December 16, 2016

Michael P. Pfeifer
Kansas State University
Manhattan, Kansas, USA
Mike5454@ksu.edu

Dear Dr. Jeremy Roberts,

The final report on the material editor to be used for MCNP is completed and attached. I have made some major and minor changes since the review. To reiterate the use of my code I have made a python script that will take molecular inputs and percent's to make corresponding material cards for either photons or neutrons. The purpose of this code is to test the effects water composition will have on neutron albedo. In the review, I received questions and criticism that I plan to fully cover to avoid any miscommunication.

[1] I was asked to look into using other variables than water to test how composition can affect shielding properties. While my code is capable of doing this, I am using neutron albedo as a part of my personal research goals. If given a shielding problem this code would be well suited for solving such a case.

[2] One reviewer wanted me to specify the energy of the neutrons to be simulated. The energy used in this paper was thermal energy neutrons. I chose to do so because it had a more drastic effect on the produced plot.

[3] Another reviewer pointed out the need for cross section libraries to be stated. For the neutron material card, I updated my data text file to include libraries for all naturally occurring isotopes at approximately 300°K. For photons the atomic number is enough to specify the material.

[4] I was addressed about lowering the geometry of the detector and source over the slab. In the simulations, the detector was just above the slab at 50 cm. above the slab is also a void, which will have no attenuating effect on the particles.

[5] A reviewer suggested that a GUI might be helpful. While I agree, making a GUI for this application would be nice, it is extremely difficult to achieve. The code requires many parameters and some directory information that would be unique to the user. In the current set-up the python code can handle any number of molecule inputs which is another advantage over a GUI.

Other issues stated were grammatical errors, clarity, and wording suggestions that have been taken into account. I have changed the wording where necessary to be as clear to the reader as possible. With all of these issues stated, please enjoy the paper.

Sincerely,

Mike Pfeifer

ME 701/Fall 2016

MATERIAL CARD EDITOR FOR MONTE CARLO PARTICLE ALBEDO SIMULATIONS

Michael P. Pfeifer
Kansas State University
Manhattan, Kansas, USA
Mike5454@ksu.edu

ABSTRACT

MCNP was used in conjunction with Python 2.7 to simulate dose rates for neutrons interacting with various water weight fractions present within the surface of both Earth and Mars. In the Python script, the user defines the molecular composition of the material for the "dry" surface then give the code an array of water weight fractions to be assessed. The code then creates material cards based off these values and creates a material card based on the mass fraction then inputs it into MCNP files, which are automatically, ran. After lengthy simulation, Python then extracts the data and creates a plot of collided/un-collided dose vs the weight fraction of water present. This is done for the standard earth surface as well as for the Martian surface. The results show that (Will add more on results upon completion)

INTRODUCTION

Extensive atmospheric showering due to galactic cosmic rays (GCR's) is known to cause a cascade of secondary particles that can contribute to radiation dose experience at the planet surface. On earth, much of the dose from (GCR's) comes from secondary neutrons (product of high-energy protons) that reach the planetary surface at thermal energies. Dose rates caused from particle albedo (reflected dose) are an important consideration when simulating a radiation environment; this is especially true for thermal energy neutron interacting with elements of low atomic mass such as the hydrogen atoms in water. In radiation shielding and environment simulations, Monte Carlo computing techniques are commonly used to estimate dose rates to ensure a safe environment for humans. This can range from a wide variety of professions such as for astronauts, airline pilots, and radiation workers. This paper, aims to demonstrate how neutron dose rates will change based off the weight fraction of water present in a reflecting medium. To do this Monte Carlo N-Particle Transport code (MCNP) is used in conjunction with python 2.7 to simulate an isotropic mono-energetic point source interacting with the surface of Earth and Mars for various weight fractions of water present. This code seeks to simplify problems with MCNP in defining material cards for mixtures of materials as well as allowing rapid calculations of material cards for various qualities or percent enrichments of molecules and elements.

EXPLAINING ZAID NUMBERS

The MCNP material card is comprised of ZAID numbers that will call the proper cross section data for the given isotope. For photons, you may specify this material with the element number followed by three zeros for natural isotope abundances. For neutrons, you must include the element number followed by the atomic mass of the isotope. For example, natural Uranium is given the ZAID number 92000 for photons, and U-235 is given the ZAID number 92235 for neutrons since Uranium is element 92 with the atomic weight is 235. ZAID numbers must also include a reference to a cross section library, which is given by a period two numbers, and a c. The most common ZAID libraries for isotopes at room temperature are .60c and .70c. For more obscure isotopes, other cross section libraries are referenced. It is easy to see how for neutrons making material cards can get complicated since they must include the ZAID data and library for all isotopes of the given elements and their weight or atomic fraction. This can be especially true when making material cards for a mixture since it will include many isotopes and require calculations to find its weight or atomic fraction. For these materials, you must also define a density in the cell card of the input file. The cell card consists of a cell number, material number, density, followed by your cell geometry that is defined by the numbers in the surface card. Assuming a working MCNP file, the python code developed will fill in a blank material card and change the density of the cell card(s) for the material specified. This program also allows the user to create multiple materials and input files for an

array of molecular percent's for a given molecule. It should be noted that this code is limited to make material cards based off the natural abundances of elements. Isotopes and elements that are manmade, do not have cross sections, or are immeasurable are not included in this script.

