

Study of the Production of Isotopes in an Urban Nuclear Post-Detonation Environment

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For my wife, SarahBeth.

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Abstract

In order to model the activated isotopes and resulting dose from a nuclear detonation in an urban environment, the Activation and Transmutation of Isotopes in an Unstructured Mesh (ACTIUM) Python toolkit has been developed to combine the unstructured mesh-based particle transport capability of MCNP6 with the CINDER2008 transmutation code to produce quantities of interest for the post-detonation nuclear forensics and weapons effects communities. The ACTIUM toolkit has been implemented and validated with a number of test cases from a simple analytic model to a case study of the urban detonation in Nagasaki, Japan. The ACTIUM approach is the first of its kind to couple the latest release of CINDER2008 as a part of the Activation in Accelerator Radiation Environments (AARE) package with MCNP6 and produce transmuted quantities per time step on an unstructured mesh for the nuclear forensics and weapon effects communities. ACTIUM uses the latest ENDF/B-VIII.0, TENDL2017, and JENDL4 cross section libraries for the transmutation calculations, and includes methods for producing material cards for the initial MCNP6 unstructured mesh calculation based on highly detailed materials often found in urban environments on a city specific basis. In the event of an urban nuclear detonation, the identification of these isotopic ratios provides insight for the radio-analytical chemistry and mass-spectrometry communities as they develop measurement techniques to analyze some of the ratios that have the highest sensitivities to source attributes. A process of how to create an unstructured mesh representation of the overall geometry of buildings along with their material compositions, and the corresponding layers of concrete and soil in an urban environment for use in neutron transport calculations, and subsequent transmutation calculations are also discussed in this work.

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Chapter 1

Introduction

The field of post-detonation nuclear forensics continues to be an area of research to combat an ever changing threat basis of nuclear terrorism and state actors around the world [92, 136, 70, 80, 102]. The Nuclear Forensics Attribution Act (NFAA) codified into law the need for technological readiness through an interagency and academic collaboration in the event of a nuclear detonation [pub]. The Technical Nuclear Forensics field was created to directly address the technological challenges associated with the analysis of pre-detonation and post-detonation nuclear materials [159]. As a part of the analysis of post-detonation materials, the isotopic composition and location of the debris is of interest to many agencies [15, 82, 80]. Much work has been done over the years to develop nuclear fallout-analysis codes that predict the particle size and resulting dose distributions, and the spatial dispersion of the fallout particulates in the event of a detonation [7]. Recently, there has been an interest in the production of activated isotopes in the surrounding environment due to prompt and delayed neutrons [50, 153, 65, 72, 73, 74]. In the event of a nuclear detonation in an urban environment, minimizing dose to first responders is of the utmost importance. When it comes to response planning, decision makers within the government need to have the most up-to-date information regarding several quantities of interest so that the maximum amount of lives can be saved. Quantities of interest in a post-detonation scenario include the spatial distribution of neutron-induced stable and radioactive isotopes in the environment, fallout patterns, blast and fire damage zones [134]. Dose is directly related to the spatial distribution of neutron-induced radioactive isotopes

in the environment and fallout patterns. The ACTIUM toolkit is developed to calculate the prompt neutron-induced stable and radioactive isotopes in the surrounding environment in post-detonation scenario. The distribution of these isotopes in the environment can be used to provide guidance in determining best routes for first responders in order to minimize dose, debris sample collection routes for subsequent radiochemical analysis, and provide initial radionuclide inventories to fallout codes in order to improve fallout zone fidelity. Other methods have approached isotope transmutation on unstructured mesh for the fusion community concerning shutdown dose rates associated with fusion reactors. ACTIUM is the first method to be focused on calculating some of the quantities of interest for the nuclear forensics and weapon effects communities. One of these quantities of interest is the change in isotopic ratios from the natural isotopic ratios in the surrounding environment due to neutron activation. These changes in isotopic ratios are common metrics used in analysis for the post-detonation nuclear forensics community [67, 79, 82, 126, 138]. For surface and sub-surface detonations, a portion of the materials that contain significant changes in isotopic ratios are incorporated into melt glass material. Much work has been done to characterize the isotopic ratio changes in the melt glass material [138, 11, 24, 36, 42, 51, 125, 172]. During a nuclear detonation, extreme temperatures are generated in the fireball as energy is released from the nuclear interactions occurring inside the device. Melt glass is formed as the fireball cools and the amalgamation of fission products, bomb debris, and environmental materials begins to fractionate and condense out of the fireball. The materials in the environment that are not consumed in the fireball still contain significant isotopic ratio changes, and the characterization of these ratios is a major focus of this work.

Air pollution has become a major topic of interest as shown by the amount of scientific literature and federal research that focuses on the health effects of exposure and how to mitigate the issues [25, 33, 83, 143, 44, 45, 46, 182]. Prolonged exposure to polluted-air has been linked to cardiovascular and respiratory disease, cancer, pregnancy complication, adverse birth outcomes, impairment of brain development, and childhood asthma development [143, 182, 83, 25, 33]. In an effort to characterize the polluted-air constituents, many studies have measured the gaseous and particulate matter components at various pollution concentrations for several cities around the world [5, 71, 154, 112, 16, 17,

183, 173, 37]. The work presented in Chapter 5 focuses on Houston, TX. Using the detailed pollution composition in Houston, TX, the work discussed in Chapter 5 characterizes the effects on effective dose from the activated radionuclides in the polluted air as compared with non-polluted air because of an urban nuclear detonation.

Chapter 2

Literature Review

Since the inception of atomic weaponry, experts from around the world have conducted tests of these devices in order to fully understand the physics and chemistry associated with a nuclear detonation. A major sampling and measurement campaign went alongside the tests in order to characterize the neutron induced activity in the environment from fission and activation products. Since the two urban detonations in Hiroshima and Nagasaki, many have attempted to model exactly what occurred during and shortly after those detonations.

An understanding of previous research is of the utmost importance in order to fully understand how to model an urban environment and calculate the neutron-induced stable and radioactive nuclei in the environment.

2.1 Review of Previous Studies of Nuclear Detonation Neutron-Induced Environmental Radioactivity

2.1.1 Mandeville Study

In the early 1950s, the slow neutron-induced radioactivities of nuclear explosions was investigated by Mandeville [104]. Mandeville cites that Glasstone’s “The Effects of Atomic Weapons” includes many references to the activities due to the neutrons from nuclear detonations, but never quantifies the amount of radioactivity induced [52]. Mandeville conducts two investigative cases where he looks at the radioactivity induced by slow neutrons

in the cases of an underwater detonation and underground detonation. Mandeville comes to the conclusion that the radioactivities induced by slow neutrons are on the order of 10^6 less than the radioactivities of the fallout for the underwater case and 10^8 for the underground case. Additionally, Mandeville states that he expects that the fast neutron-induced radioactivities are negligible and can therefore be ignored. The composition of the soil used in Mandeville's study is very simple when compared to more recent studies of the composition of the soil and leaves out elements that are major contributors to the long term radioactivity of post-detonation soil [61]. Mandeville's composition of the water is much like his composition of the soil in that it is missing key activated components with longer half lives [153].

2.1.2 Batzel Study

In the early 1960s, the radioactivities of underground nuclear detonations were revisited by Batzel [9]. Batzel used the entire fission energy spectrum to calculate radioactivities and used a more detailed model of the soil. Batzel concludes that induced radioactivities are 20-25 percent of the fission product radioactivity at the end of 1 day, and states that rare earth elements such as Nd, Pr, and Ce contribute anywhere from 1.0 to 5.0 percent of the total radioactivity after 1 hour.

2.1.3 Hiroshima and Nagasaki Reconstruction

DS86 and DS02

The US-Japan Joint Reassessment of Atomic Bomb Radiation Dosimetry in Hiroshima and Nagasaki, Dosimetry System 1986 (DS86) and Reassessment of Atomic Bomb Radiation Dosimetry in Hiroshima and Nagasaki, Dosimetry System 2002 (DS02) were created to provide a comprehensive overview of the work done to characterize the Hiroshima and Nagasaki detonations and resulting dosimetry from 1945 until 2002. Many of the studies included in these works are currently state-of-the-art in terms of Hiroshima and Nagasaki reconstruction efforts. DS86 and DS02 include details of the latest attempts to reconstruct the only urban detonations to ever occur. DS02 provides updates to many sections of DS86.

DS02 Source Term Evaluations

In an effort to characterize the prompt radiation leakage spectra from the Fat Man and Little Boy devices detonated over Nagasaki and Hiroshima, DS02 describes the brief history of source term calculations and provides the latest update to these calculations. Source term calculations utilize computer codes that simulate the explosion of the bomb and track the radiation from birth to its ultimate escape across a leakage boundary [184]. DS02 provides the latest source term calculation with 200 neutron energy groups and 43 gamma energy groups subdivided into 40 directional bins [184]. This updated source term is calculated by nuclear weapon design codes that have been heavily validated against atmospheric and underground nuclear tests [184].

DS02 Radiation Transport Calculations for Hiroshima and Nagasaki

DS02 details the prompt and delayed radiation transport for both Hiroshima and Nagasaki using the source terms described in above. In modeling both Hiroshima and Nagasaki, DS02 assumes a flat ground approximation and calculated flux values at discrete points.

Measurements of Neutron Fluences at Hiroshima and Nagasaki

The neutrons from the Hiroshima and Nagasaki detonations created many radionuclides in the environment and their activities were measurable 41 years after the detonation when the compilation of DS86 was finished [147]. DS86 documents that the neutron fluence can be roughly reconstructed based on the activation products in the environment. DS86 describes measurements of the activated ^{32}P in the adhesive for insulators on electric power poles in Nagasaki that was used to calculate the high energy neutron fluence. Cobalt from rebar in concrete and europium from natural sources provides the measurement basis for calculating the incident prompt neutron spectra for thermal neutrons.

DS02 provides updates to the measurements in DS86 by describing 1991 measurements to reconstruct the incident neutron spectrum. Nakanishi conducted a study comparing the measured and calculated neutron-induced radionuclides produced by the nuclear

detonation over Hiroshima, Japan [129]. In the study, Nakanishi focused on the neutron-induced activation products ^{152}Eu , ^{154}Eu , and ^{60}Co , and found that even in 1991 there were still measurable quantities of each isotope in the samples taken around Hiroshima. Nakanishi calculated and measured the neutron-induced production of ^{152}Eu from the nuclear detonation in some 14 samples taken from typical building materials, such as roof tiles and wall materials, located anywhere from 580 to 1450 m away from ground zero. From these ^{152}Eu ratio measurements, Nakanishi was able to reconstruct the ratio of thermal to epithermal neutron flux as a function of distance from the epicenter.

Review of Dose Related Factors for the Evaluation of Exposures to Residual Radiation at Hiroshima

Kerr’s review of the radiation dose reconstruction effort for Hiroshima bridges the gap between the end of DS02 and the most current status of the effort [81]. Kerr cites that there have been improvements in the activated isotopes measurements in the soil that allow for better characterization of the incident source neutrons. Kerr summarized the work done to characterize fission product contribution to the dose on the ground and concluded that there were no considerable fission products within 1 km of the hypocenter and that most fission products remained lofted for long periods of time. None of the models presented in the Kerr’s review for dose calculations involve a full physics particle transport calculation with the terrain topography included in the model.

2.1.4 Johnson Study

Recently, Johnson has been investigating the use of neutron-induced activation in Li-ion batteries for nuclear forensics applications [72, 73, 74]. Johnson notes that the neutron flux energy spectrum can be reconstructed depending on the level of activation of the isotopes within the battery, citing that the ratio of ^{24}Na to ^{58}Co can be an indicator of the hardness of the spectrum. In this study, Johnson only reports isotopes with $Z < 29$. Recent reports show that there are a number of rare earth elements within Li-ion batteries that were not considered by this research [127]. Johnson also notes that his research only used four reactions

from two batteries to reconstruct the incident neutron spectrum and that the accuracy of the reconstruction can be improved if more reactions are considered [74]. The research outlined in this proposal will focus on the rare earth elements from La to Lu.

2.1.5 Burnett Underground Radionuclide Production Studies

In support of the Comprehensive Nuclear-Test-Ban Treaty (CTBT), Burnett studied the radionuclides produced from an underground detonation in both fictional and historical underground test scenarios [21, 23]. In both cases, Burnett only accounted for two radionuclides produced from environmental neutron activation. Instead, Burnett’s articles focused on the radionuclides produced from activated bomb components and fission products that escape the underground chamber and are detectable in the air or on the surface. Burnett estimates the amount of activity from fission products in both scenarios with a scaling rule of thumb of $A = 1.45 \times 10^{23} f \lambda$ where A is the activity of the fission product per kT of weapon yield, f is the fission production production fraction and λ is the decay constant of the fission product.

2.1.6 Burnett Underwater Radionuclide Production Study

Burnett calculates the production of radionuclides in the event of a 1 kT underwater detonation in an effort to inform sample collections in support of the CTBT [22]. Burnett estimates the activities of each radioisotope by extrapolating measurements of activated seawater up to the same neutron fluence observed from a 1 kT weapon. Burnett assumes that water molecules do not contribute to the overall activity of the seawater because of the assumption that water consists of only ^1H and ^{16}O . Burnett notes that ^1H and ^{16}O capture to make stable ^2H and ^{17}O but they fail to account for the natural abundance of H and O where ^2H is present in the water at 0.0115 percent and ^{17}O and ^{18}O are present at 0.038 and 0.205 percent. ^2H and ^{18}O undergo (n, γ) reactions to produce radionuclides and Burnett is not accounting for these significant contributions to the overall activity.

2.2 Review of Monte Carlo Neutron Transport with MCNP on Unstructured Mesh

The history of the Monte Carlo N-Particle (MCNP) code is illustrious and has its inception at Los Alamos National Laboratory (LANL). The first formulations of the Monte Carlo Method are found in a letter from John von Neumann to the Theoretical Division leader in 1947 [57]. Since that time, several Monte Carlo codes have been developed by the leaders in Monte Carlo at LANL that have ultimately become MCNP6. Goorley provides a comprehensive history of MCNP up to the release of MCNP Code Version 6.0 [57].

MCNP has been extensively validated and verified in shielding, criticality safety, weapons effects, reactor safety and many more application areas [117, 35, 39, 57, 111, 84, 167, 175]. The unstructured mesh geometry capability in MCNP was first introduced with the release of MCNP Code Version 6.0 [57, 106]. MCNP6 developers have validated first and second order mesh element tracking of neutrons through unstructured mesh geometry in MCNP Code Version 6.2 [94, 95, 106, 110, 109]. Kulesza’s work of benchmarking neutron tracking through unstructured mesh geometry highlights the validity of deep neutron penetration type problems on an unstructured mesh representation of the geometry and the ability to view results directly on the model geometry [94].

Many other Monte Carlo codes have been developed by teams of developers from around the world. Some of the most prominent codes, other than MCNP, are Geant4, TRIPOLI, FLUKA, SERPENT, and SCALE and all but GEANT4 reference MCNP when showing validation results in their seminal journal publications [3, 19, 144, 8, 100]. Many publications benchmark new features in their Monte Carlo codes with MCNP results [62, 63, 163, 139, 180, 75]. Figure 2.1 shows the number of MCNP packages distributed by RSICC compared with all other Monte Carlo codes and illustrates MCNP’s popularity among user’s choice in Monte Carlo transport codes [158]. As of 2017, over 20,000 copies of MCNP licenses have been distributed by the Radiation Safety Information Computational Center (RSICC) [158]. GEANT4 usage statistics are not included in Figure 2.1 because RSICC does not manage the distribution of GEANT4.

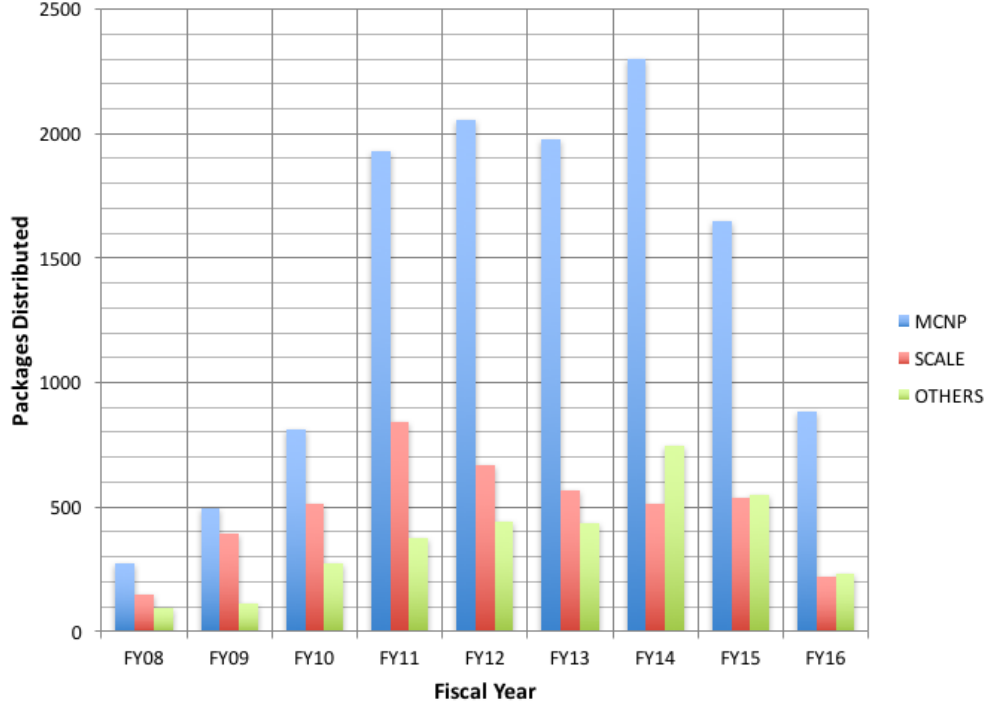


Figure 2.1: Overview of the Number of Distributed Packages of Monte Carlo Codes [158]

2.3 Review of the CINDER Transmutation Code

The CINDER transmutation code has its origins at the Bettis Atomic Power Laboratory and was originally developed by T. R. England in support of naval reactor design [43]. The original CINDER code used 4-group neutron fluxes to transmute < 250 nuclides included with the original cross section set [43]. In the 1990s, the CINDER data and code were updated to CINDER90 for accelerator applications by W.B. Wilson at LANL to include 3400 nuclides and transmute these nuclides with a 66-group neutron flux [49]. A mechanism for including the high-energy spallation products was developed for CINDER90 [49]. CINDER90 was incorporated into the MCNPX code as a built-in physics module that would do on-the-fly transmutation calculations for each neutron capture interaction and allow the transport of the delayed radiation from the transmuted nuclei [142]. The delayed particle production, treatment, and transport within MCNP using CINDER90 has been heavily validated [39, 40, 166, 167, 175, 115]. The MONTEBURNS code couples

MCNP and CINDER90 to calculate time-resolved reactor burnup quantities [14, 28, 99]. In the latest version of the code, CINDER2008, CINDER90's code base was updated to "modern" Fortran 90, implemented new solver algorithms, and added more post-processing options [66, 122, 121, 123]. CINDER2008 has been validated in both neutron- and photon- induced transmutation [123, 98, 62, 105]. Hecht concludes that Geant4 and MCNP6 coupled with CINDER2008 compare well with activation and fission product experiments [62]. CINDER2008 is now distributed with the Activation in Accelerator Radiation Environments (AARE) available through RSICC [120, 124]. CINDER2008 has been adopted by the community and has been extended with a "easy-to-use" graphical user interface for CINDER2008 transmutation calculations [97]. Other transmutation or burnup codes such as FISPACTII and ORIGEN are developed for reactor-based transmutation or burnup calculations [160, 38, 155, 177].

2.4 Review of R2S Methods

Originally, the rigorous 2-step (R2S) computational system was developed to calculate the fusion reactor shutdown dose rates [27]. R2S used MCNP4C to do the initial neutron transport, they translated the resulting fluxes into FISPACT99 input, performed the transmutation of each cell in the MCNP geometry using FISPACT99, and translated the decay gamma output from FISPACT99 into the source for another MCNP4C run to calculate the shutdown dose rates [27]. The ACTIVATION script that accompanies CINDER90 applies the R2S method using MCNPX as the transport code and CINDER90 as the transmutation code [49]. The next renditions of the R2S approach, such as the R2Smesh code system and Advanced-D1S method focus on refining the spatial resolution of the calculations by using fine MCNP mesh tallies that overlay the geometry to calculate the shutdown dose rates [103, 171]. As the evolution of the R2S system continues, there has been significant development utilizing unstructured mesh geometry representations instead of structured mesh tallies to calculate the fusion reactor shutdown dose rates [47, 145, 41, 12, 34, 85, 78]. The MCR2S approach uses MCNP6 as the transport software and FISPACTII as the transmutation solver where the unstructured mesh representation of the geometry is also used to tally the flux. The fluxes

on each mesh element are then translated into individual FISPACTII runs where the decay gamma spectrum is recorded and used as the source in a subsequent MCNP6 run to calculate dose rates [41]. The results from the unstructured mesh based code systems compare well to traditional constructed solid geometry (CSG) based analysis of fusion systems [69].

2.5 Review of Modeling Urban Environments for Particle Transport

Modeling urban environments for particle transport began by using satellite images and LIDAR scans to create a CSG representation of the city from right parallelepiped surfaces [54, 56, 55]. In these early urban environmental studies, the prompt and delayed absorbed human dose were tallied using mesh tallies in MCNPX. As modeling developed, the use of 3-D lattices allowed for more detailed geometries and material definitions [91]. The Hazus database is used to provide the type of building and LIDAR data provides the geometry of the buildings. The LIDAR data is then converted to 3-D voxels to be included in the structured lattice geometry and dose is tallied with mesh tallies. The most advanced method of modeling urban environments is using unstructured mesh representations of the LIDAR city building data [113, 114, 108]. The unstructured mesh approach allows the dose to be tallied directly on the geometry and allows for straight-forward modifications of the model in a CAD program. In all of the modeling techniques described above, the building material composition is subjective and at best an approximation. There have not been any effort to model the underground infrastructure that exists in most urban environments.

Chapter 3

Hiroshima and Nagasaki Verification of an Unstructured Mesh based Transmutation Toolkit

A version of this chapter has been accepted by the ANS Nuclear Technology Journal submitted by Tucker McClanahan, Tim Goorley, and John Auxier II.

Dr. Goorley and Dr. Auxier II provided guidance and necessary review of the document. The data presented in this chapter has been review by LANL and has been granted an unlimited release corresponding to LA-UR-19-31806.

3.1 Abstract

In order to model the activated isotopes and resulting dose from a nuclear detonation in an urban environment, the Activation and Transmutation of Isotopes in an Unstructured Mesh (ACTIUM) Python toolkit has been developed to combine the unstructured mesh-based particle transport capability of MCNP6 with the CINDER2008 transmutation code to produce quantities of interest for the post-detonation nuclear forensics and weapons effects communities. The ACTIUM toolkit has been implemented and validated with a number of test cases from a simple analytic model to a case study of the urban detonation in Nagasaki, Japan. The ACTIUM approach is the first of its kind to couple the latest

release of CINDER2008 as a part of the Activation in Accelerator Radiation Environments (AARE) package with MCNP6 and produce transmuted quantities per time step on an unstructured mesh for the nuclear forensics and weapon effects communities. ACTIUM uses the latest ENDF/B-VIII.0, TENDL2017, and JENDL4 cross section libraries for the transmutation calculations, and includes methods for producing material cards for the initial MCNP6 unstructured mesh calculation based on highly detailed materials often found in urban environments on a city specific basis.

3.2 Introduction

As stated in the introduction to the thesis, characterizing the environmental transmuted isotopes in the event of an urban detonation is of the utmost importance to provide estimates of dose rates to first responders, inform decision makers, and guide radiochemical collections. The Activation and Transmutation of Isotopes in an Unstructured Mesh (ACTIUM) Python toolkit has been developed to calculate the environmental transmuted isotopes by combining the transmutation solver of CINDER2008 with the unstructured mesh transport capability of MCNP6. ACTIUM is the first method to be focused on calculating some of the quantities of interest for the nuclear forensics and weapon effects communities.

The unstructured mesh capability in MCNP6 allows the user to transport both charged and neutral particles through an unstructured mesh representation of the geometry of interest and tally the flux and energy deposition on the unstructured mesh [107]. Unstructured meshes can be created by any number of computer aided engineering (CAE) tools where the CAE tool splits apart a solid into several small pieces called elements, and these elements are defined by a series of points called nodes and matrices containing information on how the nodes are connected called connectivity data. MCNP6 is designed to work with an Abaqus/CAE input file that contains the nodal and connectivity information of the mesh. Martz’s guide provides more information on the usage of the unstructured mesh feature in MCNP6 [107].

The ACTIUM toolkit is similar to the unstructured mesh based R2S systems with some notable improvements and application specific functionalities. The ACTIUM toolkit has

built-in memory management methods to allow processing of unstructured mesh models with any number of mesh elements and cover model extents out to hundreds of kilometers. The cross section set included in the ACTIUM toolkit is specifically designed to include as many cross sections relevant to the transmutation of isotopes in an urban environment. While the goal of the fusion based R2S systems is the total shutdown dose rates, the ACTIUM toolkit provides dose rates along with transmuted and time binned isotopic inventories, decay heat, and contributions by specific nuclides to the overall dose. This chapter provides the details of the ACTIUM toolkit as well as verification exercises.

3.3 Methods

The ACTIUM toolkit includes two main modules: the Material Processing module and the Activation module. The Material Processing module pulls material data from various material composition databases and publications to provide homogenized materials for the initial MCNP6 run. The Activation module couples MCNP6.2 and latest release of CINDER2008 as apart of the AARE package using a Python wrapper to translate the fluxes on the unstructured mesh geometry from the initial MCNP6 run into input files for CINDER2008. The Activation module then executes individual CINDER2008 runs in parallel using OpenMP or MPI, and post-processes the outputs from the CINDER2008 runs for direct analysis. Currently, MCNP6 does not have the capability to define a unique material for each mesh element.

During the calculation of the transmuted quantities for each mesh element, ACTIUM assumes that the flux over each time bin is constant and largely unaffected by the transmuted nuclei. Future work includes the implementation of an iterative approach that would make burn-up style calculations possible with ACTIUM. However, CINDER2008 within ACTIUM does allow for the newly transmuted nuclei to transmute. For example, if there is an $^{28}\text{Al}(n,\gamma)$ reaction producing ^{29}Al , ^{29}Al has the possibility of capturing a neutron and resulting in ^{30}Al .

Dose rate conversion factors for specific isotopes produced during the initial neutron burst are included with the ACTIUM package [89]. These dose conversion factors are associated with converting the activity of a specific isotope over a surface area of contaminated ground

to a dose rate at one meter from the ground surface. The ACTIUM package includes a series of Python packages to implement these dose rate conversion factors for each mesh element during an optional post-processing step. It is the user’s responsibility to mesh the geometry appropriately in order to correctly represent the physics of the model.

The Material Processing module is included with the toolkit to help set up the original MCNP6 run with materials often found in an urban environment: soil composition based on latitude and longitude interpolated from USGS data, building construction materials separated by building type, homogenized materials of the building interior based on building type, and homogenized materials of various electronics, e.g. laptops, cellphones, hard disks, etc. The output of the Material Processing module is a set of highly detailed MCNP material cards that are ready to be used as input in the neutron flux calculation. As a part of the Material Processing module, there are a suite of scripts for parallel-processing the raw cross section data in ENDF-B/VI format using NJOY2016 and producing grouped cross section sets in a user-defined energy bin structure. These grouped cross sections can then be translated into CINDER cross section library format by the Library Maker Code distributed with CINDER2008 [66]. Two cross section sets that include a combination of ENDF-B/VIII, JENDL4, and TENDL2017 data grouped to 66-Group and 321-Group energy bin structures are included in the ACTIUM toolkit to demonstrate the result of the cross section processing described above [18, 156, 90]. These cross section have the following prioritization order: ENDF-B/VIII, JENDL4, and TENDL2017 meaning that if the reaction had ENDF-B/VIII cross sections, the ENDF-B/VIII cross section was incorporated into the set. If a reaction was not present in the ENDF-B/VIII or JENDL4 cross sections, the TENDL2017 cross section would be incorporated into the set.

3.3.1 Activation Module Overview

The Activation Module implements a solution strategy similar to the R2S system with the exception that the end goal is an isotopic inventory for each mesh element for subsequent analysis. The Activation Module allows the user to calculate the isotopic inventory for each mesh element in the model, and when all of the processes have finished the transmutation

runs, it produces a HDF5 database coupled with a XDMF file for direct viewing of results in ParaView or VisIT [32, 48, 29, 4].

