ARMY RESEARCH LABORATORY



Parametric Study of Beta-Endpoint Energy in Direct Energy Converters

by Kara Blaine and Marc Litz

ARL-TR-4034

January 2007

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January 2007

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Kara Blaine and Marc Litz Sensors and Electron Devices Directorate, ARL

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| 1. REPORT DATE (DL | D-MM-YYYY) | 2. REPORT TYPE | | | 3. DATES COVERED (From - To) | | |
| January 2007 | | Progress | | | May 2006 | | |
| 4. TITLE AND SUBTI | ΓLE | | | | 5a. CONTRACT NUMBER | | |
| Parametric Stu | dy of Beta-Endpo | oint Energy in Direc | t Energy Conver | ters | | | |
| | | | | | 5b. GRANT NUMBER | | |
| | | | | | 5c. PROGRAM ELEMENT NUMBER | | |
| 6. AUTHOR(S) Kara Blaine an | d Marc Litz | | | | 5d. PROJECT NUMBER | | |
| | | | | | 5e. TASK NUMBER | | |
| | | | | | 5f. WORK UNIT NUMBER | | |
| 7. PERFORMING ORG | GANIZATION NAME(S) A | ND ADDRESS(ES) | | | 8. PERFORMING ORGANIZATION | | |
| U.S. Army Res | earch Laboratory | | | | REPORT NUMBER | | |
| | D-ARL-SE-DE | | | | ARL-TR-4034 | | |
| 2800 Powder N | | | | | | | |
| Adelphi, MD 2 | 20783-1197 | | | | | | |
| | NITORING AGENCY NAM | | | | 10. SPONSOR/MONITOR'S ACRONYM(S) | | |
| | earch Laboratory | | | | | | |
| 2800 Powder N | | | | | 11. SPONSOR/MONITOR'S REPORT NUMBER(S) | | |
| Adelphi, MD 2 | .0783-1197 | | | | | | |
| 12. DISTRIBUTION/A | VAILABILITY STATEME | ENT | | | | | |
| Approved for p | public release; dis | tribution unlimited. | | | | | |
| 13. SUPPLEMENTAR | Y NOTES | | | | | | |
| batteries. Num energy deposite spectrum illum energy constan DEC devices c have most impa | nerical simulations ed in the material inating layers of s t. The goal of the an be fabricated f | s, using a nuclear so . Two different par silicon-carbide (SiC e simulations is to it or higher efficiency ttky devices, generation | cattering code (M ametric studies v C), 2) the other va dentify the region 7. The results sho | ICNPX), have vere performe rying the mat as within the pow that 50 ke | y-converter (DEC) for isotope-based e been performed to determine the electron ed 1) varying β -endpoint energy of a terial layers while keeping the β -endpoint materials of maximum energy deposition so V and 100 keV β -endpoint energies stand to ty of carriers, and highest energy deposition | | |
| 15. SUBJECT TERMS | | | | | | | |
| SiC, DEC, isot | ope | | | 10 100 00 | 1 | | |
| 16. SECURITY CLASS | | | 17. LIMITATION OF ABSTRACT SAR | 18. NUMBER OF PAGES 60 | 19a. NAME OF RESPONSIBLE PERSON Marc Litz | | |
| a. REPORT Unclassified | b. ABSTRACT Unclassified | c. THIS PAGE Unclassified | SAK | | 19b. TELEPHONE NUMBER (Include area code) 301-394-5556 | | |
| | | | | | Standard Form 298 (Rev. 8/98 | | |

Standard Form 298 (Rev. 8/98) Prescribed by ANSI Std. Z39.18

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1. Background

Direct energy conversion in isotope batteries can yield steady low-power over ten to twenty years without significant degradation. Low-power sensors can benefit from nuclear batteries by harvesting from the high-density storage. The energy density of isotopes is 5 to 9 orders of magnitude more dense than the energy stored in chemical bonds. With isotope batteries, the opportunity exists for sensors to be left unattended for the duration of their lifetimes-decades for some applications. Chemical batteries cannot last that long, even unused, because of degradation of the chemistry. Low maintenance of the unattended sensors keeps them unobtrusive. Unattended underwater sensors, which can be dropped into the ocean, can also benefit from long-lived, low-maintenance isotope batteries. Replacement issues in the field would be non-existent. Embedded sensors would also be feasible, such as sensors buried in the earth which could detect seismic pulses or sensors built into building foundations or bridges which could detect structural damage.

Chemical batteries vary depending upon the chemistry. However their basic components are all the same. They have a positive anode and a negative cathode with an electrolytic separator between them. Electrons and holes flow through the electrolyte. The difference between single use batteries and rechargeable batteries lies in whether the electrochemical reaction that occurs is reversible or not. If the reaction is reversible, the application of a potential between the electrodes (cathode and anode) adds energy to the circuit, and allows the process to repeat, where in single-use (primary) batteries it cannot (1).

The design concept of a nuclear battery involving direct energy conversion would consist of alternating layers of a direct energy converter (DEC), most likely silicon-carbide (SiC) diodes, and a nuclear isotope, which would serve as the energy source. This can be seen in figure 1. The theory is similar to the first voltaic cell (2), where the more layers are stacked together; the higher the voltage can be expected.



Figure 1. Alternating layers of isotope energy source and SiC direct-energy-converter (DEC) in a AA-battery package.

MCNPX is a general-purpose Monte Carlo N-Particle code which supports 34 particle types, contains cross section libraries, and includes the ability to use physics models for energies where tabular data are not available (*3*). MCNPX treats an arbitrary three-dimensional configuration of materials in geometric cells. Pointwise continuous-energy cross section data for scattering in materials are used. Source and tally structures with extensive statistical analysis of convergence are integral to the output parameters. Rapid convergence is enabled by a wide variety of variance reduction methods. MCNPX includes libraries for neutrons, photons, electrons, protons and photonuclear interactions. "Mesh" and "radiography" tallies are included for 2 and 3-dimensional imaging purposes. An auxiliary program, GRIDCONV, converts the mesh and radiography tally as well as standard mtal-file results for viewing by independent graphics packages.

Monte Carlo algorithms calculate a statistically valid, most likely results of a series of events, based on the known probability-density-functions of the events (4). These algorithms are useful if you want to ask what will be the outcome of a complex series of events. This is particularly useful in complex series of molecular motions or a sequential series of events as in photon scattering through a material. Each event has its own probability of occurrence. It can take days to run, in order to test as many events and outcomes as possible and keep the statistics low.

These algorithms use random number generators to create the space for variety in the complexity and follow with variance reduction techniques to develop statistics that give guidance as to the value or weight of the answer. Credit for inventing the algorithm often goes to Stanislaw Ulam.

Unlike Monte Carlo simulation, deterministic transport methods require that the phase-space be discretized in space, energy and angle, introducing a substantial degree of complication in terms of algorithm development, problem set-up, and requires a significant amount of computer memory in order to store the spatial, angular and energy dependent flux information. The large demand placed on computer memory by deterministic transport codes has limited their use. However, with the rapid increase in computer processing power, memory capacity, and reduction in unit cost, three-dimensional, time-independent, deterministic transport codes are now becoming available as production codes (*5*).

Forty-eight different isotopes have been identified in the literature, for application to nuclear batteries, as shown in table 1 (*6 through 9*). From this list, the isotope that best falls within the ideal beta-energy range can be picked for efficiency optimization. Simulations testing the ideal DEC are also described, using four different DEC's for comparison, as shown in table 2.

| A | | Z | N | Halflife (yr) | alpha | beta pk (kev) | IT,ec |
|-----|---------|----|----|---------------|-------|------------------|------------|
| 3 | H(T) | 1 | 2 | 12.32 | | 18.6 | |
| 14 | C(PMMA) | 6 | 8 | 5710 | | 156 | |
| 32 | Р | 15 | 17 | 0.04 | | 1711 | |
| 35 | S | 16 | 19 | 0.239 | | 167.4 | |
| 42 | Ar | 18 | 24 | 32.9 | | 600 | |
| 44 | Ti | 22 | 22 | 49.3 | | 266 | |
| 55 | Fe | 26 | 29 | 2.73 | | 232 | |
| 60 | Co | 27 | 33 | 5.24 | | 310 | 1170,1330 |
| 63 | Ni | 28 | 35 | 101 | | 66.9 | |
| 85 | Kr | 36 | 49 | 10.755 | | 687 | |
| 90 | Sr | 38 | 52 | 28.77 | | 546 | |
| 106 | Ru | 44 | 62 | 1.0234 | | 39 | |
| 109 | Cd | 48 | 61 | 1.2674 | | 184 | |
| 113 | Cd | 48 | 65 | 14.1 | | 58 | |
| 121 | Sn m | 50 | 71 | 55 | | 6 | |
| 137 | Cs | 55 | 82 | 30 | | 190 | |
| 145 | Pm | 61 | 84 | 17.7 | | 161 | |
| 147 | Pm | 61 | 86 | 2.624 | | 225 | |
| 108 | Ag m | 47 | 61 | 418.25 | | | 109.5,2027 |
| 108 | Ag g | 47 | 61 | 4.50913E-06 | | 1649 | |
| 148 | Gd | 64 | 84 | 75 | 3271 | | |
| 151 | Sm | 62 | 89 | 90 | | 76 | |
| 155 | Eu | 63 | 92 | 4.67 | | 253 | |
| 157 | Tb | 65 | 92 | 99 | | 63 | |

 Table 1. Table of isotopes that have been considered in the literature for application to nuclear batteries.

| 171 | Tm | 69 | 102 | 1.92 | | 96 | |
|-----|------|----|-----|-------------|------|-----|------|
| 178 | Hf m | 72 | 106 | 31 | | | 2445 |
| 179 | Та | 73 | 106 | 1.79 | | 110 | |
| 198 | Au | 79 | 119 | 8.56164E-08 | | 980 | |
| 193 | Pt | 78 | 115 | 50 | | 56 | |
| 204 | Tl | 81 | 123 | 3.78 | | 763 | |
| 210 | Pb | 82 | 128 | 22.29 | | 63 | |
| 208 | Ро | 84 | 124 | 2.8979 | 5216 | | |
| 210 | Ро | 84 | 126 | 0.379 | 5304 | | |
| 228 | Ra | 88 | 140 | 5.75 | | 46 | |
| 227 | Ac | 89 | 138 | 21.773 | | 44 | |
| 228 | Th | 90 | 138 | 1.9131 | 5520 | | |
| 232 | U | 92 | 140 | 68.9 | 5414 | | |
| 235 | Np | 93 | 142 | 1.085 | 123 | | |
| 236 | Pu | 94 | 142 | 2.857 | 5867 | | |
| 238 | Pu | 94 | 144 | 87.74 | 5593 | | |
| 241 | Pu | 94 | 147 | 14.35 | | 21 | |
| 241 | Am | 95 | 146 | 432 | 5500 | | |
| 242 | Am | 95 | 147 | 0.001826484 | | 645 | |
| 242 | Am m | 95 | 147 | 141 | | | 49 |
| 243 | Am | 95 | 148 | 7370 | 5280 | | |
| 244 | Cm | 96 | 148 | 18.1 | 5902 | | |
| 248 | Bk | 97 | 151 | 9 | 5793 | | |
| 250 | Cf | 98 | 152 | 13.07 | 6128 | | |

Table 1. Table of isotopes that have been considered in the literature for application to nuclear batteries (cont'd).

