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CUSTOMIZED MULTI-GROUP CROSS SECTION GENERATION WITH NJOY
FOR DISCRETE ORDINATES COMPUTED TOMOGRAPHY AND RADIOGRAPHY
SIMULATION

by

STEVEN MICHAEL WAGSTAFF

A THESIS

Presented to the Faculty of the Graduate School of the
MISSOURI UNIVERSITY OF SCIENCE AND TECHNOLOGY

In Partial Fulfillment of the Requirements for the Degree

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2018

Approved by

Xin Liu, Advisor
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Ayodeji B. Alajo

ABSTRACT

The purpose of this work was to explore the creation of photoatomic multi-group cross section libraries to be used with a software package DOCTORS (Discrete Ordinates Computed TOMography and Radiography Simulator). This software solves the linear Boltzmann equation using the discrete ordinates method [1]. To create these libraries, NJOY2016 was used, creating both fine and broad energy multi-group cross section files. The cross section's accuracy was tested against an equivalent Monte Carlo simulation using MCNP6.

Two simulation geometries were used. The first, a cylindrical water phantom with a single source projection placed in front, simulating an X-ray radiography. The second used the same water phantom with 16 cone beam sources placed evenly around the phantom to simulate a computed tomography (CT) scan. The accuracy of the fine energy multi-group cross sections when used in DOCTORS has been verified. The accuracy of the broad energy multi-group cross sections when used in DOCTORS shows that more work must be done before they can be used reliably.

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I would like to thank my advisor Dr. Xin Liu for giving me this opportunity. I would also like to thank Dr. Hyoung K. Lee and Dr. Ayodeji B. Alajo for sitting on my committee and offering invaluable advice and insights. Dr. Wim Haeck at Los Alamos National Laboratory for helping me learn about the NJOY program. The Nuclear Engineering faculty at MS&T for the education which that allowed me to move into this work. Finally, I would like to thank my family for the support they gave me throughout this journey.

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1. INTRODUCTION

Software which allows the simulation of neutronics in nuclear engineering has existed for decades. These software packages require the use of particle-material interaction data called cross section libraries. There are many libraries which cater to different materials and situations related to neutronics and nuclear reactors. There is currently no multi-group library dedicated to low energy ($E < 1$ MeV) X-ray imaging, including radiography and CT. These are important non-destructive testing and evaluation techniques used in numerous industrial and medical applications.

The creation of these multi-group cross section libraries can be achieved using the software package NJOY [2]. These cross sections will be used with the DOCTORS program, which solves the linear Boltzmann equation using the discrete ordinates method [1]. The results of these simulations performed with DOCTORS will be compared to Monte Carlo simulations using MCNP6 [3]. All MCNP6 simulations were completed and NJOY multi-group cross sections were created using the photon library from ENDF/B-VII.1. This work will test the accuracy and viability of creating fine and broad energy multi-group cross section libraries using NJOY and their use with DOCTORS.

2. LITERATURE REVIEW

This section will review the relevant literature for this work. This review is split into 3 sections covering discrete ordinates methodology used by DOCTORS, Monte Carlo simulation with MCNP6, and NJOY2016.

2.1. DISCRETE ORDINATES SOFTWARE

The discrete ordinates method has been around since the 1950's when Chandrasekhar used it for radiation transport in atmospheres [4]. There have been several computer codes developed to solve discrete ordinates since that time. This started with the computer code DORT which was eventually replaced by TORT, DORT's 3D counterpart [5]. Denovo, relatively recently created, solves discrete ordinates utilizing modern programming standards and replaced TORT [6]. Denovo also utilized the Ex nihilo package for data processing solution methods [7].

DOCTORS, created in 2017, computes the effective dose in a patient using the discrete ordinates method [1]. This code attempts to increase processing speed through use of the graphical processing unit (GPU). The current version of DOCTORS uses parallel ray-tracing and voxel sweeping algorithms implemented on a single GPU through the CUDA language [8]

2.2. MONTE CARLO SIMULATION

Monte Carlo simulations (stochastic methods) have been used repeatedly in the past [9]. The Monte Carlo method does not solve the transport equation directly for

particle behavior instead tracking individual particles and recording aspects of their average behavior [10]. Due to the stochastic nature of particle transport, Monte Carlo simulations are typically considered the gold standard and are often used as benchmarks for simulating photon transport with other methods. Unfortunately, computation time for these simulations can be very high due to the required large number of particle histories to keep the relative uncertainty acceptable.

When choosing to run a Monte Carlo simulations MCNP is a commonly used software package. MCNP is a general-purpose, continuous-energy, generalized-geometry, time-dependent Monte Carlo radiation-transport code [3]. MCNP's primary source of nuclear data is Evaluated Nuclear Data Files (ENDF) [11]. This evaluated data is processed into a format appropriate for MCNP by codes such as NJOY [12].

2.3. NJOY

The NJOY nuclear data processing system is a comprehensive computer code package for producing pointwise and multigroup nuclear cross sections from data in the ENDF format [13]. NJOY originally started as a successor to the code package Multigroup Interpretation of Nuclear X-sections more commonly known at the time as MINX [14]. Early in NJOY's life, the mid 1970's, development was supported by the U.S. Fast Breeder Reactor and Weapons Programs [2]. The current release is NJOY2016, an open source code which is freely available to the public.

NJOY2016 is a modular program consisting of the primary program module NJOY and 23 sub modules used by the primary program. The major modules used to create the multi-group cross section files for DOCTORS are RECONR, GAMINR, and DTFR. MCNP cross section files can also be created using NJOY2016 using the ACER module.

3. METHODS

This section will cover the methods used during this work. Section 3.1 will discuss the theory behind multi-group approximation. Section 3.2 will discuss the methods used for creating multi-group cross section files with NJOY 2016. Section 3.3 and 3.4 will cover the set up used for all simulation and the methods used to compare the results respectively.

3.1. MULTI-GROUP ENERGY APPROXIMATION

In particle transport simulation, the assumption is often made that the energy range 0 to E_0 is made of G intervals with the width $\Delta E_g = E_g - E_{g+1}$, for $g = 1, \dots, G$. [15]. The convention of increasing group number corresponding with decreasing energy is generally accepted. When the particle flux and interaction cross sections over each energy group are averaged, they become functions of group index rather than energy [16]. The group averaged total cross section, $\sigma_{t,g}(r)$, can be calculated with equation (1).

$$\sigma_{t,g}(r) = \frac{\int_{\Delta E_g} \sigma_t(r,E) \phi(r,E) dE}{\phi_g(r)} \quad (1)$$

where $\sigma_t(r, E)$ is the continuous energy total cross section, and $\phi(r, E)$ is the scalar flux (distribution of the particle fluence with respect to energy in the ICRU nomenclature [17]).

The group scalar flux $\phi_g(r)$ corresponds to the scalar flux by equation (2).

$$\phi_g(r) = \int_{\Delta E_g} \phi(r,E) dE \quad (2)$$

Group cross sections are created by approximating the problem specific scalar flux which is typically unknown. This scalar flux is known as the spectral weighting function $f(E)$, with energy separability assumed in equation (3) [16].

$$\phi(r,E) \approx f(E)\phi_g(r), E_{g+1} \leq E < E_g \quad (3)$$

When equation (2) and (3) are substituted into equation (1) the group cross section $\sigma_{t,g}(r)$ becomes equation (4).

$$\sigma_{t,g} = \frac{\int_{\Delta E_g} \sigma_t(r,E) f(E) dE}{\int_{\Delta E_g} f(E) dE} \quad (4)$$

The spectral weighting information will be obtained through the use of the fine multi-group (90 energy groups) cross section file created with NJOY and run with DOCTORS. This fluence data will then be used to create the broad energy multi-group cross section file using the custom weighting option in NJOY.

3.2. NJOY2016

The creation of multi-group cross section files was handled by the NJOY software package. There were three modules primarily used when creating photoatomic multi-group cross section data for use in DOCTORS: RECONR, GAMINR, and DTFR. These

modules must be run in sequence as the output from one module is required to run the next. The final output from DTFR must be modified with a header before it can be used in DOCTORS. The NJOY input file used to create the weighted 7 group water phantom data table can be found in appendix A.

3.2.1. RECONR Module. Creating a cross section file starts with data in an ENDF/B-VII file which must be input into the RECONR module. This module is used to reconstruct resonance cross sections from resonance parameters and reconstruct cross sections from ENDF nonlinear interpolation schemes [2]. There are several options which must be input by the user to run this module. Those inputs are: the input/output files, a label for the file, the ENDF material number, the number of descriptive cards used, and the fractional reconstruction tolerance desired. This step is required primarily because the output format for this module is a pointwise ENDF (PENDF) which is required to run the GAMINR module.

3.2.2. GAMINR Module. The GAMINR module was created to produce complete and accurate multigroup photoatomic cross sections [2]. As with RECONR, this module has inputs which must be defined by the user. GAMINR requires the input of the original ENDF file as well as the PENDF output file created from RECONR as well as a designated output file. The basic options which must be defined are: ENDF material number, gamma group structure, weighting option, Legendre order, and the ENDF file/section to be processed.

There are pre-defined options in NJOY for the gamma group structure and weighting option. When either of these options are set as user defined addition inputs

must be added to the input file. The energy group option requires the number of desired groups and a number of energy boundaries equal to the number of desired groups plus one, input in eV. The weighting information must be entered as a TAB1 record. The following format is used for a single interpolation range:

Float, Float, INT, INT, NR, NP

NBT, INT

E(1) C(1) ...

where Float is a double value, INT is an integer, NR is the number of interpolation ranges, NP is the number of (E, C(E)) pairs, NBT is the index of the (E, C(E)) pair corresponding to the end of an interpolation range, and the last INT value is the interpolation law used [2]. The output file from GAMINR is in the form of a groupwise ENDF file (GENDF).

3.2.3. DTFR Module. The DTFR module is used to prepare libraries for discrete-ordinate transport codes that accept the format designed for the S_N code DTF-IV [2]. The transport table output of DTFR must be modified with a header before use in DOCTORS. This header contains a label, number of energy groups, energy group boundary information, Legendre order, number of materials, and ENDF material numbers for all materials.

The DTFR module requires the input of the GENDF and PENDF files which were created from the RECONR and GAMINR modules. The output file for the tables must be defined as well as the number of tables desired along with the number of energy groups.

DTFR is also used as a quick plotting tool requiring several printing options which must be included in the input file but will not be discussed.

In addition, the user must also enter table information. The position of the total cross section, in-group scattering, and total table length. DTFR also allows for special edits which, in this case, were used for three reactions: photon coherent scattering MT 502 (ENDF reaction type numbers), photon incoherent scattering MT 504, and photoelectric absorption MT 522. Finally, a material description, ENDF material number, index number, and temperature must be entered.

3.3. SIMULATION SETUP

There were two models used to create the data for this study. The first, had an isotropic point source placed in front of the phantom simulating radiography. The second, used 16 cone beam sources placed uniformly around the phantom to simulate a CT scan [18]. A simple diagram of the water phantom and cone beam setup can be found in Figure 3.1, the cone angle is 30° for each cone beam.

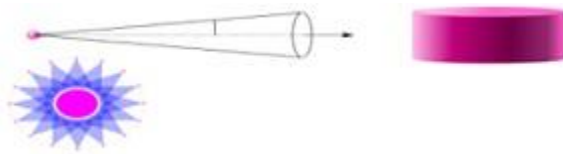


Figure 3.1. Cone Beam Simulation Setup, Side and Top Down View
[19]

The input file for the MCNP6 simulation was created using DOCTORS. The user defined geometry, material data, and source specifications input into DOCTORS is automatically used to create the MCNP6 input file. Currently the only supported file format for a Monte Carlo simulation is the MCNP6 input file format [20].

The water phantom is a cylinder with a diameter of 35 cm and is 12.5 cm long. The phantom is located at the center of a rectangular empty space with a volume of 50 x 50 x 12.5 cm in the x, y, and z directions respectively. The mesh dimensions for the volume is 64 x 64 x 16 for a total of 65,536 voxels with a pitch of 7.81 mm. As indicated by previous study, isotropic scattering dominates at these low (<100 KeV) energies [21]. This led to using quadrature set S_6 and isotropic scattering (0th Legendre expansion) in all simulations.