In order to execute the activation module the user specifies the file path and name of the MCNP6 output file, EEOU file, CINDER2008 BIGZA file, CINDER2008 decay gamma library, CINDER2008 cross section library, and the CINDER2008 executable in the input file. The user also specifies the transmutation time steps along with the specific particle and elemental edit number. These transmutation time steps do not correspond to time bins, but are the exact snapshots in time that CINDER2008 will calculate the transmuted isotopes in a given mesh element. The default will choose the first particle and elemental edit. The last line in the input file should be the command to run the activation calculation.

The Activation Module initializes the transmutation calculation by loading in the material definitions from the MCNP6 output file, elemental fluxes on the MCNP6 EEOU file, and isotopic natural abundances and other elemental data from the CINDER2008 BIGZA file. The Activation Module translates the MCNP6 material definitions into CINDER2008 material definitions by breaking up the element definitions, if present, into their natural isotopics and assigning each nuclide their own atom fractions. If specific isotopes are specified, the code directly translates the atom fractions from the MCNP6 material definitions to CINDER2008 material definitions. Energy binned fluxes from the EEOU file are linearly interpolated to match the CINDER cross section energy group structure. The user is free to choose any arbitrary energy bin structure when binning the fluxes in MCNP6 but in order to minimize interpolation error, the MCNP6.2 energy bin structure should be the same as the CINDER cross section library used in the transmutation calculation (shown in Section 3.4). The Activation Module fully automates the production of the CINDER2008 input files and parallelizes the transmutation calculations by executing CINDER2008 on several parallel computer processes. Figure 3.1 shows an overview of the activation module and Figure 3.2 shows an overview of the individual worker function. The individual worker function is where the CINDER2008 calculation is performed, and this function is executed by each worker in both Multiprocessing and OpenMPI mode.

Once the transmutation calculation has been initialized, the parallelization scheme is set up depending on whether the user elects to use Python’s multiprocessing package (default)

or Open MPI [170, 59]. Sections 3.3.1 & 3.3.1 describe the parallelization schemes in more detail where the CINDER2008 calculations are executed. The inputs for one mesh element of each material in the calculation whose neutron flux is zero along with all of the mesh elements whose neutron flux is non-zero are added to either the queue in Multiprocessing mode or the list of inputs in OpenMPI mode for processing by the workers; either subprocesses or MPI processes. The results from the zero-flux runs are used to get place holder data for the rest of the zero-flux mesh elements with the corresponding material. The place holder data consists of nuclide data for mesh elements that receive zero flux. This nuclide data includes the nuclides from the MCNP material cards that have not been transmuted because they were in mesh elements that received zero flux. The place holder data is essential for correct visualization of the data. Without the place holder data, it is possible that whole parts will not appear in the final HDF5 database and thus will not be visualized. Once the multiprocessing or MPI task has completed a CINDER2008 run for a single mesh element, the worker writes the results to its own HDF5 database. Zero flux mesh elements stem from mesh elements in the model that are not sampled.

Once all of the transmutation calculations have been executed, all of the worker HDF5 databases are merged into one main HDF5 database. The place holder data of the mesh elements whose neutron flux is zero is then added to the master HDF5 database. Finally, a XDMF file is written to accompany the main HDF5 database. The XDMF file is used to point to the data in the HDF5 database without having to load the entire HDF5 database. The HDF5 database contains activity, activity density, mass, and decay heat for each nuclide in each mesh element from the CINDER2008 calculations along with the mass density, atom density, and volume of each mesh element from the MCNP6 output file. The XDMF file breaks down the information in the HDF5 database by part and information category for easier data viewing. The Activation module also includes some ParaView post-processing macros that allow the user to create custom datasets within ParaView like isotopic ratios and elemental concentrations.

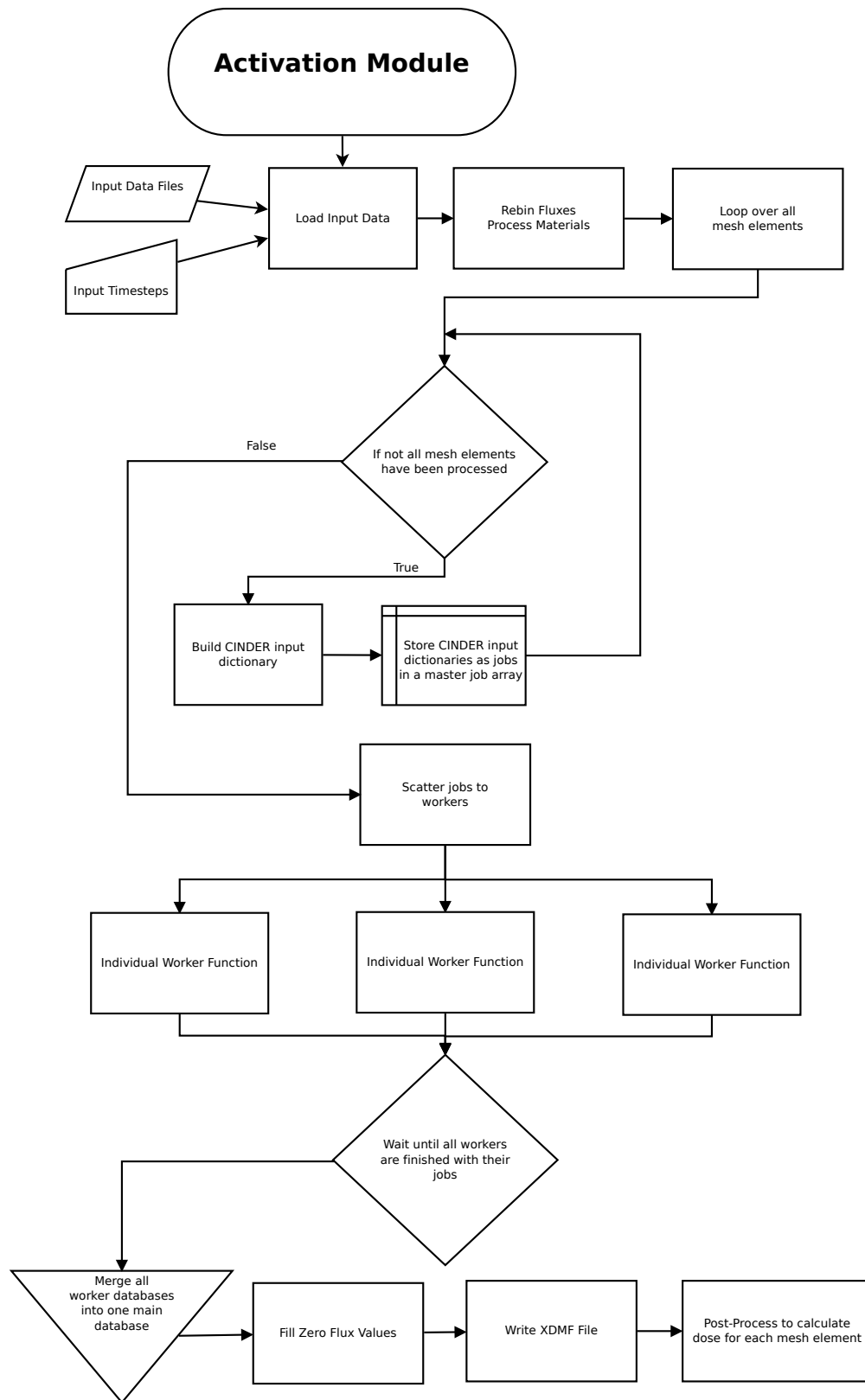


Figure 3.1: Overview of the Activation Module

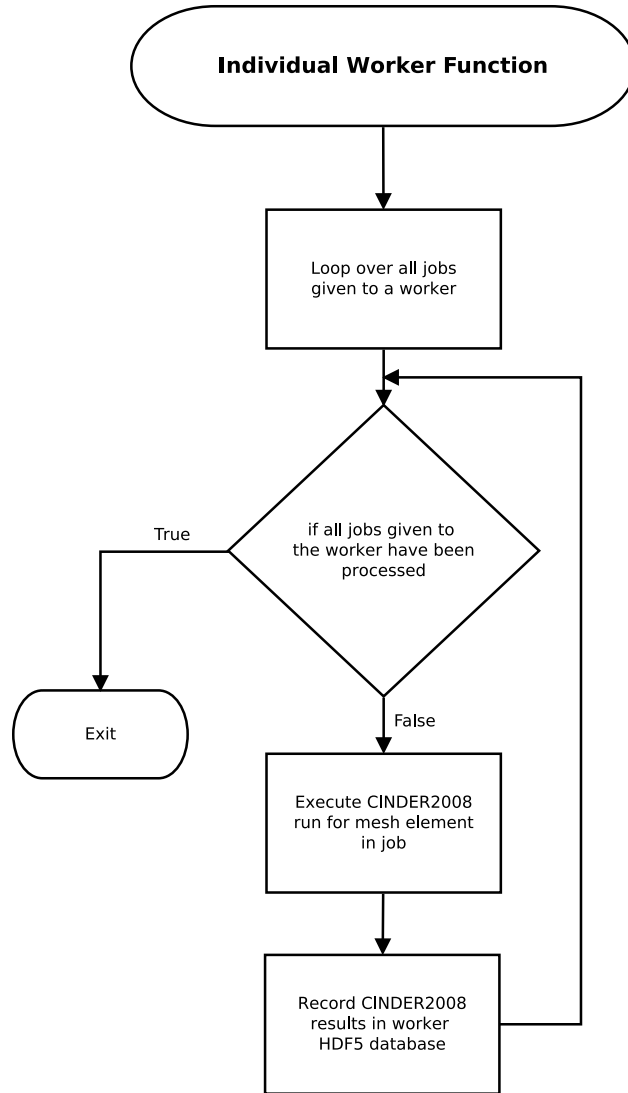


Figure 3.2: Overview of the Individual Worker Function

Multiprocessing Mode

Python’s multiprocessing package allows the code to leverage the full extent of the processors on the machine by spawning individual subprocesses instead of threads [170]. Multiprocessing mode is the preferred mode of operation if the user has a smaller calculation and is working on one computer because the overhead associated with the multiprocessing package is much less than the Open MPI overhead. For calculations using Python’s multiprocessing package, the inputs for a transmutation calculation, such as the flux, CINDER material definition, and mesh element number are passed as an input dictionary

into a queue. Inputs for mesh elements whose flux are zero are not put into the queue and their mesh element number and material number are recorded in lists for later processing. Once the queue has been constructed, a user-defined number of subprocesses are initialized and each subprocess takes an input dictionary from the queue and executes a CINDER2008 run. Each subprocess loads in the CINDER2008 output files and writes the results to the subprocess' HDF5 database. The subprocesses continue to process inputs from the queue until the queue is empty.

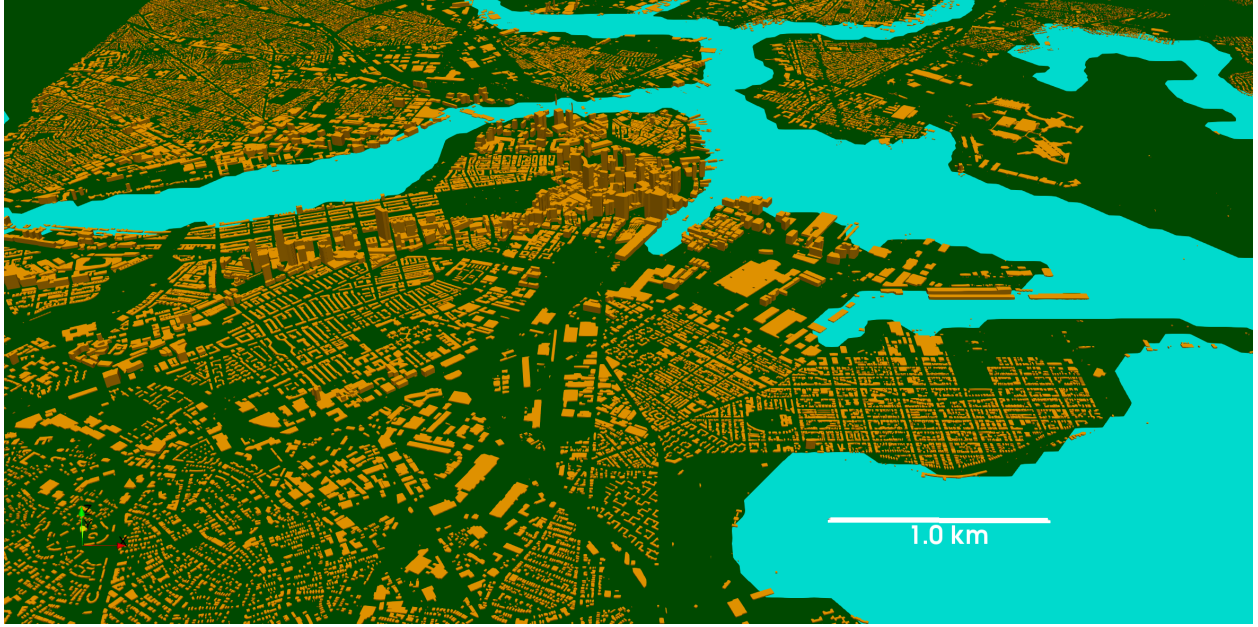
OpenMPI Mode

Open MPI is the parallelization option of choice for users running on computing clusters with multiple nodes. Even if the user is running on one machine, the user is encouraged to use the Open MPI option for larger calculations that push the memory limits of the machine because it has a number of methods built-in that help with memory management. Calculations with large mesh element counts can easily overrun the computer's local memory without these memory management schemes implemented with the Open MPI option. The initialization process described above only occurs on the lowest MPI process in order to conserve memory. After the initialization, the lowest MPI process constructs a dictionary of a list of the CINDER cross section library energy group structure and the name of the CINDER working directory for later broadcast to the other MPI processes. The MPI option constructs a list of input dictionaries where each input dictionary contains the inputs, such as the CINDER material definition, flux, volume, and mesh element number for one mesh element with a non-zero flux. Mesh elements that have a neutron flux equal to zero are not added to the list of inputs, and their mesh element number and material number are added to another list for later processing. The Activation module then splits the list of inputs into chunks with no more than 50000 input dictionaries. Chunking the list of inputs ensures that the size of the MPI messages will not exceed the 2GB message buffer size. The broadcast dictionary is then broadcast to all MPI processes once and for each chunk of input dictionaries, the inputs are divided evenly amongst the MPI processes where the MPI processes execute a CINDER2008 run for each input. Each MPI process creates a HDF5 database and writes the results from each CINDER2008 run to the database. In OpenMPI

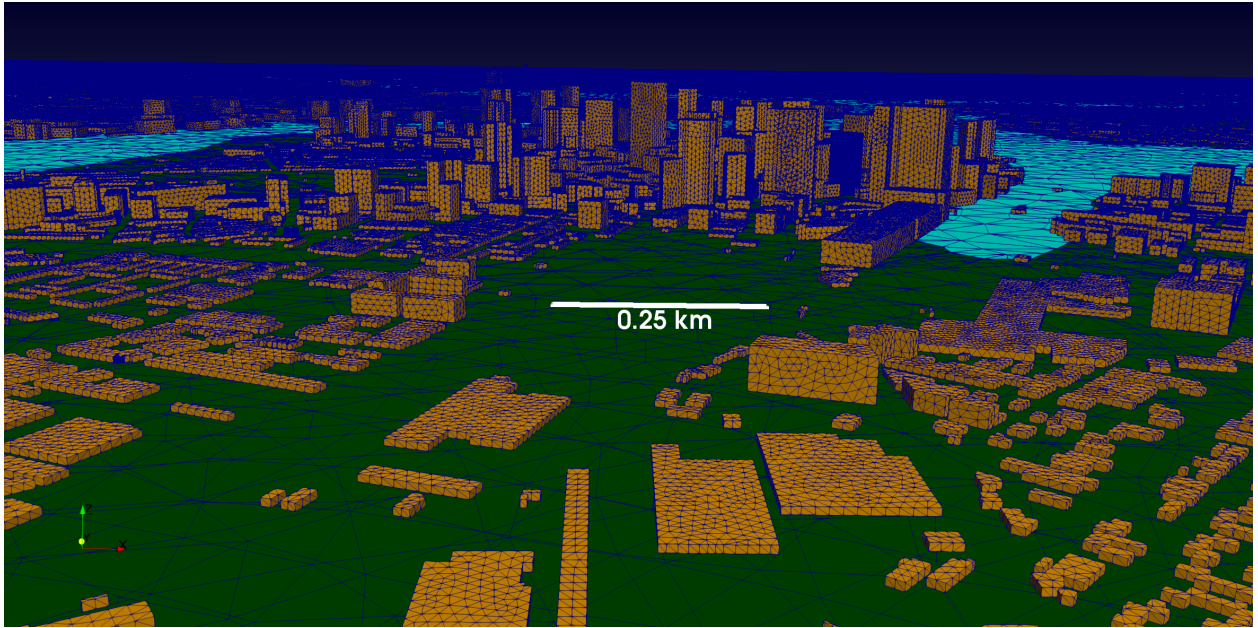
Mode, each worker reads their own HDF5 database into memory during the worker database merging routine in order to transmit the workers' results to the main process. Once the main process has received the data from the MPI Reduce command, it writes the data into the main HDF5 database. By having each worker read in the results from their databases, run times for creating the main database are drastically reduced.

3.3.2 Urban Geometry Creation Procedure

In order to calculate the stable and radioactive isotopes produced by a nuclear detonation in an urban environment, the geometry of the city needs to be constructed and converted to a format conducive for particle transport with MCNP6. Figure 3.3 shows an unstructured mesh representation of the city of Boston, MA created by the procedure outlined below.



(a) Downtown Boston, MA



(b) Unstructured Mesh Elements in the Boston, MA model

Figure 3.3: Overview of Boston, MA Unstructured Mesh Model

The general building and terrain footprints of an urban environment can be gathered from OpenStreetMap[®] directly or purchased in an importable CAD format from CADMAPPER[®] [60]. The CADMAPPER[®] website provides a user interface to create 3D CAD models of the

terrain, buildings, roads, parks, waterways, etc. for any user-selected region of the map. Once the user has selected a region of the map, a 3D CAD model can be generated and imported into the user’s CAD program of choice. The data downloaded directly from OpenStreetMap has to be edited and converted before the user can import it into a CAD program. JOSM is an open source extensible editor for OpenStreetMap data, and within JOSM, the user can edit the OpenStreetMap data to delete certain features not necessary for valid representation of the urban environment; such as lines representing roads, subway tracks, park benches, trees etc. [151]. Once the OpenStreetMap data is cleaned up in JOSM, the user can then open the OpenStreetMap data in OSM2World to convert the data into a importable CAD file format [88]. Once the urban environment data is imported into a CAD program, the user must clean-up the model to ensure that there are no overlaps, interferences, or spline surfaces in the model and make sure the overall model is “water-tight.” A “water-tight” model is one that does not have any gaps or interferences between parts, and every region of the model is defined and assigned a material.

Once the model is “water-tight” the user must create an unstructured mesh (UM) representation of the CAD model, and write the mesh as an Abaqus/CAE[®] input file. There are a number of methods to generate the UM representation of the CAD model, but this chapter will focus on the most prominent methods. Abaqus/CAE[®] is able to import the CAD model and generate a UM representation. Kulesza’s UM tutorial using Abaqus/CAE[®] 6.12-1 provides a detailed procedure for generating the UM Abaqus/CAE[®] input file for MCNP6 [93]. Silver Fir’s Atilla4MC software is designed for UM generation specifically for particle transport with MCNP6 [47]. Atilla4MC allows the user to generate the UM representation of the CAD model and write the Abaqus/CAE[®] input file. Once the Abaqus/CAE[®] input file is generated, a MCNP6 calculation can be set up by following the procedure described in Martz’s overview of the usage of UM in MCNP6, and using the material cards from the Material Processing Module [107]. Figure 3.4 shows a high level overview of the pre-processing procedure.

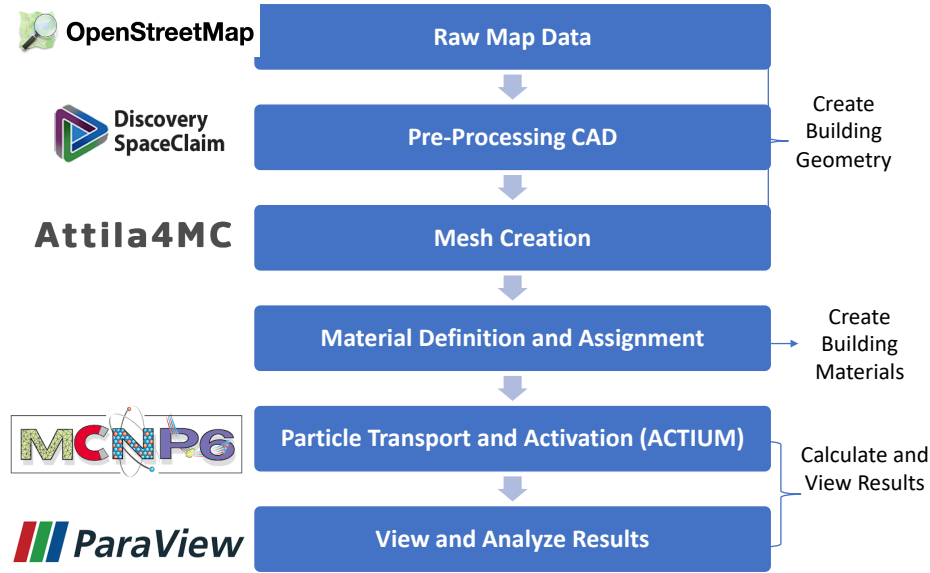


Figure 3.4: Overview of the Calculation Procedure

3.4 Validation and Results

The activation of a simple aluminum cube and a case study of the Nagasaki detonation are used to validate and demonstrate the capabilities of ACTIUM. The results and discussions of each validation effort are detailed in Sections 3.4.1 & 3.4.2.

3.4.1 Simple Cube Validation

Validation Study Description

The geometry consists of a simple ^{27}Al cube centered about the origin, that is meshed with eight equally sized hexahedral mesh elements with a total volume of 1 cm^3 . This cube is irradiated with an isotropic 1 MeV neutron point source located just outside of the top, right-most corner of the cube for $1 \mu\text{s}$ in the first time step, and then allowed to decay for six minutes without the neutron source in the second time step. The simple cube geometry setup is shown in Figure 3.5. Figures 3.5, 3.6 & 3.7 are in the same orientation.

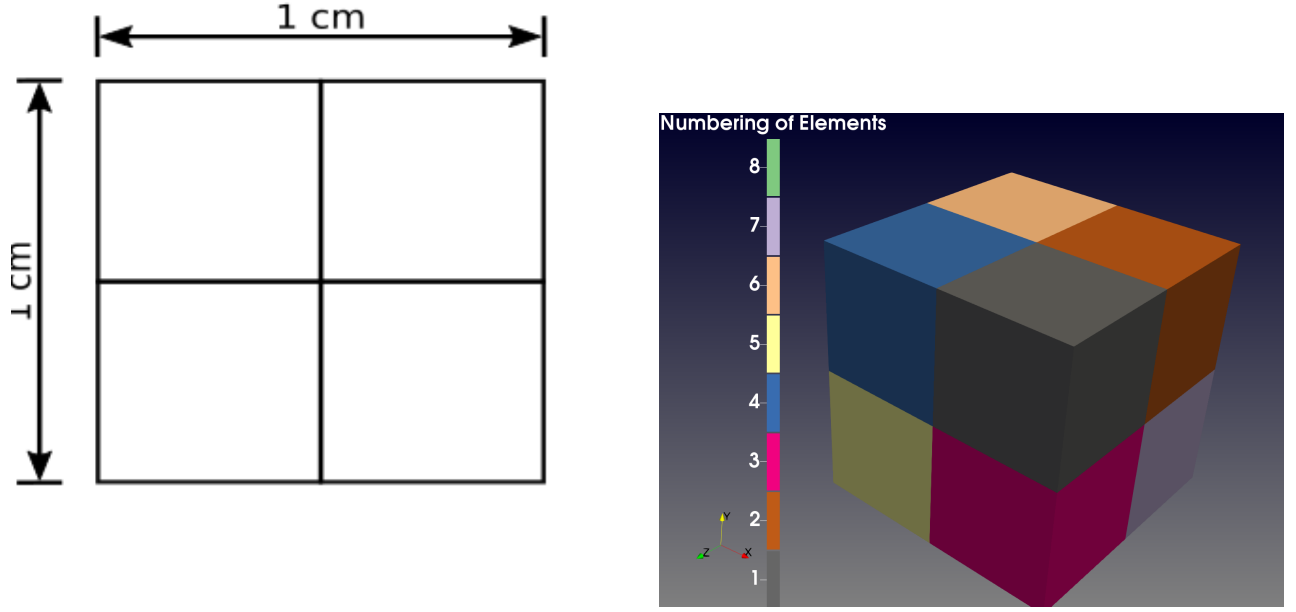


Figure 3.5: Overview of the Simple Cube Geometry

The simplified production and destruction of an isotope in a neutron induced activation scenario can be described by Equation 3.1.

$$\begin{aligned}
 \frac{dN_p}{dt} &= \text{production-destruction-decay} \\
 &= N_t(t) \int_0^\infty \sigma_t(E) \phi(E) dE - N_p(t) \int_0^\infty \sigma_p(E) \phi(E) dE - \lambda_p N_p(t) \quad (3.1)
 \end{aligned}$$

where $N_p(t)$ is the number of atoms of the nuclide being produced, $N_t(t)$ is the number of atoms of a target nuclide, $\sigma_p(E)$ is the energy dependent neutron cross section (sum of any cross section that changes the nuclide to another nuclide) of the nuclide being produced, $\sigma_t(E)$ is the energy dependent neutron cross section (sum of any cross section that changes the nuclide to another nuclide) of the target nuclide, λ_p is the decay constant for the nuclide being produced, and $\phi(E)$ is the energy dependent neutron flux. For the simple aluminum cube and calculating the ^{28}Al production, many terms in Equation 3.1 can be simplified due

to the mono-energetic neutron source and a simplified version of Equation 3.1 is shown in Equation 3.2, which is Eq. 14.15 from Tsoulfanidis' textbook [165].

$$\frac{dN_p}{dt} = N_t(t)\sigma_t\phi - N_p(t)\sigma_p\phi - \lambda_p N_p \quad (3.2)$$

Given that there is only one isotope, ^{27}Al in the simple aluminum cube, the solution of Equation 3.2 is shown in Equation 3.3 which is Eq. 14.16 from Tsoulfanidis' textbook.

$$N_p(t) = \frac{\sigma_t N_t(0)\phi}{\lambda_p + \sigma_p\phi - \sigma_t\phi} \{\exp(-\sigma_t\phi t) - \exp[-(\lambda_p + \sigma_p\phi)t]\} \quad (3.3)$$

The fluxes in the cube are tallied on a per mesh element basis in energy, and group cross sections are calculated from ENDF-B/VIII.0 and TENDL2017 data that match the energy bin structure of the tallied fluxes [18, 90]. Table 3.1 shows the energy binned fluxes tallied in each mesh element that are used in the analytical calculation of the ^{28}Al production in the cube. The cross sections shown in Table 3.2 are grouped cross sections weighted with a uniform flux distribution where the $\text{Al}^{27}(\text{n},\gamma)$ cross section is used as the target cross section, σ_t and the $\text{Al}^{28}(\text{n},\gamma)$ cross section is used as the cross section of the nuclide being produced, σ_p in Equation 3.3.