Table 2. Table of DEC that have beenconsidered in this parametric study.

| Material | Density [g/cc] |
|--------------------------|-------------------|
| Silicon (Si) | 2.3 |
| Silicon Carbide (SiC) | 3.2 |
| cvd diamond (cvd) | 3.52 |
| Gallium Nitride GaN | 6.15 |

This report describes a series of numerical simulations using MCNPX, with the goal of matching the characteristics of isotope energy deposition and range with DEC material properties. Fabrication of devices can be optimized to place p-n junctions in regions of maximum energy deposited by the betas from the various isotopes. This capability will increase the efficiency of the DEC electrical output for given choice of isotope.

2. Numerical Simulations

The two different parametric studies were performed in this study: 1) varying the beta-endpointenergy while keeping the material parameters constant, and 2) varying the material while keeping the beta-endpoint-energy constant. A table of the materials and beta-endpoint-energies matrix is shown in table 3.

| | | DEC | | | | | |
|-----------------------------|-----|-----------------|--------------------------|----------------------|--------------------------|--|--|
| | | Silicon (Si) | Silicon Carbide (SiC) | cvd diamond (cvd) | Gallium Nitride (GaN) | | |
| Dete | 20 | | Х | | | | |
| Beta Endmoint | 50 | Х | Х | Х | Х | | |
| Endpoint Energy [keV] | 100 | | Х | | | | |
| | 200 | | Х | | | | |
| | 500 | | Х | | | | |

Table 3. Table of runs done through MXCNPX.

The first half of the project, which varied endpoint energy while keeping the DEC material constant, was performed by selecting various endpoint energies on a logarithmic scale in a range suitable to electron energies found in beta emitters of table 1. A discussion of the spectrum that was input for each endpoint energy, can be found in section 2.1 of this paper. The endpoint energy parameter was varied for SiC as DEC material. It is currently the most likely candidate for a nuclear battery as it is available and known to be radiation resistant. Silicon Carbide has a relatively large band gap (3.3 eV), which usually results in low leakage currents.

The second half of the parametric study varied the DEC material properties at a constant betaendpoint energy of 50 keV. This particular energy was chosen for the material study because of its closeness in value to the endpoint energy of nickel-63 (Ni63), whose endpoint energy is 66 keV. Only an approximation is sought. Nickel-63 is an easily available isotope that may have future practical applications in experimentation.

2.1 Monte-Carlo Neutron Particle eXtended (MCNPX)

The first stage in the process of running simulations using MCNPX is to create an input deck, which consists of surfaces (shapes within the defined geometry) and cells (combinations of the surfaces). Each cell is assigned a density, as well as a material element specification, which is stated in the input deck by atomic percentage of molecular makeup, atomic number and mass. The user also specifies which particles are to be tracked through each cell.

The geometry design of the following simulations used 30 DEC layers measuring 5 mm \times 5 mm \times 5 μ m, for a total of 150 μ m of DEC stacked together. In select cases, when higher energy spectrums were used, additional simulations were run using 5 mm \times 5 mm \times 50 μ m layers for a total coverage of 1500 μ m in order to ascertain the stopping power of the DEC. In all cases, only

beta particles were tracked throughout the model, and the source was located 1mm away. The geometry of the general input deck is shown below in figure 2 for clarification.



Figure 2. Model of the geometry created within MCNPX.

The beta spectrum of the simulation coded into the MCNPX input deck is based off on a Strontium-90 (Sr90) beta-emitter (9), and normalized for the appropriate endpoint energy. The spectrum emitted from Sr-90, like many other beta-emitters, has been shown to peak at approximately one third of the endpoint energy (10), although the number used for the peak in the calculations is actually less than one third. An example of one such spectrum is shown in figure 3.



Figure 3. Beta spectra from MCNPX input deck all have the same shape, with the peak occurring just before one third of the endpoint energy. The area under the curve is normalized to one, and each varies only in endpoint. Shown above is the 50 keV beta spectrum used.

Although the Sr90 beta spectrum was the basis for the calculations performed, its spectrum is similar to many other isotopes' beta spectrum that may be used for future experimentation. Nickel-63 is known to vary from Sr90's spectrum, where instead of peaking at approximately one third of the endpoint energy, the peak of Ni63's output spectrum occurs at the extreme low end of the spectrum (10). It has been shown that the low energy electrons (<100 keV) deposit more of their energy into the materials than the high energy (>100 keV) electrons. The lower energy electrons are more likely to be captured by the depletion region of DECs and converted into usable power in a circuit (11). This study's purpose is to give an approximation of what to expect in future experimentation. MCNPX is a nuclear scattering code showing conversion of electron and photon incident energy into scattered electrons and photons. In parallel, a drift-diffusion circuit model is in the process of being verified. This parametric study calculates the efficiency of energy absorbed by the DEC material, as a function of isotope input-energy-spectrum and material.

The output of MCNPX includes tallies and mesh calculations of particle flux, energy deposition and dose; along with mesh calculations of similar metrics. The tallies are dumped into an output text file along with a set of default data and tables. The mesh data is dumped into a separate mesh file, and needs to be converted into text format through another program, called gridconv, which comes with the MCNPX package.

The text file outputted by MCNPX contains useful tables, including one which shows the tracks entering and the population in each layer for each particle tracked in the simulation. The tracks entering a layer show all electrons entering a layer including the source particles; if an electron exited a layer and reentered, it would be counted again. The population of a layer shows the number of tracks entering a layer plus source particles and does not include reentrant electrons, and thus population vs. tracks entering indicates backscatter. Population was useful in determining whether or not electrons were created, and up to what layer the electrons penetrated the DEC.

Delta rays, or fast moving electrons which pass through a material, cause secondary ionization. Delta rays knock orbiting electrons out of their corresponding atom, and MCNPX measures the number of free electrons generated, distinguishing them as knock-on electrons. The number of knock-on electrons produced was useful in distinguishing between properties of the endpoint energy and DEC.

There are two tallies of MCNPX which were found useful. Tally 4 measures the flux averaged over the layer and is measured in particles/cm², where tally 6 measures the energy deposition averaged over a cell in units of MeV/gram. Tally 4 and tally 6 are both scaled to the number of source or input particles, and have energy bins defined by the user in the input deck. The energy bins make it possible to plot the tallies as a function of energy bin and layer.

Where a tally measurement occurs in the region of a layer, a mesh measurement occurs over a grid in any defined area of the geometry of input deck. In other words, the mesh is independent of the geometry and can cover several different materials and layers if needed. There are several types of mesh measurements that are possible to make, but the one found most useful was a track averaged mesh tally, or a type 1 mesh, called pedep, which measures energy deposition in MeV/cm³ and is also normalized by source particles. Although pedep is close to the tally 6 measurement, pedep normalizes to mesh unit volume as opposed to weight. This is because of pedep's ability to cross into regions of different densities. In both the cases of tally 6 and pedep, the amount of electron energy deposition can be used to calculate the approximate number of electrons deposited.

3. Results

There was a noticeable trend in the data gathered from the simulation of the endpoint energy study. The penetration depth of the electrons increased as expected with an increase of endpoint energy, from 5 μ m in the case of 20 keV to 750 μ m in the case of 500 keV. The resolution of the simulation had to be adjusted for the 200 keV and 500 keV runs from 5 μ m to 50 μ m in order to see the penetration depth. However, all other analysis was done for using the 5 μ m layer size.

Numerical values such as population, electron activity (population – total flux), and total energy deposited were the largest in layer 1 for the 100 keV run. Population and electron activity were largest in layer 2 (5 to 10 μ m) with the 500 keV endpoint, while most of the energy was deposited in layer 2 for 200 keV. The change between maximum energy deposition from 100 keV endpoint in the first layer to 200 keV endpoint in the second layer is most likely due to the stopping power of SiC, the DEC used in the simulation, to stop the lower energy betas better than the higher energy betas. However, because the low energy electrons are absorbed faster than higher energy deposited in the layer/peak energy of the input electrons), and the 100 keV run was found to have the highest efficiency in the second layer. The data from the endpoint energy study is summarized in table 4(a).

Table 4. The above tables, describing the Endpoint Energy Parametric Study (a) and the Density Parametric Study (b), show a summary of results from the simulations. The results from table 4(a) show that 100keV has the highest efficiency down to the second layer of SiC. Table 4(b) shows that Si has the highest efficiency of the different materials at 50keV.

| Resolution | 5 µm | | | | |
|---|----------|----------|----------|----------|-----------|
| Number of Histories | 1.E+07 | | | | |
| Denisty of Material (g/cc) | 3.2 | | | | |
| Material | SiC | | | | |
| Area of One Layer (cm ²) (5µm thick layers) | 0.25 | | | | |
| Mass Per Layer (g) | 0.0004 | | | | |
| End Point Energy | 20 keV | 50 keV | 100 keV | 200 keV | 500 keV |
| Peak Energy | 4.98 keV | 12.5 keV | 24.9 keV | 49.8 keV | 125 keV |
| Average Energy | 8.2 keV | 20.4 keV | 40.8 keV | 81.5 keV | 203.8 keV |
| Penetration Depth | 5 µm | 25 µm | 65 µm | 200 µm | 750 µm |
| Population in Layer 1 | 13467551 | 20522916 | 24131201 | 22824814 | 18019896 |
| Flux of Layer 1 (1/cm ² /history) | 0.562606 | 2.4465 | 4.4667 | 5.5590 | 5.4766 |
| Total Flux of Layer 1 | 1406515 | 6116275 | 11166825 | 13897500 | 13691550 |
| Electron Activity in Layer 1 | 12061036 | 14406641 | 12964376 | 8927314 | 4328346 |
| Tracks Entering Layer 1 | 1000000 | 10215748 | 10922921 | 11534130 | 11593980 |
| Total Energy Deposited in Layer 1 (MeV/g) | 13.8765 | 31.9846 | 40.1016 | 35.7448 | 22.5743 |
| Total Energy Deposited in Layer 1 (keV) | 5.5506 | 12.79384 | 16.04064 | 14.29792 | 9.02972 |
| Efficiency | 68% | 63% | 39% | 18% | 4% |
| Population in Layer 2 | 0 | 1772867 | 8895986 | 15191634 | 16175905 |
| Flux of Layer 2 (1/cm ² /history) | 0 | 0.276493 | 2.19591 | 4.5713 | 5.7305 |
| Total Flux of Layer 2 | 0 | 691233 | 5489775 | 11428175 | 14326225 |
| Electron Activity in Layer 2 | 0 | 1081635 | 3406211 | 3763459 | 1849680 |
| Tracks Entering Layer 2 | 0 | 762513 | 3920085 | 7763246 | 10425602 |
| Total Energy Deposited in Layer 2 (MeV/g) | 0 | 3.0785 | 15.411 | 24.5396 | 21.2363 |
| Total Energy Deposited in Layer 2 (keV) | 0 | 1.23E+00 | 6.16E+00 | 9.82E+00 | 8.49E+00 |
| Efficiency | 0% | 6% | 15% | 12% | 4% |

Endpoint Energy Parametric Study

(a) Endpoint Energy Study

The data gathered from the simulation of the density of the DEC had less obvious results than the endpoint energy study. However, the penetration depth was shown to increase with a decreasing density. Silicon stood out as having the highest efficiency; it both absorbed the most energy and allowed the most electrons to pass. The data from the density study is summarized in table 4(b).