Both the isotropic point source and cone beam setups were used 3 times. The first simulation in DOCTORS was performed using a 90 group cross section. The energy range was from 10 to 100 KeV with group sizes of 1 KeV and the constant weighting function option chosen in NJOY.

The second and third simulations used 7 energy groups, with energy ranges: 10-20, 20-30, 30-45, 45-60, 60-70, 70-75, and 75-100 KeV. The second simulation used the constant weighting function option. The third simulation used the fluence information obtained from the first simulation in the custom weighting option used in NJOY. The fluence information was obtained from the central point of the middle slice of the water phantom at (32, 32, 16). Figure 3.2 shows the central slice of the water phantom and the 5 points sampled for fluence data. The MCNP6 simulations were completed using the photon library from ENDF/B VII.1.

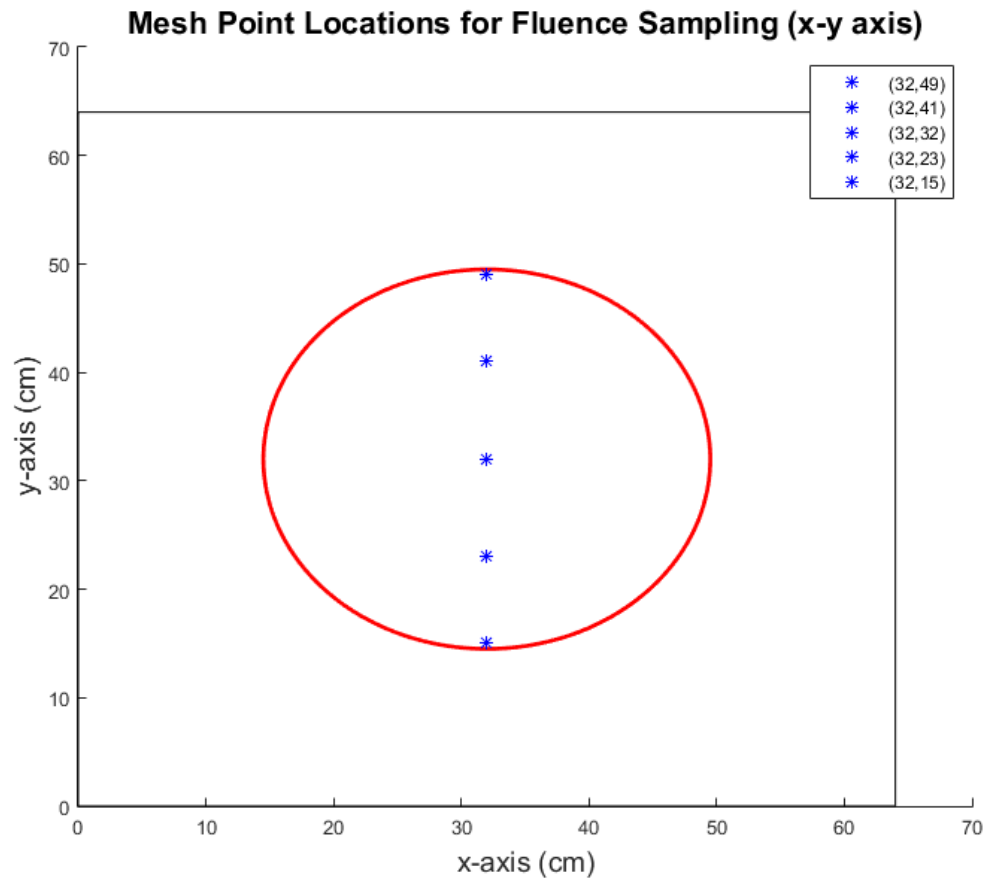


Figure 3.2. Fluence Sample Points (x-y axis)

3.4. VERIFICATION PROCESS

Matlab was used to analyze the data output from DOCTORS and MCNP6. The uncollided, collided, and total fluence data was compared. The total fluence was obtained by adding the uncollided and collided data. The MCNP6 data also has relative error and for all simulations the tolerance threshold was set to 5%. The total error was also calculated by adding the uncollided and collided error together. The propagation of error can be defined using equation (5) which for the case of addition becomes equation (6).

$$\sigma_f^2 = \left(\frac{\delta f}{\delta A}\right)^2 \sigma_A^2 + \left(\frac{\delta f}{\delta B}\right)^2 \sigma_B^2 \quad (5)$$

$$\sigma_f = \sqrt{\sigma_A^2 + \sigma_B^2} \quad (6)$$

where A and B are the error numbers and σ_A , and σ_B are the associated standard deviations of the error data [22].

The analysis was conducted on the central slice along the z-axis. The data from DOCTORS was unpacked into a cell with dimensions 16 x 64 x 64. The MCNP6 data was output as one column and required the use of the reshape function in Matlab. This function allowed the conversion of the column to the 16 x 64 x 64 matrix shape. Both sets of data were then reduced to the central slice with the squeeze function. Squeeze allows the removal of a dimension from a matrix converting the 16 x 64 x 64 into a single 64 x 64 matrix for only the 8th layer.

The raw fluence data was compared by calculating the root-mean-square-deviation (RMSD) using equation (7).

$$\text{RMSD} = \frac{1}{N} \sqrt{\sum_{n=1}^N \frac{\text{DOCTORS}_n - \text{MCNP}_n}{\text{MCNP}_n}} \quad (7)$$

where n is the current fluence value being analyzed and N is the total number of fluence values to pass the error checks. These checks ensure that only fluence values that are lower than the set tolerance and higher than 0 are evaluated.

4. RESULTS AND DISCUSSION

This section will present the results from the six trial simulations covering single projection and multi-projection cone beam. The resulting RMSD values from MCNP6 and DOCTORS will be compared and discussed.

4.1. RESULTS

4.1.1. Single Projection. The isotropic point source positioned in front of the phantom was a single projection source. The single projection simulation was performed using both MCNP6 and DOCTORS. The phantom's central slice was compared by examining the fluence values of the central energy group and the RMSD values were calculated. The MCNP6 simulations used 1×10^9 histories to achieve error results under 5% in most areas. Regions with relative error higher than 5% were discarded as unreliable.

4.1.1.1. 90 group. Data was examined from the 45th energy group corresponding to the 54-55 KeV range. Figures 3.3 to 3.5 are cross section views of the fluence in the water phantom for DOCTORS and MCNP6. These figures also include a difference map as well as the relative error from MCNP6. The fluence values shown are from 0 to 3×10^{-6} phtons/cm² per source particle from the single projection. The difference and MCNP6 error maps are shown in percentage values. The RMSD values in Figure 3.6 are only calculated for energy groups in which the MCNP6 relative error was under 5%.