These cross sections are calculated with Equation 3.4 where σ_G is the grouped cross section for energy group G with upper and lower energy bound E_0 , E_1 , $\phi(E)$ is the flux that is set to one, σ is the (n,γ) cross section, E is energy, ΔE_i is energy bin width of the raw cross section data σ_i that has energy bounds within the energy bounds of the group, and ΔE_G is the energy bin width of the energy group. Other types of interactions such as (n,α) and (n,p) are considered negligible for this validation exercise, and are not included in Table 3.2

$$\sigma_G = \frac{\int_{E_0}^{E_1} \phi(E)\sigma(E)dE}{\int_{E_0}^{E_1} \phi(E)dE} = \frac{\int_{E_0}^{E_1} \sigma(E)dE}{\int_{E_0}^{E_1} dE} = \frac{\sum \sigma_i \Delta E_i}{\Delta E_G} \quad (3.4)$$

Table 3.1: ^{27}Al Cube Case Study Fluxes (n/cm²/s)

Upper Energy Bin (MeV)	1.11E-01	1.83E-01	8.21E-01	1.11E+00
Element 1 Flux (n/cm ² /s)	1.77E+13	1.29E+13	1.21E+13	2.97E+16
Element 2 Flux (n/cm ² /s)	1.17E+13	1.20E+13	1.05E+13	2.04E+16
Element 3 Flux (n/cm ² /s)	8.65E+12	1.43E+13	1.04E+13	2.05E+16
Element 4 Flux (n/cm ² /s)	9.80E+12	1.88E+13	1.09E+13	1.54E+16
Element 5 Flux (n/cm ² /s)	1.05E+13	1.21E+13	1.14E+13	2.03E+16
Element 6 Flux (n/cm ² /s)	6.36E+12	1.22E+13	6.94E+12	1.55E+16
Element 7 Flux (n/cm ² /s)	7.50E+12	1.50E+13	7.92E+12	1.54E+16
Element 8 Flux (n/cm ² /s)	4.84E+12	1.62E+13	7.18E+12	1.18E+16

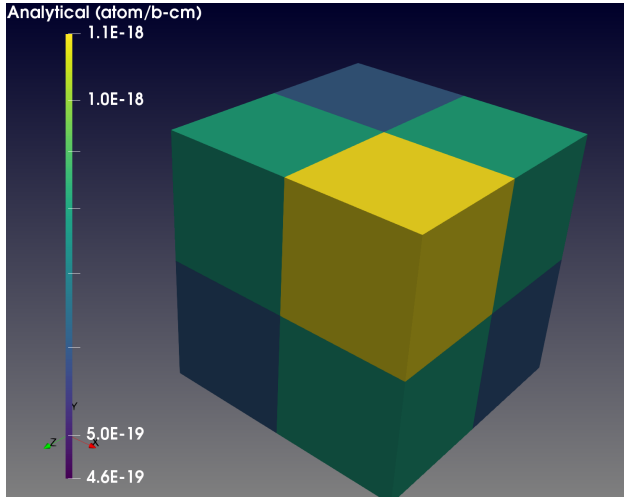
Table 3.2: ^{27}Al Cube Case Study Cross Sections

Lower Energy (MeV)	Upper Energy (MeV)	^{27}Al (n, γ) ENDF-B/VIII (barn)	^{28}Al (n, γ) TENDL2017 (barn)
7.738E-02	1.111E-01	1.981E-3	2.870E-3
1.111E-01	1.832E-01	1.628E-3	9.913E-3
1.832E-01	8.208E-01	3.299E-4	1.260E-4
8.208E-01	1.108E+00	6.396E-4	1.130E-4

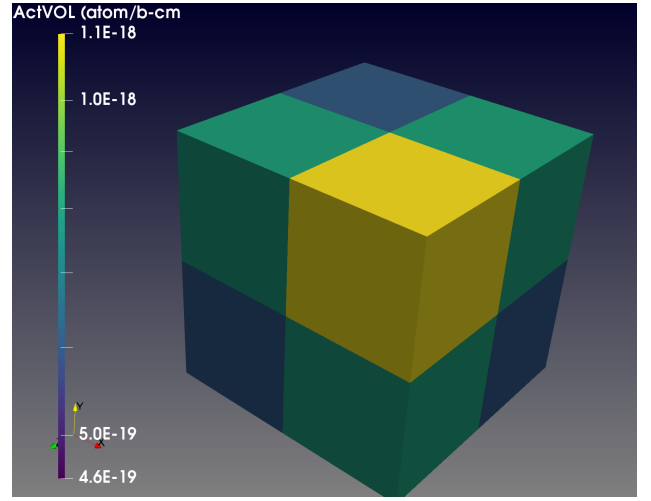
Results

Figures 3.6 & 3.7 show the results for the ^{28}Al production as calculated analytically by Equation 3.3 and calculated by ACTIUM. The fluxes in the EEOUT file used in Equation 3.3 for Figure 3.6 are converted to a XML-based VTK file for viewing and manipulation in ParaView with a LANL post-processing script [96]. The analytical solution in Figure 3.7 is calculated by multiplying the initial production of ^{28}Al by an exponential decay term. The

analytical and ACTIUM solutions closely match to within the precision of CINDER2008. Significant figures are lost while solving the Marchov equations in CINDER2008 due to round off and other approximations. A more detailed discussion of CINDER2008's precision can be found in CINDER2008's manual. Table 3.3 shows the numerical values of the atom densities calculated analytically and by the ACTIUM package. The fraction value in Table 3.3 is the ACTIUM solution divided by the analytical solution and shows excellent agreement between the two solutions.

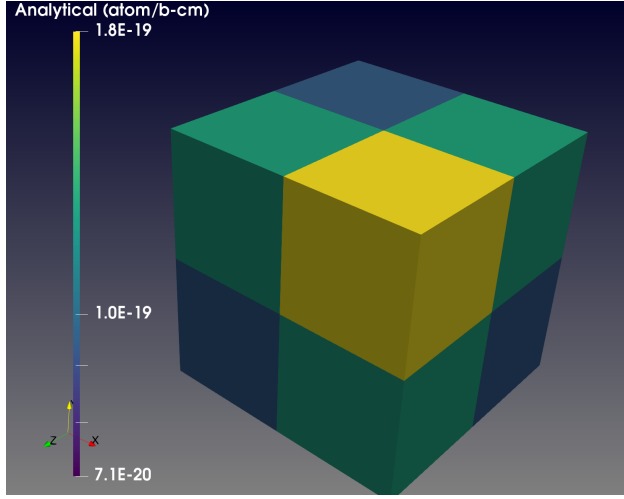


(a) Analytical Calculation

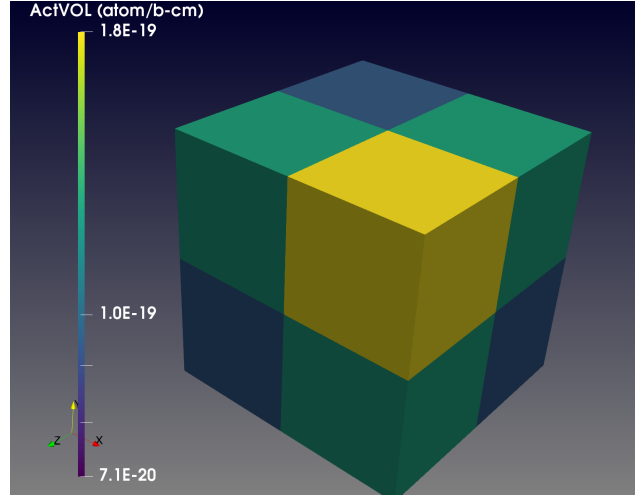


(b) ActVOL Calculation

Figure 3.6: Comparison of ^{28}Al Production for the Initial Production time step



(a) Analytical Calculation



(b) ActVOL Calculation

Figure 3.7: Comparison of ^{28}Al Production for the 6 min decay time step

Table 3.3: ^{28}Al Atom Density Validation Results

	Initial Time Step			Decay Time Step		
Element Number	ACTIUM $\left(\frac{\text{atom}}{\text{barn-cm}}\right)$	Analytical $\left(\frac{\text{atom}}{\text{barn-cm}}\right)$	Fraction $\left(\frac{\text{ACTIUM}}{\text{Analytical}}\right)$	ACTIUM $\left(\frac{\text{atom}}{\text{barn-cm}}\right)$	Analytical $\left(\frac{\text{atom}}{\text{barn-cm}}\right)$	Fraction $\left(\frac{\text{ACTIUM}}{\text{Analytical}}\right)$
1	1.15E-18	1.15E-18	1.00	1.79E-19	1.79E-19	1.00
2	7.90E-19	7.90E-19	1.00	1.24E-19	1.24E-19	1.00
3	7.90E-19	7.90E-19	1.00	1.24E-19	1.24E-19	1.00
4	5.95E-19	5.95E-19	1.00	9.30E-20	9.31E-20	1.00
5	7.85E-19	7.85E-19	1.00	1.23E-19	1.23E-19	1.00
6	5.99E-19	5.99E-19	1.00	9.37E-20	9.37E-20	1.00
7	5.96E-19	5.97E-19	1.00	9.33E-20	9.33E-20	1.00
8	4.57E-19	4.57E-19	1.00	7.15E-20	7.15E-20	1.00

3.4.2 Nagasaki Validation

The urban detonations occurring in Hiroshima and Nagasaki are the only two examples of nuclear detonations in urban environments. Many studies of these detonations have been conducted over the last 70+ years and much of that work has been documented in the DS86 and DS02 reports [147, 148, 184, 185]. The results and analysis shown in this section are meant to validate the ACTIUM package and not to replicate the large body of work in DS86 and DS02.

Dose measurements taken days after the events are used to validate the ACTIUM package [118]. Two teams of surveyors were sent out on separate occasions to measure the dose fields around the hypocenters of Hiroshima and Nagasaki; one team from the Naval Medical Research Institute (NMRI) and the other team organized by the Manhattan Engineer District. The team from NMRI took measurements at Hiroshima on November 1-2, 1945, and Nagasaki on October 15-27, 1945 using a Geiger-Muller type instrument, and made a majority of the measurements at a height of 1 m above the ground [118]. The group of scientists organized by the Manhattan Engineer District conducted surveys using Lauritzen-Wollan electrosopes positioned 5 cm above the ground. The NMRI team noted that there was no notable change in the measured dose when measurement height was changed from 5 cm to 1 m above ground.

In both validation cases, the same CINDER2008 cross section library is used during the transmutation portion of the calculations. This CINDER2008 cross section library consists of ENDF/B-VIII.0, JENDL4, and TENDL2017 cross section data that are first made into 66-Group cross sections using the suite of scripts accompanying the ACTIUM package to execute NJOY2016 and then processed into CINDER2008 cross section library format using the Library Maker code distributed with CINDER2008.

Dose rates are calculated using dose conversion factors for specific isotopes produced during the initial neutron burst [89]. These dose conversion factors are associated with converting the activity of a specific isotope over a surface area of contaminated ground to a dose rate at one meter from the ground surface. The layering of the terrain models for both Hiroshima and Nagasaki allow for the calculation of the surface area of each tetrahedral mesh

element based on the known height of the tetrahedral mesh elements (set by the height of the layer) and the volume of each mesh element. During post-processing, these dose conversion factors are applied to the surface areas of each mesh element, and the resulting dose dataset is stored alongside the other quantities of interest.

The results from the Hiroshima validation exercise are not included in this article due to a number of external factors that render the correct reproduction of the dose contours out of the scope of the ACTIUM package. The ACTIUM calculation does not account for the “black rain” phenomenon that certainly would have deposited fission and activation products from the weapon downwind of ground zero. Given that the Nagasaki detonation occurred at a fallout-free height of burst, minimal fission products fell to the ground in the immediate vicinity of the hypocenter except for the “black rain” phenomenon [118, 147, 148, 184, 185]. The ACTIUM calculation is only showing the contribution to the dose rate from the prompt neutron induced activation in the soil. Only activation from prompt neutrons is shown in the following sections.

Calculation Description

Figure 3.8 shows the energy dependent neutron leakage for the Fat Man device used as an isotropic source in the initial MCNP6 neutron flux calculation and is held constant in time for 1 μ s [68, 53]. The Fat Man source is binned with 200 energy bins. A yield of 20 kT was chosen for the initial neutron flux calculation.

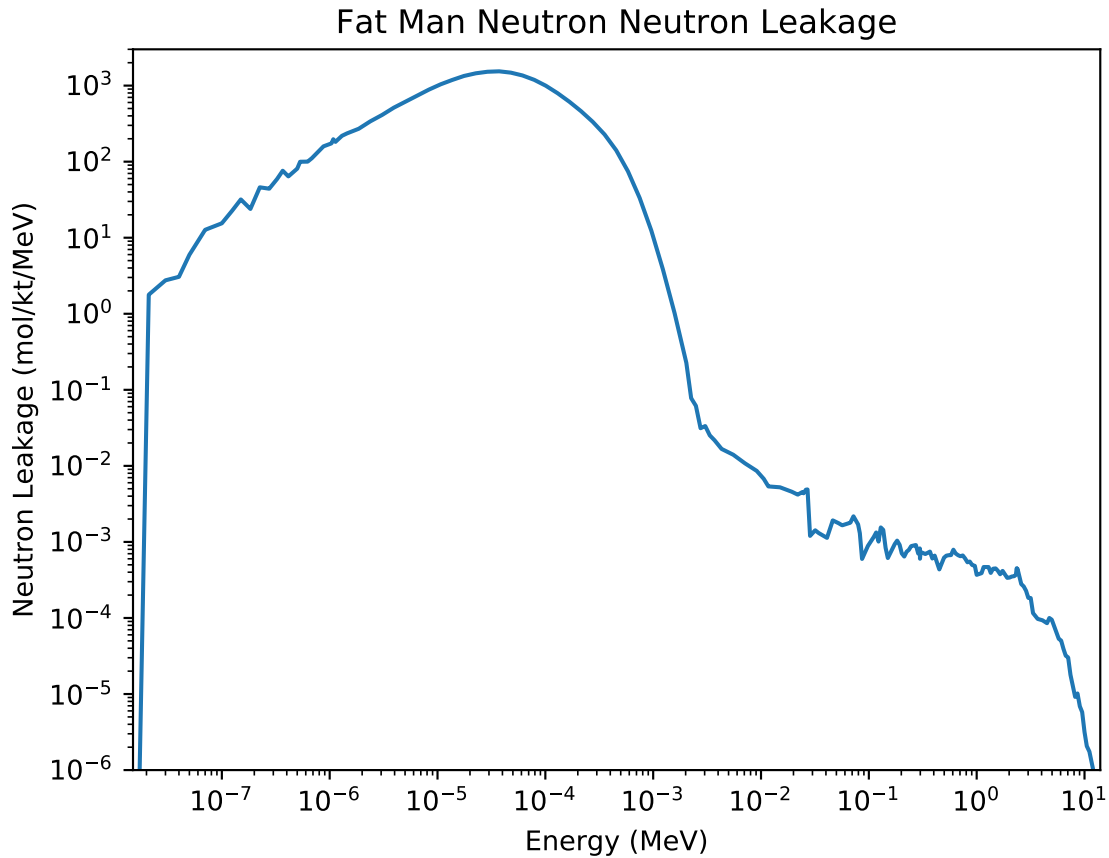


Figure 3.8: Energy Dependent Fat Man Neutron Leakage

The terrain composition for Hiroshima and Nagasaki, shown in Table 3.4, is chosen from the Hiroshima Castle and Nagasaki Hypocenter Monument sample where the elemental composition was measured to the PPM level with atomic emission spectrometry and neutron activation analysis [147]. Water is added to both elemental compositions at the recommended value of 30 percent [147]. The totals deviate from 1000 mg because of errors in gravimetric measurements of the oxygen in the samples [147].

Table 3.4: Hiroshima and Nagasaki Soil Composition [147]

Element	Hiroshima Relative Mass (mg per g)	Nagasaki Relative Mass (mg per g)	Element	Hiroshima Relative Mass (mg per g)	Nagasaki Relative Mass (mg per g)
H	10.1	10.0	Ga	0.022	0.023
Li	0.026	0.026	As	0.0066	0.009
B	0.0040	0.0022	Se	0.0012	0.002
C	26.3	24.4	Rb	0.225	0.07
N	1.6	1.5	Sr	0.070	0.134
O	447	503	Y	0.014	0.02
Na	12.4	7.89	Zr	0.035	0.126
Mg	2.71	8.20	Nb	0.005	0.01
Al	64.9	99.6	Mo	0.0014	0.002
Si	328	245	Ag	0.0002	0.0014
P	0.512	1.07	Sb	0.0008	0.006
Cl	0.115	0.340	Cs	0.005	0.004
K	31.1	7.64	Ba	0.535	0.37
Ca	5.4	11.6	La	0.021	0.023
Sc	0.005	0.02	Ce	0.036	0.043
Ti	1.52	5.86	Sm	0.003	0.0039
V	0.0253	0.167	Eu	0.0009	0.0015
Cr	0.0273	0.151	Tb	0.0006	0.0004
Mn	0.587	1.31	Hf	0.0040	0.0060
Fe	20.6	57.3	Ta	0.0008	0.0006
Co	0.0038	0.0227	Pb	0.066	0.062
Ni	0.009	0.053	Th	0.0099	0.007
Cu	0.034	0.057	U	0.0026	0.0025
Zn	0.335	0.256	Total	954.3794	986.3922

The Nagasaki terrain geometry consists of a CAD-importable model generated by Terrain2STL[®] using the NASA Shuttle Radar Topography Mission (SRTM3) dataset that encompasses over 55 km² [77]. This CAD-importable model is then pre-processed using the methods described in Section 3.3.2. The terrain model has 90 m resolution and is segmented into layers for proper calculation of the dose one meter from the ground. Figure 3.9 shows the ground zero location on the terrain model where the Nagasaki neutron isotropic point source is placed 503 m above ground zero. Overall, the Nagasaki terrain model consists of 740,000 tetrahedral mesh elements spread over four sections: two six cm thick top-most layers of water and soil and two bottom-most layers of water and soil of varying thicknesses. A six cm thickness of water and soil allow for most of the incident neutrons to be captured without appreciably attenuating the resulting delayed gamma. A one MeV neutron has a mean free path (MFP) of 1.31 cm and a one MeV gamma has a MFP of 5.88 cm in Nagasaki soil. Some of the water features of the Nagasaki terrain were not captured in the model due to the resolution of the SRTM3 data. The terrain model is sliced in the same fashion as the Hiroshima model to correctly represent the physics when viewing the dose results. Humid air is included in the model as a traditional constructive solid geometry (CSG) cell that encompasses the unstructured mesh model. Some limitations of this model are that the terrain has a resolution of 90 m and neutronic effects from the buildings is not captured in this model. The model is only mesh elements of terrain and seawater and a CSG cell for the atmosphere.

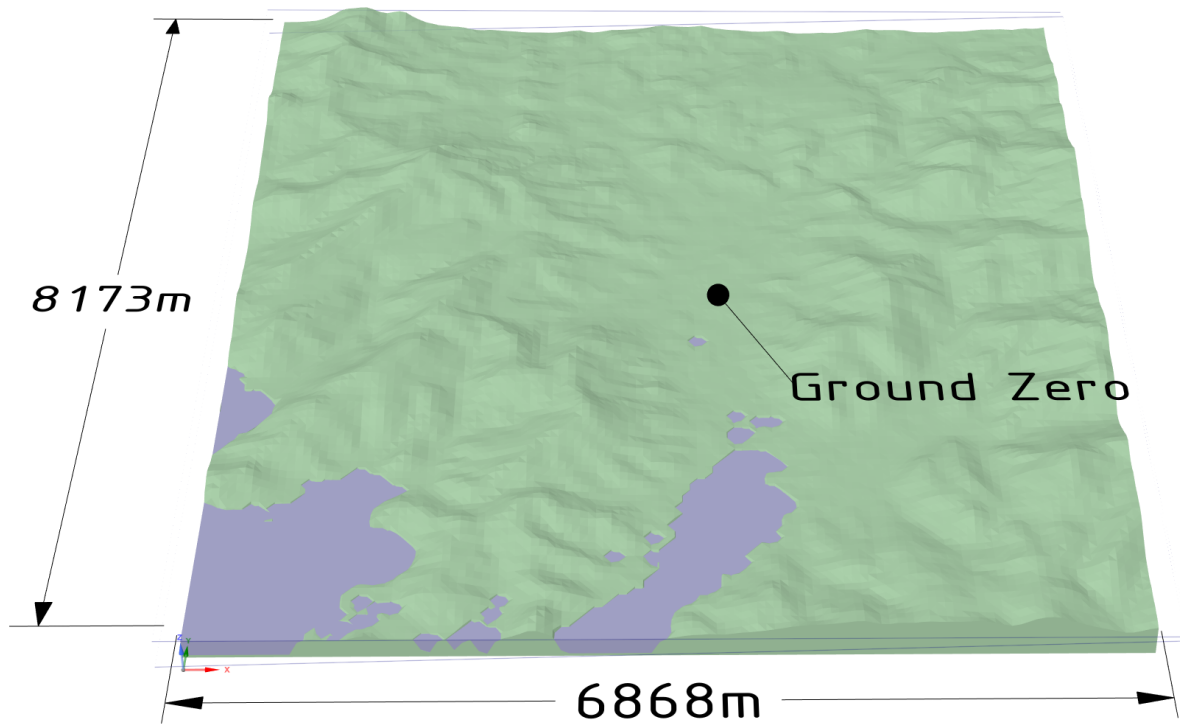


Figure 3.9: Nagasaki terrain model showing ground zero

Nagasaki Validation Study Results

Figures 3.10 & 3.11 show the results for the ACTIUM calculation (colored rings) of the residual dose rates due to the activated soil at the same times as the measurements taken by the Manhattan District Survey team and Naval Medical Research Institute Survey team, respectively (black rings). The discrepancies shown in these two figures can be attributed to a set of external factors such as wash out by over a meter of rain that accumulated between the detonation and measurement time, and debris clearing by the Japanese before, during, and after the time of the measurements were taken. A “yellow-brown rain” was observed at Nagasaki that consisted of much less fission and activation products from the weapon [146]. These “black” or “yellow-brown” rain phenomenon are not considered fallout in the classical sense. The Hiroshima and Nagasaki heights of burst were chosen to be fallout free, meaning that the upward lofting of the dust and debris do not enter the fireball as it is rising. The distance between contours of the same dose value in the ACTIUM calculation versus the

measurements for Figures 3.10 & 3.11 is less than 500 yards. Mesh elements that received fluxes $> 1\text{E-}6$ below the peak flux have relative statistical errors less than 10 percent.

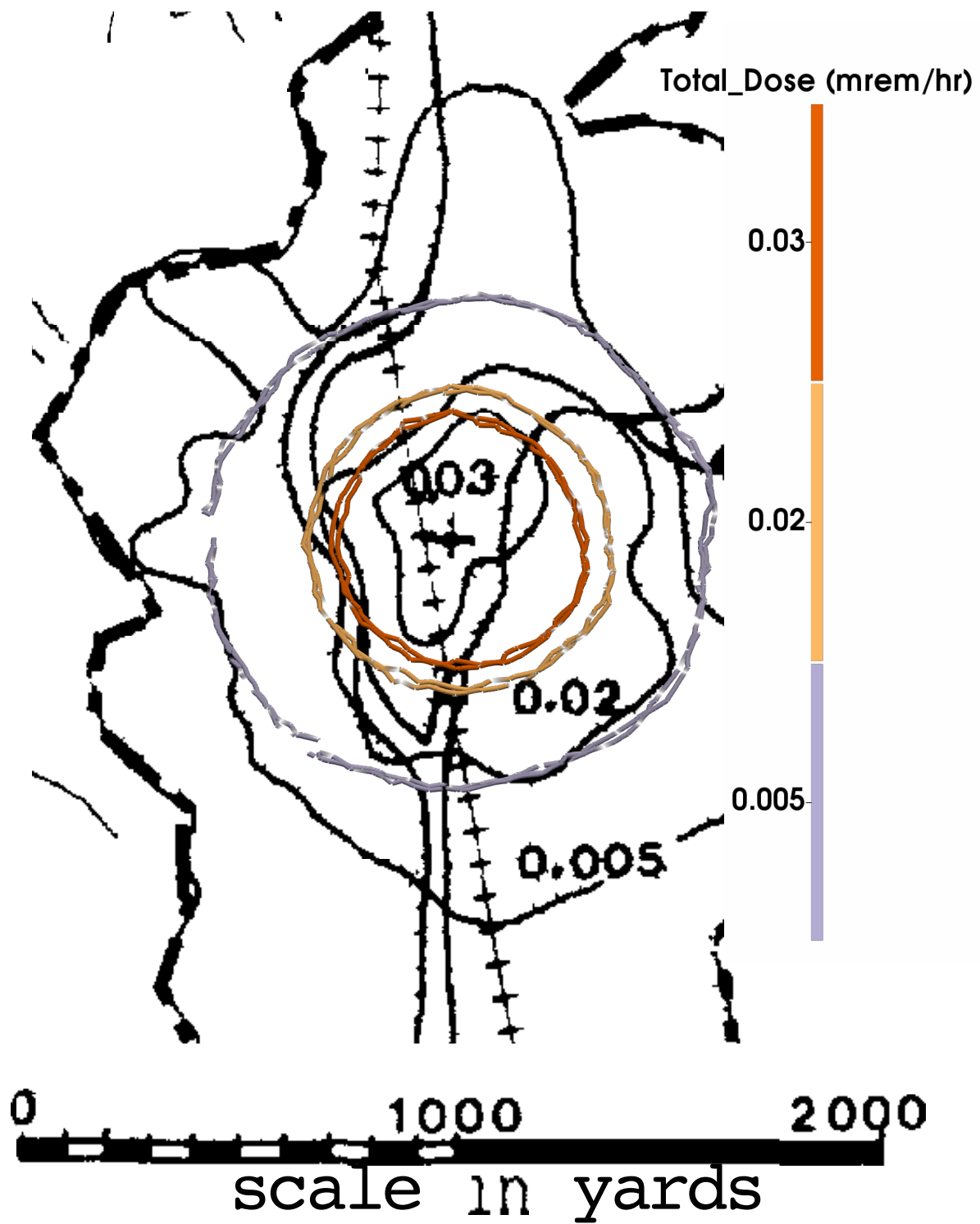


Figure 3.10: Comparison between dose rate measurements by the Manhattan District Survey (black rings) and the ACTIUM code (colored rings) 50 days after the detonation in Nagasaki.

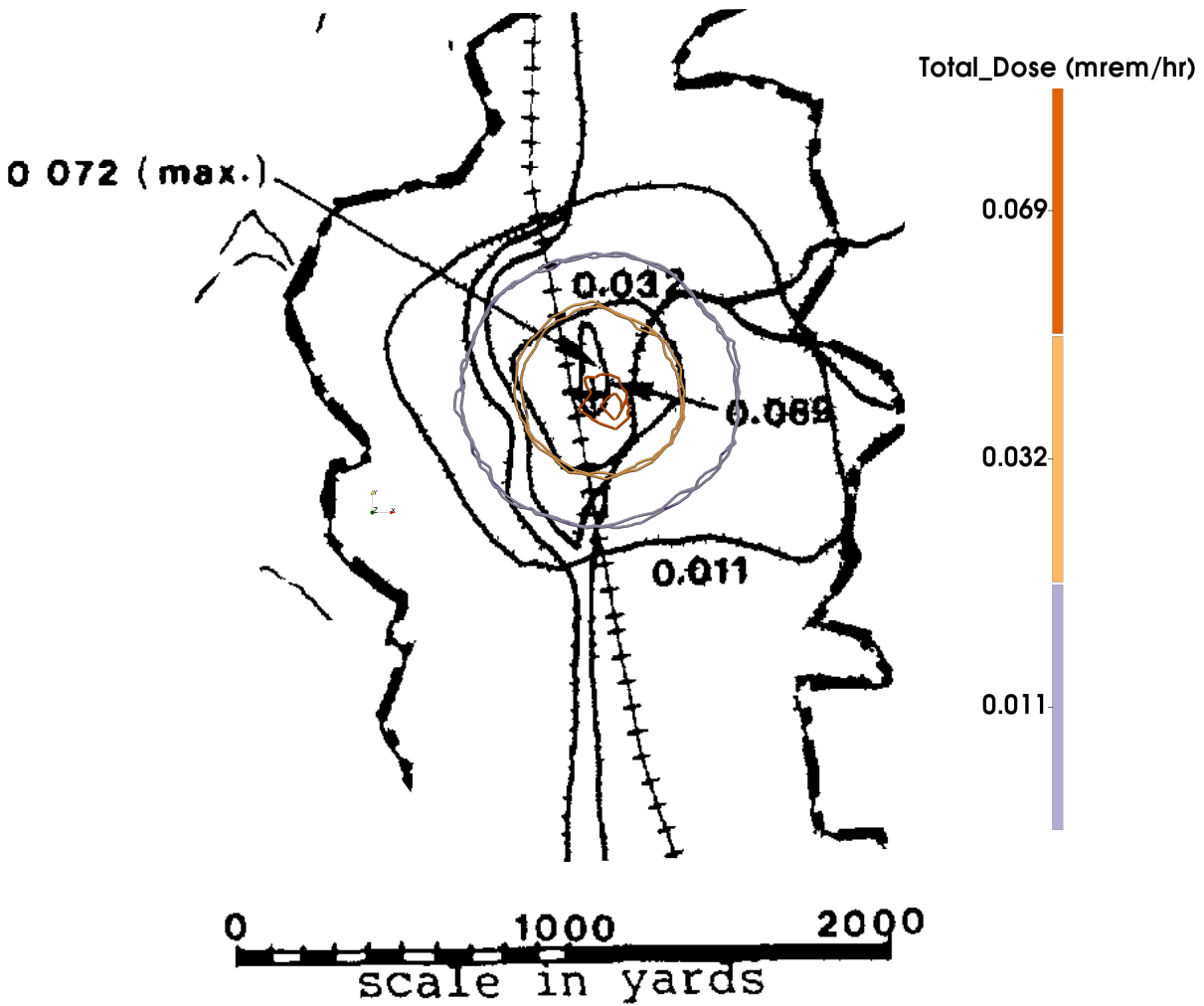


Figure 3.11: Comparison between dose rate measurements by the Naval Medical Research Institute Survey (black rings) and the ACTIUM code (colored rings) 74 days after the detonation in Nagasaki.