Table 4. The above tables, describing the Endpoint Energy Parametric Study (a) and the Density Parametric Study (b), show a summary of results from the simulations. The results from table 4(a) show that 100keV has the highest efficiency down to the second layer of SiC. Table 4(b) shows that Si has the highest efficiency of the different materials at 50keV (cont'd).

Density Parametric Study

| Resolution | 5 µm | | | |
|---|----------|----------|----------------|----------|
| Number of Histories | 1.E+07 | | | |
| Endpoint Energy | 50 keV | | | |
| Peak Energy | 12.5 keV | | | |
| Average Energy | 20.4 keV | | | |
| Area of One Layer (cm^2) (5µm thick layers) | 0.25 | | | |
| Material | Si | SiC | cvd diamond | GaN |
| Denisty of Material (g/cc) | 2.3 | 3.2 | 3.52 | 6.15 |
| Mass Per Layer (g) | 2.9E-04 | 4.0E-04 | 4.4E-04 | 7.7E-04 |
| Penetration Depth | 30 µm | 25 µm | 20 µm | 15 µm |
| Population in Layer 1 | 19748290 | 20522916 | 19117877 | 22469743 |
| Flux of Layer 1 (1/cm ² /history) | 3.11999 | 2.4465 | 1.9275 | 1.6944 |
| Total Flux of Layer 1 | 7799975 | 6116275 | 4818750 | 4235900 |
| Electron Activity in Layer 1 | 11948315 | 14406641 | 14299127 | 18233843 |
| Tracks Entering Layer 1 | 10404071 | 10215748 | 10119837 | 10032005 |
| Total Energy Deposited in Layer 1 (MeV/g) | 40.3031 | 31.9846 | 30.9761 | 15.8747 |
| Total Energy Deposited in Layer 1 (keV) | 16.12124 | 12.79384 | 12.39044 | 6.34988 |
| Efficiency | 79.03% | 62.71% | 60.74% | 31.13% |
| Population in Layer 2 | 2830682 | 1772867 | 1723081 | 160593 |
| Flux of Layer 2 (1/cm ² /history) | 0.609659 | 0.276493 | 0.221778 | 0.0138 |
| Total Flux of Layer 2 | 1524148 | 691233 | 554445 | 34479 |
| Electron Activity in Layer 2 | 1306535 | 1081635 | 1168636 | 126114 |
| Tracks Entering Layer 2 | 1352110 | 762513 | 751796 | 72939 |
| Total Energy Deposited in Layer 2 (MeV/g) | 6.41721 | 3.0785 | 3.13765 | 0.1240 |
| Total Energy Deposited in Layer 2 (keV) | 2.566884 | 1.23E+00 | 1.26E+00 | 4.96E-02 |
| Efficiency | 12.58% | 6.04% | 6.15% | 0.24% |

(b) Material Density Study

The percent energy deposition curves shown in figure 4 were created by the matlab routine, plot_edep_pk_layers.m, which is shown in appendix C. The percent energy deposition can normalizes the total energy deposition per layer with the average energy.

For the endpoint energy study, the endpoint energies of 20 keV and 50 keV stand out as leaving the most energy behind, with the 100 keV not far behind. Although the 20 keV endpoint energy data is found to deposit a significant amount of energy in the first layer, it is the only layer that the electrons penetrate. This is shown in figure 4(a).

For the material density study, the generated curves from the exponential fits are very similar, as seen in figure 4(b). Only the GaN curve deviates from the other curves with any significance, and this is most likely because its density has the greatest difference from any of the other densities. However, this deviation is small, and the similarities show that the greatest contribution of energy deposition is due largely in part to the endpoint energy of the input beta spectrum.



Figure 4. (a) Endpoint energies of 20 keV and 50 keV stand out as leaving the most energy behind in SiC with the 100 keV endpoint energy not far behind. (b) The similarities in the curves regardless of density show that the greatest contribution of energy deposition is due to endpoint energy. GaN is shown to vary the most from the other curves, because its density varies the most from the other densities.

More knock-on electrons are generated with higher endpoint energies on a nearly linear scale, as shown in figure 5(a). More than 10 times the number of knock-ons are created by 500 keV endpoint betas than 20 keV endpoint betas.

GaN generated the largest number of knock-on electrons of the four materials varied in the simulations. Figure 5b shows that GaN generated 7% more knock-on electrons (for 50 keV incident betas) than in SiC. While knock-on electron energies are always less energetic than the incoming electrons, the lower the energy of the knock-on, the higher probability that the energy deposited can be collected and converted to electrical current. The comparison-of-material study does not provide such clear cut results, however, as the endpoint energy study, and the number of knock-on electrons generated varies as much as 24% with the density and type of the material.

A valuable result is the number of energy deposited from electrons below 20 keV because the lower energy electrons are more easily collected by the junction, contributing to electrical current in the circuit. As shown in figure 6(a), more energy of this high efficient range is deposited from lower energy spectra. This is partly because the input electrons themselves are close to the ideal range, as well as the knock-on electrons produced are of a low energy. One interesting result was that although the percentage decreases, as expected with increasing endpoint energy, the maximum energy deposition within this range occurred with a 100 keV endpoint energy.

Silicon is shown to absorb the most energy at the low range in figure 6(b), which is consistent with the results listed in table 4(b). The material density results all fall within 0.5% of each other, although they do not correspond linearly, which is a common theme of the study.



Figure 5. (a) With higher energy endpoints, more electrons are generated, but they are too high of an energy to be collected, and therefore to be useful. There is more energy lost with higher energy endpoints. (b) The density of the material seems to have no trend in its effect on the number of knock-on electrons generated.



Figure 6. (a) There are more lower energy electrons deposited in the DEC as a function of the total energy deposition with lower energy endpoint energies. (b) Lower density materials absorb the energy from 20 keV electrons better than higher density materials.

4. Conclusions

Small isotope batteries (I-bat devices) would be capable of providing low levels of power for an extremely long period of time (i.e., >100 years) and would be capable of operating over a wide range of operational environments with little if any loss of performance, most notably at extremely low temperatures (i.e., <100 K), but also in harsh biological environments. They would be ideal for distributed power applications such as MEMS devices or sensors on small (i.e., nano) sensors.

Through the use of MCNPX simulations and Matlab post-processing evaluations, we were able to discern the variation in the DEC material appears to have no definite bearing on efficiency of energy deposition. The material choice will likely play a larger role in later calculations of a drift diffusion model as well as actual experimental data. Known properties of a material will also play a role in its choice. Silicon, for example, although shown to have the highest efficiency per density, will not be a likely candidate as a DEC for a nuclear battery because of its inability to withstand degradation. At the moment, SiC seems to be the better choice because many studies have been done with SiC, and it is known to be a robust material.

The variations of energy deposition, unlike in the material study, were directly affected by beta source endpoint energy. The 20 keV endpoint energy betas provided the greatest efficiency in layer one as well as percentage of energy deposition per layer, when normalized to the average energy. However, the 20 keV betas only penetrated 5 μ m into SiC, and the realistic energy output would not be high enough.

| | 20keV | 50keV | 100keV | 200keV | 500keV | Si | SiC | cvd diamond | GaN |
|----------------------------|---------|---------|---------|---------|---------|---------|---------|----------------|---------|
| Energy Flux [MeV] | 0.0011 | 0.0113 | 0.0364 | 0.0790 | 0.1826 | 0.0142 | 0.0113 | 0.0091 | 0.0079 |
| Energy Deposition [MeV] | 2.78e-5 | 1.35e-4 | 2.75e-4 | 3.97e-4 | 5.44e-4 | 1.20e-4 | 1.35e-4 | 1.48e-4 | 1.29e-4 |
| Efficiency Ratio (%) | 2.492 | 1.194 | 0.755 | 0.502 | 0.298 | 0.844 | 1.194 | 1.625 | 1.632 |

Table 5. Energy Flux compared to Energy Deposition yields an Efficiency Ratio. Though the 20 keV yields the
highest ratio, the 50 keV in SiC has the highest percentage of energy deposition.

A comparison of the energy flux and the energy deposition yields an efficiency of how much energy passes through the DEC to how much is deposited, and can be seen in table 5. The energy flux is averaged over the surface area of the layer of DEC, and because the source definition of the simulation covered approximately half of the area, the efficiency could theoretically be doubled if the source covered closer to the whole diode. The 20 keV endpoint energy generates the highest efficiency, 2.5%, but there is actually the highest percentage of energy deposited from the 50 keV endpoint energy, whose efficiency is only 1.2%. These efficiencies represent a very simplified model; it is most relevant to schottky diodes.

A closer evaluation of the results showed that endpoint energies of 50 keV or 100 keV would be ideal. The 100 keV endpoint energy betas were shown to have the highest efficiency in the second layer of SiC, or after passing through 10 μ m. Both energies, however, have low penetration, making them ideal for use in Schottky diodes. The low energies with high absorption would not require additional shielding in batteries that could otherwise make them heavy and bulky.

Ni-63 falls right in the range of the idea endpoint energy, having an endpoint energy of 66 keV. According to this study, though the beta spectrum of Ni-63 varies from the beta spectrum used in the simulations, we should see high efficiencies of energy absorption. Additionally, only about 40 μ m of SiC should be necessary as stopping power for Ni-63.

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Appendix A. Additional Figures

Parametric study of a) beta-end-point energy and b) material type have been described in the body of this report. The figures graphically shown in this appendix pictorially show more of the details described in the paper. Figures A-1 through A-5 show the a) flux and b) energy deposition in the 30 SiC layers (if electrons got that far), as a function of beta endpoint energy [20, 50, 100, 200, and 500 keV]. Figures A-6 through A-8 show the variation of flux and energy deposition as a function of the material [Si, cvd diamond, GaN]. Figure A-9 shows the number density of electrons generated, in the SiC layers. The contour plots differ by the input source of the five beta endpoint energies. Figure A-10 shows penetration depth of 50 keV betas as a function of beta endpoint energy and material type. Figure A-11 shows the energy flux efficiency ratios as a function of beta endpoint energy and material type.



Figure A-1. (a) Shows the input beta spectrum for the 20 keV simulation as well as the resulting flux with SiC as the DEC. (b) Shows the energy distribution for the same simulation. The data is shown for layer one for both cases (the only penetrated layer).



Figure A-2. (a) Shows the input beta spectrum for the 50 keV simulation as well as the resulting flux with SiC as the DEC. (b) Shows the energy distribution for the same simulation. The data is shown for layers 1-5 in both cases (the only penetrated layers).



Figure A-3. (a) Shows the input beta spectrum for the 100 keV simulation as well as the resulting flux with SiC as the DEC. (b) Shows the energy distribution for the same simulation. The data is shown for layers 1-13 in both cases (the only penetrated layers).