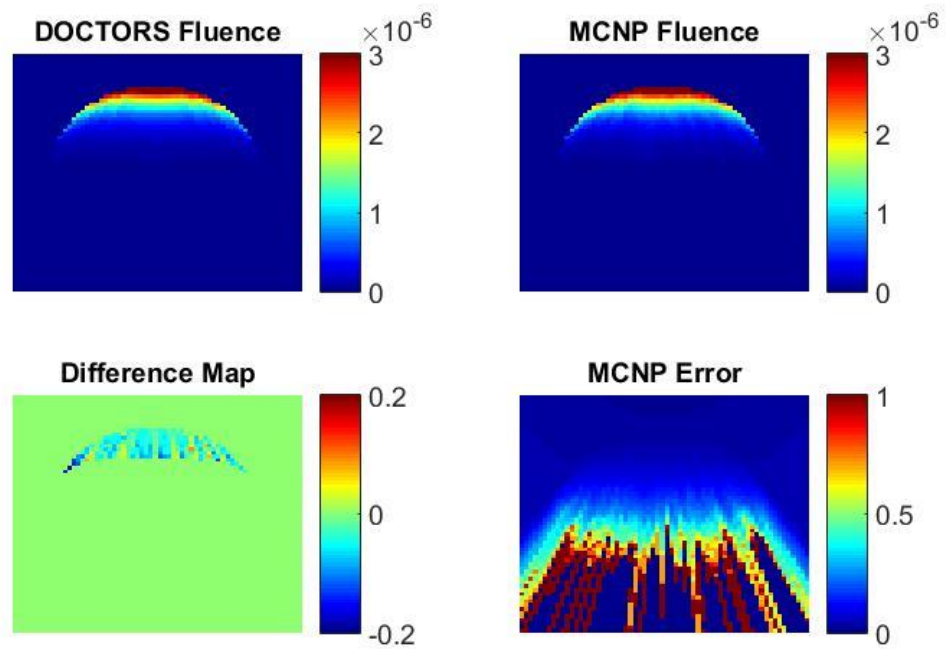


Figure 3.3. 90 Group Single Source Constant Weight Uncollided Fluence

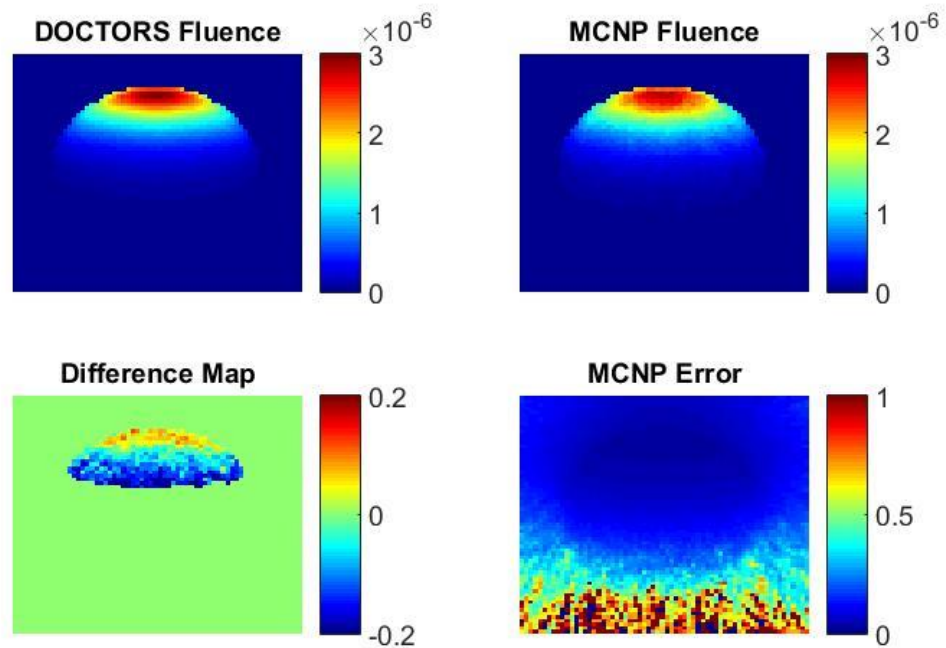


Figure 3.4. 90 Group Single Source Constant Weight Collided Fluence

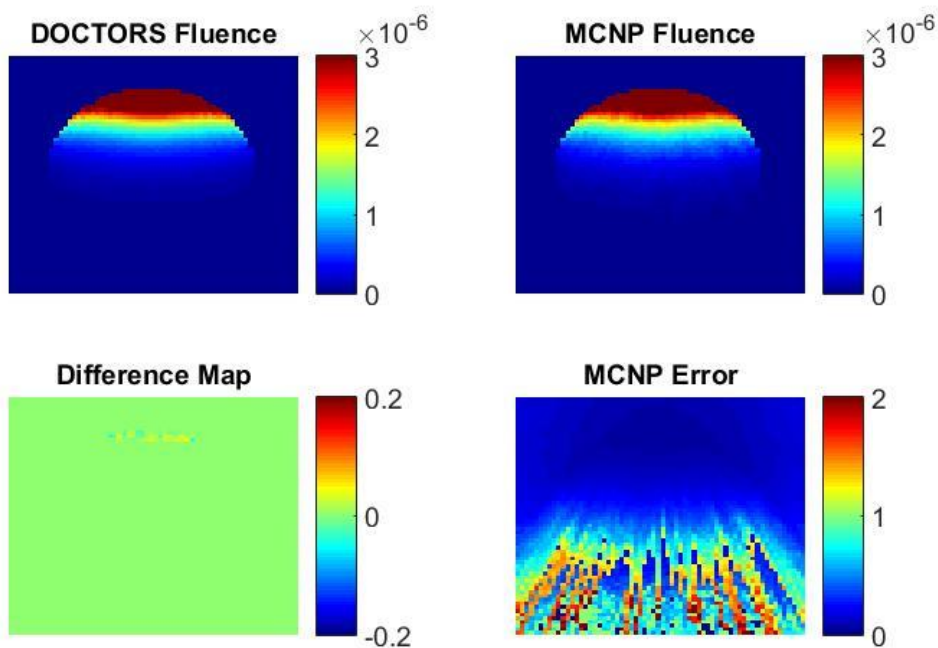


Figure 3.5. 90 Group Single Source Constant Weight Total Fluence

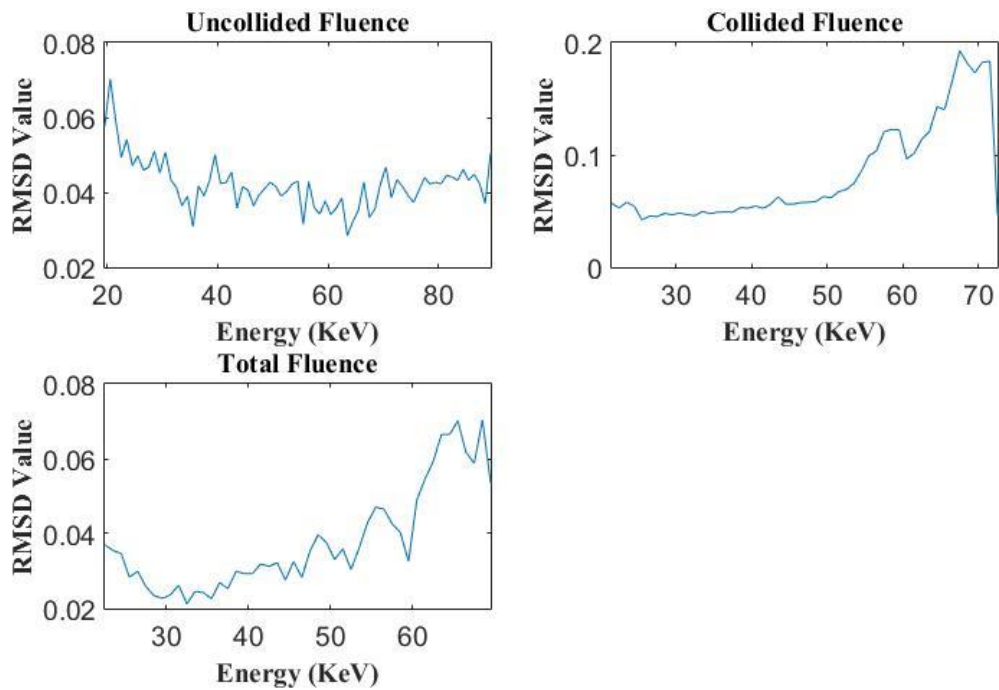


Figure 3.6. 90 Group Single Source Constant Weight RMSD Values

4.1.1.2. 7 group constant weighting. Data was examined from the 4th energy group of the 7 group single projection simulation with constant weighting. This group corresponds to the 45-60 KeV range. This simulation was conducted using the constant weighting option when creating the cross section with NJOY. Figures 3.7 to 3.9 are cross section views of the fluence in the water phantom for DOCTORS and MCNP6. These figures also include a difference map as well as the relative error from MCNP6. The fluence values are shown from 0 to 3×10^{-6} phtons/cm² per source particle from the single projection. The difference and MCNP6 error maps are shown in percentage values. The RMSD values in Figure 3.10 were only calculated for energy groups in which the MCNP6 relative error was under 5%.

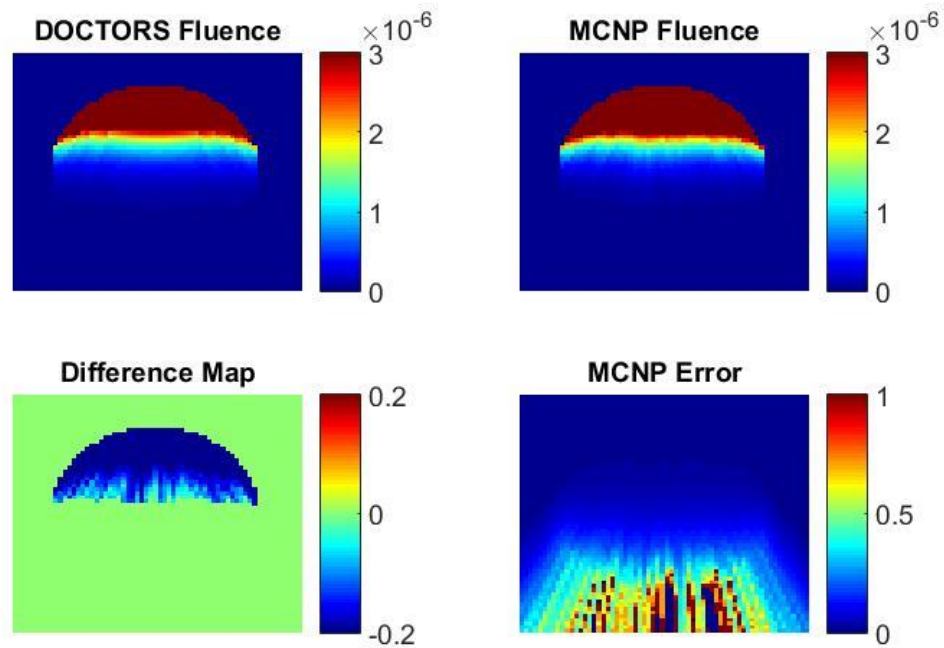


Figure 3.7. 7 Group Single Source Constant Weight Uncollided Fluence

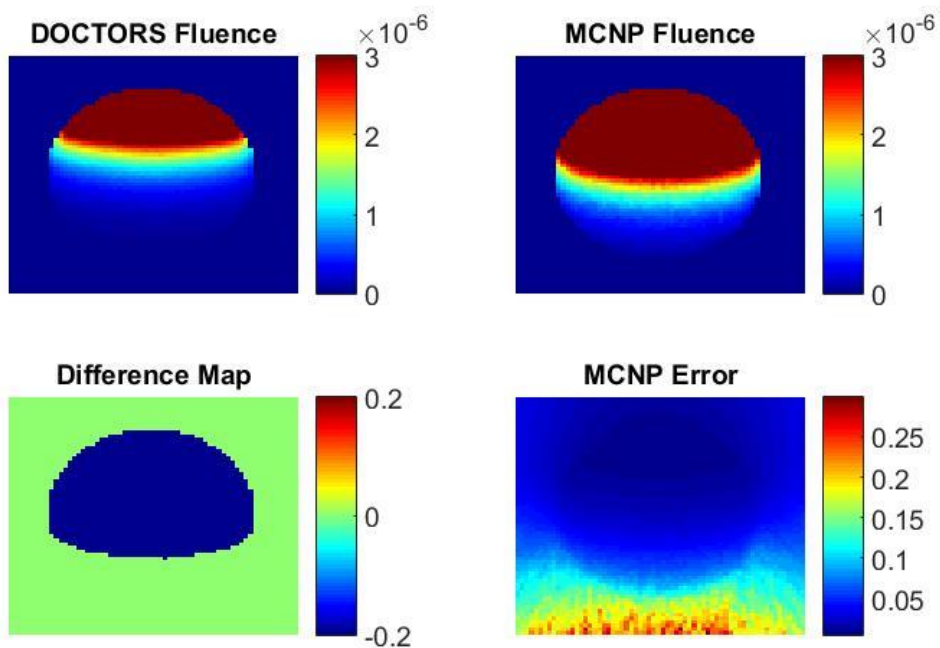


Figure 3.8. 7 Group Single Source Constant Weight Collided Fluence

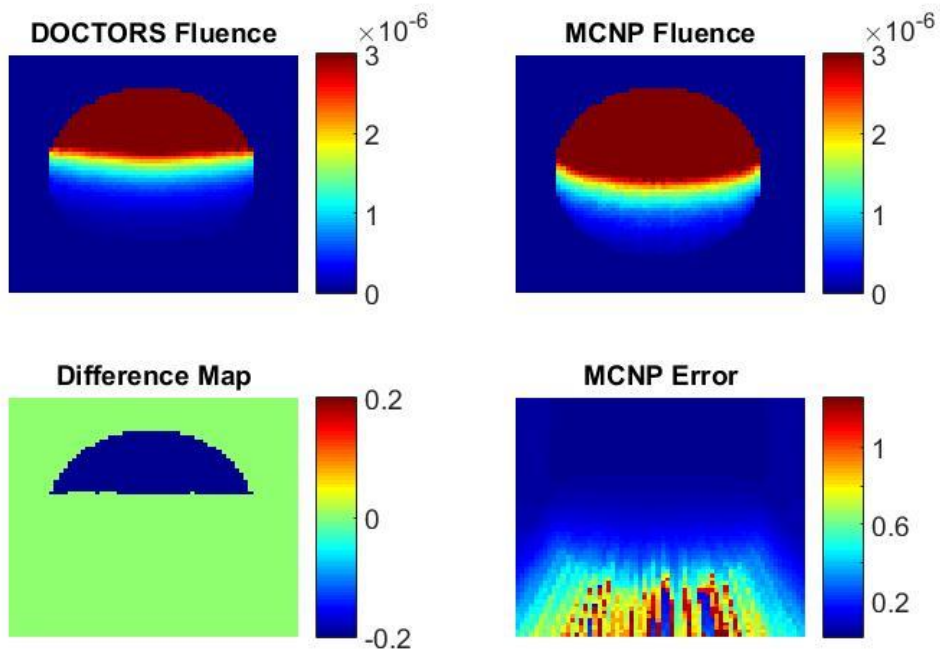


Figure 3.9. 7 Group Single Source Constant Weight Total Fluence

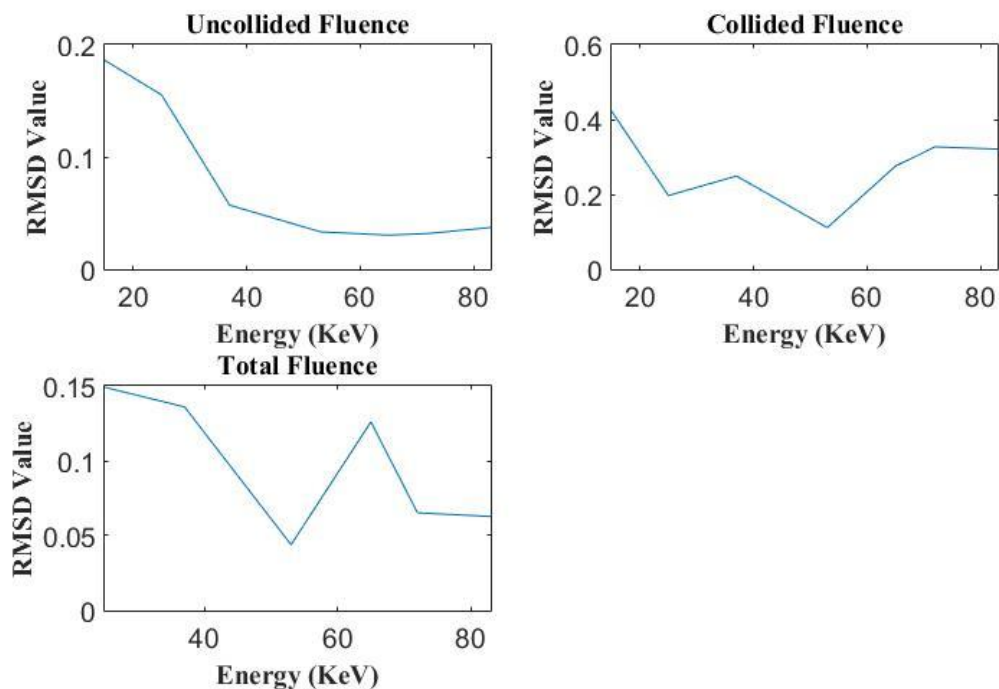


Figure 3.10. 7 Group Single Source Constant Weight RMSD Values

4.1.1.3. 7 group custom weighting. Data was examined from the 4th group of the 7 group single projection simulation with custom weighting. This group corresponds to the 45-60 KeV range. The custom weighting option was used when creating the cross section in NJOY. The weighting data used to construct the cross section was the fluence data of the 90 group single source simulation. The normalized fluence spectrum from multiple positions in the 90 group simulation is shown in Figure 3.11. The points (32,23), (32,32), and (32,41) are very close together and form the purple line. The points (32,15) and (32,49) are also close together and form the green line. The data from the point (32,32) was used to create the weighted cross section. Figures 3.12 to 3.14 are cross section views of the fluence in the water phantom for DOCTORS and MCNP6. These figures also include a difference map as well as the relative error from

MCNP6. The fluence values are shown from 0 to 3×10^{-6} phtons/cm² per source particle from the single projection. The difference map and MCNP6 error map are shown in percentage values. The RMSD values in Figure 3.15 were only calculated when the energy group in MCNP6 had a relative error was under 5%.