Table 3.5 shows the top dose contributors from the activated soil as a function of time after detonation for both Hiroshima and Nagasaki along with their parent isotope's concentration in the original soil. The parent isotope is the isotope that would undergo a (n,γ) reaction to produce the nuclide shown in the table. The percent of total dose is calculated by summing the dose contributions of the nuclide over every mesh element and dividing by the sum of the dose over all mesh elements. Some of the isotopes that make up a significant portion of the total dose are originally single PPM levels in the original soil. The results shown in Table 3.5

could be used to inform the material inputs of subsequent fire or fallout calculations where these nuclides could be lofted and transported far from their place of origin.

Table 3.5: Calculated Isotopic Contributions to Total Dose from the Soil

Nuclide	Nagasaki % Total Dose (%)	Nagasaki Parent Soil Concentration (mg per g)	Nuclide	Hiroshima % Total Dose (%)	Hiroshima Parent Soil Concentration (mg per g)	Time
⁵⁶ Mn	88.8	1.02	⁵⁶ Mn	70.1	0.47	1 hr
²⁴ Na	10.4	6.12	²⁴ Na	28.0	9.94	
³⁸ Cl	0.28	0.06	⁴² K	1.06	1.68	
⁴² K	0.15	0.39	¹⁴⁰ La	0.19	0.01	
¹⁴⁰ La	0.12	0.02	⁷² Ga	0.17	0.007	
²⁴ Na	90.8	6.12	²⁴ Na	93.7	9.94	1 day
⁵⁶ Mn	4.66	1.02	⁴² K	2.84	1.68	
¹⁴⁰ La	2.00	0.02	⁵⁶ Mn	1.41	0.47	
⁴² K	1.05	0.39	¹⁴⁰ La	1.23	0.01	
⁷² Ga	0.79	0.007	⁷² Ga	0.54	0.007	
¹⁴⁰ La	31.5	0.02	²⁴ Na	42.0	9.94	1 week
⁴⁶ Sc	25.0	0.02	¹⁴⁰ La	36.6	0.01	
²⁴ Na	21.6	6.12	⁴⁶ Sc	7.89	0.004	
⁵⁹ Fe	9.99	0.12	⁵⁹ Fe	4.56	0.04	
¹²² Sb	2.49	0.003	²³³ Pa	2.04	0.008	
⁴⁶ Sc	58.1	0.02	⁴⁶ Sc	45.6	0.004	1 month
⁵⁹ Fe	19.5	0.12	⁵⁹ Fe	22.1	0.04	
⁶⁰ Co	6.16	0.018	¹³⁴ Cs	9.02	0.004	
¹²⁴ Sb	2.71	0.002	²³³ Pa	7.77	0.008	
¹³⁴ Cs	2.03	0.003	⁶⁵ Zn	5.15	0.13	

Figure 3.12 shows the distribution of neutron-activated isotopes that are the top contributor to neutron-activated gamma dose for each mesh element. The naturally occurring radioactive isotopes have been subtracted from Figure 3.12 so that the neutron-activated isotopes would not be clouded by the mesh elements that have background levels of dose. ^{56}Mn , ^{27}Mg , and ^{88}Rb are dominant in the terrain while ^{38}Cl , ^{24}Na , ^{82}Br , and ^{80}Br are dominant in the water mesh elements. ^{27}Mg and ^{88}Rb are mostly dominant around the tops of the mountains surrounding the hypocenter. The spatial distribution of ^{27}Mg and ^{88}Rb show that depending on the relative location to the detonation location, the shape of the incident neutron energy flux spectrum may be significantly different.

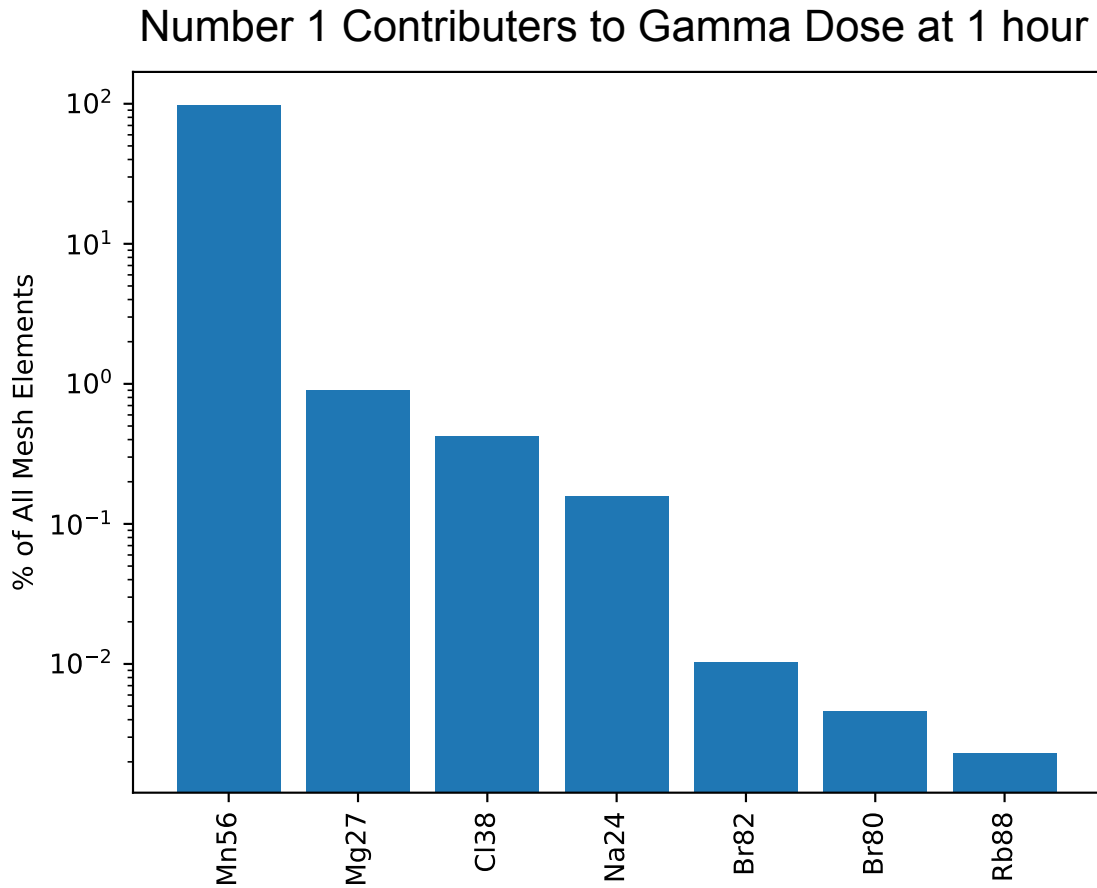


Figure 3.12: Isotopes that contribute most to gamma dose at 1 hour post-detonation

3.5 Conclusions

The ACTIUM toolkit provides a unique set of analysis tools to calculate the production and destruction of isotopes from a nuclear detonation in an unstructured mesh model of an urban environment. Validation case studies have shown that the results from the ACTIUM toolkit agree with analytical methods and measured results. Future work includes the implementation of an iterative processes whereby the newly transmuted isotopes in the unstructured mesh are used as input to a subsequent MCNP6 calculation so that an updated neutron flux may be calculated and used to further transmute the materials in the unstructured mesh.

3.6 Acknowledgements

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Chapter 4

Comparison of Isotopic Ratios for Isotopes in an Urban Post-Detonation Environment

4.1 Abstract

This chapter establishes sets of isotopic ratios that are the results of the series of calculations show sensitivities to specific aspects of the source and environmental parameters. The isotopic ratios are calculated using the neutron fluxes from MCNP6 and the CINDER2008 transmutation code that utilizes a 66-group cross section library that has cross sections for over 4000 nuclides. In the event of an urban nuclear detonation, the identification of these isotopic ratios provides insight for the radio-analytical chemistry and mass-spectrometry communities as they develop measurement techniques to analyze some of the ratios that have the highest sensitivities to source attributes. A process of how to create an unstructured mesh representation of the overall geometry of buildings along with their material compositions, and the corresponding layers of concrete and soil in an urban environment for use in neutron transport calculations, and subsequent transmutation calculations is also discussed in this chapter.

4.2 Introduction

The latest Nuclear Posture Review (NPR) enforces the need for the United States to maintain and hone advanced nuclear forensics capabilities along with the ability to readily attribute the source of the detonation to either a nation-state or terrorist group [136]. In the event of an urban nuclear detonation, there are a number of post-detonation signatures that may be measured in order to inform attribution and decision makers on how to direct first-responder efforts. One of these signatures is the change in isotopic ratios from the natural isotopic ratios in the surrounding environment because of neutron activation. These changes in isotopic ratios are common metrics used in analysis for the post-detonation nuclear forensics community [67, 79, 82, 126, 138]. For surface and sub-surface detonations, a portion of the materials that contain significant changes in isotopic ratios are incorporated into melt glass material. Much work has been done to characterize the isotopic ratio changes in the melt glass material [138, 11, 24, 36, 42, 51, 125, 172]. During a nuclear detonation, extreme temperatures are generated in the fireball as energy is released from the nuclear interactions occurring inside the device. Melt glass is formed as the fireball cools and the amalgamation of fission products, bomb debris, and environmental materials begins to fractionate and condense out of the fireball. The materials in the environment that are not consumed in the fireball still contain significant isotopic ratio changes, and the characterization of these ratios is the impetus of this chapter. This chapter focuses on characterizing the spatial, yield, and material definition effects on isotopic ratios produced in the time-frame after initial neutron irradiation and before blast or x-ray heating occur. A portion of the work presented is a literature review of the detailed elemental composition of urban materials. One of the key goals of this chapter is to establish the importance of the inclusion of electronics (e.g. computer monitors and consoles, mobile phones, television screens, etc.) in the materials used to model urban environments for weapons effects calculations. The reported isotopic ratio values in this chapter may provide insight for the mass spectrometry or radio-analytical chemistry communities to guide the chemistry as to which isotopic ratios may provide significant information about the detonated device.

The work presented in this chapter is a result of a full forward radiation transport simulation coupled with a transmutation solver where the model consists of a soil, concrete, and atmospheric layers with fully rendered buildings constructed from LIDAR data with specific building material definitions. Another impetus of this work is to observe whether or not the inclusion of electronics in the building material definitions alter the isotopic ratios in the different building, soil, and concrete materials. These isotopic ratios may have impacts on how the radio-analytical chemistry communities attribute the source of the detonation.

Previous work by Johnson et al. have demonstrated that measurements of isotopes produced in irradiated lithium-ion batteries found in an urban environment can be used to reconstruct the neutron energy spectrum at that location, when the sample is collected [74]. In order to reconstruct the source neutron spectrum in the event of an urban detonation, one would have to deconvolve the air and building scattering and building and human albedo contributions from the reconstructed incident neutron spectrum when considering reconstructing the incident neutron spectrum for a cell phone.

4.3 Methods

A sensitivity study process is detailed in following sections where Section 4.3.1 discusses the composition of the materials used in the sensitivity study, Section 4.3.2 details the neutron sources, and Section 4.3.3 describes how the results are processed into usable data. The sensitivity study characterizes the changes in isotopic ratios by varying the neutron source, yield, and height of burst (HOB) of the detonation, and investigates the spatial and time dependence of the ratios. The study presented in this chapter utilizes the ACTIUM Python Toolkit described in Chapter 3 to facilitate the calculation of the production of isotopes per mesh element by CINDER2008 due to an incident neutron flux that is calculated by MCNP6 [66, 176]. The city of Atlanta, GA is modeled by a tetrahedral unstructured mesh representation of the city. Figures 4.1 & 4.2 show an overview of the model of Atlanta, GA and a detailed view of the unstructured tetrahedral mesh representation. Figure 4.3 provides an example of the ^{147}Nd activity shortly after time of detonation initiated by a 100 KT detonation at a 6 ft HOB on the unstructured mesh representation of Atlanta, GA.

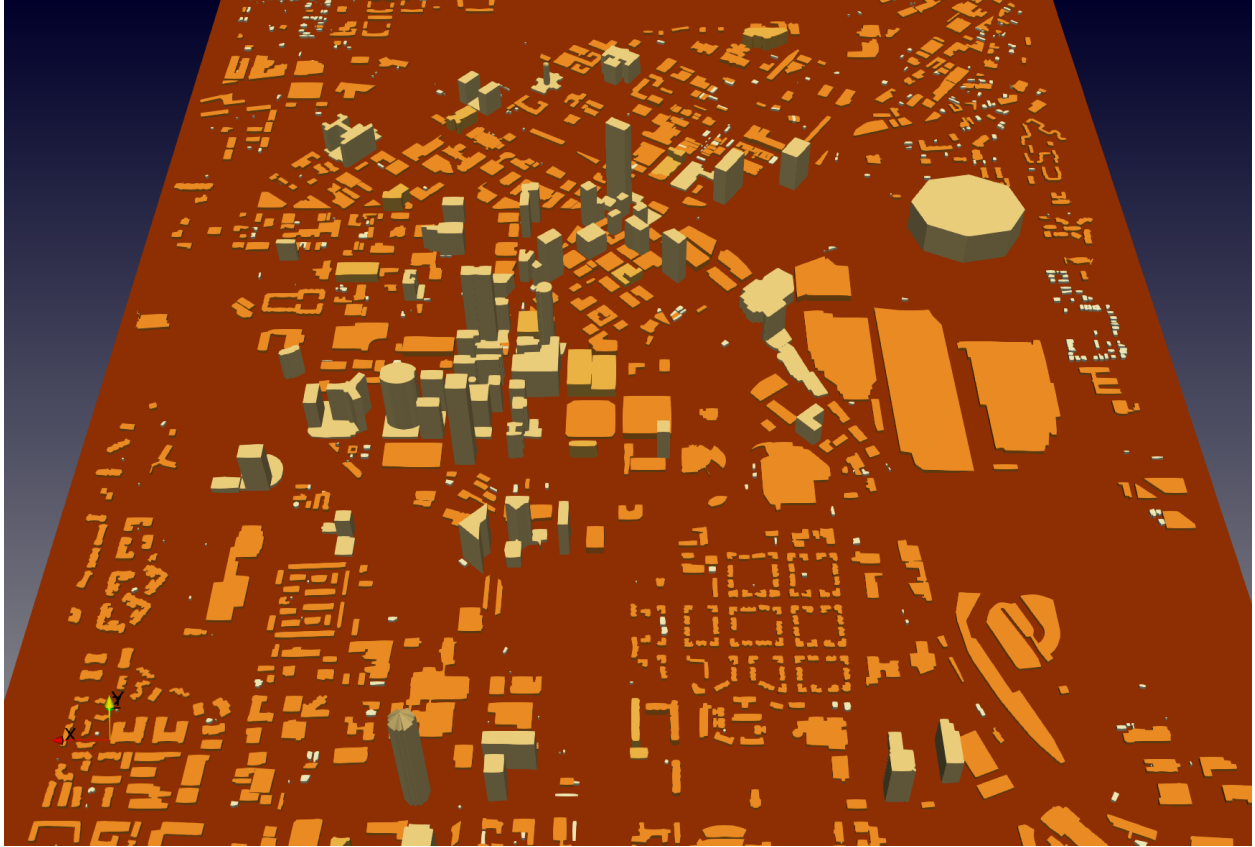


Figure 4.1: The 2.7 km x 3.5 km model of Atlanta, Ga is shown with different colors representing various building types corresponding to their material composition.

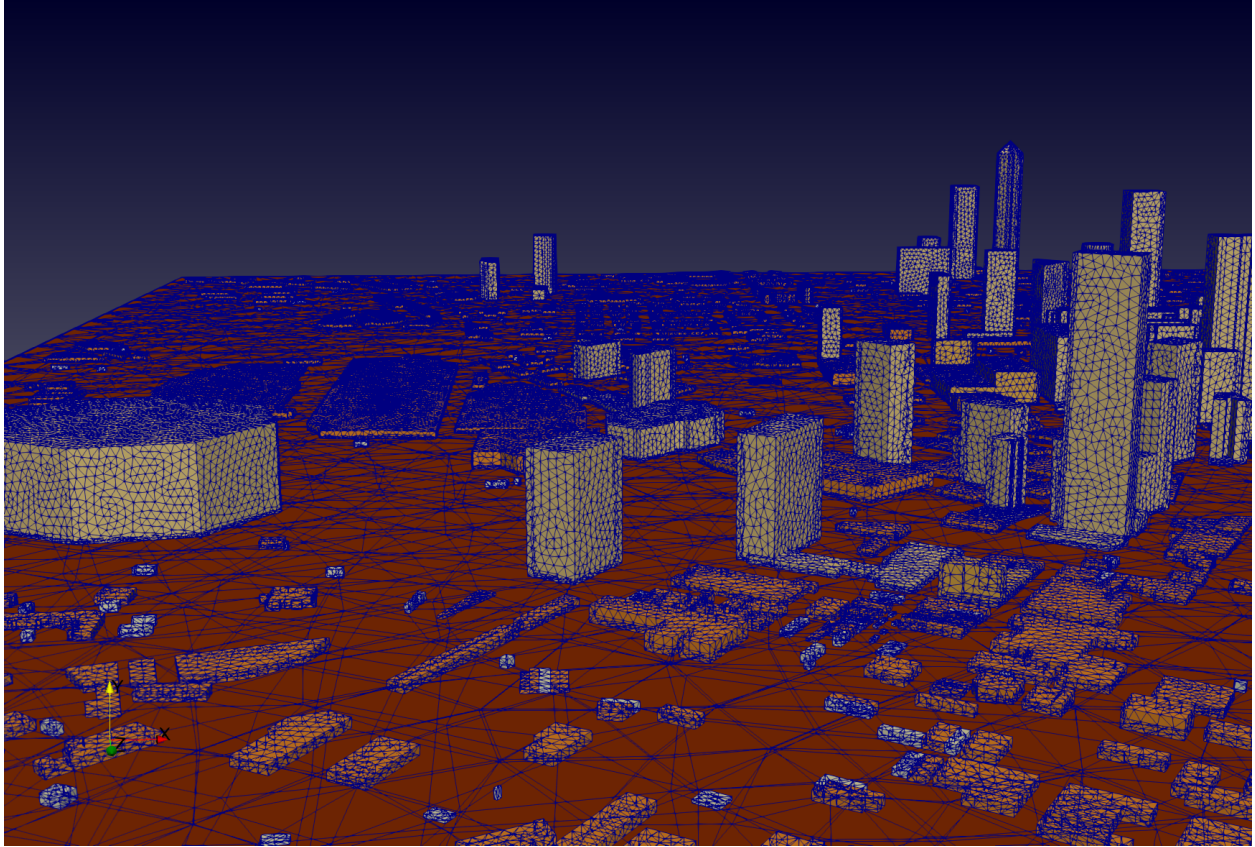


Figure 4.2: Detailed view of the mesh model of Atlanta, GA is shown with different colors representing various building types corresponding to their material composition and the blue color corresponding to the mesh outline.

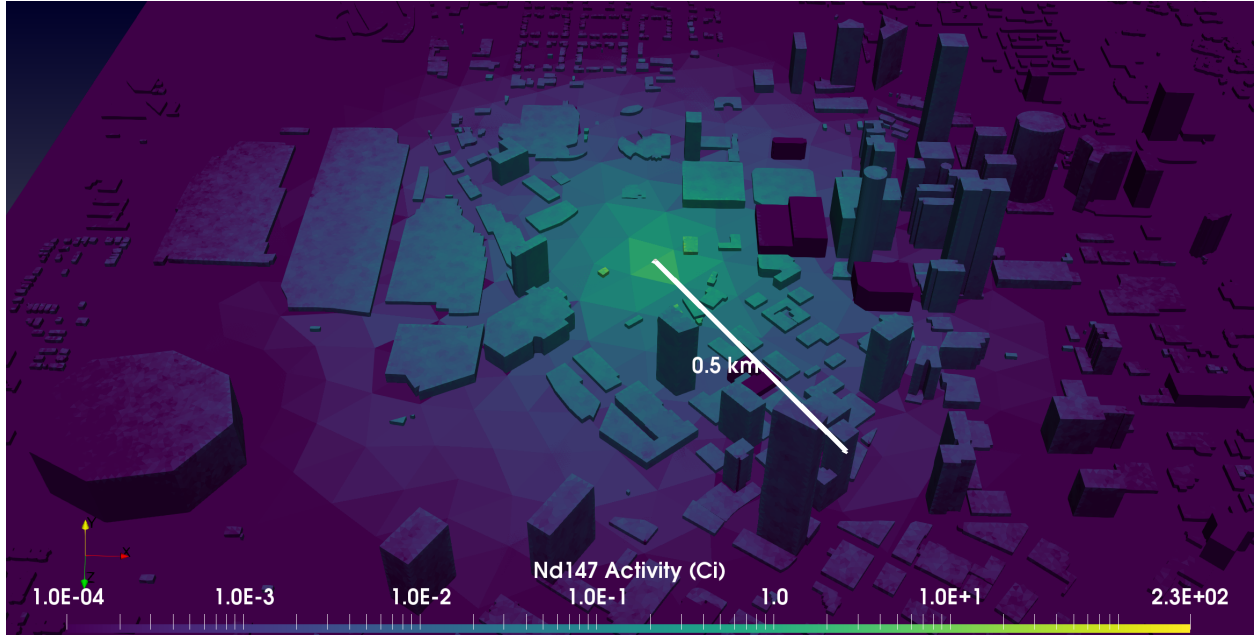


Figure 4.3: ^{147}Nd Activity shortly after time of detonation from a 100 KT detonation with a HOB of 6 ft

The unstructured mesh was generated by converting OpenStreetMap building information to a CAD-importable format, and then meshing the CAD parts with Attila4MC by following the procedure outlined in this thesis [60, 47]. The model consists of terrain, a 6 inch layer of concrete that is conformal to the terrain top-most surface, and distinct wood, brick, concrete or steel/glass buildings. There were no significant water features in the immediate vicinity of downtown Atlanta. Therefore, there is no water modeled except for the humidity included in the air. The procedure for converting LIDAR terrain elevation data to unstructured mesh is able to include water features with surface areas larger than 8100 m^2 . The mesh resolution on each part is limited by the meshing algorithm used by Attila along with memory limitations of the high-performance computing resources. The terrain was meshed to with a maximum mesh element edge-length of 100 m while the concrete layer on top of the terrain and the buildings were meshed with a max mesh element edge-length of 10 m. This unstructured mesh model was used as the geometry for subsequent MCNP6 neutron transport calculations. The air is not meshed in this process but is included as a standard cell in the MCNP geometry.

4.3.1 Materials

The material definitions used in the model are a conglomeration of the detailed composition of building stock and common urban materials. Section 4.3.1, 4.3.1 & 4.3.1, detail the literature reviews used to assimilate material databases for structural, soil, and electronic materials respectively. Section 4.3.1 discusses the Material Processing Python package as a part of the ACTIUM Python Toolkit. The Material Processing module pulls from the material composition databases to provide homogenized materials for the initial MCNP6.2 run.

Structural Building Materials

Table 4.1 tabulates a summary of the structural building and soil materials that are included in the Material Processing Python Toolkit along with a short description of the origin of the material composition.

Table 4.1: Material Processing Data Summary Table where ppm is parts per million and MA is most abundant

Name	Density (g/cm ³)	Level of Detail	Reference
Notebook Computer	1.42	ppm	Figure 2 [168] and Table 1 [137]
Lithium Ion Battery	1.73	ppm	Table 2 [127]
Hard Drive Disk	2.37	ppm	Figures 4 & 7 [168]
NdFeB Magnets	7.5	ppm	Table 2 [168]
PCB	1.85	ppm	Table 1 PCB-1 [161]
Mobile Phone	2.177	ppm	Table 4 Average [127]
LCD/LED Display	-	ppm	Table 1 [150] and Table 7 [58]
Carbon Steel	7.82	MA	[116]
Dry Air	0.001205	MA	[116]
Suburban Air	0.001205	ppm	Table 7 Average [31]
Fired Brick	2.1	MA	[116]
ppm Fired Brick	2.1	ppm	[131]
Southern Pine Wood	0.64	MA	[116]
Average Northern Wood	0.64	ppm	Table 3 Spruce [164] Table 5 Mean [119]
Spruce Wood	0.45	ppm	Tables 2 & 3 [164] & Table 1 [181]
Fir Wood	0.51	ppm	Tables 2 & 3 [164]
NIST SRM 612 Glass	2.4	ppm	[140]
Plate Glass	2.4	ppm	MA [116] and ppm [64]
Fly Ash Concrete	1.83	ppm	MF30 Table 1 [186] and Table S7 [162]
Silica Fume Concrete	2.02	ppm	MS10 Table 1 [186]
Blast Furnace Slag Concrete	1.89	ppm	MB30 Table 1 [186]

Suburban air from the average of Table 7 of Chung’s article on the elemental composition of airborne particulate matter sampled from a suburban area located outside of Seoul, South Korea [31]. In Chung’s experiment, samples were collected in air particulate filters from May

1993 to February of 1994 and analyzed using Instrumental Neutron Activation Analysis to provide the parts per million (ppm) level elemental composition.

The Average Northern Wood material is a combination of the organic elements in Table 3 of Tejada's article and the trace elements from Table 5 Mean column of Meier's article [164, 119]. Tejada performed a literature review of the trace element concentrations of wood fuels for a variety of tree species in order to provide a basis for the environmental impacts of the wood ash described later in the article. Spruce and Fir wood materials pull the organic related elements from Table 2 and the trace elements from Table 3 in Tejada's article. Rare earth element concentrations from Table 1 of Wyttenbach's article are added to the Spruce Wood material [181].

In order to evaluate a worst case scenario where all of the glass in the buildings is loaded with contaminants, NIST SRM 612 glass is available in the Material Processing Module [140]. Pearce's article provides a detailed analysis of the constituents of the NIST SRM 612 in Tables 2 & 4. The NIST SRM 612 glass included in the Material Processing Module combines the major composition from Table 2 and the trace composition from Table 4. Trace elements from Table 4 were selected for completeness of the elemental composition thereby taking the data where available for each element and averaging the concentrations if more than one are provided. Plate glass with an elemental composition at the ppm level is also available in the Material Processing Module. Plate glass defined with isotopes at the ppm level combines the major composition from the Plate Glass material in Pacific Northwest National Laboratory's (PNNL) report and the trace element composition from Hickman's paper by taking the average of the 15 samples in Table 1 [64].

Fly Ash, Silica Fume, and Blast Furnace concrete from Yilmaz's Article are available in the Material Processing Module [186]. In an effort to evaluate the gamma attenuation coefficients and fast neutron removal cross sections of concrete, Yilmaz characterizes several varieties of concrete and provides the detailed elemental composition of each evaluated sample of concrete. The composition of the concrete samples were in accordance to a number of standards.

A variety of standard building materials such as PVC, laminate, polystyrene, ceramic, sand, granite, mineral wool, etc. are also included in the structural materials portion of the database. These materials are not included in Table [4.1](#).

Soil Material

Soil data from the United States Geological Survey (USGS) Data Series 801 is included in the Material Processing Module [[157](#)]. The USGS soil composition data is a result of an extensive study by the USGS where they deployed many teams all over the conterminous United States to collect over 4000 samples of soil. The elemental composition of each sample of soil was determined by a number of analytical chemistry techniques including inductively coupled plasma-atomic emission spectrometry and inductively coupled plasma-mass spectrometry. References for the elemental composition of the generic categories of soil such as Quartz, Kaolin, Chlorite, etc. is displayed in Table [4.2](#).