Figure A-4. (a) Shows the input beta spectrum for the 200 keV simulation as well as the resulting flux with SiC as the DEC. (b) Shows the energy distribution for the same simulation. The data is shown for all 30 layers in both cases (5 μm layer width simulation is used for best comparison).



Figure A-5. (a) Shows the input beta spectrum for the 500 keV simulation as well as the resulting flux with SiC as the DEC.
(b) Shows the energy distribution for the same simulation. The data is shown for all 30 layers in both cases (5 μm layer width simulation is used for best comparison).



Figure A-6. (a) Shows the input beta spectrum for the 50 keV simulation with as well as the resulting flux Si as the DEC. (b) Shows the energy distribution for the same simulation. The data is shown for layers 1-6 in both cases (the only penetrated layers).



Figure A-7. (a) Shows the input beta spectrum for the 50 keV simulation as well as the resulting flux with cvd diamond as the DEC. (b) Shows the energy distribution for the same simulation. The data is shown for layers 1-6 in both cases (the only penetrated layers).



Figure A-8. (a) Shows the input beta spectrum for the 50 keV simulation as well as the resulting flux with GaN as the DEC. (b) Shows the energy distribution for the same simulation. The data is shown for layers 1-3 in both cases (the only penetrated layers).



Figure A-9. Shows the mesh plots of the endpoint energy simulations. (a) 20 keV zoomed in over 5 μm (equivalent of one layer), (b) 50 keV zoomed in over 5 μm, (c) 100 keV zoomed in over 15 μm (equivalent of 3 layers), (d) 200 keV zoomed in over 50 μm (equivalent of 10 layers), and (e) 500 keV showing all 30 layers. The zoomed in region does not always denote the region in which penetration ends, only in which the mesh plot had enough variance to be interesting.



Figure A-10. These graphs show the penetration depth in the DEC as a function of (a) endpoint energy and (b) material density



Figure A-11. Energy Flux compared to Energy Deposition yields an Efficiency Ratio. (a) Shows endpoint energy and (b) shows material density ratios.

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Appendix B. MCNPX Input Deck

The details of the MCNPX input deck (shown below) include geometry definition statements (surfaces or volumes), materials parameters (element and density), source definition statements (beam, surface, particle type), which physics algorithms should be used during the numerical simulations, and which diagnostic results should be calculated and displayed (flux, dose, energy deposited). All of these choices have an effect on the a) complexity of the model, b) error-bars associated with the results, and c) the run-time of the simulation.

\$25th SiC layer 25 3 -3.2 Model of Silicon Carbide with Sr source -25 imp:e 1 u=1 c 5um layers 26 3 -3.2 -26 imp:e 1 u=1\$26th SiC layer c (MCNPX scaled in cm) 27 3 -3.2 -27 imp:e 1 u=1 \$27th SiC layer 28 3 -3.2 -28 imp:e 1 u=1 \$28th SiC layer с c -----29 3 -3.2 -29 imp:e 1 u=1\$29th SiC layer c This is a model of the way electrons would be generated 30 3 -3.2 -30 imp:e 1 u=1 \$30th SiC layer c in the SiC after being hit by electrons from a strontium с c source. c air encasing $31 \ 2 \quad -0.00129 \quad -31 \ 1 \ 2 \ 3 \ 4 \ 5 \ 6 \ 7 \ 8 \ 9 \ 10 \ 11 \ 12 \ 13 \ 14 \ 15$ c ----с 16 17 18 19 & c +----+ 20 21 22 23 24 25 26 27 28 29 30 imp:e 1 u=1 c с Cell Cards 32 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 & c 18 19 20 21 22 23 24 25 26 27 28 29 30 cl & c +----+ imp:e 1 u=133 0 imp:e 1 u=1c # mat density surface data 31 c SiC c room 34 2 -0.00129 -32 imp:e 1 fill=1 1 3 -3.2 -1 imp:e 1 u=1 \$SiC closest to 35 0 source 32 imp:e 0 \$outside world 2 3 -3.2 -2 imp:e 1 u=1\$2nd SiC layer 3 3 -3.2 -3 imp:e 1 u=1 \$3rd SiC layer c +----imp:e 1 u=1 \$4th SiC layer 4 3 -3.2 -4 cl 5 3 -3.2 -5 imp:e 1 u=1 \$5th SiC layer c Surface Cards 6 3 -3.2 imp:e 1 u=1 \$6th SiC layer -6 c c +-----+ 7 3 -3.2 -7 imp:e 1 u=1 \$7th SiC layer 8 3 -3.2 imp:e 1 u=1 \$8th SiC layer c # type params -8 9 3 -3.2 -9 imp:e 1 u=1 \$9th SiC layer c SiC 1 rpp 708.75 709.25 493.9995 494 10 3 -3.2 -10 imp:e 1 u=1 \$10th SiC layer 117.25 117.75 11 3 -3.2 \$11th SiC layer c \$SiC layer closest to source -11 imp:e 1 u=1 12 3 -3.2 imp:e 1 u=1 \$12th SiC layer 2 rpp 708.75 709.25 493.9990 493.9995 117.25 117.75 -12 13 3 -3.2 -13 imp:e 1 u=1 \$13th SiC layer c \$2nd SiC layer 3 rpp 708.75 709.25 493.9985 493.9990 117.25 117.75 14 3 -3.2 -14 imp:e 1 u=1\$14th SiC layer 15 3 -3.2 -15 imp:e 1 u=1 \$15th SiC layer c \$3rd SiC layer 16 3 -3.2 -16 imp:e 1 u=1\$16th SiC layer 4 rpp 708.75 709.25 493.9980 493.9985 117.25 117.75 17 3 -3.2 -17 imp:e 1 u=1\$17th SiC layer c \$4th SiC layer 18 3 -3.2 \$18th SiC layer 5 rpp 708.75 709.25 493.9975 493.9980 117.25 117.75 -18 imp:e 1 u=1 19 3 \$19th SiC layer c \$5th SiC layer -3.2 -19 imp:e 1 u=120 3 -3.2 -20 \$20th SiC layer 6 rpp 708.75 709.25 493.9970 493.9975 117.25 117.75 imp:e 1 u=121 3 -3.2 c \$6th SiC layer -21 imp:e 1 u=1\$21th SiC layer 22 3 -3.2 7 rpp 708.75 709.25 493.9965 493.9970 117.25 117.75 -22 imp:e 1 u=1 \$22th SiC layer 23 3 -3.2 -23 imp:e 1 u=1 \$23th SiC layer c \$7th SiC layer 24 3 -3.2 -24 imp:e 1 u=1 \$24th SiC layer 8 rpp 708.75 709.25 493.9960 493.9965 117.25 117.75

c \$8th SiC layer 9 rpp 708.75 709.25 493.9955 493.9960 117.25 117.75 c \$9th SiC layer 10 rpp 708.75 709.25 493.9950 493.9955 117.25 117.75 c \$10th SiC layer 11 rpp 708.75 709.25 493.9945 493.9950 117.25 117.75 c \$11th SiC layer 12 rpp 708.75 709.25 493.9940 493.9945 117.25 117.75 c \$12th SiC layer 13 rpp 708.75 709.25 493.9935 493.9940 117.25 117.75 c \$13th SiC layer 14 rpp 708.75 709.25 493.9930 493.9935 117.25 117.75 c \$14th SiC layer 15 rpp 708.75 709.25 493.9925 493.9930 117.25 117.75 c \$15th SiC layer 16 rpp 708.75 709.25 493.9920 493.9925 117.25 117.75 c \$16th SiC layer 17 rpp 708.75 709.25 493.9915 493.9920 117.25 117.75 c \$17th SiC layer 18 rpp 708.75 709.25 493.9910 493.9915 117.25 117.75 c \$18th SiC layer 19 rpp 708.75 709.25 493.9905 493.9910 117.25 117.75 c \$19th SiC layer 20 rpp 708.75 709.25 493.9900 493.9905 117.25 117.75 c \$20th SiC layer 21 rpp 708.75 709.25 493.9895 493.9900 117.25 117.75 c \$21th SiC layer 22 rpp 708.75 709.25 493.9890 493.9895 117.25 117.75 c \$22th SiC layer 23 rpp 708.75 709.25 493.9885 493.9890 117.25 117.75 c \$23th SiC layer 24 rpp 708.75 709.25 493.9880 493.9885 117.25 117.75 c \$24th SiC layer 25 rpp 708.75 709.25 493.9875 493.9880 117.25 117.75 c \$25th SiC layer 26 rpp 708.75 709.25 493.9870 493.9875 117.25 117.75 c \$26th SiC layer 27 rpp 708.75 709.25 493.9865 493.9870 117.25 117.75 c \$27th SiC layer 28 rpp 708.75 709.25 493.9860 493.9865 117.25 117.75 c \$28th SiC layer 29 rpp 708.75 709.25 493.9855 493.9860 117.25 117.75 c \$29th SiC layer 30 rpp 708.75 709.25 493.9850 493.9855 117.25 117.75 c \$30th SiC layer c lead block to encase silicon carbide 31 rpp 708.5 709.5 493.850 494 117 118 c room dimensions 32 rpp 0 1419 0 1984 0 466 c +-----+ c Material Cards c c c +-----+ c m# isotope percent & c m1 82000 1.0 \$lead 11.34 g/cc m2 8016 .3 & 7014 .7 \$air 0.00129 g/cc

m3 6012 .43 & .57 \$SiC 3.2 g/cc 14028 c m4 14028 1.0 \$Si 2.3 g/cc \$C 2.3 g/cc c m13 6012 1.0 c m5 90000 1.0 \$Sr с c +-----+ | c Source Definition c c c +----sdef & dir=1 & erg= d2 & vec=0 -1 0 & par=e & rad=d1 & pos=709 494.1 117.5 с si1 0 .1 sp1 -21 с c energy distribution taken from now strontium c (old: 280kv-8ma-12may-aft.spe) si2 9.16E-05 0.000549 0.00412 0.00833 0.0125 0.0167 & 0.0208 0.025 0.0291 0.0333 0.0375 0.0417 0.0459 0.05 sp2 0 1000 3405 4692 4768 3900 2775 & 2234 1725 1331 1007 764 556 378 с c si3 h .707 1 c sp3 d 0 1 с c +-----+ c Data Cards c | c | c +----+ mode e nps 10000000 \$10Mh~100min с c +-----c Tallies c c c +-----+ с c fc2 electron flux over a surface in particles/cm^2 c f2:e 1.4 2.4 3.4 c e2 0 98i .51 с fc4 electron flux averaged over the cell in particles/cm^2 f4:e 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 & 18 19 20 21 22 23 24 25 26 27 28 29 30 e4 0 498i .51 с fc6 electron energy deposition averaged over the cell in MeV/g f6:e 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 &