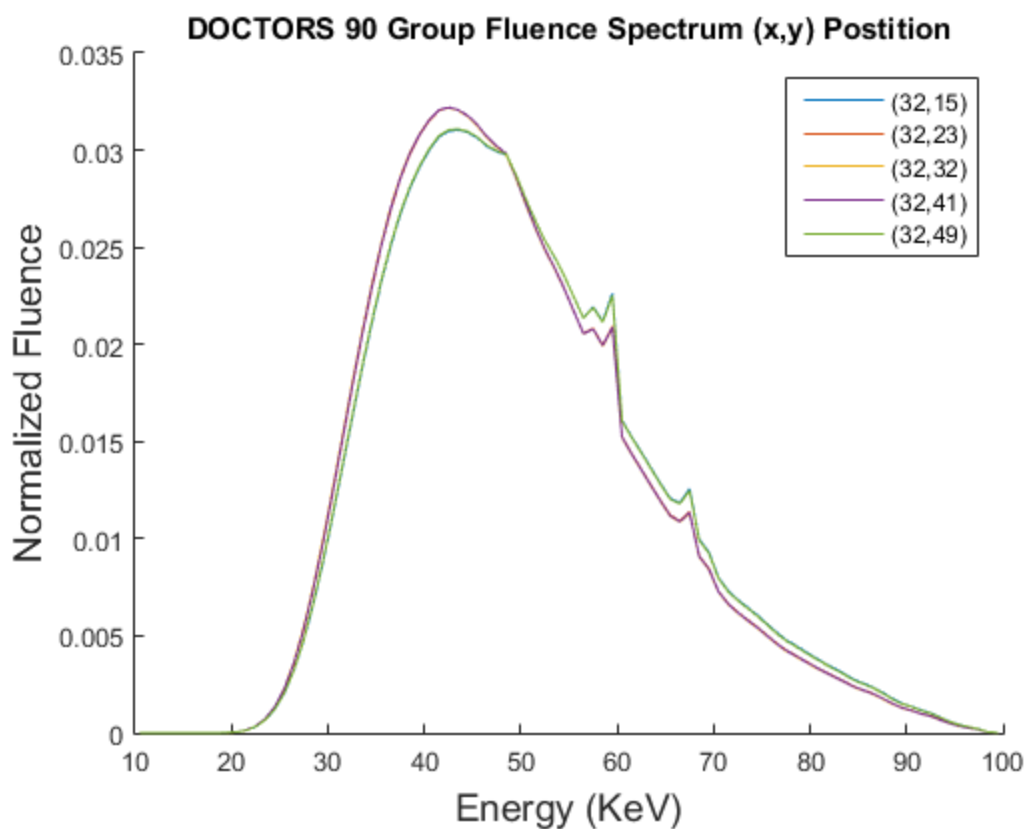


Figure 3.11. 90 Group Single Source Normalized Fluence Spectrum

4.1.2. Multiple Projection (CT). The CT simulation consisted of 16 cone beam sources around the same water phantom as used in the single source simulation. This simulation was performed using both DOCTORS and MCNP6.

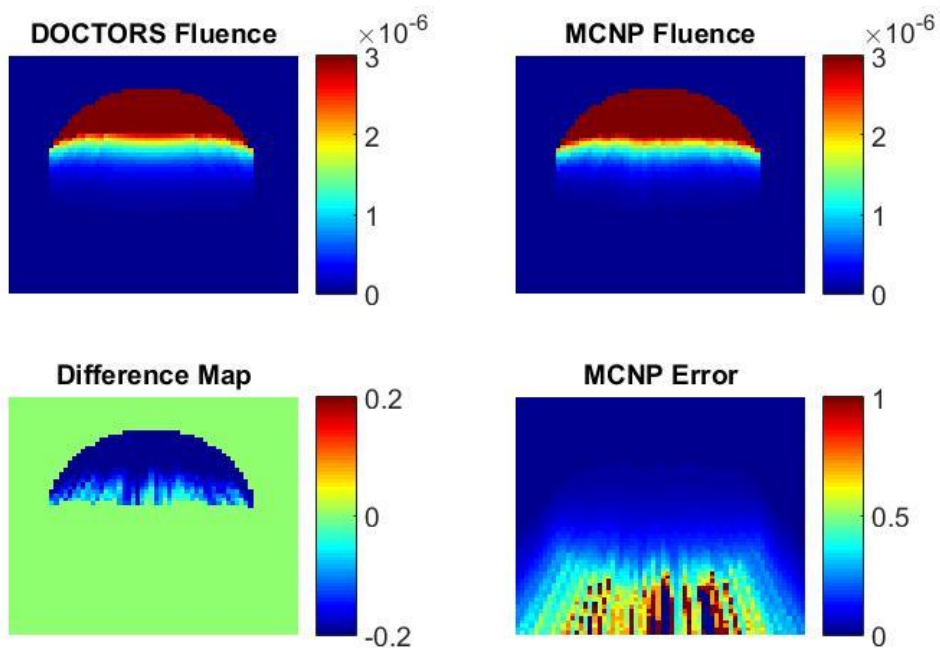


Figure 3.12. 7 Group Single Source Custom Weight Uncollided Fluence

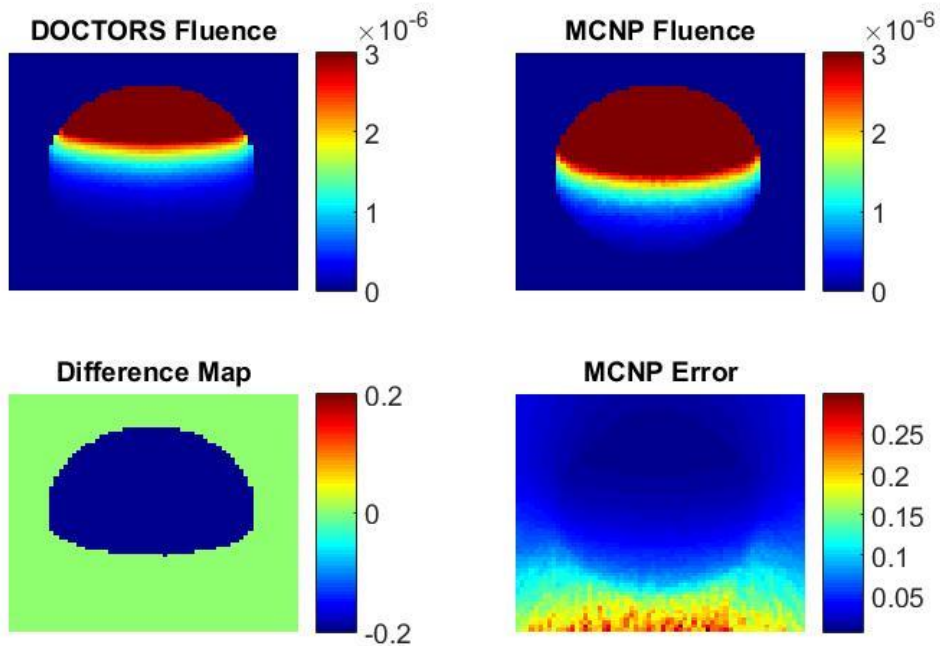


Figure 3.13. 7 Group Single Source Custom Weight Collided Fluence

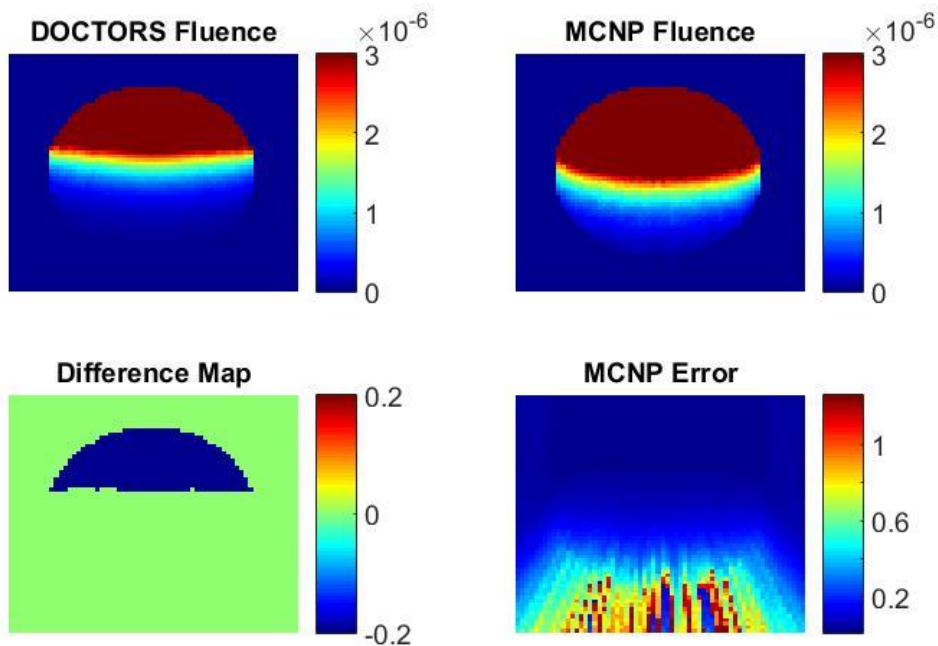


Figure 3.14. 7 Group Single Source Custom Weight Total Fluence

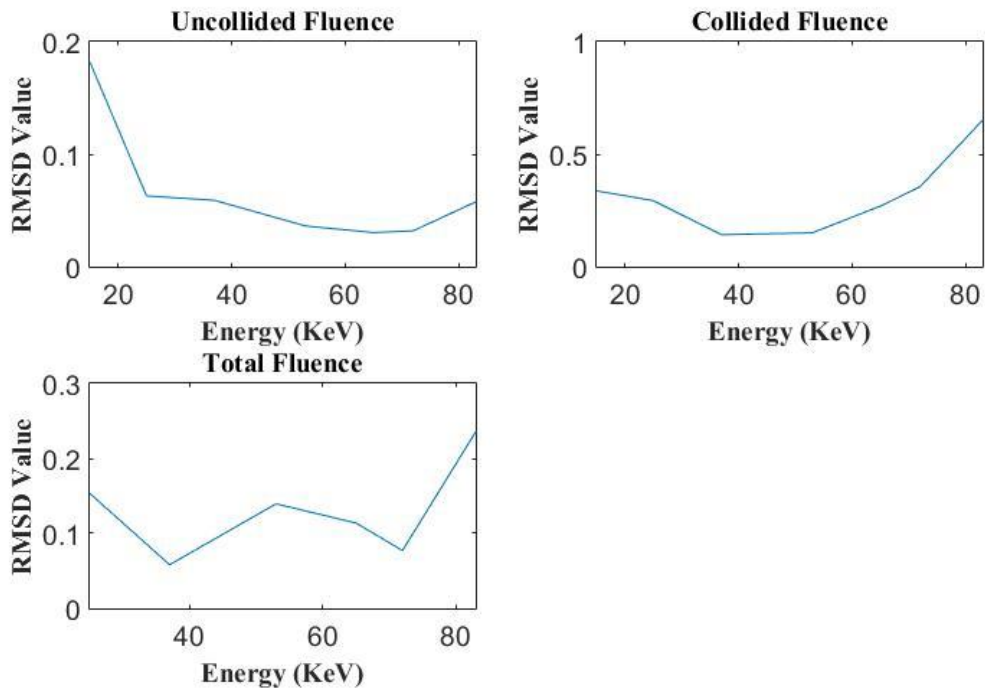


Figure 3.15. 7 Group Single Source Custom Weight RMSD Values

The central slice of the phantom was compared by examining the fluence values of the central energy group. The central energy group for the 90 group simulation was group 45 corresponding to 54-55 KeV. For the 7 group simulation group 4 was evaluated corresponding to 45-65 KeV. The RMSD values were calculated from this data and compared. The MCNP6 simulation required the use of 1×10^9 histories to achieve error results under 5% in most areas. Regions with relative error higher than 5% were discarded as unreliable.