Table 4.2: Material Processing Terrain Data Summary Table where all materials only include the most abundant material components

Name	Reference
Quartz	[132]
Kaolin	[128]
Chlorite	[128]
Sepiolite	[128]
Calcitep	[132]
Gibbsite	[132]
Dolomite	[152]
Aragonite	[174]
Zeolite	[178]
Gypsum	[132]
Talc	[132]
Hornblende	[6]
Serpentine	[132]
Hematite	[132]
Goethite	[132]
Pyroxene	[157]
K Feldspar	[157]
Plagioclase Feldspar	[157]
Pyrite	[157]

Electronic Materials

The weight percentages of specific components of notebook computers in Ueberschaar and Oguchi’s articles were used to identify key components of a notebook computer (e.g. hard disk, battery, etc.) and allow for proper reconstruction of a notebook computer based on the elemental composition of its components [168, 137]. Ueberschaar and Oguchi dismantled

several computers in order to create distributions of the weight percents of each major component in a computer. The average notebook computer material is a conglomeration of various tables and figures in Ueberschaar and Oguchi’s articles.

Printed circuit boards (PCB) account for an average of 13.7 wt% of the weight of a typical notebook computer. The elemental composition of a PCB is included in the Material Processing Python Toolkit from Szalatikiewicz’s article [161]. In an effort to develop new ways of recycling electric and electronic PCB, Szalatikiewicz performed a literature review and compiled a table of the elemental composition of PCBs in desktop computers, mobile phones, and other electronics. PCB-1 in Table 1 of Szalatikiewicz’s article is included in the Material Processing Python Toolkit for the composition of the PCB in the notebook computer material.

Hard disk drives make up on average 8.0 wt% of a typical notebook computer [168]. Figure 4 from Ueberschaar’s article shows the heterogeneity of disassembled hard disk drives along with Figure 7 that details the material composition of a average hard disk drive. These figures from Ueberschaar’s article are included in the Material Processing Python Toolkit to calculate the average elemental composition of a typical hard disk found in a notebook computer.

Another major component of a notebook computer is the battery. Muller’s report on the chemistry of a sampling of mobile phones provides the detailed elemental composition of an average lithium-ion battery [127]. Muller’s composition of an average lithium-ion battery is included in the notebook computer material at 14.4 wt% based on Table 1 that details the material composition of several electronics in Oguchi’s article.

Muller’s study on the chemistry of mobile phones includes how the mobile phones were prepared and analyzed with a number of methods to provide a comprehensive elemental composition of the three mobile phone samples. Table 4 in Muller’s report provides the average composition of almost 50 elements found in the mobile phone samples and this composition is included in the Material Processing Module for a typical mobile phone material. Another article details the effort by Blackberry to characterize the elemental composition of an average mobile phone by using inductively coupled plasma optical emission spectrometry to analyze 85 mobile phones from the years 1998-2013 [30]. Muller’s dataset is

included in the Material Processing Python Toolkit because it has a more complete elemental composition even though fewer samples were analyzed.

Another key piece of technology that has been incorporated into the electronics database is the liquid crystal display (LCD)/ light emitting diode (LED) display. A report by the Energy Information Agency (EIA) estimates that there are on average one or more LCD/LED displays in the workplace per worker in the United States [169]. The LCD/LED display used in the electronics database is a combination of Table 7 from Gora’s article and Table 1 from Ruiz-Mercado’s article detailing the elemental composition of a sampling of deconstructed LCD/LED displays [58, 150]. Gora’s article focuses on the characteristics of concrete after adding LCD waste to the concrete mixture as a recycling application of LCD waste. Scanning electron microscopy with energy dispersive spectroscopy (SEM/EDS) was used to measure the chemical composition shown in Table 7 of Gora’s article. Table 1 of Ruiz-Mercado’s article is a result of the characterization of an LED display to establish the mass of elements of interest in a typical LED display. This characterization is then used by Ruiz-Mercado as an example of the hypothetical recycling process proposed in the article.

Material Processing Methods

The soil composition data is linearly interpolated between the sample locations using SciPy’s `interpolate.griddata` function for the location of interest for the user [76]. The output of the terrain processing portion of the Material Processing Module is three MCNP6 material cards detailing the ppm level elemental composition of the soil for the three USGS categories of soil: Top 5 cm, A horizon (5-10 cm), and C horizon (80-100 cm). B horizon data is not provided in the USGS soil composition data. Figure 4.4 illustrates the Quartz wt % at sample locations across the United States and the sampling density that is included in the USGS soil composition data. The density of the interpolated soil composition is 1.52 g/cm^3 based on generic soil from PNNL’s report.

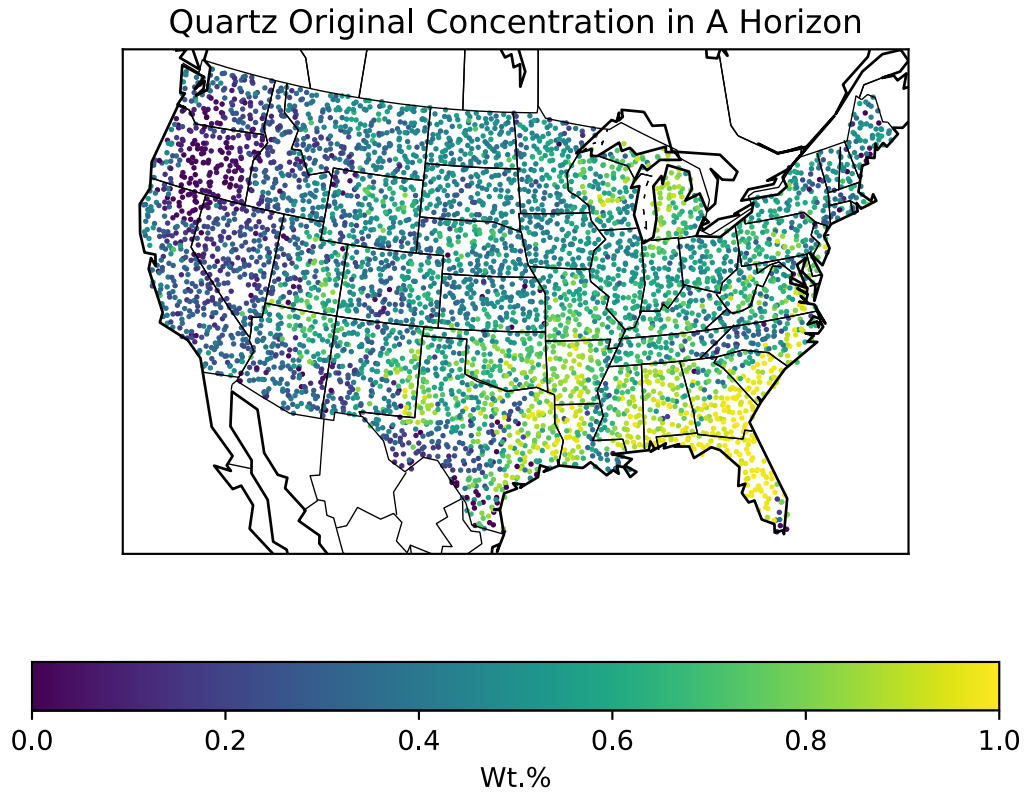


Figure 4.4: Example of the quartz concentration raw data from USGS soil composition data [157]

In order to properly represent a homogeneous building, the relative abundances of structural materials were incorporated into the Material Processing Module from Kleemann and colleagues' studies that characterize the gross composition of buildings for demolition purposes [86, 87]. Building categories from Kleemann and colleagues are applied to the city models based on building size. The building size is related to rough building type by associating the height of the building with the limits set for specific construction type by the city building code. The Python scripting interface in SpaceClaim[®] was used to characterize each building by height and overall volume by constructing a bounding box around for each building and determining the maximum height of the buildings. If the height of the building is lower than three stories, the volume of the building was considered in order to differentiate

from warehouse-type buildings and residential buildings. Characterizing the buildings by maximum height and volume is chosen over characterization by the Global Building Stock (GBS) database as apart of FEMA’s HAZUS code [2]. The GBS database is a collection of building characteristics and parameters from the Census 2010 for residential structures and Dun & Bradstreet for non-residential structures [2]. The GBS database contains percentages of building type per census block and not on a per building basis. For example, the GBS might contain information for a census block that may span a few city blocks in projected ground area, and state that 60 percent of the buildings are wood construction, 20 percent are reinforced steel concrete construction, and 20 percent are masonry construction without associating the construction type to any particular building.

The number of occupants in each type of building is based on findings from a survey by the EIA where they polled over five million buildings in the United States containing more than 88 million workers for information regarding energy consumption [169]. EIA separated the buildings into five categories corresponding to 1, 2, 3, 4 to 9, and more than 10 stories per building and these categories directly map to the categories of buildings used in SpaceClaim® to assign building materials. In each category, the survey recorded a distribution of workers per square footage of a given category so that they differentiated between warehouse-type structures with relatively large amounts of workers and smaller office buildings with fewer workers. Using the distributions of workers, the average number of workers per building type is calculated and converted to average number of workers per unit volume by dividing by the average volume of each building category based on the average height of a story in the city. For the 4 to 9 and more than 10 stories categories, the number of stories was assumed to be 6.5 and 40, respectively, based on average heights in each category. The average number of workers per unit volume is then converted to average number of cell phones, computers, or displays per person for each building category by applying the data from the EIA survey. In order get the relative density of these electronics in the building, the average mass of each type of electronic is multiplied to the number density of the electronics per building type.

The building materials used in this sensitivity study have a cutoff value for the isotopic material composition where the isotopic concentration must be above 10 parts per billion (ppb) to be included in the calculations. The cutoff value is well within the margin of error

associated with the calculations. The systematic error that goes along with estimating the composition of a building is unquantifiable when considering the exact components of a building at the time of detonation. The building composition data used in this sensitivity study stems from sources that focus on European cities, and when this study tries to apply the same building composition to an American city, the systematic error is well beyond the 10 ppb limit imposed on the material composition. I could not identify similar detailed building composition data like what is included in Kleemann’s articles for American cities.

Table 4.3 shows the isotopes that are added to the material definitions when electronics are added to the material mixture for each building type. The concentrations of all isotopes not listed in Table 4.3 do not change by more than 1 % when electronics are added to the building materials. Overall concentrations of all isotopes in the material composition decrease by less than 1 % to accommodate the inclusion of the isotopes shown in Table 4.3.

Table 4.3: Isotopes Added by Electronics Inclusion

Wood Buildings	Concrete Buildings	Steel/Glass Buildings	Brick Buildings
^{19}F	^{19}F	^{79}Br	^{19}F
^{79}Br	^{79}Br	^{81}Br	^{79}Br
^{81}Br	^{81}Br	^{116}Sn	^{81}Br
^{115}In	^{116}Sn	^{118}Sn	^{116}Sn
^{112}Sn	^{117}Sn	^{120}Sn	^{117}Sn
^{114}Sn	^{118}Sn		^{118}Sn
^{115}Sn	^{119}Sn		^{119}Sn
^{116}Sn	^{120}Sn		^{120}Sn
^{117}Sn	^{122}Sn		^{122}Sn
^{118}Sn	^{124}Sn		^{124}Sn
^{119}Sn	^{181}Ta		^{181}Ta
^{120}Sn			
^{122}Sn			
^{124}Sn			
^{141}Pr			
^{181}Ta			
^{197}Au			

4.3.2 Neutron Sources

The sensitivity study varies the neutron source spectra between four spectra ranging in overall hardness of the energy spectra from Table 8.5 in the Northrop textbook [133]. Figure 4.5 shows the neutron spectra from Figures 8.116a and 8.116b of the Glasstone textbook that are similar to the sources in Table 8.5 of Northrop [53]. The Thermonuclear Weapon spectrum has higher contributions from high energy neutrons whereas the Fission Weapon spectrum has no high energy neutron component to the spectrum. Source 3 from

the Northrop textbook is similar to the Fission Weapon spectrum whereas Sources 5, 8 & 13 are similar to the Thermonuclear Weapon spectrum. The yield is set to 100 kT and 500 kT at varying heights of burst, 6 ft, 1000 ft and 5000 ft above ground level. Ground zero location was chosen to be in the middle of a park that is surrounded by buildings in order to capture the effects of buildings and flat terrain in the same simulation.

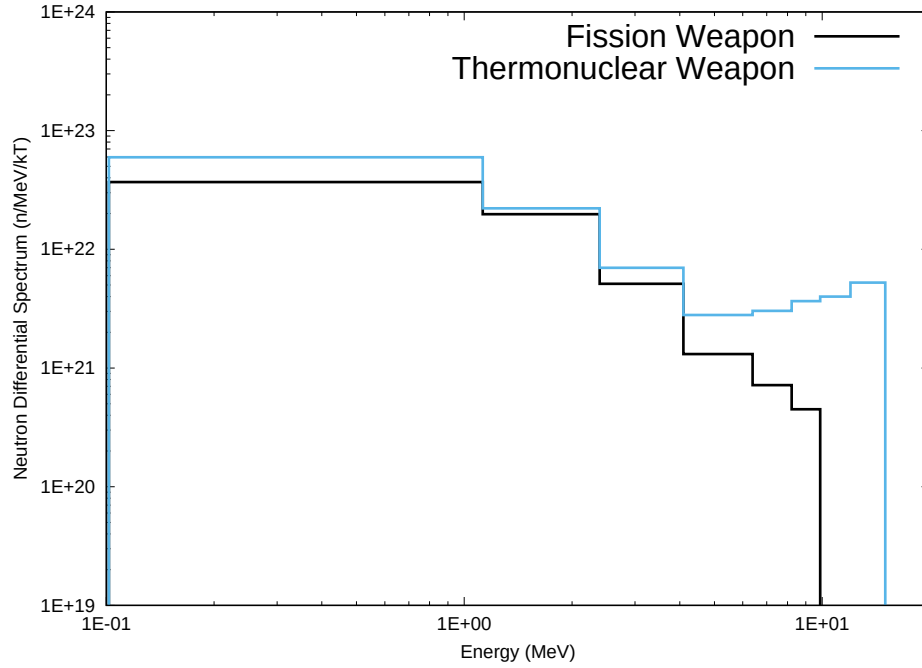


Figure 4.5: Neutron source spectra from Figures 8.116a & 8.116b [53]

4.3.3 Post-Processing of Calculations

The transmutation results from each CINDER2008 calculation including atom density, mass, activity, decay heat, etc. for each isotope on a per-mesh-element basis are stored in a HDF5 database. After the ACTIUM Python Toolkit has finished run execution, the mass data for each isotope in each mesh element is processed, and the isotopic mass ratios are stored in a 2-D matrix for each element on the periodic table. The constituents of the matrix are the

mass ratios of every isotope of an element to every other stable isotope of the same element. Only stable isotopes are stored in these matrices to lessen the time dependency on the measurement of the isotopic ratios. 2-D matrices of isotopic ratios are constructed for each scenario in the sensitivity study and these matrices are then compared between scenarios to establish ratio sensitivities to changes in the parameter space. Table 4.4 outlines the parameters and their respective value ranges.

Table 4.4: Isotopic Ratio Sensitivity Study Parameter Phase Space

Parameter	Values
Height of Burst	6, 1000, 5000 ft
Neutron Source Type	3, 5, 8, 13
Weapon Yield	100, 500 kT
Electronics Included in Building Materials	True/False
Bulk building composition types	brick, steel/glass, concrete, wood

All possible combinations of two ratios are created so that cluster analysis techniques could be used to access the most sensitive ratios to the change in parameters. Overall, more than 500,000 unique combinations of isotopic ratios are analyzed as a part of this study. For a given set of two ratios, each sensitivity study scenario is represented as a single data point in the dataset. The silhouette representation of the clusters of scenario data points provides a metric to compare sets of ratios together to determine which set of ratios is the most sensitive to the parameter change [149]. The silhouette value is calculated for each data point in the dataset and the average value for the dataset is what is used in ratio set comparisons. Equation 4.1 shows the equation for the silhouette value of a single sample where a is the average distance of all samples of an assigned cluster to the centroid of the assigned cluster, and b is the minimum distance of the sample to any other sample belonging to any other cluster that has not been assigned to the sample.

$$s = \frac{b - a}{\max(a, b)} \quad (4.1)$$

An average silhouette value of 1 is the best and means that the samples in the clusters are tightly grouped and the clusters are sufficiently separated with no overlaps between clusters. An average silhouette value of 0 signifies that there is some ambiguity as to whether the samples are properly categorized, and a value of -1 represents poorly categorized samples. Figure 4.6 shows an example plot of increasing silhouette factors from left to right where the clusters of data have greater cluster-cluster separation with decreasing overlaps between clusters, and less inner-cluster sample spreading from Lovmar's article [101]. The silhouette factors corresponding to the clustering of samples is located in the top right of each sub-figure in Figure 4.6.

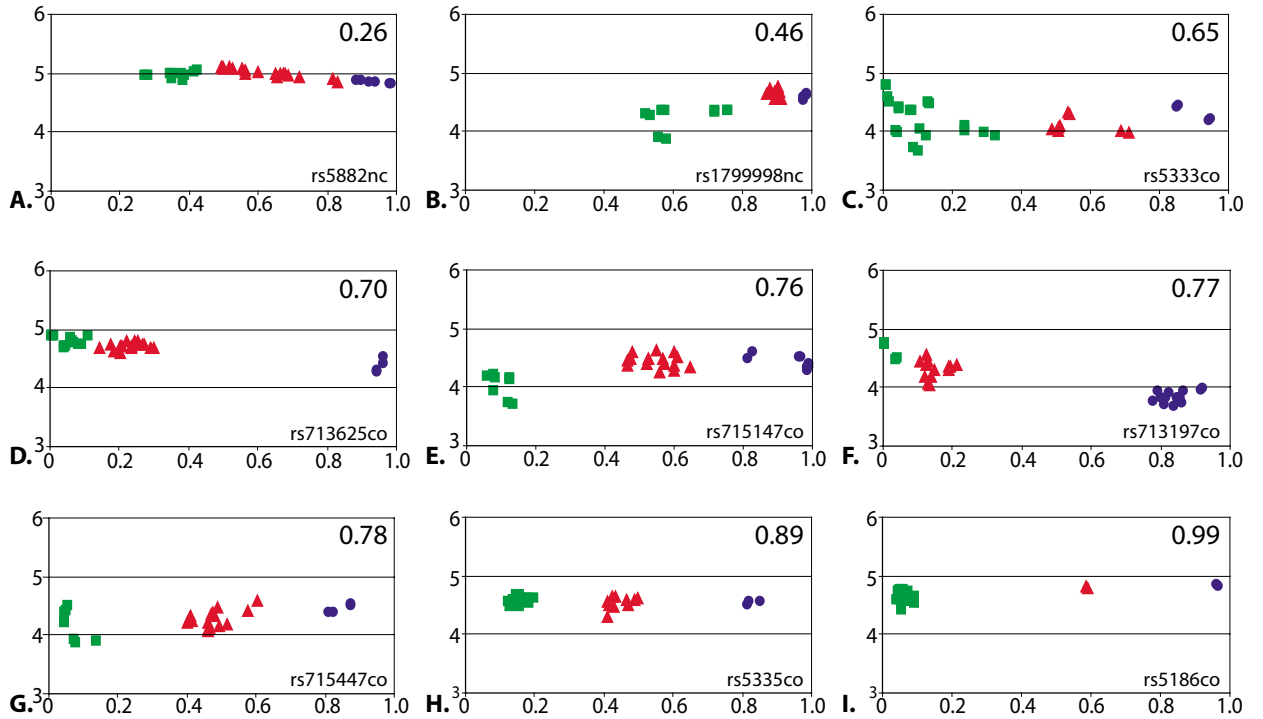


Figure 4.6: Silhouette factor examples showing increasing silhouette factors [101]

For the sensitivity study, average silhouette values of 1 indicate that there are strong groupings of scenarios when assigned specific parameter categories. The parameters used in

each scenario are known and the clustering categories that are used in the silhouette value calculation are assigned based on the specifics of the scenario. The average silhouette values are calculated with a scikit-learn’s machine learning Python package [141].

4.4 Results

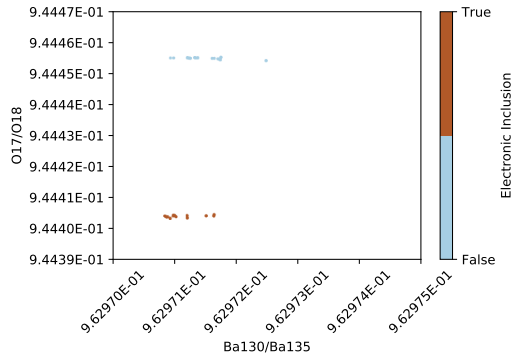
Two groups of isotopic ratios are investigated in Sections 4.4.1 & 4.4.2: building specific isotopic ratios that encompass the entire model and total isotopic ratios over all materials that could possibly be consumed by the fireball and present themselves in melt glass. The dominate source of error in Sections 4.4.1 & 4.4.2 is the statistical error inherent to the Monte Carlo methods used to calculate the incident neutron flux. For each neutron transport calculation, more than 80 % of the mesh elements that have significant flux ($> 1\text{E-}5$ of peak flux) have errors less than 10 %. The systematic error associated with the composition of buildings is negated by the use of isotopic ratios.

4.4.1 Building Specific Isotopic Ratios

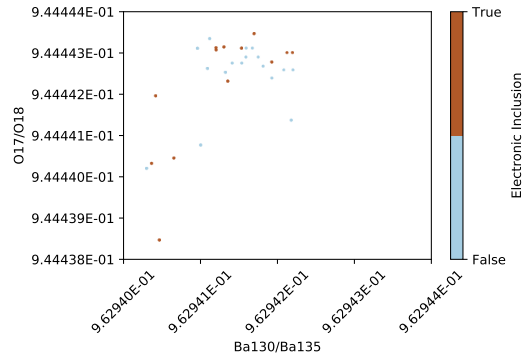
Isotopic ratios were calculated for more than 250 stable isotopes for each of the 48 scenarios evaluated for the building specific isotopic ratios sensitivity study. The sets of isotopic ratios shown in this section are selected based on their relative average silhouette values, and are filtered based on their overall spread of the data. All combinations of all stable isotopic ratios were computed, and some of the stable isotopes have radioactive parent nuclei that leads to the ratio changing over time. The ratios shown in this section are calculated at 1 day post-detonation. The sensitivities of these ratios to the parameters of interest are only valid at the 1 day time-frame due to the potential disproportional growth of one isotope over another in the ratio. The overall spread of the data for a specific set of isotopic ratios is filtered to show the sets of isotopic ratios that have a minimum spread of $1\text{E-}4$. The ratios shown in this section are fractions of the natural isotopic ratios shown in Equation 4.2 where $R_{Calculated}$ is the calculated isotopic ratio and $R_{Natural}$ is the natural isotopic ratio.

$$R_{fraction} = \frac{R_{Calculated}}{R_{Natural}} \quad (4.2)$$

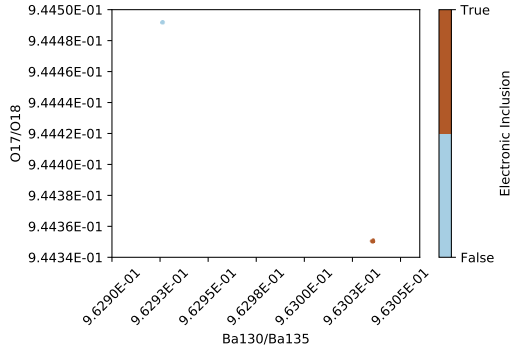
In modern cities, electronics are ubiquitous, and may influence how a neutron navigates through an urban environment. Electronics contain significant amounts of elements that have high neutron absorption cross sections compared with other common building materials. Some of the scenarios in this sensitivity study include electronics in the building materials and some do not. Figure 4.7 shows the most sensitive set of two ratios to whether or not electronics were included in the building materials based on the filtering criteria described above. An average of two computers and one LCD display per worker were included in the building materials with electronics. The clear separation in the two clusters for the brick and steel/glass buildings in Figure 4.7 shows that there are isotopic ratios that are sensitive to the changes in neutronics when electronics are introduced to the building material. However, not all building materials were sensitive to electronics being included in the building material definition. Table 4.5 shows that the best set of ratios for wood buildings when categorized by the inclusion of electronics resulted in a silhouette factor of -0.03 signifying that there is not a clear distinction between wood building with or without electronics included in the material definition, and is shown by the wood buildings ratio plot in Figure 4.7. The inconsistency in the sensitivity of a set of isotopic ratios to whether or not electronics are included in the material definition could be a result of nuclide precursors present in one material to produce a specific isotopic ratio may not be present in all building materials. These precursors may have existing significant cross sections that reside in the energy range that would be affected by the introduction of neutron absorbing nuclei in the electronics.



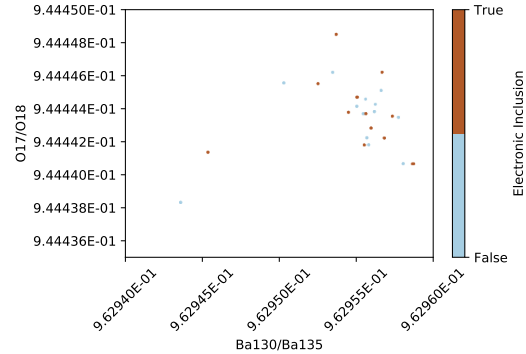
(a) Brick Buildings



(b) Concrete Buildings



(c) Steel/Glass Buildings



(d) Wood Buildings

Figure 4.7: $^{17}\text{O}/^{18}\text{O}$ vs. $^{130}\text{Ba}/^{135}\text{Ba}$ fractions of natural ratios at 1 day post-detonation clustered by electronic inclusion where each subfigure contains ratios from all 48 scenarios

Figure 4.8 shows the $^{130}\text{Xe}/^{132}\text{Xe}$ vs. $^{166}\text{Er}/^{167}\text{Er}$ ratios that are sensitive to the highest HOB for the brick buildings. The silhouette factors for sensitivity to HOB for all building types are relatively low when compared to the greater sensitivity of other ratios to other parameters of interest. When the scenarios are characterized by HOB for the wood, steel/glass concrete buildings, there are some overlaps between clusters as demonstrated in Figure 4.8. When the scenarios were characterized by yield, there were no ratios that showed clear sensitivity to the change in parameters. Yield insensitivity indicates that multiple

neutron interactions by a single nuclide are very unlikely. The sensitivities to neutron source are also not shown.