18 19 20 21 22 23 24 25 26 27 28 29 30

28
e6 0 498i .51 с c fc8 electron energy deposition in MeV c *f8:e 1 2 3 c e8 0 1e-5 97i .51 с c +----+ c Mesh c c | c +----+ с tmesh с c (a)radial meshes (b)zaxis(symmetry) (c)angles counterclockwise с c flux=#/cm2 \$dose=rem/hr \$pedep=MeV/cm3 с c flux: flux c pedep: total energy deposition/unit vol c dose: dose over cross planes с rmesh1:e flux pedep popul dose c layer 1 SiC cora1 708.75 18i 709.25 corb1 493.9995 494 corc1 117.25 18i 117.75 с rmesh21:e flux pedep popul dose c layer 1 SiC cora21 708.75 18i 709.25 corb21 493.9995 18i 494 corc21 117.25 117.75 с rmesh31:e flux pedep popul dose c layer 1 SiC cora31 708.75 709.25 corb31 493.9995 18i 494 corc31 117.25 18i 117.75 с с rmesh41:e flux pedep popul dose c layer 2 SiC cora41 708.75 18i 709.25 corb41 493.999 493.9995 corc41 117.25 18i 117.75 с rmesh51:e flux pedep popul dose c layer 2 SiC cora51 708.75 18i 709.25 corb51 493.999 18i 493.9995 117.75 corc51 117.25 с rmesh61:e flux pedep popul dose c layer 2 SiC cora61 708.75 709.25 corb61 493.999 18i 493.9995 corc61 117.25 18i 117.75

с с rmesh71:e flux pedep popul dose c layer 3 SiC cora71 708.75 18i 709.25 corb71 493.9985 493.999 corc71 117.25 18i 117.75 с rmesh81:e flux pedep popul dose c layer 3 SiC cora81 708.75 18i 709.25 corb81 493.9985 18i 493.999 corc81 117.25 117.75 с rmesh91:e flux pedep popul dose c layer 3 SiC cora91 708.75 709.25 corb91 493.9985 18i 493.999 corc91 117.25 18i 117.75 с с rmesh101:e flux pedep popul dose c all SiC layers (30) cora101 708.75 18i 709.25 corb101 493.985 29i 494 corc101 117.4925 117.5075 с endmd

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Appendix C. Matlab Routines

In order to analyze the information gained from the MCNPX simulations, routines were written in Matlab that could efficiently read in the data files. The analysis routines include:

- read_mcnpx.m
 - reads in the data from the text file
- tally_convertF6_plot.m
 - uses read_mcnpx.m to plot out the data by tally number
 - o converts tally 6 from units of MeV/gram to keV
- energyDistribution.m
 - o inputs and normalizes the beta/gamma spectrum in use
- plot_espec_edep_tally.m
 - o calls tally_convertF6_plot.m, which calls read_mcnpx.m
 - o calls energyDistribution.m
 - yields plots of tally_convertF6_plot.m as well as a plot of tally 4 data with the normalized energy spectrum
- tally_compareF6_cell1.m
 - o calls read_mcnpx.m
 - plots the converted tally 6 data (in keV instead of MeV/gram) from the first layer of multiple simulations, allowing for easy comparison
- plot_edep_pk_layers.m
 - o calls read_mcnpx.m
 - plots the percent energy deposition for specified files, which equals the total energy deposition for a layer divided by the energy peak of the input beta spectrum as well as a fitted exponential curve (with the equation)
- mcnpx_mesh_energy_convert.m
 - reads in the data from the mesh text file after conversion using the MCNPX gridconv
 - o plots the mesh data in contour form
 - \circ converts the energy deposition mesh from MeV/cm³ to #/cc

The actual Matlab code follows.

read_mcnpx.m

```
function [filnam,prefix,E,T,fom,num,cell,titles,units,type,Nenergybins]=read_mcnpx
%
% format:
% read_mcnpx
%
% input:
% - mcnpx output file
%
% output:
% - E : the energy bins of the various tallies stored in cell
```

% arrays and matrices... for example, if there are 3 different % tally calls within a run, E will be a 1x3 cell array. the size % of each cell is based on the number of energy bins for the % individual tally and the number of layers calculated in the % different tallies. the benefit of cell arrays is that each cell % does not have to be the same size. % - T : the actual data taken from the tallies. it is stored in % the same manner as the E array % - fom : the statistics corresponding to the tallies. stored in % the same way as E and T. - num : the tally number, corresponding to F2,4,6,8... etc. num % should be the same dimensions as E, however stored as a matrix. % % for instance, if there are 3 different tallies, num should be a % 1x3 matrix where each entry is a number % - cell : cell is a cell array which holds the cell numbers of % the different layers corresponding to the data. in the case of % 3 different tallies, cell would be a 1x3 cell array, where each % cell would contain a 1xn matrix where n is the number of layers % being calculated in the tally % - titles : cell array which stores the titles corresponding to % the data % - units : cell array which stores the units of the data % - type : stores the particle type of the data in a cell array % % This routine has been written to be used in conjunction with other % plotting routines. % % % Pick an output file to read the data from % suffix='.': prefix='C:\MCNPX\scratch\'; %prefix='C:\Documents and Settings\dag\Desktop\air.water.SiC\'; if nargin==0 ;filnam='outp';end pathfilename=prefix; [filnam,prefix,filterindex] = uigetfile([pathfilename, '*.*']); if filterindex==0, filnam=0; prefix=0; E=[]; T=[]; fom=[]; num=[]; cell=[]; titles=[]; units=[]; type=[]; Nenergybins=0; return: end: % % Initialize Data Matrices % ncell=0; Nlines=20000; Nenergybins=800; % Initialize only one column, and concatenate additional columns later to % accomodate more data E tally=zeros(Nenergybins,1); T_tally=E_tally; fom tally=E tally; ruler='123456789 123456789 123456789 123456789 123456789 123456789 123456789 123456789 123456789 123456789 123456789 123456789 123456789;

```
nlin=0;
tally num=0;
ntot=0;
end_loop=0;
num=\{\};
cell=\{\}; \quad E=\{\};
titles={}; T={};
units={}; fom={};
type={};
%
% Read the Data
%
filnamcomp=[prefix,filnam];
fid=fopen(filnamcomp);
while end loop==0
  line = fgetl(fid); nlin=nlin+1;
  % Get out at end of input
  if ~isstr(line), break, end
  % Indicates that next diagnostic found
  % All tallies have this '1tally' marker
  [n,m]=size(line);
  if m==32
     stchar2=findstr('1tally',line);
     if ~isempty(stchar2)
       % Need to derive tally number from '1tally' line
       C=textscan(line, '%s %n %s %s %n');
       % We know for each case C{1}(1)='1tally'
       % However, these are still considered cells, so need to convert to matrix
       tally num=C{2};
       % Skip two lines to get to line beginning with 'tally type'
       % **Had trouble getting program to find this string on its own**
       line = fgetl(fid); nlin=nlin+1;
       line = fgetl(fid); nlin=nlin+1;
       % Scan the line to read in the data (reads in the data into a cell)
       C=textscan(line,'%s');
       % We know for each case C{1}(1)='tally', C{1}(2)='type',
       % and C{1}(3)= modified tally number
       [n,m]=size(C{1});
       space=' ';
       tally_title=cell2mat(C{1}(4));
       for tmp=5:n-2, tally_title=[tally_title, space, cell2mat(C{1}(tmp))]; end
       tally_units=cell2mat(C{1}(n));
       % Read the next line to get the particle type
       line = fgetl(fid); nlin=nlin+1;
       C=textscan(line,'%s');
       % We know for each case C{1}(1)='particle(s):'
       particle type=cell2mat(C{1}(2));
     end
  end
  % Find Cell Number
  stchar3=findstr(' cell ',line);
```

```
if isempty(stchar3), stchar3=findstr(' surface ',line); end
  if ~isempty(stchar3)
     if stchar3==1
       C=textscan(line,'%s %n');
       cell_num(ntot+1)=C{2};
     end
  end
  % Now that we know what we are looking at, we need to look for 'energy'
  % Should only be the line after ' cell '/' surface '
  stchar=findstr('energy',line);
  if ~isempty(stchar)
     %
     % Generic Reading of Data.
     % The string 'energy' is found at the 7th position on the line
    if stchar==7
       ntot=ntot+1;
       for dlin=1:Nenergybins
          line=fgetl(fid); nlin=nlin+1;
          stchar1=findstr('total',line);
          if ntot==1
            % First time only, find arraylegnth
            if ~isempty(stchar1)
               % The string 'total' is found at the 7th position on the line
               if stchar1 == 7
                  Nenergybins=dlin-1;
                  disp(['modified Nenergybins ',num2str(Nenergybins)]);
                  E tally=[];
                  T tally=[];
                  fom_tally=[];
                  break
               end
            end
          end
          a=sscanf(line(1:15),'%f');
          b=sscanf(line(16:29), \frac{1}{6});
          c=sscanf(line(30:35),'%f');
          temp1(dlin,1)=a;
          temp2(dlin,1)=b;
          temp3(dlin,1)=c;
       end
       E_tally=cat(2,E_tally,temp1);
       T_tally=cat(2,T_tally,temp2);
       fom_tally=cat(2,fom_tally,temp3);
       disp(['....data from ',num2str(ntot),'th tally, Cell number ',num2str(cell_num)]);
       disp(['taken from tally ',num2str(tally num),', ',num2str(tally title),' in
',num2str(tally units)]);
       disp(['read..... nlin=',num2str(nlin)]);
     end
  end
  % All tallies have '1analysis' to denote the end of the tally
  stchar4=findstr('1analysis',line);
  % restart counting for the next tally
  if ~isempty(stchar4)
     % is under the assumption that all tallys are of the same legnth
    ntot=0;
```

```
E=[E,E_tally]; E_tally=[];
```

```
T=[T,T_tally]; T_tally=[];
fom=[fom,fom_tally]; fom_tally=[];
num=[num,tally_num];
cell=[cell,cell_num];
titles=[titles,tally_title];
units=[units,tally_units];
type=[type,particle_type];
clear cell_num;
end
% All tallies have 'terminated' to denote the end of the file
stchar0=findstr('terminated',line);
if stchar0==6, end_loop=1; end
end
fclose(fid);
```

tally_convertF6_plot.m

function [filnam,prefix,E,T,fom,num,cell,titles,units,type,Nenergybins]=tally_convertF6_plot %

% This function uses the read mcnpx.m read routine to read in the output % from a run of mcnpx. % % This routine plots the tally data together in the same grouping as % outputted by MCNPX. For instance, if there are two separate F6 tally % calls within the MCNPX input deck, there will be two F6 graphs. % % This version is based off of tally_generic_plot but converts the F6 tally % from units of MeV/g to keV % % input: % % output: % - Multiple plots - the number of which depends on the number of % MCNPX tallies called in the input deck %

[filnam,prefix,E,T,fom,num,cell,titles,units,type,Nenergybins]=read_mcnpx; if filnam==0, filnam='Quit at file select'; return; end;

color_matrix = ['b';'r';'g';'c';'m';'y';'k']; scrsz = get(0,'ScreenSize');