4.1.2.1. 90 group. Data was examined from the 45th energy group corresponding to the 54-55 KeV range. Figures 3.16 to 3.18 are cross section views of the fluence in the water phantom for DOCTORS and MCNP6. These figures also include a difference map as well as the relative error from MCNP6. The fluence values are shown from 0 to 4×10^{-7} phtons/cm² per source particle from the single projection. The difference and MCNP6 error maps are shown in percentage values. The RMSD values in Figure 3.19 were only calculated for energy groups in which the MCNP6 relative error was under 5%.

4.1.2.2. 7 group constant weighting. Data was examined from the 4th group of the 7 group multi-projection simulation with constant weighting. This group corresponds to the 45-60 KeV range. This simulation was conducted using the constant weighting option when creating the cross section in NJOY. Figures 3.20 to 3.22 are cross section views of the fluence in the water phantom for DOCTORS and MCNP6. These figures also include a difference map as well as the relative error from MCNP6.

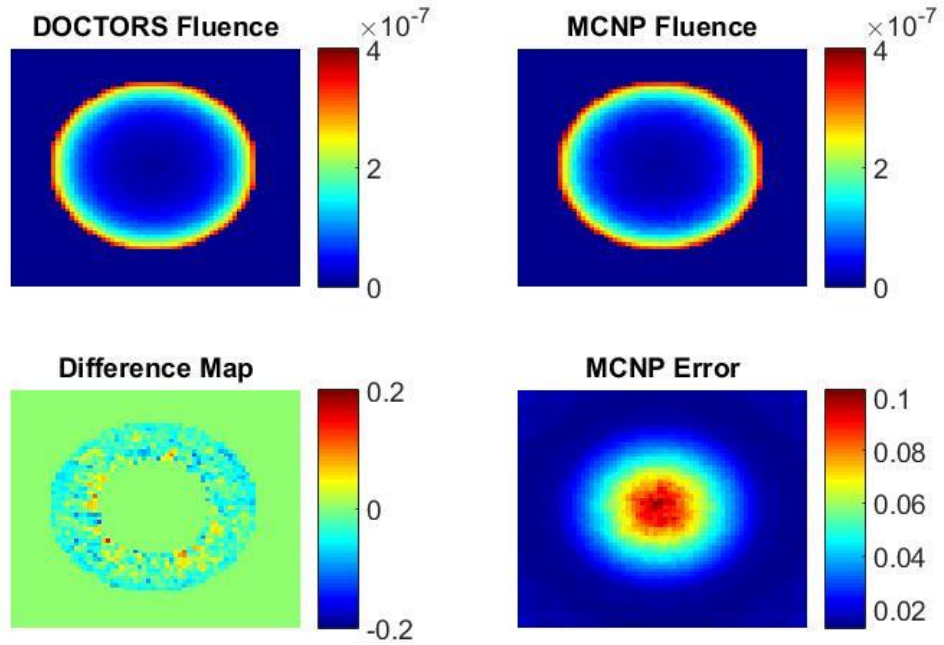


Figure 3.16. 90 Group Cone Beam Source Constant Weight Uncollided Fluence

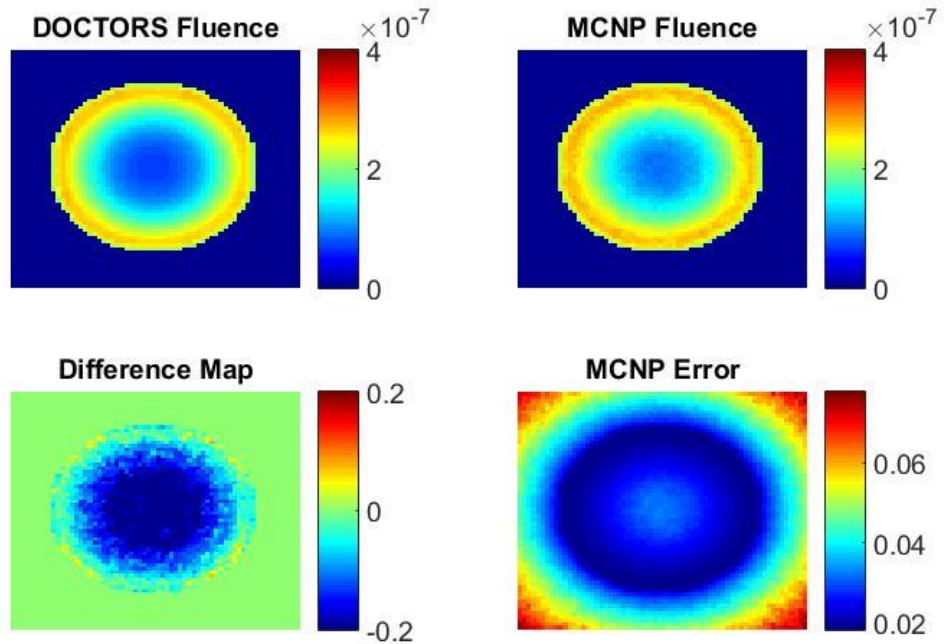


Figure 3.17. 90 Group Cone Beam Source Constant Weight Collided Fluence

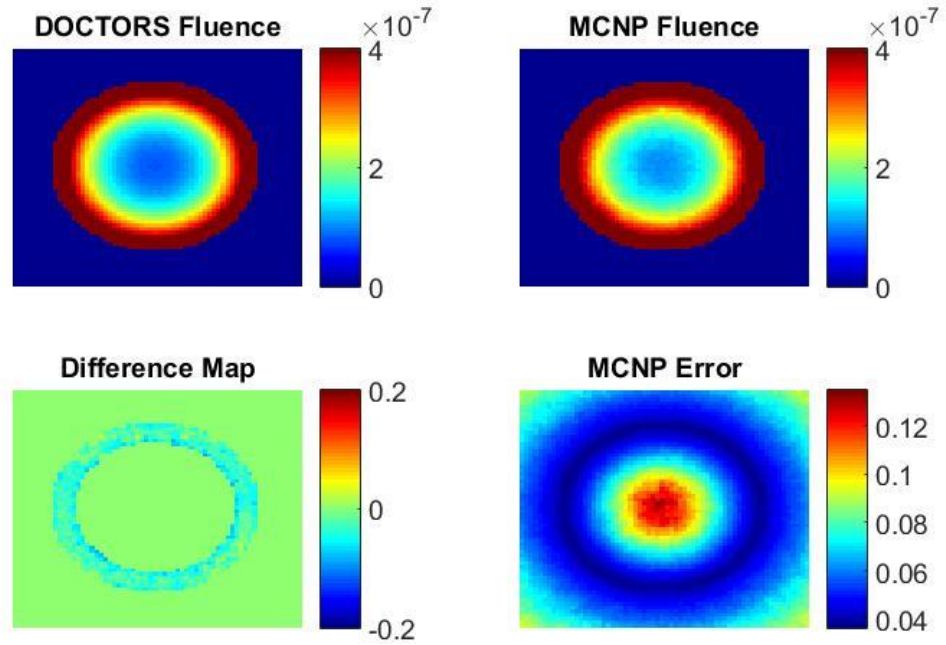


Figure 3.18. 90 Group Cone Beam Source Constant Weight Total Fluence

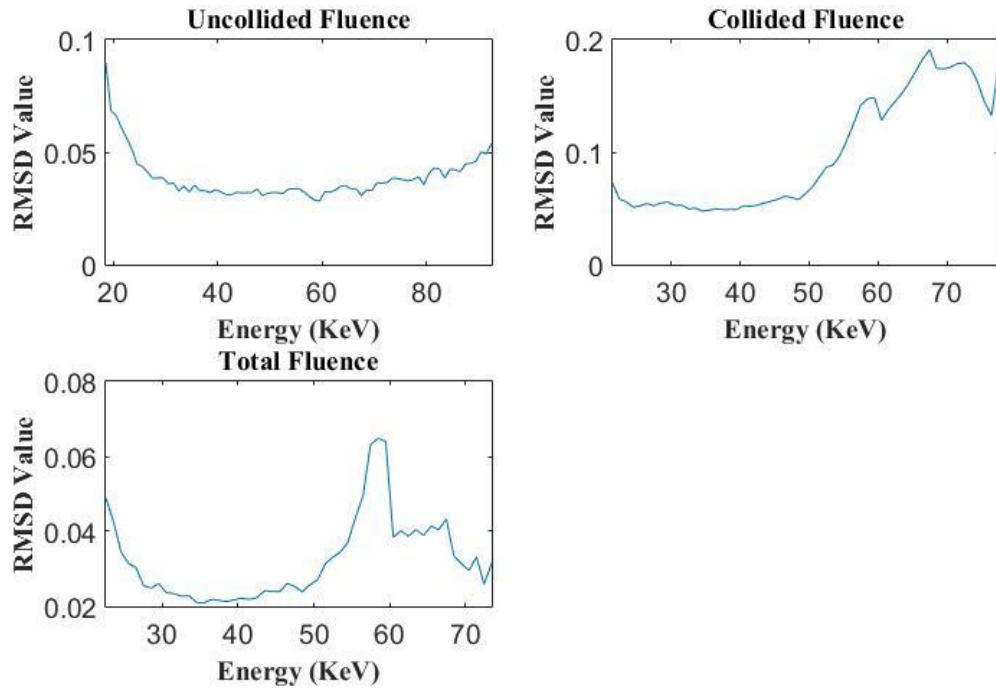


Figure 3.19. 90 Group Cone Beam Source Constant Weight RMSD Values

The fluence values are shown from 0 to 5×10^{-6} photons/cm² per source particle from the single projection. The difference map and MCNP6 error map are shown in percentage values. The RMSD values in Figure 3.23 were only calculated for energy groups in which the MCNP6 relative error was under 5%.

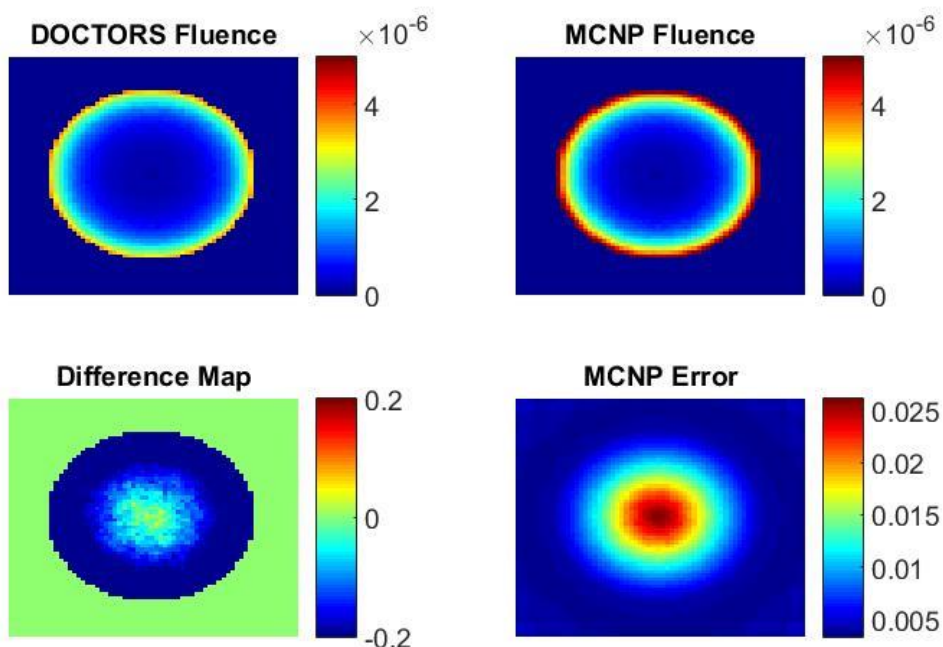


Figure 3.20. 7 Group Cone Beam Source Constant Weight Uncollided Fluence

4.1.2.3. 7 group custom weighting. Data was examined from the 4th group of the coarse group multi-projection simulation with custom weighting. This group corresponds to the 45-60 KeV range. This simulation was conducted using the custom weighting option when creating the cross section in NJOY. The data used to construct the cross section was the fluence data of the 90 group multi-projection simulation.