USING PYTHON 2.7

As a reference for the code, an Element Data text file was made that includes each element letter, photon ZAID number, a list of neutron ZAID numbers, a list for natural abundances, and the element's average atomic mass. This text file is opened in python and split so that the data is extracted into separate lists. Four dictionaries were made so the element letter would be able to reference the mass and photon/neutron ZAID data for that element. These dictionaries will allow the material strings and arrays defined by the user to communicate with each other. The user inputs molecules and their corresponding molecular percent for the non-enriched or "dry" material in their standard notation. For example, SiO2 at 1.00 is read by python as Silicon Dioxide at 100 percent purity or as the lists [Si, O] and [1, 2]. Using dictionaries python is able to connect the element letters with its ZAID numbers and average atomic mass.

When specifying an array of enriched or "wet" material to be calculated, a for loop is used to normalize the fractions of the dry material based off the array percent of the "wet" portion. This for loop passes the molecular data and percent's into the "mat" class to be interpreted as individual elements and their occurrences (such as stated earlier for SiO2). This is done for each molecule giving two lists that combined contain the elements and their element occurrence in the molecule. Using the other dictionaries, we are able to get the atomic weight of the molecules by multiplying the elements atomic mass by the number of times it occurs in the molecule stated. Totaling this up for all molecules given by the user, we are able to calculate the total atomic mass for the mixture. In this process, the code also linearly interpolates a mixture density (g/cm^3) by using the dry and wet parameters given by the user. This is inserted into the cell card where the user types "den".

Using a fifth empty dictionary that connects with the elements given by the user, we are able to combine similar elements between molecules and sum the mass results. Let us consider the case in which we want to find the weight fraction of oxygen in the mixture of 25% carbon dioxide and 75% carbon monoxide. We would end up with the calculation given below.

$$Tot.Mass(O) = 0.25 * (Mass(O)) + 0.75 * 2 * (Mass(O))$$

This is stating that the total mass for oxygen is equal to the sum of the molecular percent's multiplied by the number of occurrences in that molecule times the mass of oxygen. This calculation is done over every molecule given and added into the dictionary until we have the total atomic weights for all elements that occur. A for loop then searches the dictionary for values greater than zero and divides by the total atomic mass of the mixture to find the mass fraction of that occurring element.

APPLYING THE CODE

This code was constructed to show how collided over un-collided dose increases with water content present in Earth' and Mar's surface. The dry ground composition for Earth is taken from Tatsuhiko Sato and Koji Niita's paper *Analytical Functions to Predict Cosmic-Ray Neutron Spectra in the Atmosphere* [].The dry ground composition for Earth is given in Table 1.

Table 1: Molecular composition of dry ground for Earth.

Earth Crust Composition ρ = 2.7(g/cm^3)	
Molecule	**Percent**
SiO2	75%
Al2O3	25%

By increasing the amount of water present in the surface and normalizing, we can see how the water content will affect neutron albedo.

Similarly, for Mars we get the dry ground composition using the On-Line Tool for the Assessment of Radiation In Space (OLTARIS)[1]. OLTARIS includes some water in its composition of Martian regolith therefore; we must start by normalizing the other values around this parameter. The calculated dry ground regolith for Mars is given in Table 2.

Table 1: Molecular composition of dry ground for Mars.

Mars Regolith Composition ρ = 1.7 (g/cm^3)	
Molecule	**Percent**
SiO2	55.3%
Fe2O3	10.0%
Al2CaK2MgNa2O7	34.7%

The water content present in both the Earth and Mars surface was increased by five percent until 100% water was achieved. The python script when run creates 21 input files of various water compositions for each case to be run by MCNP.