[n,m]=size(num);

```
% -----
```

% Find out the width of the layers

% -----

% Assume that the layers are 5x5mm in the other 2D

width=str2double(inputdlg('How wide were the layers in MCNPX (cm)?','Please input a value')); volume=0.5*0.5*width;

if isempty(width),

filnam='Quit at layer width';

prefix=0; E=[]; T=[]; fom=[]; num=[]; cell=[]; titles=[]; units=[]; type=[]; Nenergybins=0;

```
return;
end
% Find out the density of the material
density={'2.3 ','3.2 ','3.52','6.15'};
[s,v]=listdlg('PromptString','Select a density of your material:','Name','Select One',...
      'SelectionMode', 'single', 'ListSize', [160 80], 'ListString', density);
if isempty(s),
  filnam='Quit at density select';
  prefix=0; E=[]; T=[]; fom=[]; num=[]; cell=[]; titles=[]; units=[]; type=[]; Nenergybins=0;
  return:
end
mass=str2double(density{s})*volume;
% -----
% Convert F6 from MeV/g to keV
% -----
for i=1:m
  if num{i}==6
    [q,r]=size(cell{i});
     for j=1:r %for each cell
       for k=1:q %for each energy bin
          T{i}(k,j)=T{i}(k,j)*1e3*mass;
       end
     end
  end
end
% -----
% Plot Each Tally Together
% -----
for i=1:m
  [q,r]=size(E{i});
  %for each different tally
     figure('Position',[1 scrsz(4)/2 scrsz(3)/2 scrsz(4)/2]);
       %for each different tally
       % Prints the plots
       semilogy(E{i}(:,1),T{i}(:,1),color_matrix(1),'LineWidth',2);
       title({[texlabel(filnam,'literal')],[titles{i}]});
       xlabel('E (MeV)');
       if num{i}==6, ylabel('keV');
       else, vlabel(units{i}); end
       text=(['Tally ', num2str(num{i}), ', Cell 0',num2str(cell{i}(1))]);
       grid on;
       hold on;
       whitebg([1,0.9841,0.9841]);
       for j=2:r
          if j==2, cc=2;
          else, cc=cc+1; end
          if cc>7, cc=1; end
          semilogy(E{i}(:,j),T{i}(:,j),color_matrix(cc),'LineWidth',2);
          if cell{i}(j)<10
            for k=1:q,
```

```
if k==1, legout=0; end
```

```
if legout==0
           if T{i}(k,j)>0
             legout=1;
             text=([text;'Tally ', num2str(num{i}), ', Cell 0',num2str(cell{i}(j))]);
           end
        end
     end
  else
     for k=1:q,
        if k==1, legout=0; end
        if legout==0
           if T{i}(k,j)>0
             legout=1;
             text=([text;'Tally ', num2str(num{i}), ', Cell ',num2str(cell{i}(j))]);
           end
        end
     end
  end
end
legend_h=legend(text,'Location','Best');
set(legend_h,'Color','w');
hold off:
```

```
end
```

energyDistribution.m

function [bin,dist]=energyDistribution(type)

%

% Asks questions to determine which preentered input spectrum to calculate % from

%

% Energy levels taken from data entered into mcnpx input card

%

% Input

% - Asks yes or no if there was a beta spectrum used

% - If a beta spectrum was used, then you select the spectrum from a

% list

- % If beta spectrum was not used, asks if gamma spectrum was used
- % If you say no to both, expect an error
- % If neither was actually used, you must manually edit the
- % program to include other spectrums
- %

% Find out if photons or electrons:

% Photons: m=6, Electrons, m=8

[n,m]=size(type);

if m==8

% Find out what energy betas were used in the run energies={'0 ','10 ','20 ','50 ','100','200','500','546'}; [s,v]=listdlg('PromptString','Select a Beta Endpoint Energy:','Name','Select One',... 'SelectionMode','single','ListSize',[160 130],'ListString',energies); if isempty(s), bin=[]; dist=[]; return; end

```
if energies{s}=='10 '
    % 10keV - beta
    bin = [1.8315E-05 0.00010989 0.000824176 0.0016666667 0.002490842 0.003333333
0.004166667 0.005 0.005824176 0.006666667 0.007490842 0.008333333 0.009175824 0.01];
  elseif energiess=='20
    % 20keV - beta
    bin = [3.663E-05 0.00021978 0.001648352 0.003333333 0.004981685 0.0066666667
0.008333333 0.01 0.011648352 0.013333333 0.014981685 0.0166666667 0.018351648 0.02];
  elseif energies{s}=='50 '
    % 50keV - beta
    bin = [9.16E-05 0.000549 0.00412 0.00833 0.0125 0.0167 0.0208 0.025 0.0291 0.0333
0.0375 0.0417 0.0459 0.05];
  elseif energies{s}=='100'
    % 100keV - beta
    bin = [0.000183 0.0011 0.00824 0.0167 0.0249 0.0333 0.0417 0.05 0.0582 0.0667 0.0749
0.0833 0.0918 0.1];
  elseif energies{s}=='200'
    % 200keV - beta
    bin = [0.000366 0.0022 0.0165 0.0333 0.0498 0.0667 0.0833 0.1 0.116 0.133 0.15 0.167
0.184 0.2];
  elseif energies{s}=='500'
    % 500keV - beta
    bin = [0.000916 0.00549 0.0412 0.0833 0.125 0.167 0.208 0.25 0.291 0.333 0.375 0.417
0.459 0.5];
  elseif energies{s}=='546'
    % 546keV - beta
    bin=[0.001 0.006 0.045 0.091 0.136 0.182 0.2275 0.273 0.318 0.364 0.409 0.455 0.501
0.546];
  else
    bin=[]; dist=[];
    return;
  end
  peak=bin(5);
  % beta dist
  dist = [0 1000 3405 4692 4768 3900 2775 2234 1725 1331 1007 764 556 378];
  % normalize the peak
  [n,m]=size(dist);
  [xi,yi,z]=int_trap(bin,dist);
  for i=1:m, dist(i)=dist(i)/z*peak; end
  return
elseif m==6
  % Find out what energy photons were used in the run
  energies={'bremsstrahlung','2.26MeV
                                          ','no radiation '};
  [s,v]=listdlg('PromptString', 'Select a Photon Spectrum:', 'Name', 'Select One',...
     'SelectionMode', 'single', 'ListSize', [160 100], 'ListString', energies);
  if isempty(s), bin=[]; dist=[]; return; end
  if energies{s}=='bremsstrahlung'
    bin=[.001.002.005.01.015.025.05.075.1.125.15.175.2.225.25.275.3];
    dist=[0 100 500 1000 2000 3405 4692 4768 3900 2775 2234 1725 1331 1007 764 556
378];
```

peak=bin(8);

```
% normalize the peak
[n,m]=size(dist);
[xi,yi,z]=int_trap(bin,dist);
for i=1:m, dist(i)=dist(i)/z*peak; end
elseif energies{s}=='2.26MeV
bin=[2.26];
dist=[1];
else
bin=[]; dist=[];
return;
end
return
end
end
```

plot_espec_edep_tally.m

```
function [filnam,prefix,E,T,fom,num,cell,titles,units,type,Nenergybins]=plot_espec_edep_tally
%
% This function uses the read mcnpx.m read routine to read in the output
% from a run of mcnpx.
%
% This routine plots the tally data together in the same grouping as
% outputted by MCNPX. For instance, if there are two separate F6 tally
% calls within the MCNPX input deck, there will be two F6 graphs.
%
% input:
%
% output:
%
        - Multiple plots - the number of which depends on the number of
        MCNPX tallies called in the input deck
%
%
```

[filnam,prefix,E,T,fom,num,cell,titles,units,type,Nenergybins]=tally_convertF6_plot;

```
% ------
% Plot the Data
% ------
color_matrix = ['b';'r';'g';'c';'m';'y';'k'];
scrsz = get(0,'ScreenSize');
```

[n,m]=size(num);

```
% ------
% Plot Energy Speectrum of Betas and Calulated Energy Distribution
% ------
legend_labels={};
for i=1:m
if mod(num{i},10)==4
[energy_bin,energy_dist]=energyDistribution(type{i});
if ~isempty(energy_bin)
```

```
figure('Position',[1 scrsz(4)/2 scrsz(3)/2 scrsz(4)/2]);
        [q,r]=size(E{i});
        for j=1:r
          if j==1
             cc=1;
             [a,b]=size(energy_dist);
             if b == 1
               params=strcat(color matrix(cc),'--p');
               semilogy(energy_bin,energy_dist,params,'LineWidth',2);
             else
               semilogy(energy_bin,energy_dist,color_matrix(cc),'LineStyle','--
','LineWidth',2,'MarkerSize',12);
             end
             xlabel('E (MeV)');
             ylabel(units{i});
             grid on;
             hold on;
             whitebg([1,0.9841,0.9841]);
             [a,b]=size(type{i});
             if b==8, text=('Beta Input Spectrum');
             elseif b==6, text=('Photon Input Spectrum'); end
             legend_labels=[legend_labels;{text}];
             cc=cc+1;
          else, cc=cc+1; end
          if cc>7, cc=1; end
          semilogy(E{i}(:,j),T{i}(:,j),color_matrix(cc),'LineWidth',2);
          for k=1:q,
             if k==1, legout=0; end
             if legout==0
               if T{i}(k,j)>0
                  legout=1;
                  text=(['Tally ',num2str(num{i}),', Cell ',num2str(cell{i}(j))]);
                  legend_labels=[legend_labels;{text}];
               end
             end
          end
        end
     end
  end
  if ~isempty(energy_bin)
     if b==8.
       title({[texlabel(filnam,'literal')],['Input Energy Distribution of Betas and Calulated Energy
Distribution']});
     elseif b==6,
        title({[texlabel(filnam,'literal')],['Input Energy Distribution of Photons and Calulated Energy
Distribution']});
     end
     legend_h=legend(legend_labels,'Location','Best');
     set(legend_h,'Color','w');
     hold off;
  end
  legend_labels={};
end
```

tally_compareF6_cell1.m

function [filnam,prefix,E,T,fom,num,cell,titles,units,type,Nenergybins]=tally_compareF6_cell1

% This function uses the read_mcnpx.m read routine to read in the output
% from a run of mcnpx.
%
% This routine plots the tally data from cell 1 of the F6 outputted by
% MCNPXplot only and asks for the next file to plot on the same graph. It

% will continue to do so, until you say "no" instead of "yes".