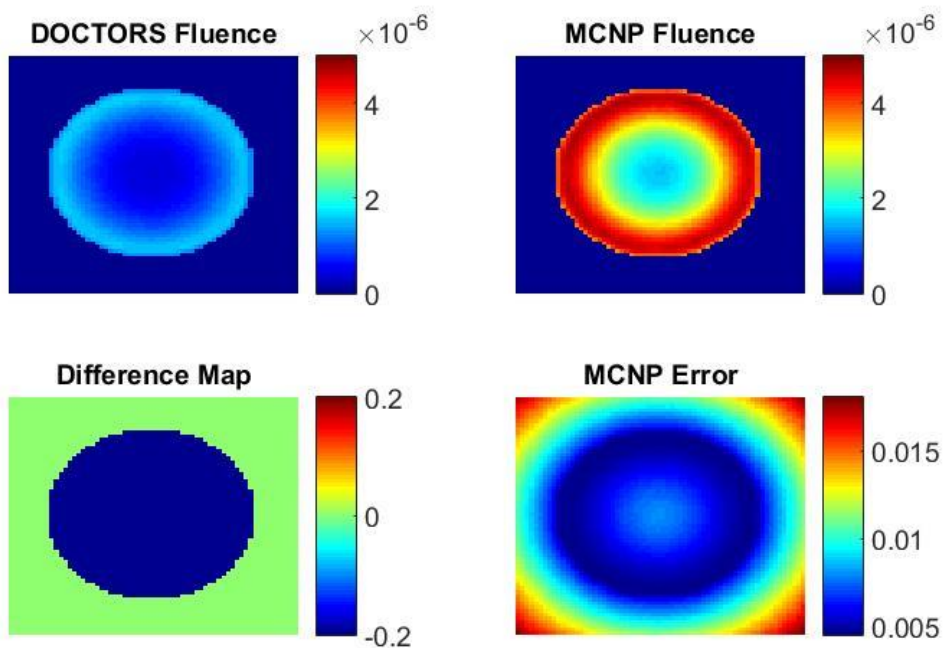


Figure 3.21. 7 Group Cone Beam Source Constant Weight Collided Fluence

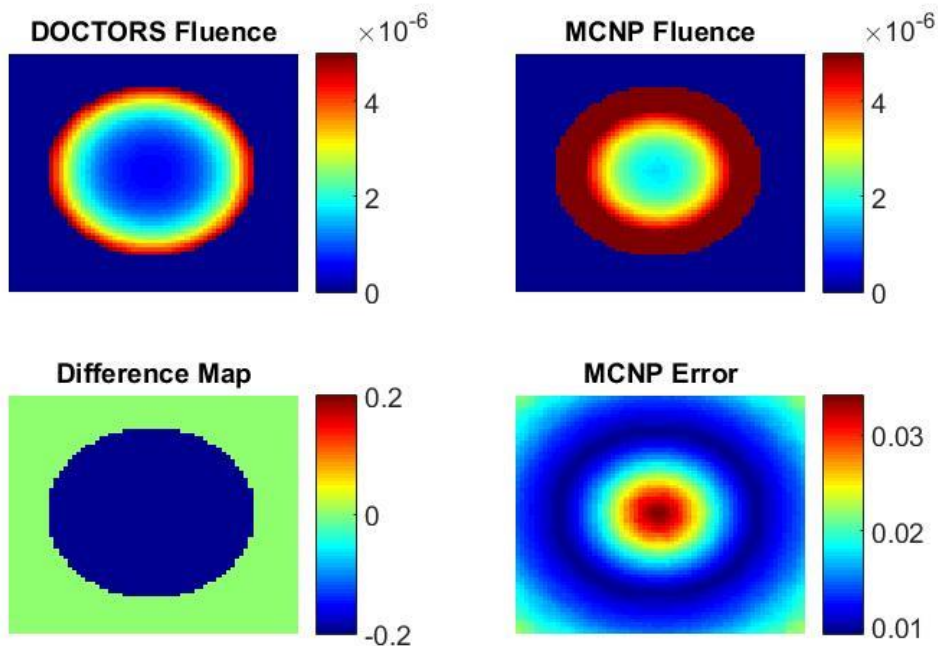


Figure 3.22. 7 Group Cone Beam Source Constant Weight Total Fluence

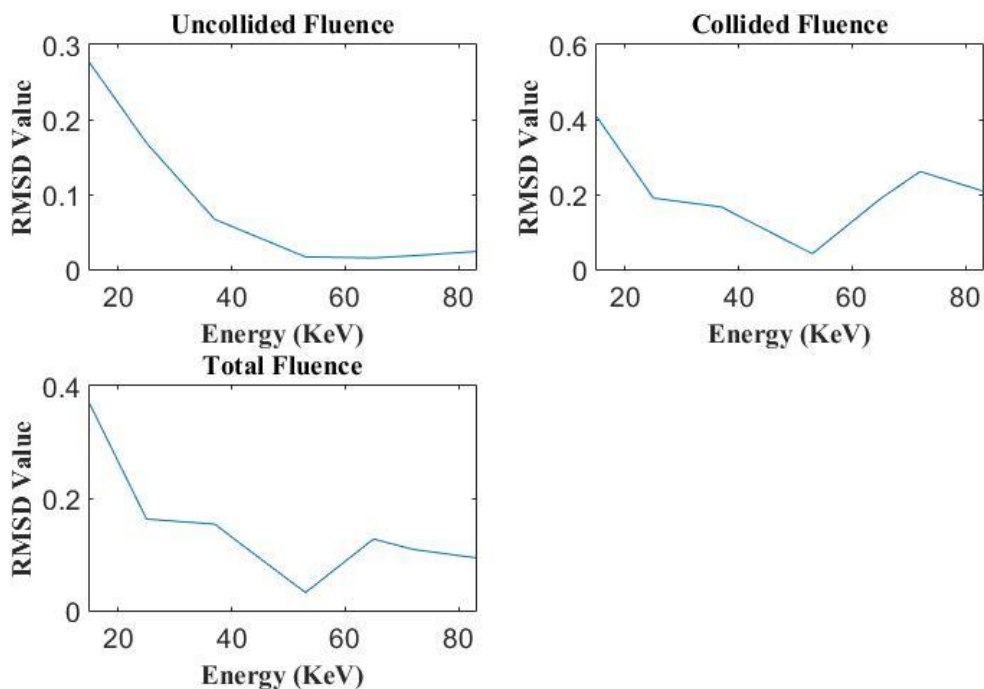


Figure 3.23. 7 Group Cone Beam Source Constant Weight RMSD Values

The normalized fluence spectrum for multiple positions in the 90 group multi-projection simulation are shown in Figure 3.24. The fluence data from point (32,15), and (32,49) are very close to one another and form the green line. The fluence data from point (32,23) and (32,41) form the purple line and the data from point (32,32) is the yellow line. Figures 3.25 to 3.27 are cross section views of the fluence in the water phantom for DOCTORS and MCNP6. These figures also include a difference map as well as the relative error from MCNP6. The fluence values are shown from 0 to 5×10^6 photons/cm² per source particle from the single projection. The difference map and MCNP6 error map are shown in percentage values. The RMSD values in Figure 3.28 were only calculated for energy groups in which the MCNP6 relative error was under 5%.