EXECUTING MCNP

A MCNP_Run definition is created that receives the directory of the input files. This definition then looks for any files ending in '.i' and runs the files in MCNP6. The amount of tasks can be changed depending on the user's computer hardware. The MCNP executable functions similarly to many compiled programs: the input file, output file, and additional arguments are specified using keyword indicators after the executable is called. For example, an

MCNP process with an input file named *sample.i* and output file *sample.o* can be initialized with the following command string:

%MCNP_Directory%/mcnp6.exe i=sample.i o=sample.o

In python, pre-constructed input files are executed by feeding the above string to the os.system() function, where *%MCNP_Directory%* is replaced with the MCNP directory specific to a given computer, and *sample.i* is replaced with the desired input file name. The sub process will automatically wait for the MCNP to execute before starting the next iteration to prevent multiple instances of MCNP running at once.

MCNP MODELING

For the MCNP model, a neutron point source was used with a thermal energy of 0.025eV. The point source and surface tally are set one meter apart and are 50cm above a slab of our defined material. Using the Monte Carlo tool Visual Editor to input the model geometries, we are able to see a representative picture of the source in detector. This is shown in Figure 1.

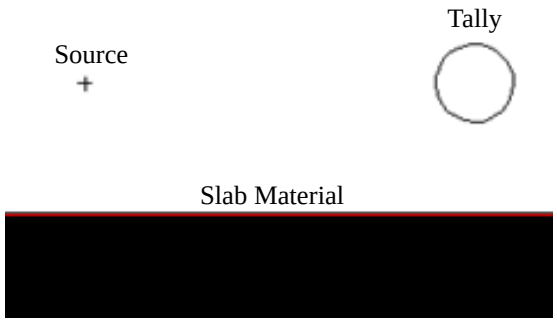

Figure 1: Point source and tally surface as shown in Visual Editor.

A run is performed with no slab present in order to obtain the un-collided dose measurement. This un-collided measurement will act as a control.

RESULTS

To plot the results a separate python file was made. This python file searches the MCNP output files for a unique line in the output file as a reference then locates itself to the dose data. The dose data for the file names given is then extracted. Using the control the collided/un-collided dose ratio was found by subtracting the un-collided control data from the data given in the runs to get the collided dose. The collided dose was then divided by the un-collided to achieve a simple ratio. The data was split into separate arrays for Earth and Mars. This data was then plotted against the percent water composition to observe the effects of neutron albedo at thermal energies. The plotted data is seen in Figure 2.

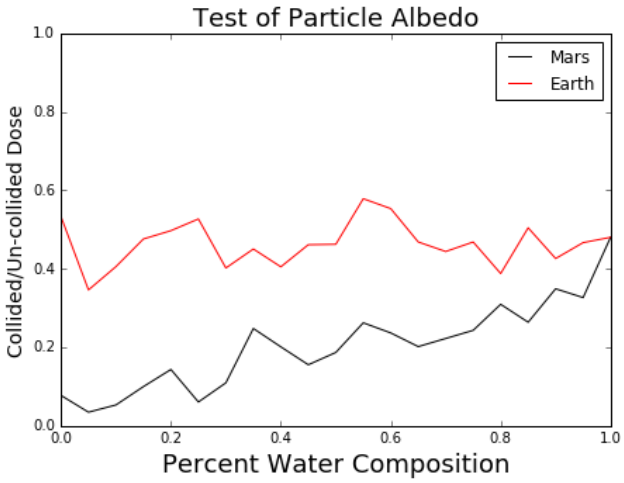

Figure 2: Collided over un-collided dose for various water compositions of the Earth and Martian surfaces.

From the figure, you can see that water in the surface has little to no impact for the Earth crust at thermal energies. On the other hand, Mars has very little albedo for the dry ground composition and an almost linear increase with water composition. Since the Martian surface provides very little water/Ice it can be assumed that for the majority of the Martian surface there would be a minimal amount of additional dose from neutron albedo.

CONCLUSION

Python is a powerful tool that can be used in conjunction with MCNP can iteratively simulate many different scenarios in order to solve large problems. From the results of the material editor, we found that at thermal energies neutron albedo is almost negligible on Mars. These results confirmed my suspicion that the maximum reflected dose would come from the presence of low z elements such as hydrogen. In the future, this work will be continued to find at what energy (if any) that we would observe a significant increase in dose from neutron albedo. I would also like to use this work in other applications such as solving for mixtures in reactor designs and optimizing shielding.

ACKNOWLEDGMENTS

I would like to thank Saqr Alshogeathri and Richard Reed for their guidance in this project.

REFERENCES

1. On-Line Tool for the Assessment of Radiation In Space (OLTARIS)." OLTARIS. March 26, 2015. Accessed December 15, 2016. https://oltaris.nasa.gov/materials/402.

2. Sato, Tatsuhiko, and Koji Niita. “Analytical Functions to Predict Cosmic-Ray Neutron Spectra in the Atmosphere.” *Radiation Research* 166, no. 3 (2006): 544–55.