%

color_matrix = ['b';'r';'g';'c';'m';'y';'k']; scrsz = get(0,'ScreenSize');

cont=1; cc=1; find_density=1; legend_labels={};

while cont>0

```
% load in the information from read_mcnpx
[filnam,prefix,E,T,fom,num,cell,titles,units,type,Nenergybins]=read_mcnpx;
```

```
% determine the size of the data you are dealing with [n,m]=size(num); [q,r]=size(E{1});
```

if cont==1

% -----

% Find out the width of the layers

% -----

% Assume that the layers are 5x5mm in the other 2D

% Assume that all runs are calculated with the same width

width=str2double(inputdlg('How wide were the layers in MCNPX (cm)?','Please input a
value'));

volume=0.5*0.5*width;

end

if find_density==1

% Find out the density of the material

% -----

density={'2.3 ','3.2 ','3.52','6.15'};

[s,v]=listdlg('PromptString','Select a density of your material:','Name','Select One',... 'SelectionMode','single','ListSize',[160 80],'ListString',density);

mass=str2double(density{s})*volume;

% Do all the files have the same density - should it ask you the density % more than once?

button = questdlg('Are all of the runs done with the same material (Does the density stay the same)?',...

```
'Please select yes or no', 'Yes', 'No ', 'Yes');
    if button=='Yes', find density=0; end
  end
  % -----
  % Convert F6 from MeV/g to keV
  % -----
  for i=1:m
    if num{i}==6
       for j=1:r %for each cell
         for k=1:q %for each energy bin
            T{i}(k,j)=T{i}(k,j)*1e3*mass;
         end
       end
    end
  end
  % -----
  % Plot Each Tally Together
  % -----
  for i=1:m
    % Only continue for Tally F6
    if num{i}==6
       % Only start a figure the 1st time
       if cont==1, figure('Position',[1 scrsz(4)/2 scrsz(3)/2 scrsz(4)/2]); end
       % Plot
       semilogy(E{i}(:,1),T{i}(:,1),color_matrix(cc),'LineWidth',2);
       % Only do the following the first time
       if cont==1
         title({'Parametric Comparison: Spectrum of Energy Deposited'});
         xlabel('E (MeV)');
         ylabel('Energy Deposited (keV)');
         grid on;
         hold on:
         whitebg([1,0.9841,0.9841]);
       end
       text=(texlabel(filnam,'literal'));
       legend labels=[legend labels;{text}];
    end
  end
  % -----
  % Decide if you want to plot another file on the same graph
  % -----
  % If so, continue, if not, finish the graph and guit
  button = questdlg('Do you want to plot another file on the same graph?','Please select yes or
no','Yes','No ','Yes');
  if isempty(button)
    legend_h=legend(legend_labels,'Location','Best');
    set(legend_h,'Color','w');
    hold off
    cont=0;
  elseif button=='No '
    legend h=legend(legend labels,'Location','Best');
    set(legend_h,'Color','w');
```

```
hold off
  cont=0:
else %button=='Yes'
  cont=cont+1;
  cc=cc+1;
  if cc>6, cc=1; end
end
```

end

plot_edep_pk_layers.m

function plot_edep_pk_layers

%

% This function uses the read_mcnpx.m read routine to read in the output % from a run of mcnpx. % % This routine plots the Percent Energy Deposition in the Layers by % calculating the total energy deposition and dividing by the peak energy % of the input spectrum used. % % input: % - Beta Endpoint Energy - 10/20/50/100/200/500 keV - from here the % peak energy can be determined % - Width - or thickness of the layers being used in the model. % Typical widths are 5e-4cm or 5e-2cm. Check the model if you are not % sure. The width is used to calculate the volume of the chip, % assuming that the other sides are 5mmx5mm (0.5cm). % - Density - The density of the chip is needed to find the mass % and to convert the units of the tally into keV from MeV/gram. % The density of % SiC=3.2g/cc % Si=2.3g/cc % GaN=6.15g/cc % cvd diamond=3.52g/cc % % output: % - A plot with one point per layer including an exponential fit. % The equation is listed in the legend. % cont=1; cc=1;while cont>0 [filnam,prefix,E,T,fom,num,cell,titles,units,type,Nenergybins]=read mcnpx; if filnam==0. ';'Quit at file select']); disp([' return:

end;

```
color matrix = ['b';'r';'m';'g';'c''k';];
scrsz = get(0,'ScreenSize');
```

```
[n,m]=size(num);
```

```
% -----
  % Plot the Energy Deposition in the Layers
  % -----
  % First Find the Tally Totals for F6
  F6 total=[];
  for i=1:m,
     if num{i}==6
       [q,r]=size(T{i});
       for k=1:r
          sum=0;
          for j=1:Nenergybins
            sum=sum+T{i}(j,k);
          end
          F6 total=[F6 total,sum];
       end
       % Find out what energy betas were used in the run
       energies={'10','20','50','100','200','500'};
       [s,v]=listdlg('PromptString', 'Select a Beta Endpoint Energy:', 'Name', 'Select One',...
          'SelectionMode', 'single', 'ListSize', [160 80], 'ListString', energies);
       if isempty(s)
                             ';'Quit in energy select']);
          disp(['
          return;
       end;
       if s==1, peak=2.49; %10keV - energies(s)
       elseif s==2, avg=8.2; %peak=4.98; %20keV
       elseif s==3, avg=20.4; %peak=12.5; %50keV
       elseif s==4, avg=40.8; %peak=24.9; %100keV
       elseif s==5, avg=81.5; %peak=49.8; %200keV
       elseif s==6, avg=203.8; %peak=125; %500keV
       end
       % Find out the width of the layers
       % Assume that the layers are 5x5mm in the other 2D
       width=str2double( inputdlg('How wide were the layers in MCNPX (cm)?','Please input a
value'));
       if isempty(width)
          disp(['
                             ';'Quit in width select']);
          return:
       end
       volume=0.5*0.5*width;
       % Find out the density of the material
       density={'2.3 ','3.2 ','3.52','6.15'};
       [t,w]=listdlg('PromptString','Select a density of your material:','Name','Select One',...
          'SelectionMode', 'single', 'ListSize', [160 80], 'ListString', density);
       if isempty(t),
                              ';'Quit in density select']);
          disp(['
          return:
       end
       mass=str2double(density{t})*volume;
```

```
%Convert F6_total from MeV/g to keV
        ratio=[]:
       for I=1:r
          edep=F6_total(l)*1e3*mass;
          %ratio(l)=edep/peak*100;
          ratio(I)=edep/avg*100;
        end
       % Plot and Fit the Data
        if cont==1
          figure('Position',[1*scrsz(3)/5 4*scrsz(4)/9 4*scrsz(3)/9 4*scrsz(4)/9]);
        end
       [estimates, model] = fitcurve(cell{i},ratio);
        properties=strcat(['*',color_matrix(cc)]);
        plot(cell{i},ratio,properties);
        if cont==1
          hold on
          grid on
          xlabel('layer');
          vlabel('Energy Deposition/Average Energy (%)');
          title('Percent Energy Deposition in Layers');
        end
        [sse, FittedCurve] = model(estimates);
        plot(cell{i}, FittedCurve, color matrix(cc))
       data{cont}=texlabel(filnam,'literal'):
        interp{cont}=texlabel(strcat(['y = ',num2str(estimates(1)),' e^',num2str(-1*estimates(2)),'
x',]),'literal');
        % Changes the background color to tan but later change the legend back to white
        whitebg([1,0.9841,0.9841]);
       % Decide if you want to plot another file on the same graph
       % If so, continue, if not, finish the graph and quit
        button = questdlq('Do you want to plot another file on the same graph?','Please select yes
or no','Yes','No ','Yes');
        if isempty(button)
          if cont==1
             title({[texlabel(filnam,'literal')],...
               ['Percent Energy Deposition in Layers']}):
             legend_h = legend('Data',texlabel(strcat(['y = ',num2str(estimates(1)),' e^/,num2str(-
1*estimates(2)),' x',]),'literal'));
             set(legend_h,'Color','w');
          else
             for i=1:cont
               if i==1, textstring={[data{i}],[interp{i}]];
               else, textstring=cat(2,textstring,{[data{i}],[interp{i}]]); end
             end
             legend_h = legend(textstring);
             set(legend h,'Color','w');
          end
          hold off
          cont=0:
        elseif button=='No '
          if cont==1
```

```
45
```

```
title({[texlabel(filnam,'literal')],...
                       ['Percent Energy Deposition in Layers']}):
                    legend h = legend('Data',texlabel(strcat(['y = ',num2str(estimates(1)),' e^/,num2str(-
        1*estimates(2)), 'x',]), 'literal'));
                    set(legend h,'Color','w');
                  else
                    for i=1:cont
                       if i==1, textstring={[data{i}],[interp{i}]];
                       else, textstring=cat(2,textstring,{[data{i}],[interp{i}]]); end
                    end
                    legend_h = legend(textstring);
                    set(legend h,'Color','w');
                  end
                  hold off
                  cont=0:
               else %button=='Yes'
                  cont=cont+1;
                  cc=cc+1:
                  if cc>6, cc=1; end
               end
             end
          end
        end
        end
mcnpx_mesh_energy_convert.m
        function mcnpx mesh energy convert
        %
        % Read mesh diagnostic output .... mdat file type after ascII conversion
        % Plot contours of energy flux or dose, and the associated statistics
        % Logic inserted for any rectangular mesh
                - organizes data into a 3D matrix representing x-y-z
        %
        %
                - looks at size of each dimension and selects biggest side of
        %
                 rectangle for the plane, under the assumption that there is
                  only one division in the other dimension
        %
                - labels on graph tell you which plane you are looking at, as
        %
                 well as the location of the corresponding value
        %
        %
                    - the mcnpx mesh output only has an accuracy of 3 decimal
        %
                     places so for smaller numbers, what looks like an error
        %
                     of a repeating number in the data lables is actually
        %
                     what the mdat file reads
        %
        % Format:
```

mcnpx_contour_read_mesh

%

%

% Inputs:

| % | - conversion_print: if the conversion_print if inputed with any number greater |
|---|--|
| % | than zero, the converted graph will be plotted in number |
| % | denisty #/cc |
| % | |
| % | statistics_print: if statistics_print is inputed with any number greater |
| % | than zero, the statisticswill be outputed as well as just the data |
| % | |

% - data_print: if data_print is inputed with any number greater

% than zero, the data will be outputed

%

% Development

```
%
        - labels of graph should read from the text and converted into
```

- % numbers, dived up manually into tick marks
- % (currently read from labels in lines 199-209)
- % - the labels of the countour plot is not always
- % accurate
- %

```
% flux in #/cm2/s
```

```
% dose in rem/hr
```

```
ncell=0; Ncells=56; Nenergybins=800; Nlines=20000;
E=zeros(Nenergybins,Ncells); MeVpg=E; fom=E;
ruler='123456789 123456789 123456789 123456789 123456789 123456789 123456789
123456789 123456789 123456789 123456789 123456789 123456789;
```

%

```
% *** read from mdat data ***
%
nlin=0; ncell=0;
suffix='.';
prefix='C:\mcnpx\scratch\';
pathfilename=prefix;
[filnam,prefix,filterindex] = uigetfile([pathfilename,'*.*']);
if filterindex==0,
  disp(['
                      ':'Quit at file select'])
  return;
end;
disp([prefix,filnam])
filnamcomp = [prefix,filnam];
fid = fopen(filnamcomp);
% find the peak energy
                       ','20
energies={'10
                                   ','50
                                     50         ',...
____'.546         '....
                          ','500
  '100
              '.'200
  'bremsstrahlung'};
[s,v]=listdlg('PromptString','Select an Endpoint Energy:','Name','Select One',...
   'SelectionMode', 'single', 'ListSize', [160 120], 'ListString', energies);
if isempty(s)
  disp(['
                       ';'Quit in energy select'])
  return:
end:
                            ', peak=2.49;
if energies\{s\} = = 10
elseif energies{s}=='20
                                 ', peak=4.98;
elseif energies{s}=='50
                                  peak=12.5;
elseif energies{s}=='100
                                  , peak=24.9;
                                  , peak=49.8;
elseif energies{s}=='200
                                  , peak=125:
elseif energies{s}=='500
elseif energies{s}=='546
                                  , peak=136;
elseif energies{s}=='bremsstrahlung', peak=75; end
peak=peak*1e-3; %convert peak from keV to MeV
```

conversion_print = questdlg('Do you want to plot the converted data?','Please select yes or no','Yes','No ','Yes'); data_print = questdlg('Do you want to plot the data before conversion?','Please select yes or no','Yes','No ','No '); statistics_print = questdlg('Do you want to plot the statistics of the data?','Please select yes or no','Yes','No ','No ');

