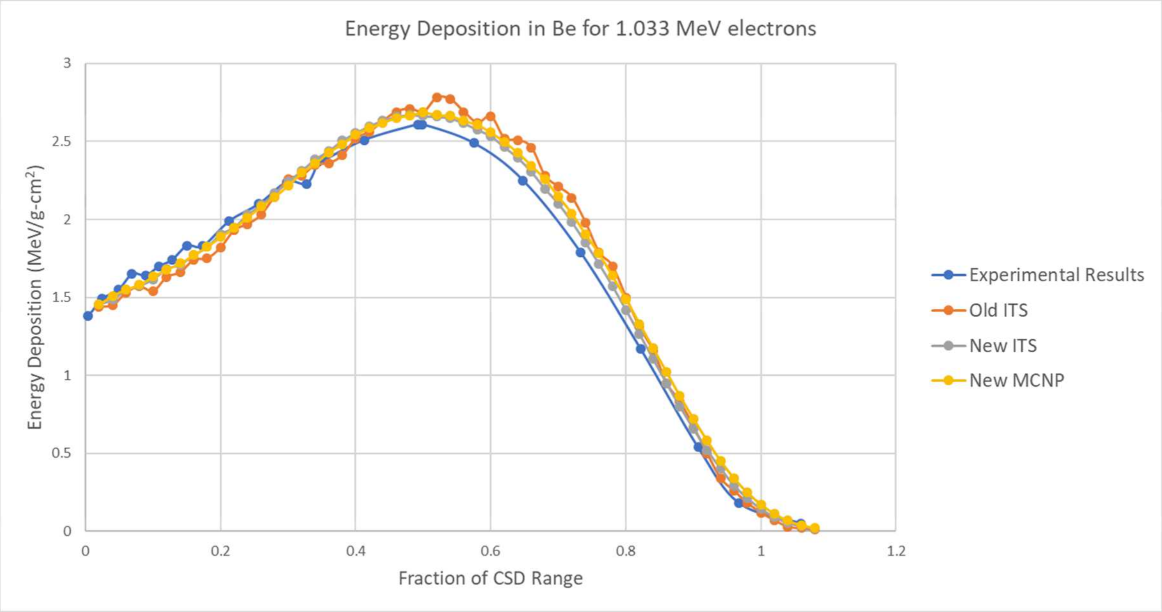
```
* material 1: Beryllium, density = 1.85 g/cc
*
********************************************************************************
* Geometry Input                                                               *
********************************************************************************
*
geometry 3
1 1 0.004672703
1 1 0.002632972
1 1 1
*
electrons
energy 1.033
cutoffs 0.001 0.001
position
 point 0.0
*
********************************************************************************
* Output options                                                               *
********************************************************************************
*
```

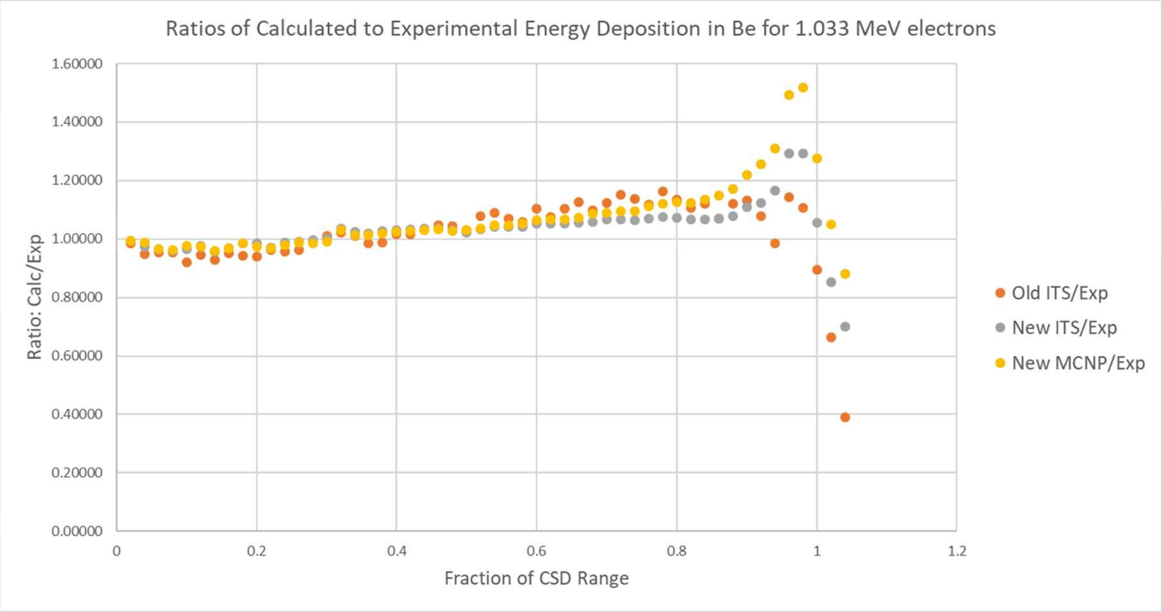
```
echo 1
title
 XSections for calorimetric measurement of electron energy deposition in Be
energy 1.1
electron-grid-length 120
*
* material 1: Beryllium, density = 1.85 g/cc
material be 1.000000
  density 1.85
*
```