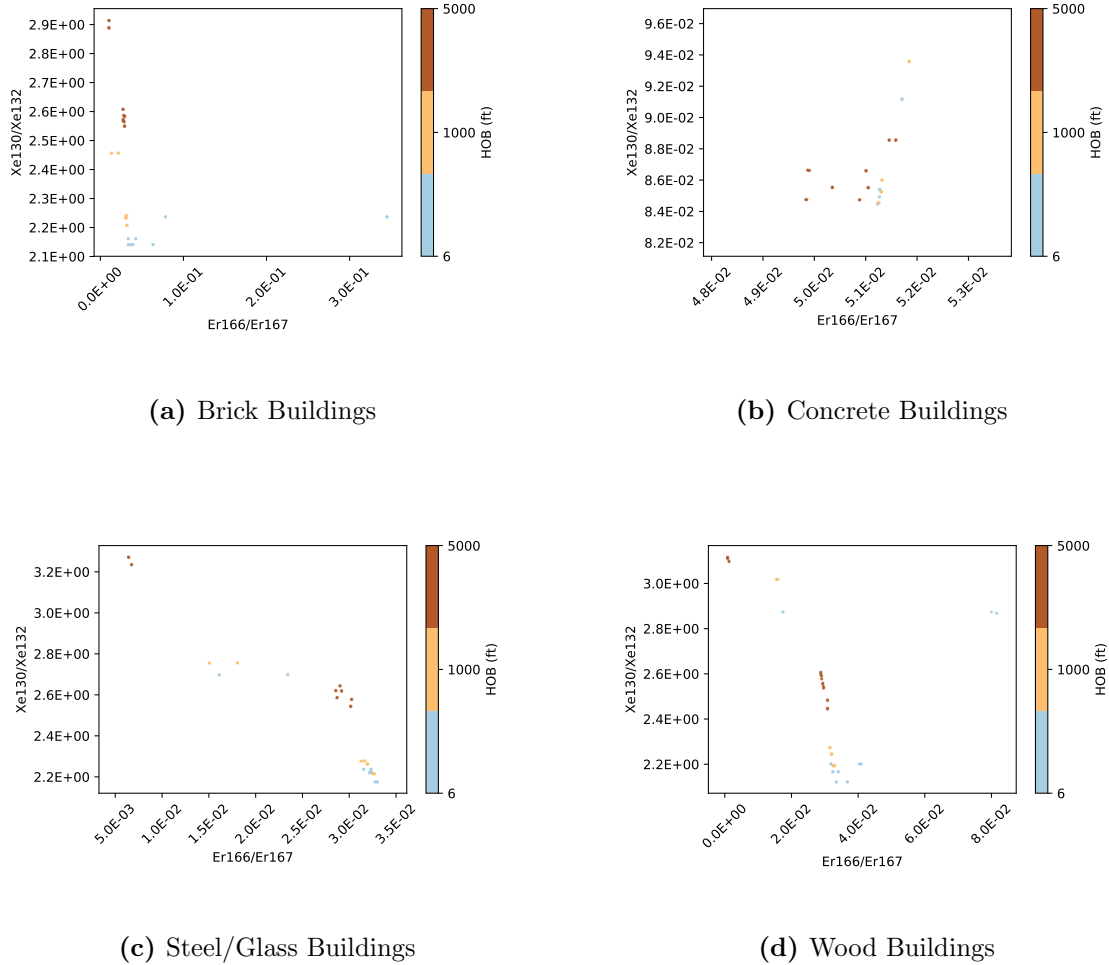


Figure 4.8: $^{130}\text{Xe}/^{132}\text{Xe}$ vs. $^{166}\text{Er}/^{167}\text{Er}$ fractions of natural ratios at 1 day post-detonation clustered by HOB where each subfigure contains ratios from all 48 scenarios

Table 4.5 provides an overview of the most sensitive isotopic ratios for each building type clustered by HOB and electronics inclusion. The sets of ratios shown in Table 4.5 were chosen from ratios of stable isotopes only for the ratios at 1 day post-detonation. The data shown in Table 4.5 has also been filtered by the overall spread of the data in the x and y space to where data that has a spread of less than $1\text{E-}4$ is not shown in the table. Isotopic

ratios that contained a zero for one or more of the scenarios were also filtered out of the ratios provided in Table 4.5. A zero recorded in the isotopic ratio for a specific scenario signifies that either the isotope in the numerator or denominator of the ratio was not produced in the material. There were sets of ratios that are more sensitive to the changes in parameters, but either did not have sufficient spread, or contained zeros in the data, and were therefore not included in Table 4.5. The average silhouette values for each combination of ratios is shown in Table 4.5 to allow for comparison between different sets of ratios. The best sets of ratios that had the highest average silhouette values when categorized by yield showed that none of the materials were sensitive to the yields evaluated in the sensitivity study, and the sets of ratios categorized by yield are not included in Table 4.5. The highest silhouette values for sets of ratios categorized by yield were mostly less than 0.06, and a silhouette factor of 0.06 indicates that there is not acceptable tightness or separability in the clusters of scenario data points. Although isotopes of Xe is a noble gasses, they are included in Table 4.5 because of the non-zero probability that they are entrained in the building material.

Table 4.5: Most Sensitive Sets of Isotopic Ratios

HOB		
Material	Ratio Set	Average Silhouette Value
Steel/Glass Buildings	$^{203}\text{Tl}/^{205}\text{Tl}$ vs. $^{130}\text{Xe}^*/^{132}\text{Xe}^*$	0.16
Brick Buildings	$^{166}\text{Er}^*/^{167}\text{Er}^*$ vs. $^{130}\text{Xe}^*/^{132}\text{Xe}^*$	0.42
Wood Buildings	$^{201}\text{Hg}/^{204}\text{Hg}$ vs. $^{104}\text{Pd}^*/^{108}\text{Pd}^*$	0.12
Concrete Buildings	$^{158}\text{Dy}^*/^{160}\text{Dy}^*$ vs. $^{101}\text{Ru}^*/^{104}\text{Ru}^*$	0.36
Electronics Inclusion		
Material	Ratio Set	Average Silhouette Value
Steel/Glass Buildings	$^{130}\text{Ba}^*/^{135}\text{Ba}^*$ vs. $^{17}\text{O}/^{18}\text{O}$	1.00
Brick Buildings	$^{174}\text{Hf}/^{180}\text{Hf}$ vs. $^{179}\text{Hf}/^{180}\text{Hf}$	1.00
Wood Buildings	$^{108}\text{Cd}^*/^{110}\text{Cd}^*$ vs. $^{167}\text{Er}^*/^{170}\text{Er}^*$	-0.03
Concrete Buildings	$^{142}\text{Nd}^*/^{145}\text{Nd}^*$ vs. $^{122}\text{Te}^*/^{124}\text{Te}^*$	0.0

* indicates fission product

Table 4.6 shows the most sensitive ratios that are not noble gases for measurement techniques that do not allow for noble gas measurements. The silhouette factor for HOB-clustered Steel/Glass buildings does not change but the silhouette factor for HOB-clustered Brick buildings decreases by a factor of two. Scenarios clustered by Electronic Inclusion are unaffected by noble gases and do not change between Table 4.5 and Table 4.6. Brick and wood buildings silhouette factors both decrease when noble gases are omitted from the table. A decrease in silhouette factor signifies that there is less sensitivity to the parameter of interest.

Table 4.6: Most Sensitive Sets of Isotopic Ratios with No Noble Gasses

HOB		
Material	Ratio Set	Average Silhouette Value
Steel/Glass Buildings	$^{72}\text{Ge}^*/^{73}\text{Ge}^*$ vs. $^{203}\text{Tl}/^{205}\text{Tl}$	0.16
Brick Buildings	$^{201}\text{Hg}/^{204}\text{Hg}$ vs. $^{104}\text{Pd}^*/^{110}\text{Pd}^*$	0.19
Wood Buildings	$^{201}\text{Hg}/^{204}\text{Hg}$ vs. $^{104}\text{Pd}^*/^{108}\text{Pd}^*$	0.12
Concrete Buildings	$^{158}\text{Dy}^*/^{160}\text{Dy}^*$ vs. $^{101}\text{Ru}^*/^{104}\text{Ru}^*$	0.36
Electronics Inclusion		
Material	Ratio Set	Average Silhouette Value
Steel/Glass Buildings	$^{130}\text{Ba}^*/^{135}\text{Ba}^*$ vs. $^{17}\text{O}/^{18}\text{O}$	1.00
Brick Buildings	$^{174}\text{Hf}/^{180}\text{Hf}$ vs. $^{179}\text{Hf}/^{180}\text{Hf}$	1.00
Wood Buildings	$^{108}\text{Cd}^*/^{110}\text{Cd}^*$ vs. $^{167}\text{Er}^*/^{170}\text{Er}^*$	-0.03
Concrete Buildings	$^{142}\text{Nd}^*/^{145}\text{Nd}^*$ vs. $^{122}\text{Te}^*/^{124}\text{Te}^*$	0.0

* indicates fission product

4.4.2 Total Isotopic Ratios Near Hypocenter

In order to calculate the isotopic ratios that may be observed in melt glass, mesh elements from all material types are selected based on the distance between the centroid of the mesh element and detonation location. For this specific study, the six feet HOB is the only HOB

analyzed for melt glass related isotopic ratios resulting in 16 scenarios considered. Assuming that all mesh elements within the radius of the fireball or within the radius of the crater are vaporized and their isotopes may be found in melt glass, the radii for fireball radius and crater radius are calculated using Equations 4.3 & 4.4 corresponding to Glasstone's equation 2.127.2 for the fireball radius at breakaway for a contact surface burst and in section 6.72 for the radius of a crater in wet hard rock [53]. The W in Equations 4.3 & 4.4 is the weapon yield in units of kiloton equivalent of TNT, and the resulting radius is in units of feet. Equation 4.4 is used as the radius of inclusion for the concrete and soil layers located directly below the detonation location, and Equation 4.3 is used for the radius of inclusion for all of the buildings in the proximity of the detonation. Table 4.7 shows the radii of inclusion for all weapon yields.

$$R_{\text{fireball}} = 145W^{0.4} \quad (4.3)$$

$$R_{\text{crater}} = 58W^{0.3} \quad (4.4)$$

Table 4.7: Radii of Inclusion

Yield (KT)	Fireball Radius (ft)	Crater Radius (ft)
100	915.9	230.9
500	1742	374.2

The masses of each stable isotope for all mesh elements located in the radius of inclusion are summed and used to calculate the ratios discussed in this section. The sets of isotopic ratios shown in this section are the most sensitive isotopic ratios after all of the sets of isotopic ratios have been filtered for ratios that are constant over time, have a overall spread of greater than 1E-4, each scenario produced a non-zero value, and the set of isotopic ratios had no duplicate isotopes. Once filtered, the sets of isotopic ratios were ordered by their

average silhouette values and the sets of isotopic ratios shown below correspond with the highest silhouette values. Figure 4.9 shows the set of isotopic ratios that have the highest sensitivity to electronics inclusion. All of these isotopic ratios have the potential to influence the ratios observed in melt glass. Table 4.8 shows the average silhouette factor for the isotopic ratios shown in Figure & 4.9. These silhouette factors signify strong inner-cluster grouping and minimal overlaps between clusters.

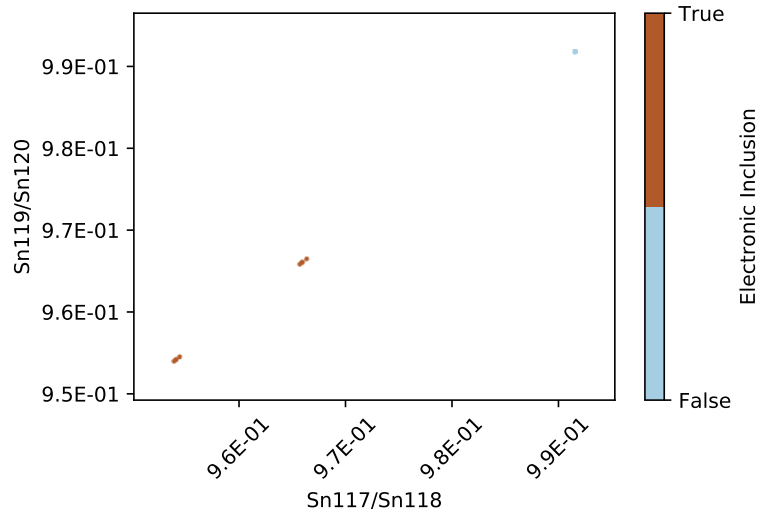


Figure 4.9: $^{117}\text{Sn}/^{118}\text{Sn}$ vs. $^{118}\text{Sn}/^{119}\text{Sn}$ fractions of natural isotopic ratios clustered by electronic inclusion for 16 scenarios

Table 4.8: Most Sensitive Sets of Isotopic Ratios

Parameter	Ratio Set	Average Silhouette Value
Electronics Inclusion	$^{117}\text{Sn}/^{118}\text{Sn}$ vs. $^{118}\text{Sn}/^{119}\text{Sn}$	0.89

4.5 Conclusions

An overview of how to model the buildings of an urban environment has been demonstrated on the city of Atlanta, GA complete with details on how to account for the composition of the structural composition of the building and the electronics that has been shown to significantly affect the neutronics in an urban environment. The isotopic ratios shown in this work are examples of ratios that proved to be some of the most sensitive stable isotopic ratios to HOB and electronics inclusion. The complete spatial distribution of stable and radioisotopes can be incorporated into other fire or atmospheric modeling codes to better understand dose distributions after the irradiated materials have been lofted into the atmosphere due to fires and/or rubblization. The results from evaluating the sensitivities of isotopes produced from an urban nuclear detonation may be used to inform first-responder triage efforts by suggesting which type of building to sample based on the answers regarding attribution. The most sensitive isotopic ratios may also be used to guide radio-analytical chemistry or mass spectrometry communities as they develop new measurement techniques.

Chapter 5

Study of Production of Radionuclides in Polluted Air

A version of this chapter has been submitted as a contributed summary to the 21st Topical Meeting of the Radiation Protection and Shielding Division of the American Nuclear Society by Tucker McClanahan.

5.1 Abstract

This study estimates the contribution to overall effective dose from the activated radionuclides in polluted air in the event of an urban nuclear detonation. Shortly after an urban nuclear detonation, decision makers need to know how to prepare first responders for what dose levels to expect and what types of contamination they may encounter. Characterizing the effective dose contribution from neutron-activated polluted air to the first responder is of great importance. The radionuclides discussed in this work are calculated using the ACTIUM Python Toolkit methodology that stitches together MCNP6's unstructured mesh neutron transport capability with CINDER2008's transmutation solver to provide isotopic inventories for each mesh element in the model. This study indicates that pollution has marginal effects on overall effective dose where the largest differences between polluted and non-polluted air occur around 3 days after detonation. At 3 days post-detonation, the

activated species in the air are sufficiently diffuse and the overall dose from the air is near terrestrial background dose levels.

5.2 Introduction

Air pollution has become a major topic of interest as shown by the amount of scientific literature and federal research that focuses on the health effects of exposure and how to mitigate the issues [25, 33, 83, 143, 44, 45, 46, 182]. Prolonged exposure to polluted-air has been linked to cardiovascular and respiratory disease, cancer, pregnancy complication, adverse birth outcomes, impairment of brain development, and childhood asthma development [143, 182, 83, 25, 33]. In an effort to characterize the polluted-air constituents, many studies have measured the gaseous and particulate matter components at various pollution concentrations for several cities around the world [5, 71, 154, 112, 16, 17, 183, 173, 37]. This study focuses on Houston, TX. Using the detailed pollution composition in Houston, TX, this study characterizes the effects on effective dose from the activated radionuclides in the polluted air as compared with non-polluted air because of an urban nuclear detonation [17].

The city of Houston, TX has received much attention due to the urban/industrial nature of the city with a sprawling urban area projected to be home to more than 2 million people, and the U.S.'s second largest shipping port [135, 20]. In the Houston area, gasoline engines are the top contributor of organic carbon (OC) emissions making up 40 percent of the OC emissions with diesel engines contributing 10 percent of OC emissions [5]. The sum contributions from diesel engines, gasoline engines, and ship emissions contribute 41 percent of the organic aerosol (OA) (mixture of sulfate, ammonium, nitrate, and chloride) emissions in the Houston area [5]. Particulate matter (PM) in the Houston area has been measured with mass spectrometry to elemental quantities of 1 ppm [17]. For this study, the composition of polluted air in Houston, TX is a conglomeration of measurements of the various aspects of polluted air: PM composition, OC, and OA composition [5, 16, 17, 37, 183]. Using the detailed composition of polluted air in Houston, TX, this study characterizes the effects on dose from the activated radionuclides in the polluted air as compared with non-polluted air due to an urban detonation.

Air pollution has been shown to affect the optical and thermal properties of the air [71, 13]. While these effects on the optical and thermal properties of the air will almost certainly affect the prompt optical flash and thermal fluence propagation through the atmosphere from the nuclear detonation, the neutron transport through the atmosphere will be largely unperturbed because of the very low concentrations of elements added by the presence of air pollution, and the relatively large distance between neutron interactions in the air. Even though the particle transport will be largely unperturbed, this work illuminates the activated radionuclides in the event of an urban detonation that are added to the air from the inclusion of pollution. The results in this work do not account for fission products and assumes that the air is static for the duration of the calculation or affected by wind currents which we assume is small compared to the time frame of activation. In reality, the activated air will have been either engulfed by the fireball, swept up into the radioactive plume and be entrained in fallout, or have been dispersed into the atmosphere by the blast wave. This work isolates and characterizes the contribution from the activated species in the polluted air from an urban nuclear detonation to the effective dose to people, and provides a potential starting activated material composition for inclusion in fallout and plume modeling codes.

5.3 Methods

A study of the radionuclides produced in polluted and non-polluted air is described in the following sections where Section 5.3.1 discusses the model geometry and the parameters of the unstructured mesh, Section 5.3.2 details the neutron sources, Section 5.3.3 discusses the material compositions used in the study, and Section 5.3.4 includes the details of how the results in Section 5.4 are calculated and post-processed.

5.3.1 Geometry

The geometry used in this study is composed of five layers of atmosphere of varying thicknesses, a thin layer of terrain and seawater, and a neutronically thick layer of terrain and seawater that spans 2 km by 2 km by 3.6 km (WxDxH). Figure 5.1 shows the atmospheric model used in this study. The thicknesses of the layers of atmosphere correspond the height of

the atmospheric boundary layer [71]. The atmospheric boundary layer and the concentration of pollution in the atmosphere have an inverse relationship. In this study, when the pollution level is ‘Severe’, only the bottom atmospheric layer has pollution in the material definition and all other layers above the severe layer are typical Houston Air with the appropriate densities per layer. The severe layer of atmosphere extends from ground surface to 460 m. Table 5.1 shows the altitude ranges of the pollution layers.

Table 5.1: Altitude Ranges of Polluted Atmospheric Layers [71]

Pollution Layer	Altitude Range (m)
Severe	0 - 460
Moderate	460 - 535
Mild	535 - 685
Slight	685 - 900

The model is meshed with hexahedral mesh elements where the pollution layers are meshed with 30-m maximum edge-lengths, air above the pollution with 250-m maximum edge-lengths, and the thick soil layer with 100-m maximum edge-lengths. The 2-m thick soil layer and air above the pollution are included in the model so that scatter contributions from these layers is captured by particle transport, and results tallied in these coarsely meshed regions are not used in the analysis of this study. The pollution layers are meshed to 30-m resolution for minimal flux drop across the mesh element while not creating so many mesh elements that the problem overruns the memory of the computer. At 30-m resolution, 70 % of the neutron flux is unattenuated through the mesh element because of the mean free path of a 1.3 MeV neutron is 70 m in air. The 30 % drop in flux across any given mesh element satisfies the assumption that the flux is constant across the volume.

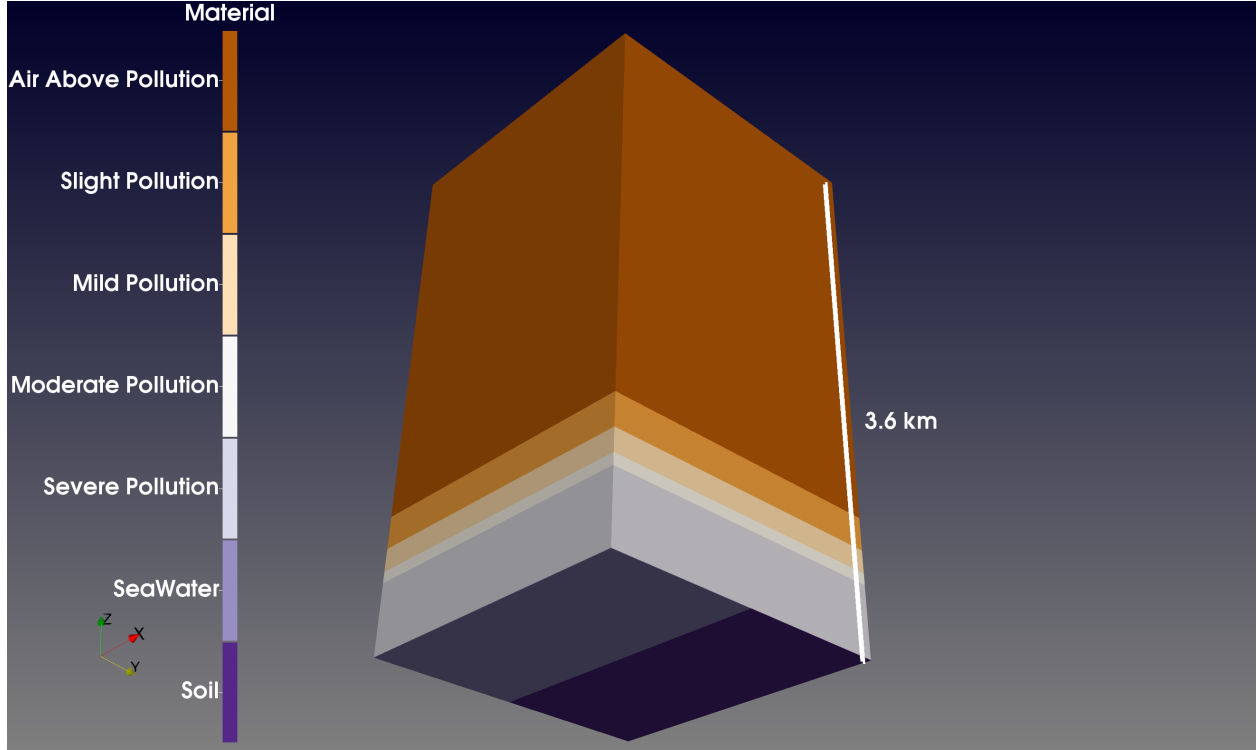


Figure 5.1: Overview of atmospheric model (2-km x 2-km x 3.6-km)

5.3.2 Neutron Sources

In order to capture the effects of neutron sources with and without high energy neutrons, the neutron sources used in this study are from Table 8.5 in the Northrop textbook [133]. Figure 5.2 shows the neutron spectra from Figures 8.116a and 8.116b of the Glasstone textbook that are similar to the sources in Table 8.5 of Northrop [53]. The Thermonuclear Weapon spectrum has higher contributions from high energy neutrons whereas the Fission Weapon spectrum has no high energy neutron component to the spectrum. Source 3 from the Northrop textbook is similar to the Fission Weapon spectrum whereas Sources 5 & 8 are similar to the Thermonuclear Weapon spectrum. The yield for all neutron source spectra is set to an arbitrary value of 100 kT, and the source location is located in the center of the ground and seawater interface where the top of the land and seawater interface is considered the origin of the model. The height-of-burst (HOB) is either 6-ft or 1000-ft in order to

evaluate the effects of a source near the ground close to the height of a human and the effects of a source height that is outside of the pollution layer in the model.

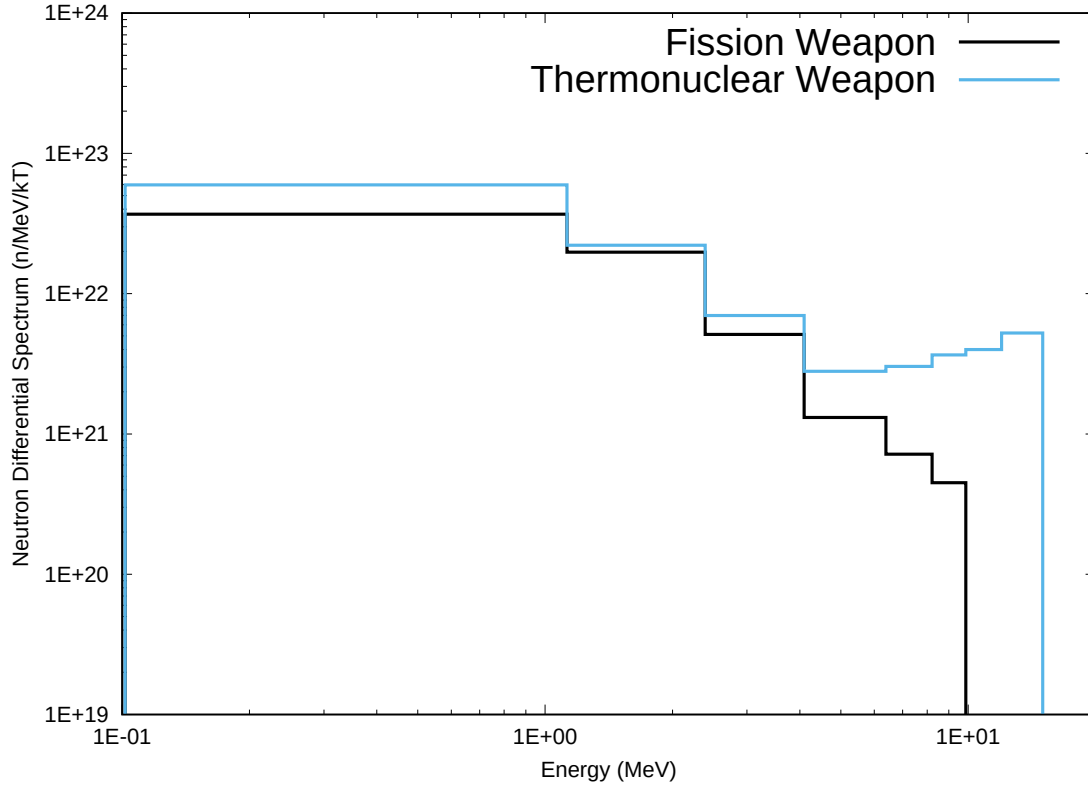


Figure 5.2: Neutron source spectra from Figures 8.116a & 8.116b [53]

5.3.3 Material Compositions

Detailed material compositions are imperative to determining the effects of pollution and seawater in the event of a detonation on a coastal urban environment.

Polluted Air

The literature categorizes PM into particulate with diameter less than $2.5 \mu\text{m}$ ($\text{PM}_{2.5}$) and diameter less than $10 \mu\text{m}$ (PM_{10}). This study only includes the $\text{PM}_{2.5}$ due to the data

available in the literature. The composition of PM_{2.5} used in this study is shown in Table 5.2, and is a combination of compositions from literature.

Table 5.2: PM_{2.5} Composition [5, 17, 37]

Component	Concentration (mg per g)	Element	Concentration (mg per g)	Element	Concentration (mg per g)
NH ₄	3.04E+01	Ni	2.87E-01	La	6.98E-02
CH ₄	2.44E+02	Co	2.14E-02	Ce	1.17E-01
Cl	2.57E+01	Cu	5.80E+00	Pr	6.50E-03
NO	2.34E+01	Zn	3.99E+00	Nd	1.96E-02
SO ₄	1.68E+02	Ga	5.97E-01	Sm	5.96E-03
C	2.95E+01	As	2.68E-01	Eu	2.75E-03
Na	4.32E+01	Se	3.55E-02	Gd	4.15E-03
Li	2.61E-02	Rb	3.74E-02	Tb	4.72E-04
Be	1.33E-03	Sr	5.95E-01	Dy	2.37E-03
Mg	7.93E+00	Y	2.03E-02	Ho	4.08E-04
Al	2.40E+01	Zr	2.27E+00	Er	1.28E-03
Si	1.07E+02	Mo	2.45E-01	Yb	1.31E-03
K	1.05E+01	Rh	7.22E-04	Lu	2.33E-04
Ca	1.63E+02	Pd	4.36E-03	W	1.20E+03
Ti	4.87E+00	Cd	3.40E-02	Pt	1.31E-03
V	3.42E-01	Sn	1.17E+00	Pb	3.03E-01
Cr	3.15E-01	Sb	9.90E-01	Th	2.40E-03
Mn	1.24E+00	Cs	2.06E-03	U	1.44E-03
Fe	1.02E+02	Ba	1.16E+01		

The elemental composition of PM_{2.5} is from Figure 1 of Bozlaker et al.'s article where they collected samples of PM_{2.5} from the Washburn tunnel in Houston, TX, and characterized the elemental composition of PM_{2.5} with an DRC-q-ICP-MS [17]. The composition of the

OA component of $\text{PM}_{2.5}$ is from Al-Naiema et al's article where the composition of the OA is measured with a HR-ToF-AMS [5]. Al-Naiema's article indicates that gasoline engine emissions is the dominant contributor to $\text{PM}_{2.5}$ concentrations in Houston, TX, and that is why this study includes the $\text{PM}_{2.5}$ composition from the Washburn Tunnel where 20,000 vehicles pass through the tunnel daily [17, 5]. Danadurai et al. provide an estimate for the sodium concentration in the particulate matter [37]. Bromine and iodine were not included in the composition of polluted air due to relatively low concentrations of at most 0.1 ng/g [183].

The composition of $\text{PM}_{2.5}$ is incorporated into the Dry Air material at various overall $\text{PM}_{2.5}$ concentration levels as described in Table 5.3 [116]. The concentration of pollution is assumed to be constant from the surface of the terrain to the height of the atmospheric boundary layer. The concentration of $\text{PM}_{2.5}$ is added to average Houston air with 75 % humidity at 80° F and 769 mmHg. A concentration cutoff limit of 0.1 ng/g is applied to the material definition used in the sensitivity study. Once the elemental concentrations have been converted to isotopic concentrations using ENDF/B-VII.1 isotopic abundances, any isotopic concentration below the concentration cutoff limit is not included in the MCNP material definition [26].