%

```
% input line detemines how many contours
%
header = fgetl(fid);
input = fgetl(fid);
line = fgetl(fid);
ncontours = str2num(input(1:3));
```

```
i=1;
```

```
while (i<=ncontours)
  %
  % determine size of different contours
  %
  A = fscanf(fid, '\%i', 19);
  B = fscanf(fid, '%g', 4); %need to step through floating numbers\
  if A(2)==2, ptype{i}='photon';
  elseif A(2)==3, ptype{i}='electron';
  else, ptype{i}="; end
  xdim{i} = A(3);
  vdim{i} = A(4):
  zdim{i} = A(5);
  totdim{i} = A(7);
  skip{i}=0;
  for j=10:19
     % check if there are more meshes written on one line to be
     % accounted for
     if A(j)>0 & j>10,
       ncontours=ncontours+1;
       ptype{i+1}=ptype{i};
       xdim{i+1}=xdim{i};
       vdim{i+1}=vdim{i};
       zdim{i+1}=zdim{i};
       totdim{i+1}=totdim{i};
       skip{i+1}=1;
       i=i+1;
     end
     if A(j)==1, type{i}='Flux in #/cm^2 per souce particle';
     elseif A(j)==3, type{i}='Population in weight times the track length';
     elseif A(j)==4, type{i}='Average Energy Deposition per Unit Volume in MeV/cm^3 per source
particle';
     elseif A(i)==5, type{i}='Dose in rem/hr per source particle';
     elseif A(j)==0, %don't do anything
     else type{i}=";
     end
  end
  i=i+1;
```

```
for i=1:ncontours
  %
  % determine labeling
  %
  if skip{i}==0
     xlabels{i} = fscanf(fid, '%13g', xdim{i});
     ylabels{i} = fscanf(fid, '%13g', ydim{i});
     zlabels{i} = fscanf(fid, '%13g', zdim{i});
  else
     xlabels{i} = xlabels{i-1};
     ylabels{i} = ylabels{i-1};
     zlabels{i} = zlabels{i-1};
  end
  %
  % read data and statistics and store in temporary locations before
  % parsing
  %
  tmp_data = fscanf(fid,'%13g',totdim{i});
  tmp_stat = fscanf(fid,'%13g',totdim{i});
  data{i} = zeros(xdim{i}-1,ydim{i}-1,zdim{i}-1);
  stat{i} = zeros(xdim{i}-1,ydim{i}-1,zdim{i}-1);
  index = 1;
  for k=1:zdim{i}-1
     for j=1:ydim{i}-1
       for ii=1:xdim{i}-1
          %sprintf('%i %i %i %i',index,ii,j,k)
          data{i}(ii,j,k) = tmp data(index);
          stat{i}(ii,j,k) = tmp_stat(index);
          index = index + 1;
       end
     end
  end
end
fclose(fid);
for i=1:ncontours
  [n,m]=size(type{i});
  % The string:
  % 'Average Energy Deposition per Unit Volume in MeV/cm^3 per source particle'
  %
            is 73 characters long, and we are searching for it - we
  %
            created type{i} ourselves based on a number from the mdat file
  if m==73
     %
     % surface plot can only handle a 2x2 matrix
     % if zdim=2 (only one z-point), then this does not matter
     % if zdim is important, then it does
     % determine which dimensions to look at
     % possibly break up into more than one contour plot
     %
```

```
sdim=zdim{i}; idim=xdim{i}; jdim=ydim{i}; order='xy'; plane='z';
if ydim{i}<sdim, sdim=ydim{i}; idim=xdim{i}; idim=zdim{i}; order='xz'; plane='y'; end
if xdim{i}<sdim, sdim=xdim{i}; idim=ydim{i}; jdim=zdim{i}; order='yz'; plane='x'; end
contour = zeros(idim-1,jdim-1,sdim-1);
statistics = zeros(idim-1,idim-1,sdim-1);
if order=='xz'
  contour = permute(data{i},[1 3 2]);
  statistics = permute(stat{i},[1 3 2]);
  ilabel=xlabels{i}; laxis='X-Axis';
  jlabel=zlabels{i}; Jaxis='Z-Axis';
  %
        klabel=ylabels{i};
elseif order=='yz'
  contour = permute(data{i}, [2 3 1]);
  statistics = permute(stat{i},[2 3 1]);
  ilabel=zlabels{i}: laxis='Z-Axis':
  ilabel=ylabels{i}; Jaxis='Y-Axis';
  %
          klabel=xlabels{i};
else
  contour = data{i};
  statistics = stat{i};
  ilabel=ylabels{i}; laxis='Y-Axis';
  jlabel=xlabels{i}; Jaxis='X-Axis';
  %
          klabel=zlabels{i};
end
%
% since we only want to make a 2D plot at this point, drop all other
% layers of contour and statistics except the first in the sdim direction.
% in most cases, there is only one layer anyway, so there are no plots
% being neglected
%
% it is important to only have a 2D array for the contourf plotting
% function
%
contour = contour(:,:,1);
statistics = statistics(:,:,1);
% Divide up the labels into 10 and 5 tick marks
[ni,mi]=size(ilabel);
[nj,mj]=size(jlabel);
if ni>5, scale_factor_i = int32(ni/5);,
else scale factor i = 1; end
if nj>10, scale factor j = int32(nj/10);
else scale factor j = 1; end
iaxis = [ilabel(1)];
jaxis = [jlabel(1)];
for iii=1+scale factor i:scale factor i:ni, iaxis = [iaxis,ilabel(iii)]; end
for jj=1+scale_factor_j:scale_factor_j:nj, jaxis = [jaxis,jlabel(jj)]; end
%
```

% plot contour and statistics % new plot for each energy distribution mesh %

```
% Move button commands into actions
     if isempty(conversion print), cp=0;
     elseif conversion print=='No ', cp=0;
     else, cp=1; end
     if isempty(data_print), dp=0;
     elseif data_print=='No ', dp=0;
     else, dp=1; end
     if isempty(statistics_print), sp=0;
     elseif statistics print=='No', sp=0;
     else, sp=1; end
     % Always print something
     if (cp==0) & (dp==0) & (sp==0), cp=1; end
     scrsz = get(0,'ScreenSize');
     if cp==1
       figure('Position',[scrsz(3)/3 scrsz(2) scrsz(3)/3 2*scrsz(4)/3]);
        [C,h] = contourf( contour/peak );
clabel(C,h,'FontSize',12,'Color','w','LabelSpacing',150,'Rotation',0);
        %[h] = imagesc( contour/peak ); colorbar;
        title({[texlabel(filnam,'literal')],...
          ['Number Density in #/cm^3'],...
          ['Taken in the ',plane,'-plane.']});
        set(gca,'XTickLabel',iaxis)
        set(gca,'YTickLabel',jaxis)
        xlabel(laxis);
       ylabel(Jaxis);
     end
     if dp==1
       figure('Position',[1 scrsz(2) scrsz(3)/3 2*scrsz(4)/3]);
        [C,h] = contourf( contour/peak );
clabel(C,h,'FontSize',12,'Color','w','LabelSpacing',150,'Rotation',0);
        %[h] = imagesc( contour/peak ); colorbar;
       title({[texlabel(filnam,'literal')],...
          [type{i}],...
          ['Taken in the ',plane,'-plane.']});
        set(gca,'XTickLabel',iaxis)
       set(gca,'YTickLabel',jaxis)
        xlabel(laxis):
       ylabel(Jaxis);
     end
     if sp==1
       figure('Position',[2*scrsz(3)/3 scrsz(2) scrsz(3)/3 2*scrsz(4)/3]);
        [C,h] = contourf( contour/peak );
clabel(C,h,'FontSize',12,'Color','w','LabelSpacing',150,'Rotation',0);
        %[h] = imagesc( contour/peak ); colorbar;
        title({[texlabel(filnam,'literal')],...
          ['Statistics '],...
          ['Taken in the ',plane,'-plane.']});
       set(gca,'XTickLabel',iaxis)
        set(gca,'YTickLabel',jaxis)
        xlabel(laxis);
        ylabel(Jaxis);
```

```
end
end
end
```

calc_energy_flux_ratio.m

```
function [eflux,edep,ratio]=calc_energy_flux_ratio
%
% This function uses the read_mcnpx.m read routine to read in the output
% from a run of mcnpx.
%
% This function calculates the energy flux - goes from #/cm2 to MeV/cc
%
% -----
% Read in the Data
% -----
[filnam,prefix,E,T,fom,num,cell,titles,units,type,Nenergybins]=read mcnpx;
if filnam==0,
                   ';'Quit at file select']);
  disp(['
  return;
end;
% -----
% Find out the width of the layers
% -----
width=str2double( inputdlg('How wide were the layers in MCNPX (cm)?', 'Please input a value') );
if isempty(width)
  disp(['
                   ';'Quit in width select']);
  return;
end
% Assume that the layers are 5x5mm in the other 2D
area=0.5*0.5;
volume=area*width;
% -----
% Find out the density of the material
% -----
den={'2.3 ','3.2 ','3.52','6.15'};
[t,w]=listdlg('PromptString','Select a density of your material:','Name','Select One',...
  'SelectionMode', 'single', 'ListSize', [160 80], 'ListString', den);
if isempty(t),
  disp(['
                    ';'Quit in density select']);
  return:
end
density=str2double(den{t});
mass=density*volume;
% -----
% Convert from #/cm2 to MeV/cc and find the sums
% -----
[n,m]=size(num);
F4_total=[]; F6_total=[];
for i=1:m
  [q,r]=size(T{i});
```

```
if mod(num{i},10)==4
    for k=1:r
       sum=0:
       for j=1:Nenergybins
         %go from units of #/cm2 to MeV/cm2 to MeV/cc to MeV/g
         T_{i}(j,k)=T_{i}(j,k)*E_{i}(j,k)/width/density;
         %go from units of #/cm2 to MeV/cm2 to MeV
         T{i}(j,k)=T{i}(j,k)*E{i}(j,k)*area;
         %calculate the sum
         sum=sum+T{i}(j,k);
       end
       %store the sums from all the cells in an array
       F4_total=[F4_total,sum];
    end
  elseif mod(num{i},10)==6
    for k=1:r
       sum=0:
       for j=1:Nenergybins
         %go from MeV/g to MeV
         T{i}(j,k)=T{i}(j,k)*E{i}(j,k)*mass;
         %calculate the sum
         sum=sum+T{i}(j,k);
       end
       %store the sums from all the cells in an array
       F6_total=[F6_total,sum];
    end
  end
end
% -----
% For the first cell only, compare the sums, and find the percentage
% difference (assume that the cell number is the same)
% -----
eflux=F4_total(1);
edep=F6_total(1);
ratio=edep/eflux*100;
disp(['F4 and F6 tallies have a ',num2str(ratio),'% ratio']);
```

```
end
```

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