Results

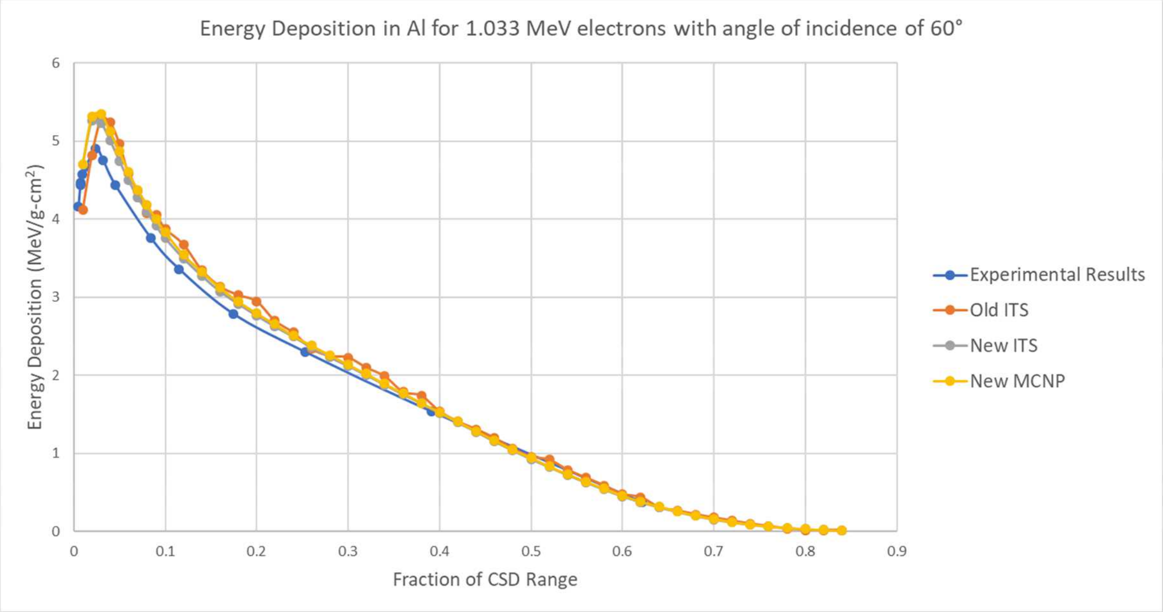
- Energy deposition is shown as a function of depth expressed as a fraction of the continuous slowing-down approximation range (or fraction of mean range, FMR).
- FMR corresponds to thickness of foils plus one-half the thickness of calorimeter.
- Materials with heat shields for thermal isolation of the calorimeter may or may not have their front shield included in calculation of FMR.