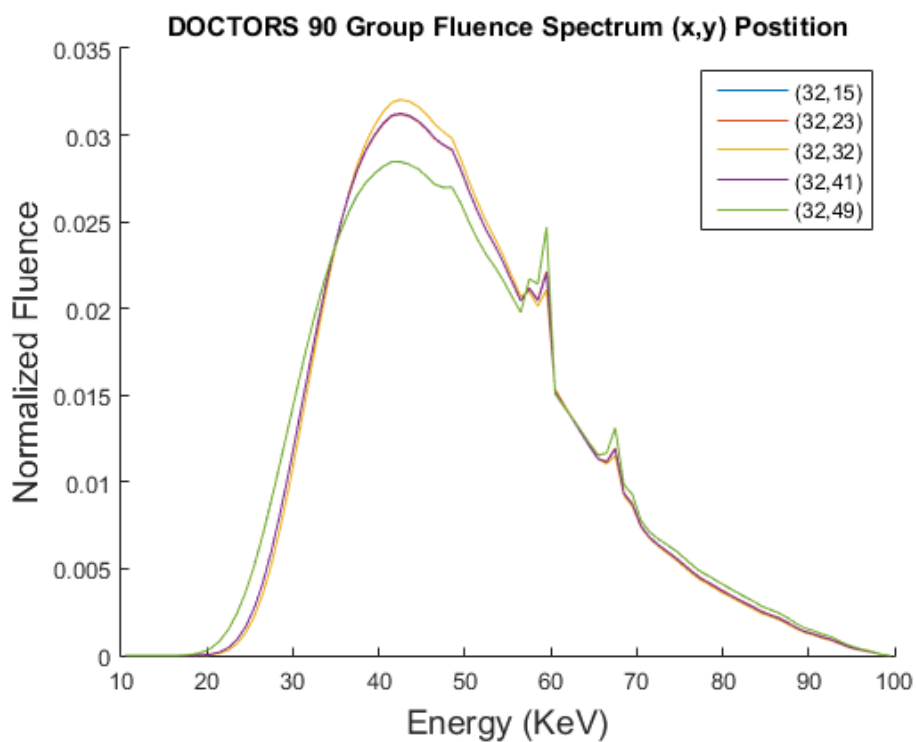


Figure 3.24. 90 Group Multiple Source Normalized Fluence Spectrum

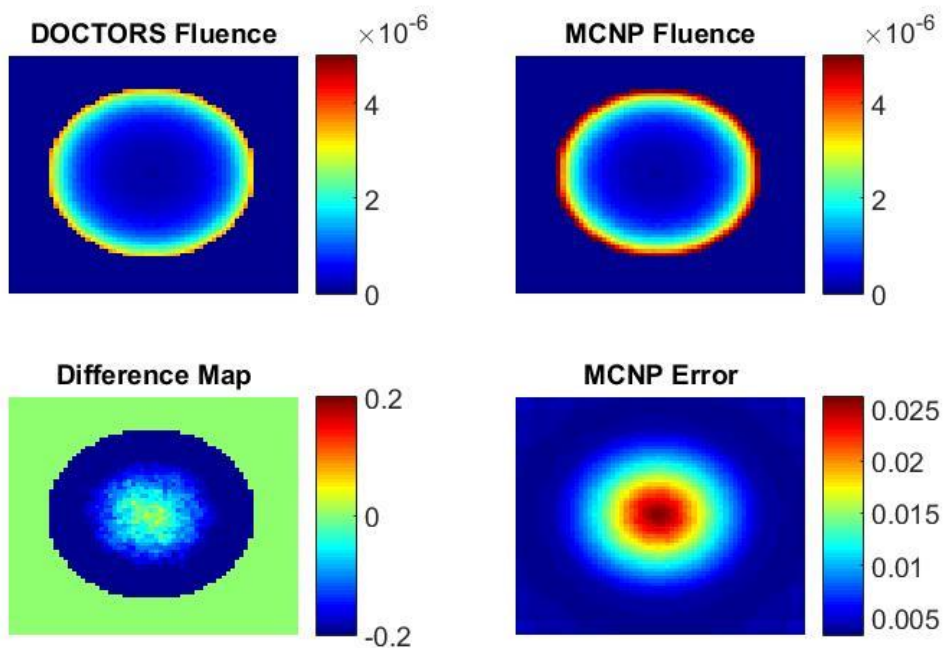


Figure 3.25. 7 Group Cone Beam Source Custom Weight Uncollided Fluence

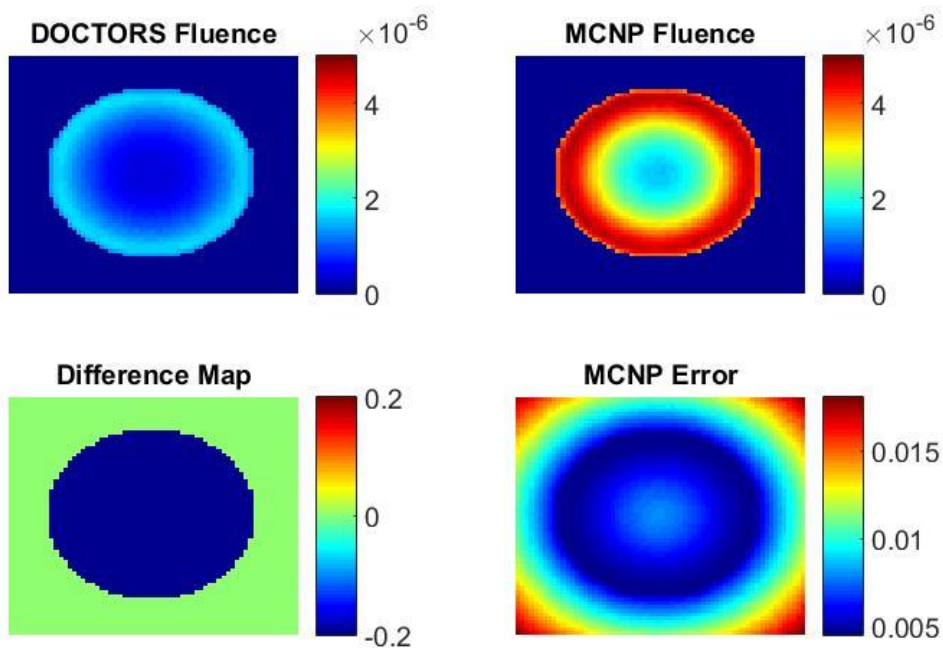


Figure 3.26. 7 Group Cone Beam Source Custom Weight Collided Fluence

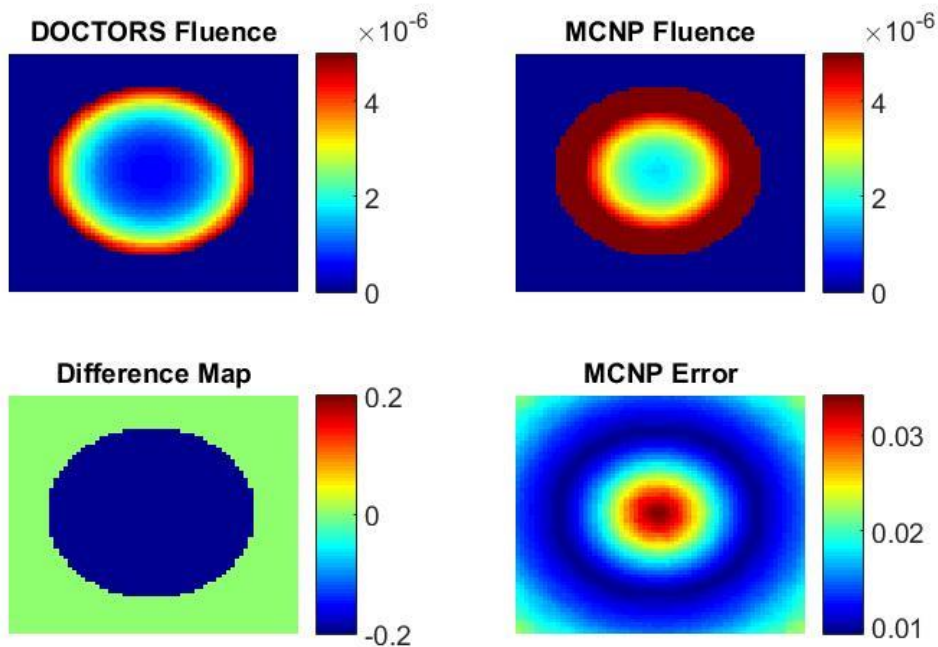


Figure 3.27. 7 Group Cone Beam Source Custom Weight Total Fluence

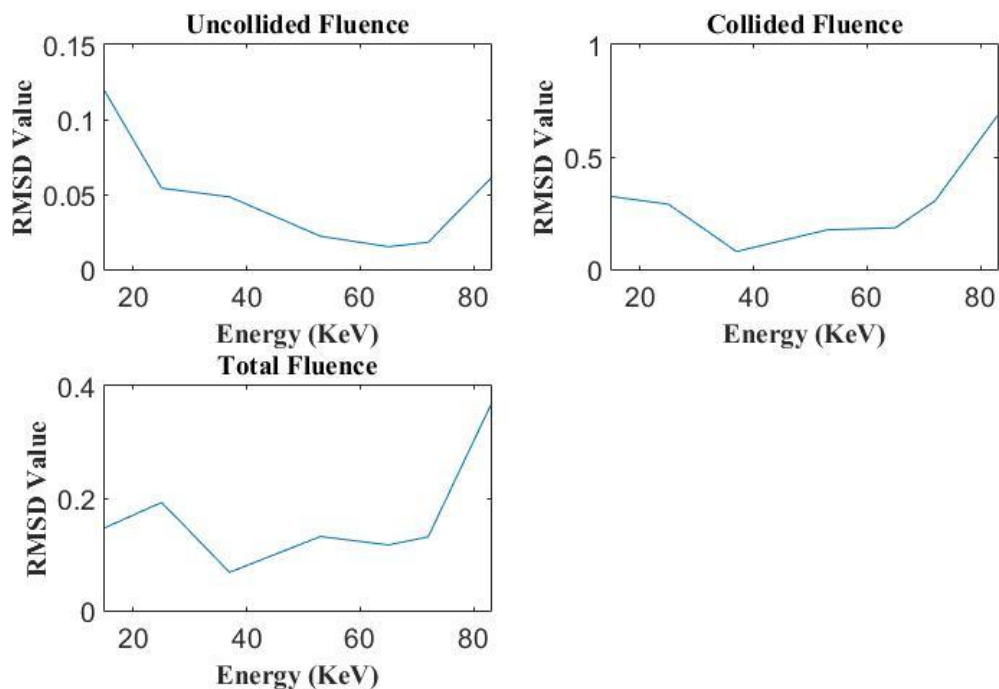


Figure 3.28. 7 Group Cone Beam Source Custom Weight RMSD Values

4.2 DISCUSSION

The RMSD values calculated from all simulations are shown in Table 3.1. The results of the 90 group single projection and cone beam simulations show that the photon fluence calculated by DOCTORS is in close agreement with MCNP6. The RMSD numbers stay under 10% in both cases with the uncollided fluence under 5%. The difference map results for the 90 group single projection simulation show that DOCTORS produced higher collided fluence than MCNP6 near the surface of the phantom and lower fluence near the middle of the phantom.

The RMSD values calculated for the 7 group simulations all followed a similar pattern. The uncollided fluence is under 10% but the collided and total fluence numbers are 2 to 3 times higher, to a maximum of 31.39%. Comparing the results from the

constant weighting to the custom weighting show that while the uncollided fluence slightly improved the collided values are higher by approximately the same margin. One explanation for this result is that the 7 energy group structure chosen was too large. Choosing smaller energy bin sizes in areas of interest will likely improve results.

Many of the RMSD values increase as energy increased. It is believed one factor in this is the use of 0th Legendre expansion in all simulations. Figure 3.29 shows the RMSD values for the single projection 90 group collided fluence for p0, p1, and p2. Increasing the Legendre order does show some improvement in the higher energy range.

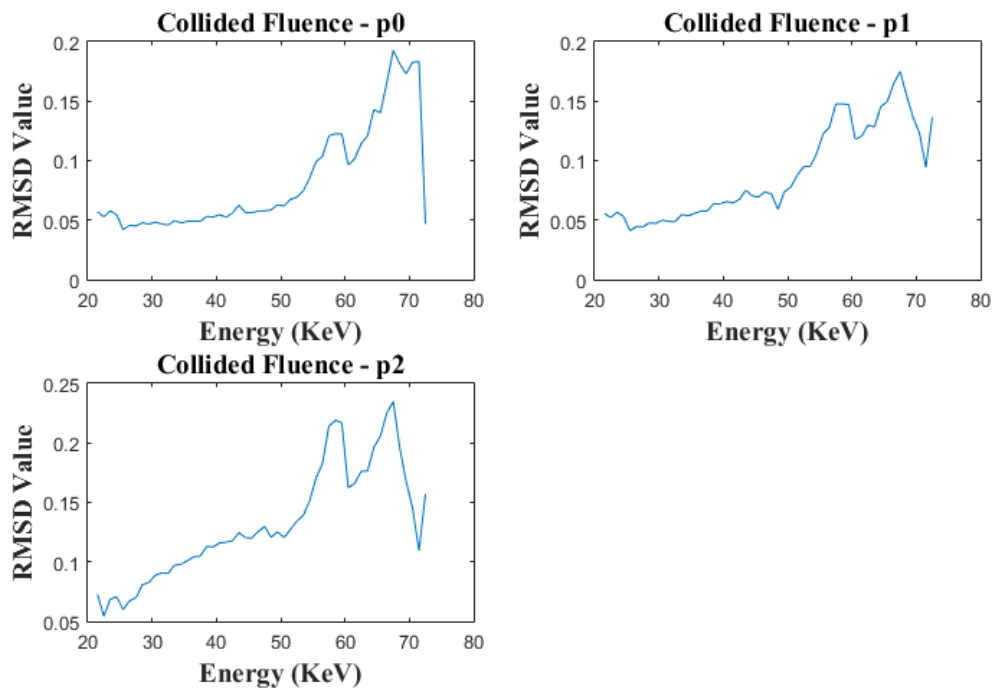


Figure 3.29. 90 Group Single Source Collided RMSD Values: p0, p1, p2

Table 3.1. RMSD Average Group Values

	RMSD Average Group Values		
	Uncollided Fluence	Collided Fluence	Total Fluence
Single Projection 90 Group	4.23%	8.24%	3.78%
Single Projection 7 Group Constant Weight	7.58%	27.17%	9.71%
Single Projection 7 Group Custom Weight	6.57%	31.39%	12.95%
Cone Beam 90 Group	3.86%	9.84%	3.23%
Cone Beam 7 Group Constant Weight	8.34%	20.90%	14.95%
Cone Beam 7 Group Custom Weight	4.82%	29.16%	16.48%

5. CONCLUSION

The amount of error observed when comparing DOCTORS and MCNP6 fine group structure simulations was reasonable. The multi-group cross section files themselves were created computationally quickly with an easily repeatable procedure using the NJOY2016 software package. Creating material specific fine multi-group cross section libraries with constant weighting is viable for use with DOCTORS.

The creation of the coarse group cross section files with custom weighting functions took significantly longer than their fine group counterparts. To create these cross sections all of the steps to create the fine group must be completed first along with a preliminary simulation run to obtain fluence data. The extra time invested along with the higher RMSD values show that more work must be done to improve this process. Custom weight multi-group cross section files created in this manner are not currently viable for use with DOCTORS.