Table 5.3: $\text{PM}_{2.5}$ Concentration in Various Levels of Polluted Air [71]

Pollution Level	Concentration ($\mu\text{g m}^{-3}$)	Atmospheric Boundary Layer Height (m)
Slight	60	900
Mild	105	685
Moderate	225	535
Severe	375	460

Seawater and Soil Compositions

The composition of the seawater used in this sensitivity study is from Table 6.1 of Wright’s chapter on seawater solution, and includes 92 elements that are naturally occurring in seawater[179]. A concentration cutoff limit of 0.1 ng/g is applied in the same manner as described in Section 5.3.3. The composition of soil for the Houston, TX area is calculated using interpolated data from the USGS Data Series 801 in the Material Processing Module from the ACTIUM Python Toolkit for a location of latitude: 29.7604° N and longitude: -95.3698° E using the same concentration cutoff limit [157, 113]. The Material Processing Module from the ACTIUM Python Toolkit reads in USGS soil composition data and interpolates the detailed composition of the soil at a user-defined latitude and longitude. The material database within the Material Processing Module includes concentrations of various elements in the soil down to ppb levels.

5.3.4 Calculation Procedure

The transmutation results presented in Section 5.4 are calculated using the ACTIUM Python Toolkit [113]. The ACTIUM Python Toolkit methodology couples the unstructured mesh neutron transport capabilities of MCNP6 with the CINDER2008 transmutation code [176, 121]. The energy-dependent neutron fluxes are tallied on each unstructured mesh element and used as input to CINDER2008 transmutation calculations. A CINDER2008 transmutation calculation is done for each mesh element with a non-zero flux. The result of the ACTIUM calculation is a database of nuclide inventories for each mesh element in the model. The nuclide inventories include activities, masses, atom densities, etc as calculated by CINDER2008. The CINDER2008 runs used a custom cross section set that prioritized ENDF/B-VIII.0, JENDL4, and TENDL2017 cross sections in 321 energy groups [18, 156, 90].

Total and isotopic-specific effective dose quantities are calculated using the nuclide specific activities in each mesh element and dose rate coefficients for contaminated air submersion [10]. These dose rate coefficients are calculated using a reference phantom energy dependent dose response function convolved with the gamma energy emission for each of the 1,252 radionuclides considered in the report. The dose coefficients are calculated assuming

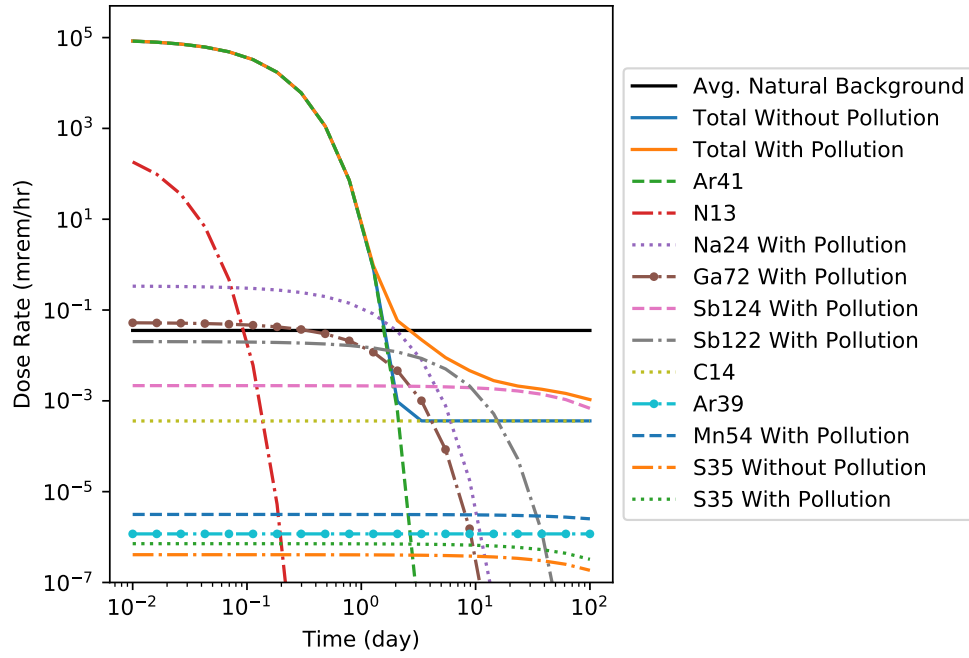
that the radionuclides are distributed uniformly throughout an infinite volume, and the reference person is completely submerged in the contaminated air. These dose coefficients also account for electron dose from bremsstrahlung radiation and direct interaction with the reference person tissue. Effective dose rate values shown in the Section 5.4 assume that the radionuclide has been uniformly distributed over an infinite volume of air and that the reference person is standing on uncontaminated flat ground and submerged in contaminated air [10].

5.4 Results

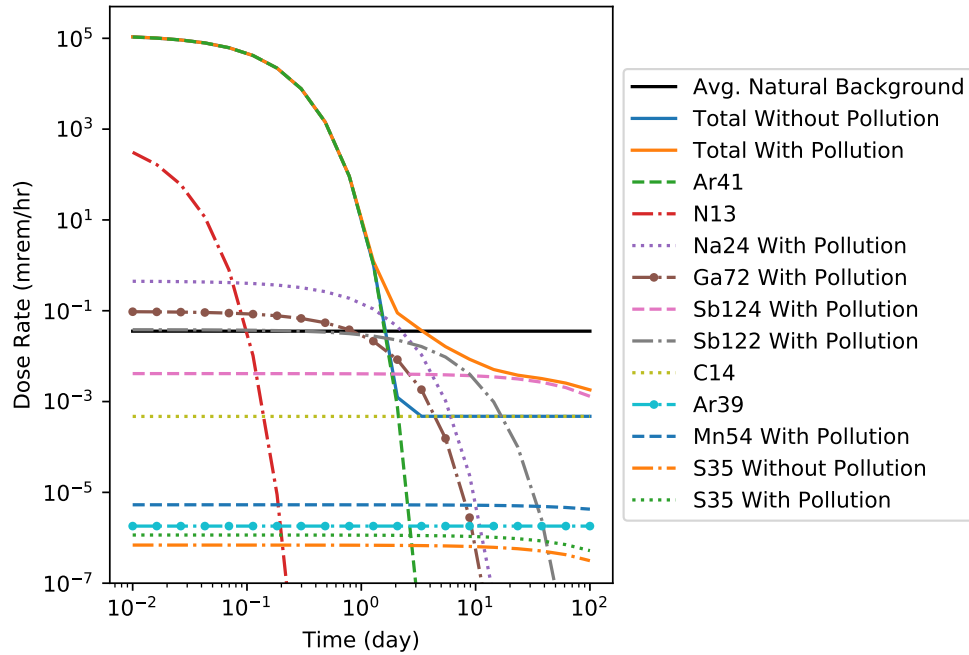
The effective dose rates only account for external effective dose from decay gammas and betas, and do not account for internal dose rate contributions. The effective dose rates provided in the figures should be interpreted as the dose rate at the time recorded in the figure and not as the differential dose rate over time. Given that the mean free path (mfp) of a 1-MeV gamma in dry air is 130 m, the overall extent of the severe pollution layer in the model in terms of number of mfp lengths is 15 x 15 x 4 mfp lengths (2 km x 2 km x 460 m). Due to the overall dimensions of the severe pollution layer, it is considered an infinite volume for the dose calculations. The activities used to calculate the dose quantities are the sum of the activities from each mesh element in the severe pollution region of the model that extends from ground surface up to 460 m. The dominant source of error for the effective dose values in this section is the statistical error associated with the Monte Carlo neutron transport used to estimate the neutron flux in each mesh element. The relative error in the neutron flux for most mesh elements is below 10%. Dose rate values for over 500 radionuclides have been calculated for each calculation using the three source spectra described in Section 5.3.2 that have varying intensities of the thermal, fast, and high-energy components of the neutron spectra for the same yield of 100 kT at 1000-ft source height. This section only includes the results for the severe pollution level. The slight, mild, and moderate levels of pollution were not included in this section due to the most severe pollution levels having minimal effect on the total effective dose. The average United States annual background effective dose rate is

shown in some figures in this section and is the sum of radon, extraterrestrial, terrestrial, and naturally occurring bodily effective dose rates [130].

Figures 5.3, 5.4 & 5.5 show dose over time from radionuclides produced by Source 3, 5, and 8 respectively. These figures include dose from severely polluted air and non-polluted air along with the isotopes that are the highest contributors to dose in either case. If the isotope in Figures 5.3, 5.4 & 5.5 does not have a “with” or “without” pollution specification, that indicates that the dose from that isotope remains unchanged with the inclusion of pollution. The total dose rate with and without pollution are largely the same across the different source spectra.

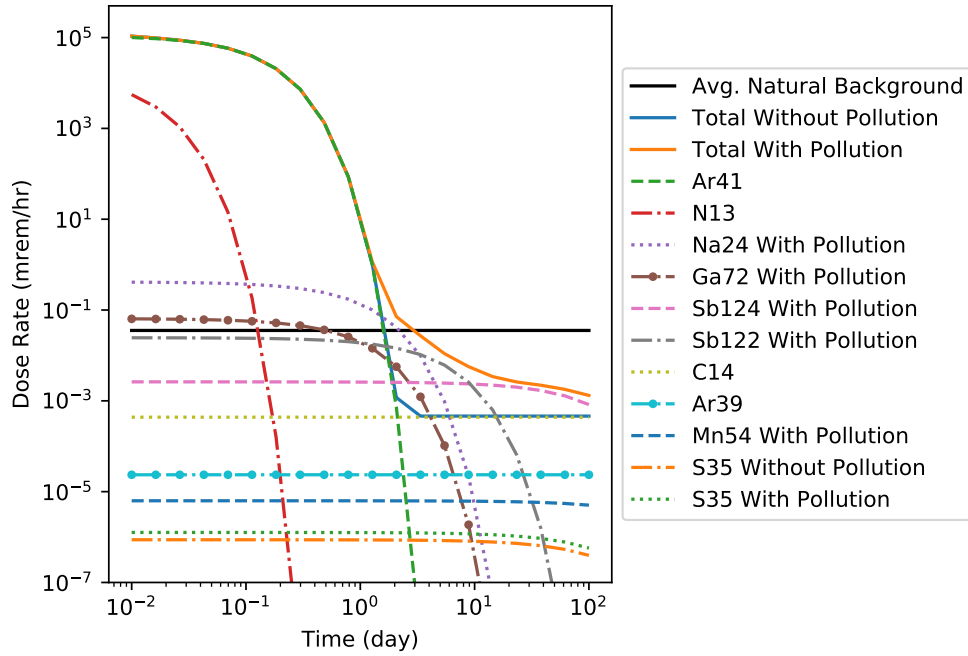


(a) 6 ft HOB

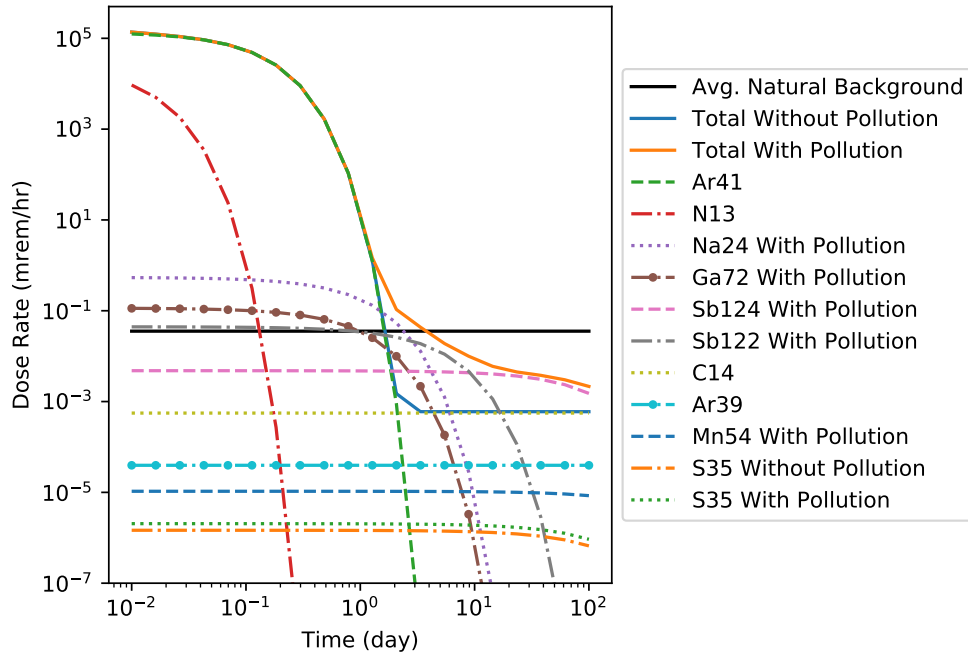


(b) 1000 ft HOB

Figure 5.3: External exposure effective dose rate over time for uniformly distributed contaminated air in an infinite volume for radionuclides activated by Source 3

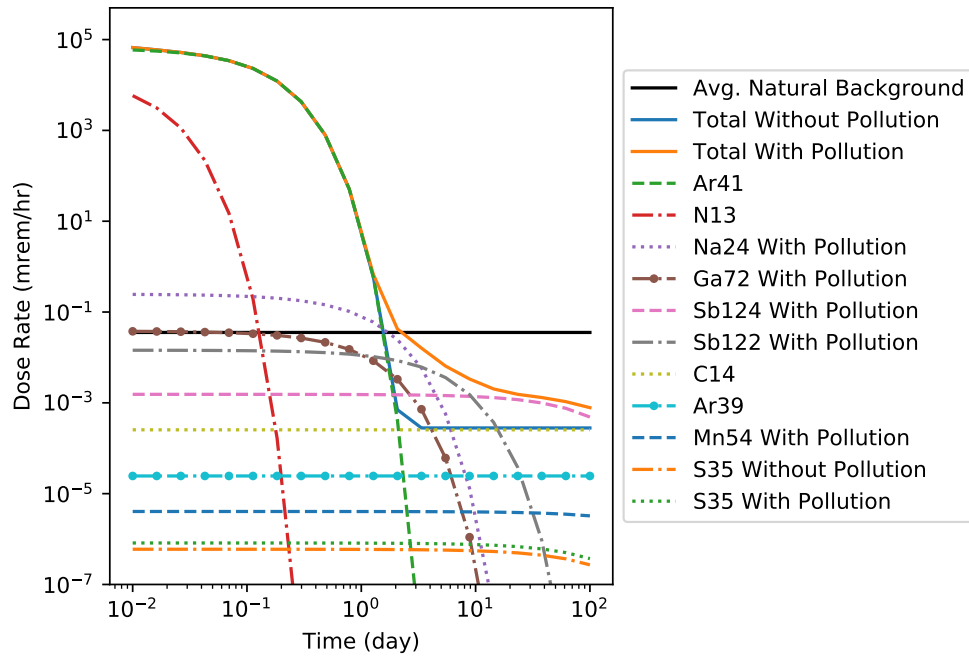


(a) 6 ft HOB

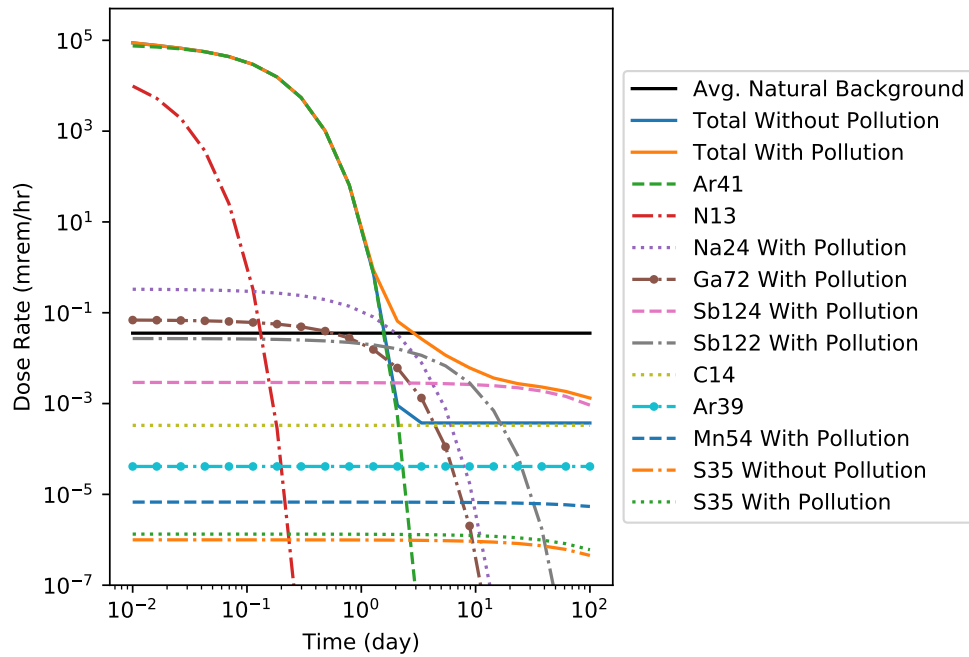


(b) 1000 ft HOB

Figure 5.4: External exposure effective dose rate over time for uniformly distributed contaminated air in an infinite volume for radionuclides activated by Source 5



(a) 6 ft HOB



(b) 1000 ft HOB

Figure 5.5: External exposure effective dose rate over time for uniformly distributed contaminated air in an infinite volume for radionuclides activated by Source 8

One major difference in the isotopic effective dose rate levels between source spectra is the increase in ^{39}Ar 's dose rate while using Source 5 and 8 over using Source 3. The dose rate from ^{39}Ar does not significantly change due to pollution. This increase is due to the presence of high energy neutrons in the source spectrum. Table 5.4 shows the most probable ^{39}Ar production mechanisms. Based on the cross sections and precursor concentration in the air shown in Table 5.4, the most probable production mechanism when high-energy neutrons are present is the $^{40}\text{Ar}(n,2n)$ reaction.

Table 5.4: ^{39}Ar Production Mechanisms [18]

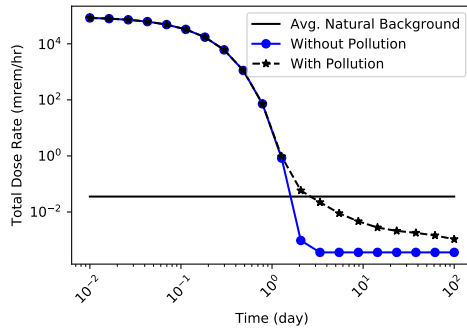
Reaction	Thermal Cross Section (b)	Fast Cross Section (b)	High-Energy Cross Section (b)	Precursor Concentration ($\mu\text{g per g}$)
$^{38}\text{Ar}(n,\gamma)$	8.0E-1	7.9E-4	1.4E-4	8.1
$^{40}\text{Ar}(n,2n)$	-	-	5.8E-1	1.3E4
$^{39}\text{K}(n,p)$	-	7.8E-3	3.9E-1	3.3E-2
$^{42}\text{Ca}(n,\alpha)$	-	5.0E-12	6.1E-2	5.1E-1

Figures 5.3, 5.4 & 5.5 show that the dose rate from ^{35}S in polluted air doubles with respect to air without pollution. However, the dose rate from ^{35}S is negligible when compared with the other isotopic dose rates. In the times less than 1 day after detonation, the dose rate contributions from the radionuclides introduced by the inclusion of pollution are superseded by the dose rate from ^{41}Ar that has a half-life of 110 minutes and its main production mechanism is the $^{40}\text{Ar}(n,\gamma)$ reaction where ^{40}Ar has a concentration of 13 mg/g in the air.

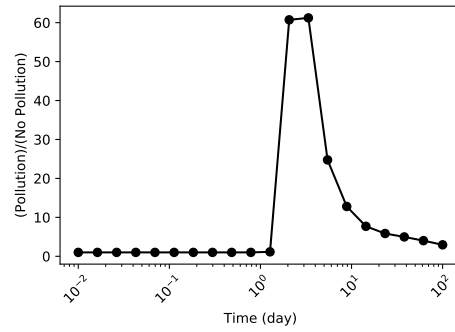
Figures 5.3, 5.4 & 5.5 all show that the total dose rate from polluted air is greater than the dose rate for air without pollution from 3 to 100 days. During these times, ^{24}Na , ^{122}Sb , ^{124}Sb dominates the effective dose rate from polluted air while ^{14}C dominates the dose rate from air without pollution.

Figures 5.6, 5.7 & 5.8 show only the total dose rates for air with and without pollution and the fraction of the two dose rates. All of the figures indicate that fractional difference in

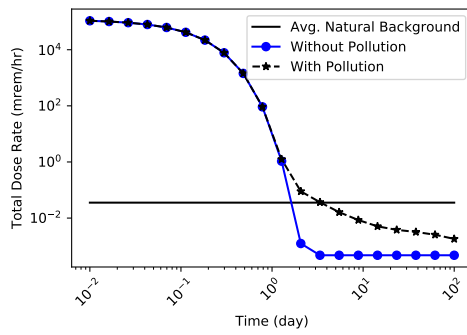
dose rates is greater for the 1000 ft HOB when compared to the fractional differences for the 6 ft HOB. This is due to more of the air being exposed to higher neutron fluxes at the 1000 ft HOB and thus producing more ^{24}Na in the polluted air. ^{14}C is present in both polluted air and air without pollution and ^{24}Na is only in the polluted air. The difference in the two material definitions is highlighted by exposing more material to neutron flux. Many of the neutrons are absorbed in the soil and seawater at the 6 ft HOB and do not contribute to the activation of the air. Even though the fractional difference between air with and without pollution is greater than a factor of 60 at 3 days after the detonation, the total dose rate is near the average annual radiation dose per person in the United States [130].



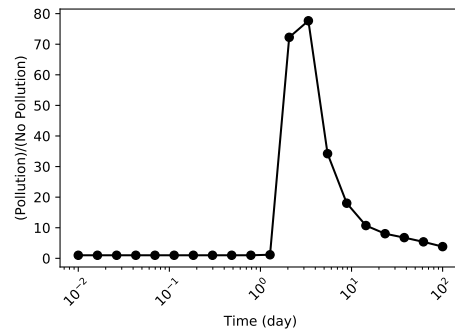
(a) Total Effective Dose, 6 ft HOB



(b) Total Effective Dose Fraction, 6 ft HOB

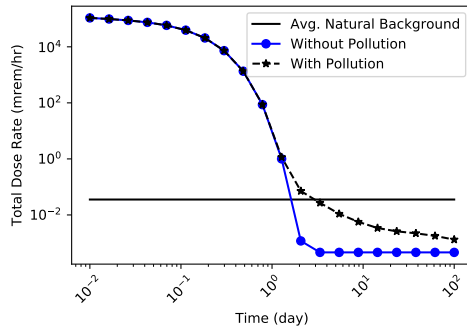


(c) Total Effective Dose, 1000 ft HOB

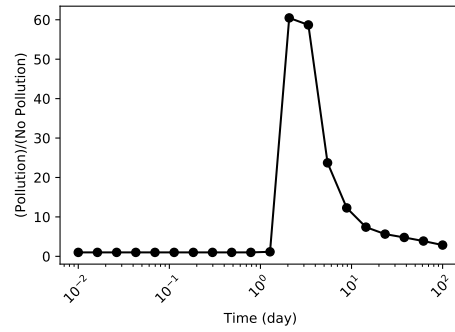


(d) Total Effective Dose Fraction, 1000 ft HOB

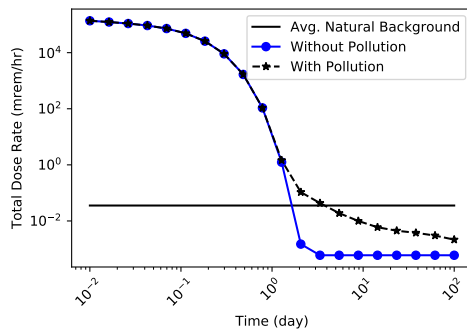
Figure 5.6: Total effective dose and total dose fractions for polluted and non-polluted air for Source 3



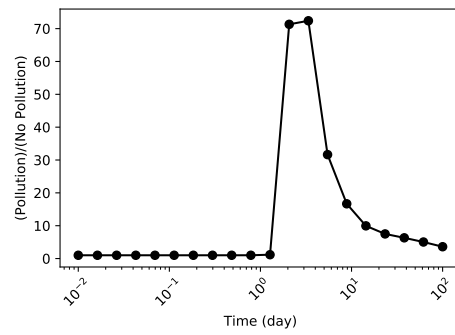
(a) Total Effective Dose, 6 ft HOB



(b) Total Effective Dose Fraction, 6 ft HOB

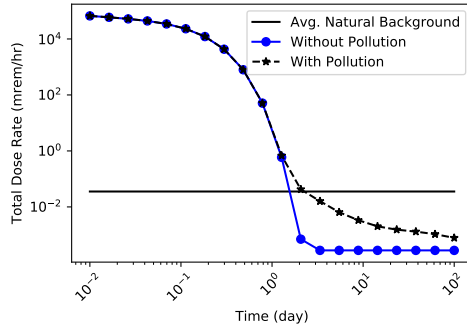


(c) Total Effective Dose, 1000 ft HOB

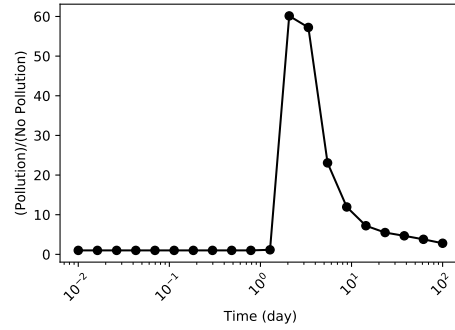


(d) Total Effective Dose Fraction, 1000 ft HOB

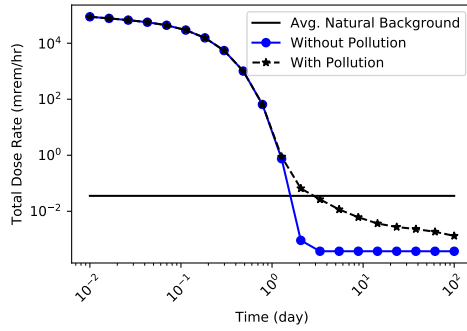
Figure 5.7: Total effective dose and total dose fractions for polluted and non-polluted air for Source 5



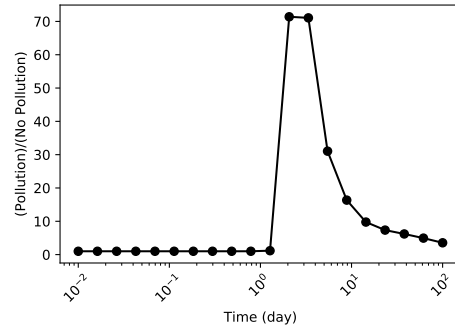
(a) Total Effective Dose, 6 ft HOB



(b) Total Effective Dose Fraction, 6 ft HOB



(c) Total Effective Dose, 1000 ft HOB



(d) Total Effective Dose Fraction, 1000 ft HOB

Figure 5.8: Total effective dose and total dose fractions for polluted and non-polluted air for Source 8

The time in which the total effective dose rates for polluted air and air without pollution are equal to the average U.S. natural background background effective dose rate differ by a factor of two where the total effective dose rate without pollution drops below natural background at 2 days and the total effective dose rate with pollution in the air drops below natural background at 4 days in Figures 5.6, 5.7 & 5.8. This may have an impact on first-responder efforts during the 2-4 day time-frame.

5.5 Conclusions

The radionuclides that are produced in both polluted and non-polluted air have been characterized for times out to 3 months post-detonation. For times less than a day, ^{41}Ar is the dominant dose contributor whether or not the air is polluted. The largest discrepancy between the total dose curves for polluted and non-polluted air is at 3 days post-detonation where the ^{24}Na in the polluted air dominates the total dose and increases the overall dose by a factor of more than 60 from non-polluted air. The time of which the total effective dose rates fall below the average U.S. natural background differ by 2 days and will need to be considered when planning first-responder action plans. Future efforts should be made to include the spatial isotopic inventories that have been calculated for various combinations of HOB, source type, and material composition into fallout and other plume modeling codes so that dispersion and entrainment effects can be captured.