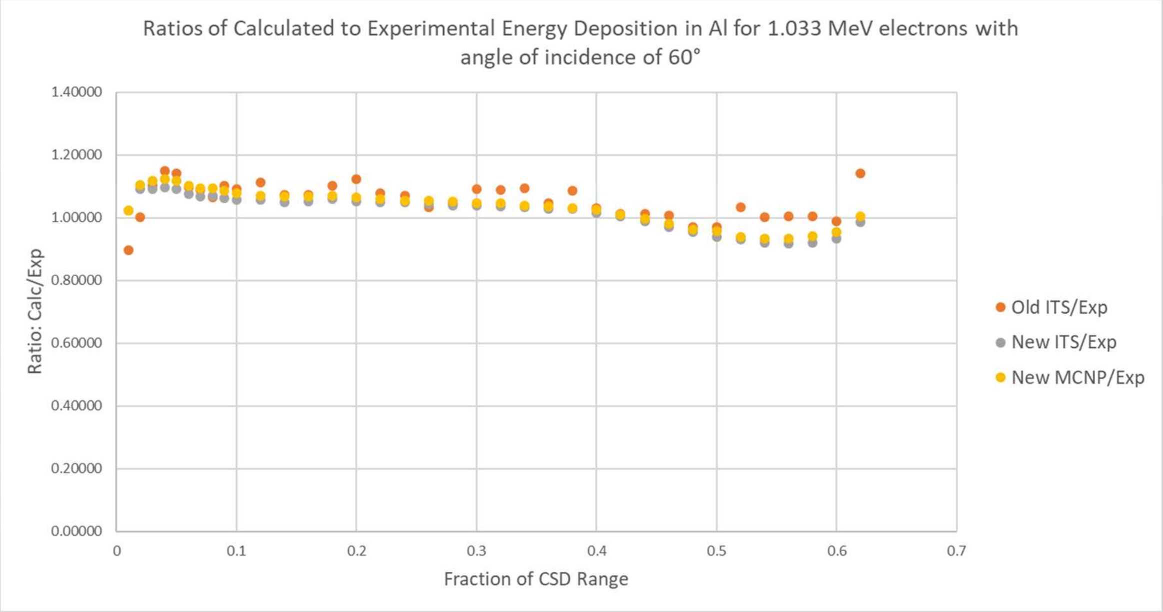
Results


Energy Deposition in Be for 1.033 MeV electrons
Energy Deposition (MeV/g-cm^2)
Fraction of CSD Range
Experimental Results
Old ITS
New ITS
New MCNP


Ratios of Calculated to Experimental Energy Deposition in Be for 1.033 MeV electrons
Ratio: Calc/Exp
Fraction of CSD Range
Old ITS/Exp
New ITS/Exp
New MCNP/Exp

Results


Energy Deposition in Al for 1.033 MeV electrons with angle of incidence of 60°
Energy Deposition (MeV/g-cm²)
Fraction of CSD Range
Experimental Results
Old ITS
New ITS
New MCNP


Ratios of Calculated to Experimental Energy Deposition in Al for 1.033 MeV electrons with angle of incidence of 60°
Ratio: Calc/Exp
Fraction of CSD Range
Old ITS/Exp
New ITS/Exp
New MCNP/Exp

Results – So far

- Generally, MCNP and ITS tend to overestimate peak dose and underestimate the tail of the energy deposition profile of a given material.
- Difficulty in identifying discrepancies: both MCNP and ITS have similar electron transport models, but dissimilar photon transport models.
  - MCNP: Doppler, Coherent, Incoherent, Pair, Photoelectric.
  - ITS: Doppler, Coherent, Incoherent, Incoherent-binding, Pair, Photoelectric, Photo-Relaxation.
  - Disabling certain models in ITS to match MCNP still gives slightly different results.

To-do

- Finish up single-layer simulations: Mo, Ta, U.
- Start multi-layer simulations: Be/Au/Be, C/Cu/C, C/Ta/C, C/Au/C, C/U/C, Al/Au/Al, Ta/Al.
- Current suggestions:
  - Perhaps expand to include Geant4.
  - Exchange photon cross section libraries with MCNP and ITS for sanity check.
  - Update FMR values to more recent values.

Questions?