APPENDIX A

NJOY2016 7 GROUP WEIGHTED INPUT FILE

reconr

20 21/ Card 1 – input:ENDF, output:PENDF

'PENDF tape for photon interaction cross sections from ENDF/B-VII.1'/ Card 2 - label

100 1/ Card 3 – material #, ncards (default = 0), ngrid (default = 0)

.001/ Card 4 – error tolerance, tempr (default = 0), errmax (default = error tolerance*10), errint (default = error/20000)

'1-Hydrogen'/ Card 5 – ncards of descriptive comments

700 1/

.001/

'7-Nitrogen'/

800 1/

.001/

'8-Oxygen'/

1800 1/

.001/

'18-Argon'/

0/ End RECONR

gaminr

20 21 0 22/ Card 1 – input:ENDF, input:PENDF, input:ngam tape (default = 0), output:GENDF (default = 0)

100 1 1 2 1/ Card 2 – material #, igg, iwt, lord, iprint (default = 1)

'7-group photon interaction library 10 to 100 keV'/ Card 3 - label

7/ Card 4 – (if igg = 1 only) ngg, egg (ngg+1 in eV)

10000 20000 30000 45000 60000 70000 75000 100000/

.0 .0 0 0 1 90 Card 5 – weight function as tab 1 record

90 1

10000 0

11000 3.51E-10

12000 1.41E-09

13000 2.19E-09

14000 3.00E-09

15000 4.19E-09

16000 5.77E-09

17000 7.44E-09

18000 8.52E-09

19000	9.98E-09
20000	1.12E-08
21000	1.31E-08
22000	1.54E-08
23000	1.74E-08
24000	1.90E-08
25000	2.06E-08
26000	2.29E-08
27000	2.50E-08
28000	2.72E-08
29000	2.95E-08
30000	3.19E-08
31000	3.44E-08
32000	3.68E-08
33000	4.00E-08
34000	4.36E-08
35000	4.71E-08
36000	5.05E-08
37000	5.38E-08
38000	5.77E-08
39000	6.32E-08
40000	7.33E-08
41000	7.89E-08
42000	9.85E-08
43000	9.46E-08
44000	9.72E-08
45000	1.04E-07
46000	1.11E-07
47000	1.18E-07
48000	1.25E-07
49000	1.32E-07
50000	1.81E-07
51000	1.73E-07
52000	1.81E-07

53000	1.79E-07
54000	1.89E-07
55000	1.99E-07
56000	2.08E-07
57000	2.17E-07
58000	2.26E-07
59000	2.37E-07
60000	2.49E-07
61000	2.59E-07
62000	2.63E-07
63000	2.67E-07
64000	2.72E-07
65000	2.76E-07
66000	2.79E-07
67000	2.80E-07
68000	2.79E-07
69000	2.75E-07
70000	2.69E-07
71000	2.60E-07
72000	2.49E-07
73000	2.36E-07
74000	2.19E-07
75000	2.00E-07
76000	1.79E-07
77000	1.56E-07
78000	1.33E-07
79000	1.09E-07
80000	8.69E-08
81000	6.61E-08
82000	4.75E-08
83000	3.21E-08
84000	2.02E-08
85000	1.17E-08
86000	6.18E-09

87000 2.88E-09
 88000 1.16E-09
 89000 4.07E-10
 90000 1.19E-10
 91000 2.76E-11
 92000 4.92E-12
 93000 6.25E-13
 94000 5.08E-14
 95000 2.78E-15
 96000 1.09E-16
 97000 2.80E-18
 98000 4.55E-20
 99000 4.65E-22
 100000 4.75E-23
 / End GAMINR
 -1 0/ Card 7 – mfd, mtd, mtname (-1 will process all files & MT 501, 502, 504, 516, 522, 525)
 700/ Card 8 – next material #, 0 will terminate
 -1 0/
 800/
 -1 0/
 1800/
 -1 0/
 0/

 dtfr
 22 23 21 24/ Card 1 – input:GROUPR, output:Tables, input PENDF, output:Plots
 1 1 0/ Card 2 – iprint, ifilm (default = 0), iedit (default = 0, cards 3-5 for iedit = 0 only)
 3 7 6 7 13 3 0/ Card 3 nmax(lord+1), ng(igg), iptotl, ipingp, itabl(# of special edits + 4 +# of groups -1) ned, ntherm
 'coh' 'incoh' 'pe'/ Card 4 - labels
 1 502 1 2 504 1 3 522 1/ Card 5 – jpos, mt, mult (sets of 3 repeated for each extra edit)
 0/ Card 7 – nptabl (default = 0), ngp (default = 0)
 'H' 100 1 0/ Card 8 – hisnam, mat (default = 0, jsigz (default = 1), dtemp (default = 300)
 'N' 700 1 0/
 'O' 800 1 0/

'Ar' 1800 1 0/

/ End DTFR

stop

APPENDIX B

MATLAB DATA ANALYSIS CODE

```

% Variables that must be set before running:
% Number of total energy groups for DOCTORS and MCNP, MCNP error tolerance, "slice" of the
% phantom in the x y plane which is to be analysed, 2 DOCTORS data input filepaths, 1 MCNP data input
% filepath

clear;
MCNP_groups = 7;
DOCTORS_groups = 7;
MCNP_tolerance = 0.05;
slice = 8;
DOC_U = % DOCTORS uncollided data filepath goes here
DOC_C = % DOCTORS collided data filepath goes here
filename = % MCNP6 data filepath goes here

DOC_raw = DOCTORS_Data_Raw(DOC_U, DOC_C);
MCNP_raw = MCNP_Data_Raw2(filename, MCNP_groups);
[DOC_flux_s, MCNP_flux_s, MCNP_error_s] = Data_Slice(DOC_raw, MCNP_raw, slice,
MCNP_groups);
[DRMSD] = Data_Comparison(DOC_flux_s, MCNP_flux_s, MCNP_error_s, MCNP_groups,
DOCTORS_groups, MCNP_tolerance);

% FUNCTIONS
%-----
% This function accepts two DOCTORS ascii files as input in string form.
% The output will be a cell containing the collided, uncollided and total
% flux.

function [DOC_out_raw] = DOCTORS_Data_Raw(DOC_filename_1_U, DOC_filename_2_C)

DOC_files = {DOC_filename_1_U, DOC_filename_2_C};

for i = 1:2
    fileID = fopen(DOC_files{i}, 'r');
    groupcount = fread(fileID, 1, 'int');    %number of groups
    xcount = fread(fileID, 1, 'int');    %number of x elements
    ycount = fread(fileID, 1, 'int');    %number of y elements
    zcount = fread(fileID, 1, 'int');    %number of z elements
    xNodes = fread(fileID, xcount, 'float');    %x positions
    yNodes = fread(fileID, ycount, 'float');    %y positions
    zNodes = fread(fileID, zcount, 'float');    %z positions
    sol = fread(fileID, xcount*ycount*zcount*groupcount, 'double');
    flux = reshape(sol, [zcount, xcount, ycount, groupcount]);
    DOC_out_raw{i} = flux; %flux of the central slice all groups
    fclose(fileID);
end

DOC_out_raw{3} = DOC_out_raw{1} + DOC_out_raw{2};

return
%-----
% This function requires an input filepath to the MCNP data file and the
% total number of group in the file. MCNP starts with the energy group 0 to
% the first specified bin so the first group will be discarded: if the user
% is looking at 90 groups MCNP will output 91, if the user is actually

```

```

% using the first group changes must be made.
% The function will return cell containing the Uncollided and
% collided raw MCNP output

function [MCNP_out_raw] = MCNP_Data_Raw2(filepath, groupnum)

N = 65536;
formatSpec = '%f %f %f %f %f %f';
fid = fopen(filepath);
Uncollided = cell(1,0);
Uncollided(1,1) = textscan( fid, formatSpec, N,'Headerlines',16, 'CollectOutput',true );

for i = 1:groupnum
    Uncollided(1,end+1) = textscan( fid, formatSpec, N, 'CollectOutput',true );
end

Collided = cell(1,0);
Collided(1,end+1) = textscan( fid, formatSpec, N, 'HeaderLines', N+14, 'CollectOutput',true );

for i = 1:groupnum
    Collided(1,end+1) = textscan( fid, formatSpec, N, 'CollectOutput',true );
end
fclose( fid );

MCNP_out_raw = cell(2,groupnum);
for i = 1:groupnum
    MCNP_out_raw{1,i} = Uncollided{1,i+1};
    MCNP_out_raw{2,i} = Collided{1,i+1};
end
return
%-----
% This function requires two cell inputs created with the functions
% MCNP_Data_Raw2 and DOCTORS_Data_Raw. This function also
% requires two integers for the "slice" of the phantom data desired in the
% x y plane and the total number of MCNP groups. The output is 3 cells
% containing the DOCTORS fluence information, MCNP fluence information, and MCNP
% error information for the desired slice.

function [DOC_flux_s, MCNP_flux_s, MCNP_error_s] = Data_Slice(DOC_data, MCNP_data, slice,
group)

% DOCTORS
% extract the data for specified slice
for i = 1:3
    DOC_flux_s{i} = squeeze(DOC_data{i}(slice, :, :, :));
end

% MCNP
% extract the flux data
for k = 1:3
    if k < 3
        for i = 1:group

            flux{k,i} = MCNP_data{k,i}(:,5);

```

```

MCNP_flux_s1{k,i} = reshape(flux{k,i}, [16,64,64]);
MCNP_flux_s{k,i} = squeeze(MCNP_flux_s1{k,i}(slice, :, :));

reler{k,i} = MCNP_data{k,i}(:,6);
MCNP_error_s1{k,i} = reshape(reler{k,i}, [16, 64, 64]);
MCNP_error_s{k,i} = squeeze(MCNP_error_s1{k,i}(slice, :, :));

end
else

for i = 1:group
    MCNP_flux_s{k,i} = MCNP_flux_s{1,i} + MCNP_flux_s{2,i};
    MCNP_error_s{k,i} = MCNP_error_s{1,i} + MCNP_error_s{2,i};
end

end
end

return
%-----
% This function requires the input of 3 cells containing the
% DOCTORS fluence, MCNP fluence, and MCNP error information. This function also
% requires 3 integers for the number of MCNP groups, number of DOCTORS
% groups, and maximum allowable MCNP error. This function will output two
% matrices containing the resulting RMSD values and fluence differences for
% the uncollided, collided and total fluence.

function [results, Flux_diff] = Data_Comparison(DOC_flux, MCNP_flux, MCNP_error, MCNP_g,
DOC_g, max)

DOC_count = DOC_g;
max_tot = sqrt(max*max + max*max);

for i = 1:MCNP_g
    DOC_flux_g = {zeros(64,64), zeros(64,64), zeros(64,64)};
    DOC_flux_g = {squeeze(DOC_flux{1}(:, :, DOC_count)), squeeze(DOC_flux{2}(:, :, DOC_count)),
squeeze(DOC_flux{3}(:, :, DOC_count))};
    DOC_count = DOC_count - 1;
    for k = 1:3
        count = 0;
        drmsd = 0.0;
        for x = 1:64
            for y = 1:64
                if k < 3
                    if (sqrt((x-32)^2+(y-32)^2)<(55-32)) % for water_simple phantom
                        if (MCNP_flux{k,i}(x,y) > 0 && MCNP_error{k,i}(x,y) < max &&
MCNP_error{k,i}(x,y) > 0)
                            count = count + 1;
                            fluxdiff{k}(x,y) = (DOC_flux_g{k}(x,y) - MCNP_flux{k,i}(x,y)) /
MCNP_flux{k,i}(x,y);
                            drmsd = drmsd + fluxdiff{k}(x,y) * fluxdiff{k}(x,y);
                        end
                    end
                end
            end
        end
    end
else

```

```

        if (sqrt((x-32)^2+(y-32)^2)<(55-32)) % for water_simple phantom
            if (MCNP_flux{k,i}(x,y) > 0 && MCNP_error{k,i}(x,y) < max_tot &&
MCNP_error{k,i}(x,y) > 0)
                count = count + 1;
                fluxdiff{k}(x,y) = (DOC_flux_g{k}(x,y) - MCNP_flux{k,i}(x,y)) /
MCNP_flux{k,i}(x,y);
                drmsd = drmsd + fluxdiff{k}(x,y) * fluxdiff{k}(x,y);
            end
        end
    end
    end

    end
end
if count == 0
    drmsd = 0;
else
    drmsd = sqrt(drmsd/count);
end
diff{k} = MCNP_flux{k,i} - DOC_flux_g{k};
results(i,k) = drmsd;

end
end
Flux_diff = diff;
return

```

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