Chapter 6

Conclusions and Future Work

The ACTIUM toolkit provides a unique set of analysis tools to calculate the production and destruction of isotopes from a nuclear detonation in an unstructured mesh model of an urban environment. Validation case studies have shown that the results from the ACTIUM toolkit agree with analytical methods and measured results. Future work includes the implementation of an iterative processes whereby the newly transmuted isotopes in the unstructured mesh are used as input to a subsequent MCNP6 calculation so that an updated neutron flux may be calculated and used to further transmute the materials in the unstructured mesh.

An overview of how to model the buildings of an urban environment has been demonstrated on the city of Atlanta, GA complete with details on how to account for the composition of the structural composition of the building and the electronics that has been shown to significantly affect the neutronics in an urban environment. The isotopic ratios shown in this work are examples of ratios that proved to be some of the most sensitive stable isotopic ratios. The complete spatial distribution of stable and radioisotopes can be incorporated into other fire or atmospheric modeling codes to better understand dose distributions after the irradiated materials have been lofted into the atmosphere due to fires and/or rubblization. The results from evaluating the sensitivities of isotopes produced from an urban nuclear detonation may be used to inform first-responder triage efforts by suggesting which type of building to sample based on the answers requested by decision makers regarding

attribution. The most sensitive isotopic ratios may also be used to guide radio-analytical chemistry or mass spectrometry communities as they develop new measurement techniques.

The radionuclides that are produced in both polluted and non-polluted air have been characterized for times out to 3 months post-detonation. For times less than a day, ^{41}Ar is the dominant dose contributor whether or not the air is polluted. The largest discrepancy between the total dose curves for polluted and non-polluted air is at 3 days post-detonation where the ^{24}Na in the polluted air dominates the total dose and increases the overall dose by a factor of more than 60 from non-polluted air. The time of which the total effective dose rates fall below the average U.S. natural background differ by 2 days and will need to be considered when planning first-responder action plans. Future efforts should be made to include the spatial isotopic inventories that have been calculated for various combinations of HOB, source type, and material composition into fallout and other plume modeling codes so that dispersion and entrainment effects can be captured.

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Appendices

A City CAD Model to MCNP6 Unstructured Mesh Tutorial

A.1 Introduction

This document serves as an overview of a procedure to convert a three dimensional (3D) computer-aided drafting (CAD) model of a city, available from the Cadmapper® website for use in the Monte Carlo N-Particle transport code (MCNP6) as a unstructured mesh (UM) for University of Tennessee, Knoxville students [176]. Martz’s overview of the usage of UM in MCNP6 and Kulesza’s UM tutorial using Abaqus/CAE® 6.12-1 are useful resources to provide a deeper understanding of UM generation and usage in MCNP6 [93, 107]. In the following sections, the reader will be guided through 3D City CAD model generation using the Cadmapper website, model cleanup using Autodesk® Inventor®, UM generation using Abaqus/CAE® 6.12.1, particle transport using MCNP6, and visualization of results using VisIT [29]. For active University of Tennessee, Knoxville students, Abaqus/CAE® 6.12.1 and Autodesk® Inventor® are available for use by visiting <https://apps.utk.edu>.

A.2 Cadmapper Operations

The Cadmapper website provides a user interface to create 3D CAD models of the terrain, buildings, roads, parks, waterways, etc. for any user selected region of the map. Once the user has selected a region on the map, a 3D CAD model can be generated and downloaded in Autodesk® 3D DXF format. The Cadmapper website uses OpenStreetMap “open data” (meaning that the users is free to use the data for any purpose as long as you credit OpenStreetMap) to create the Autodesk® 3D DXF file [60]. These 3D Autodesk® DXF files are free of cost for areas of the map less than 1 km².

Navigate to <https://cadmapper.com> and sign in to a Cadmapper account or make an account if one is not in place (the account is free). The “Create Map” webpage will be displayed once signed in where the user can navigate the map to position the highlighted region over an area of interest. Figure 1 shows the map and the highlighted portion of the map centered on downtown New York City, NY.

Create a Map

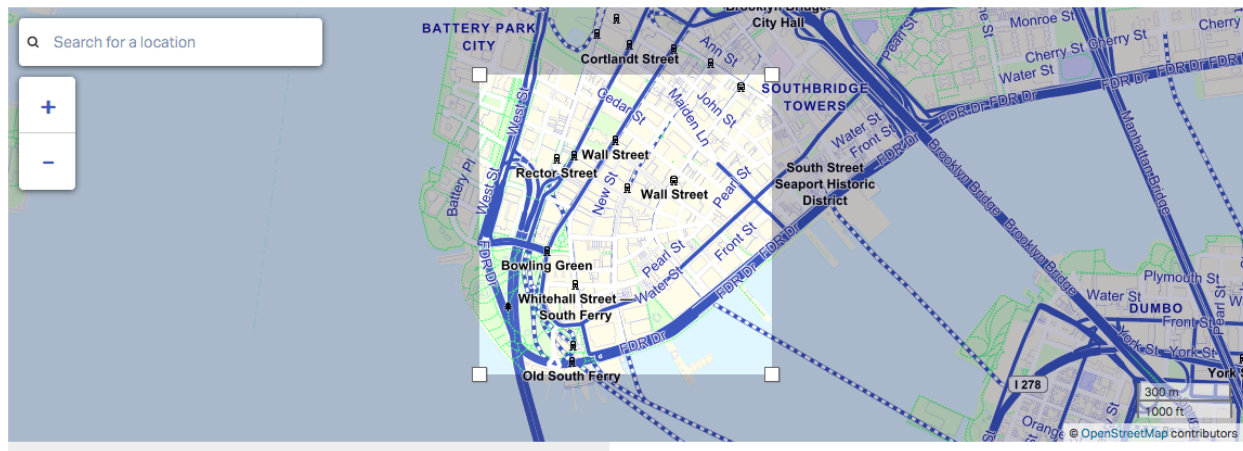


Figure 1: Highlighted portion of the map on the “Create a Map” Cadmapper webpage

Now that the highlighted region of the map is over an area of interest, make sure the settings are correct for successful import into Autodesk® Inventor®. Make sure that “Other (.DXF)” is selected in the “Select your design program” portion of the webpage, select “3D Buildings (if available)” and “Set false height if no 3D data” may be set to the average height of buildings in the area, and set the “Road Geometry” to “Centerlines” from the drop-down menu. Figure 2 shows the control panel with the correct settings.

Select your design program



AutoCAD



SketchUp 2015+



Illustrator



Rhino 5



SketchUp 8 to 2014



Other (.DXF)



Include

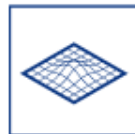


☒ 3D Buildings (if available)

☒ Set false height if no 3D data

57

meters



☐ Topography

☐ Contours

Road Geometry

Centerlines



Figure 2: Settings for downloading the 3D CAD file on Cadmapper

Click “Create File”, wait for the file to be created, and click ”Download.” Figure 3 shows the area where the newly created 3D DXF CAD file can be downloaded. Details of the 3D DXF CAD file are shown in the “Map Details” section of Figure 3. Some of these details include that the file is in units of meters and the origin is the bottom left corner of the map from the top down view.

Map near New York City, New York, US

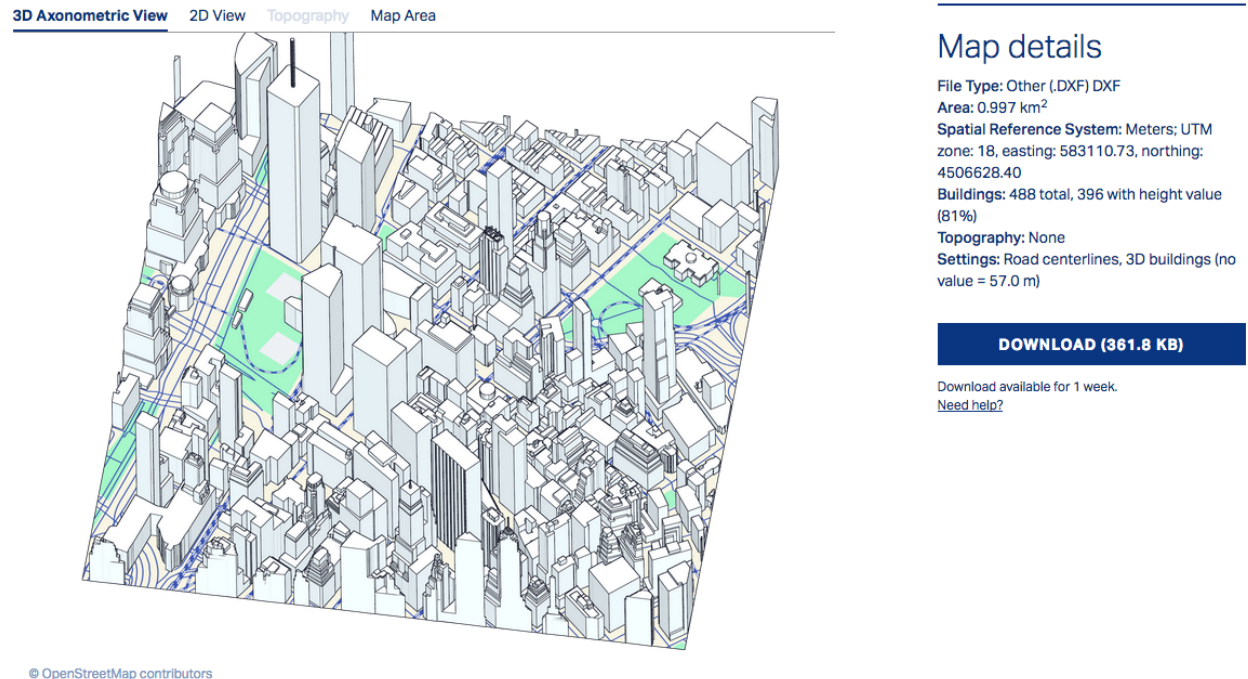


Figure 3: View of webpage where the 3D DXF CAD model can be downloaded using Cadmapper.

A.3 Autodesk® Inventor® Operations

Now that the 3D CAD model of the city generated and downloaded, the model needs to be cleaned up and solid bodies of the buildings need to be generated using Autodesk® Inventor®. Import the newly created DXF file into Autodesk® Inventor® by selecting **File** **Open (arrow)** **Import CAD Files**. This may take a few seconds as Autodesk® Inventor® loads the necessary libraries to successfully read the file. When the DXF file is opened, the prompt shown in Figure 4 is displayed. Choose the default configuration in the “Configuration” drop-down menu and click “Next.”

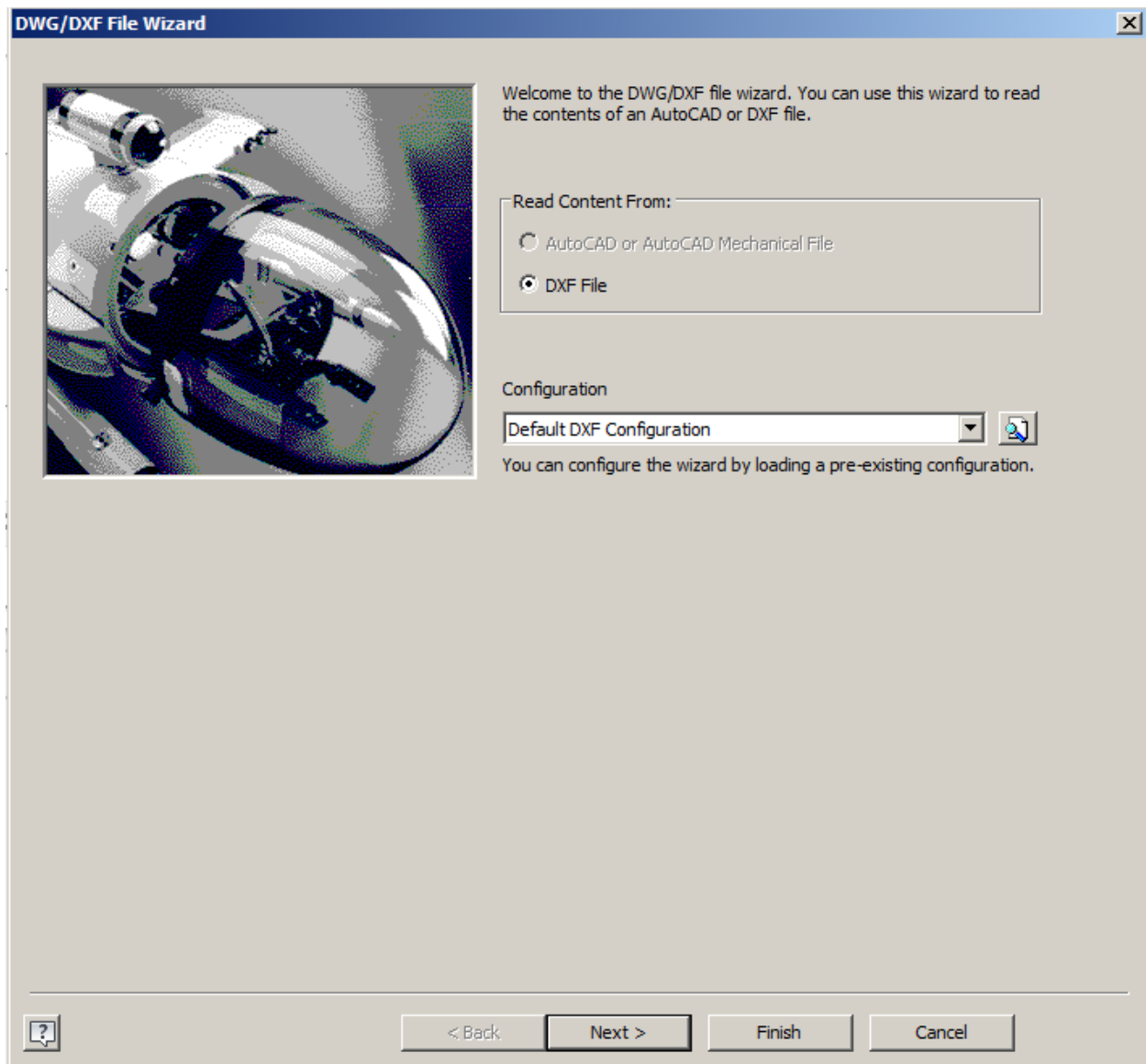


Figure 4: DXF import prompt for Autodesk Inventor

Select the layers and objects to import into Autodesk® Inventor® by selecting or deselecting the boxes in the “Layers and Objects Import Options” window shown in Figure 5 making sure that at least the “buildings” check box is selected, and click “Next.”

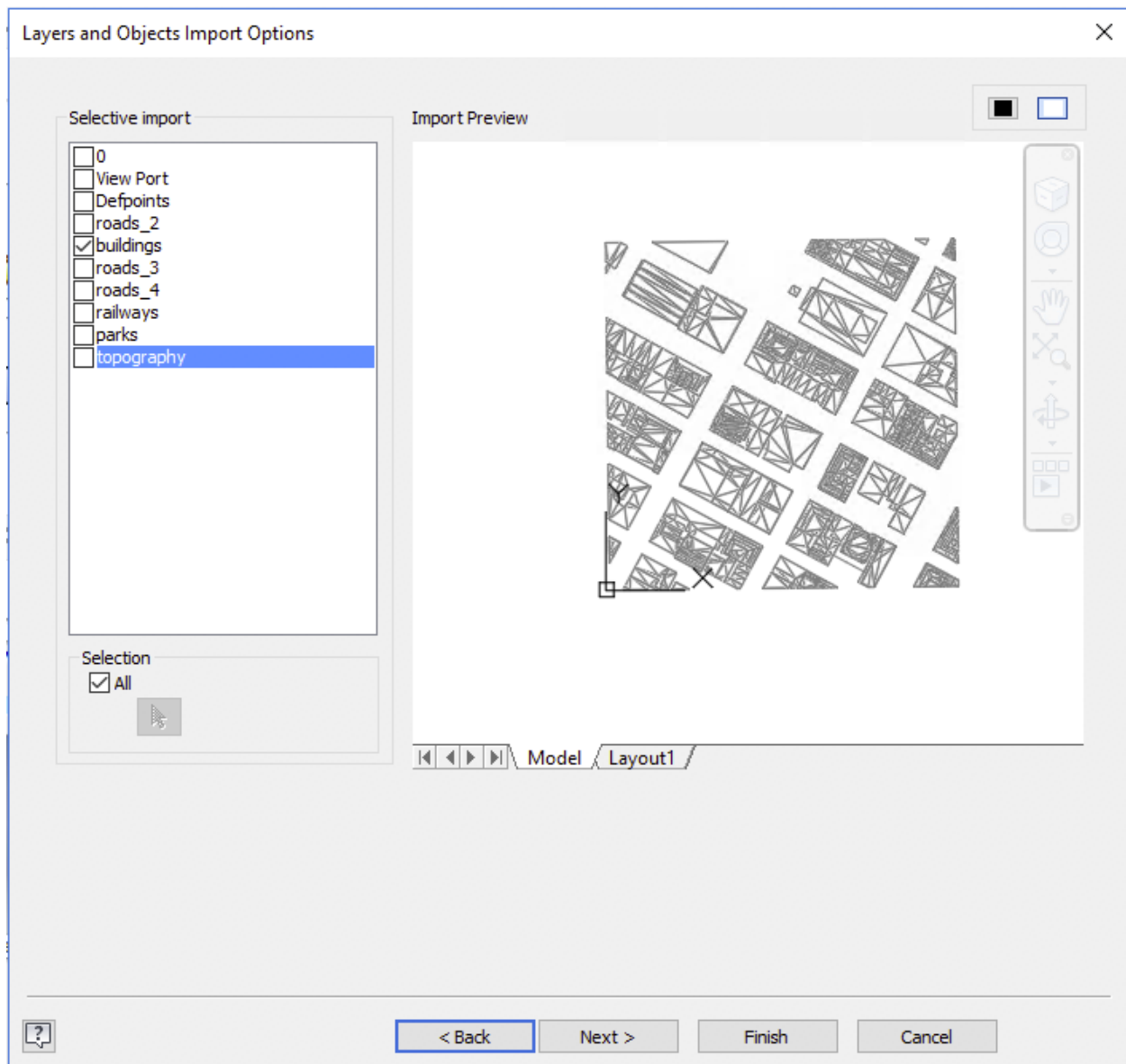


Figure 5: Layers and object selection window within Autodesk® Inventor®

If the window shown in Figure 5 does not display, completely close Autodesk® Inventor® and restart the Autodesk® Inventor® process from the beginning. In the “Import Destination Options” window shown in Figure 6, make sure that the “3D solids,” “Solids to single part file,” “Surfaces,” “Wires,” “New Part,” “Wires to 3D Sketch” boxes are selected. Also specify the units as “meter” in the drop-down menu and click “Finish.”

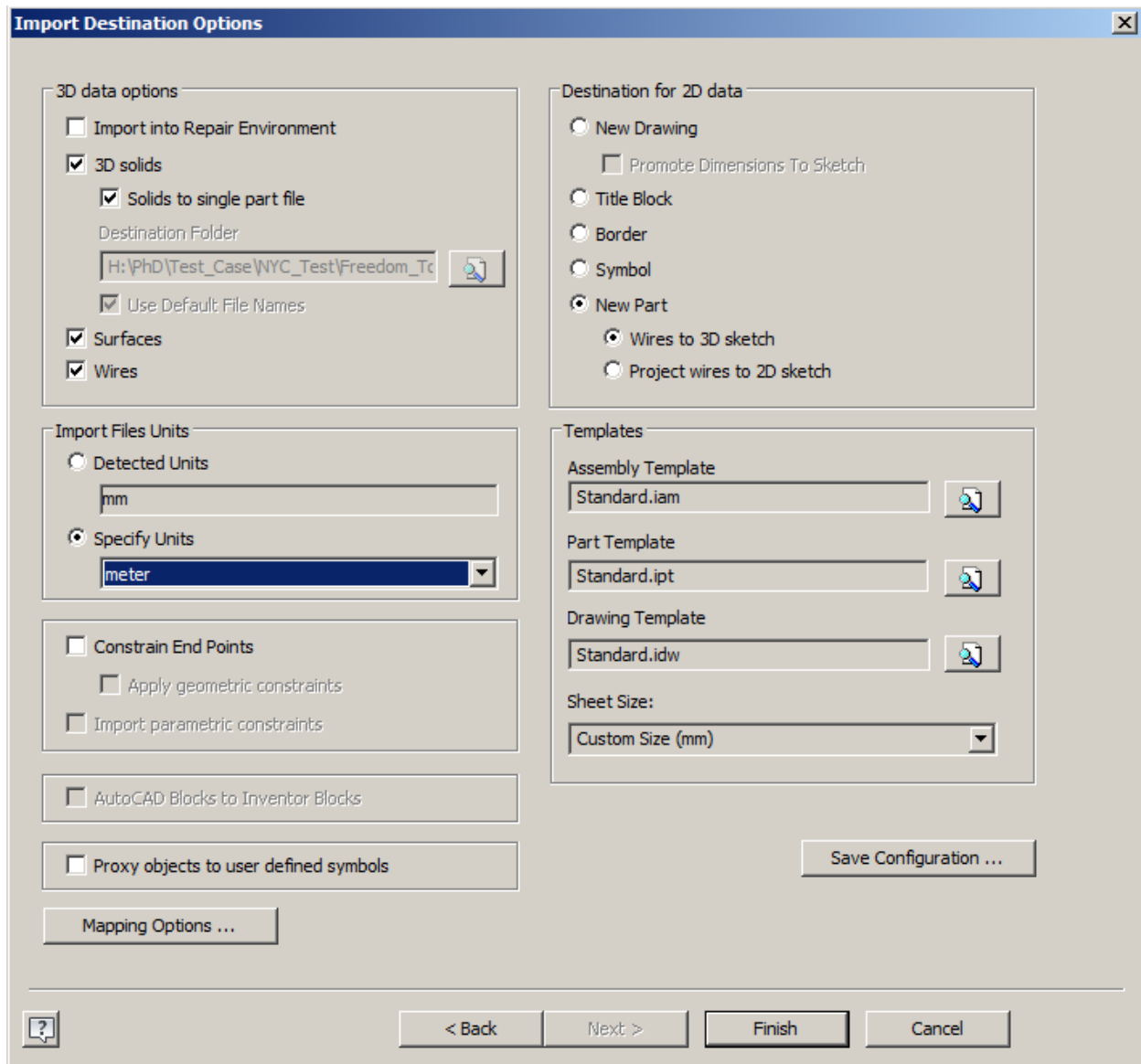


Figure 6: Import Destination Options for importing DXF files into Autodesk[®] Inventor[®]

In order to achieve the most reliable result, clean up the model by deleting the unnecessary sketches. Use the Stitch Tool to create solids from the imported surfaces by selecting the icon shown in Figure 7. Select the surfaces to be made into solid bodies and click “Apply” and “Done.”

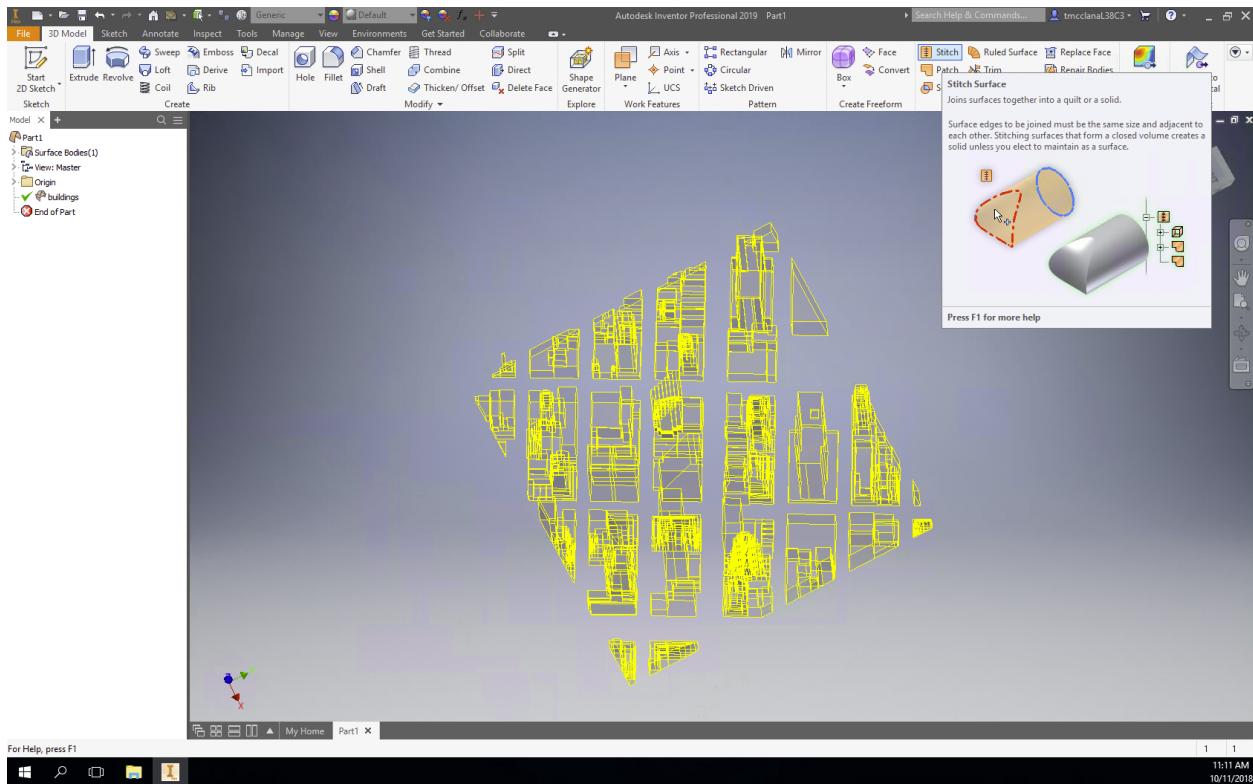


Figure 7: Stitch Tool in Autodesk® Inventor®

Change the units of the model to centimeters by navigating to **Tools** > **Document Settings** > **Units** > **cm**. The units must be centimeters because the default unit of measure in MCNP6 is centimeters. Export the model as a STEP file by selecting **File** > **Export** > **CAD Format**. In the displayed “Save As” window, select “STEP Files” from the “Save as type:” drop-down menu and click “Save.”

A.4 Abaqus Operations

Abaqus/CAE[®] 6.12-1 is an engineering analysis tool used in many engineering applications from computational fluid dynamics to finite element analysis to structured/unstructured mesh generation. For purposes of this tutorial, Abaqus/CAE[®] 6.12-1 is used to assign materials to specific regions of the model and generate an UM of the model for use in MCNP6. Start by creating a model database “With StandardExplicit Model” and setting the working directory by selecting **File** > **Set Work Directory** to the directory location of the STEP file. Import the STEP file by selecting **File** > **Import** > **Part**. Select “STEP” from the “File Filter” drop-down menu. In the “Create Part from STEP File” window shown in Figure 8, select “Import all parts,” “Combine into single part,” and click “OK.”

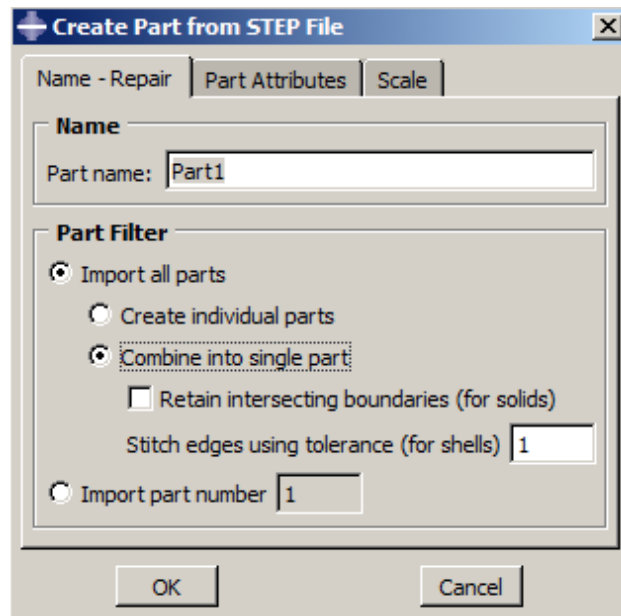


Figure 8: Create Part from STEP File window in Abaqus/CAE[®] 6.12-1

In order to assign materials to specific regions of the model, element sets must be created with the proper names and selection of geometric regions of the model. Create an element set by right clicking “Sets” and selecting “Create” as shown in Figure 9. When naming the sets make sure the proper naming conventions outlined in Kulesza’s report are followed: “Set_material_tally_###” where ### is the unique number corresponding to the material card. Then select the regions corresponding to the material that is being assigned.

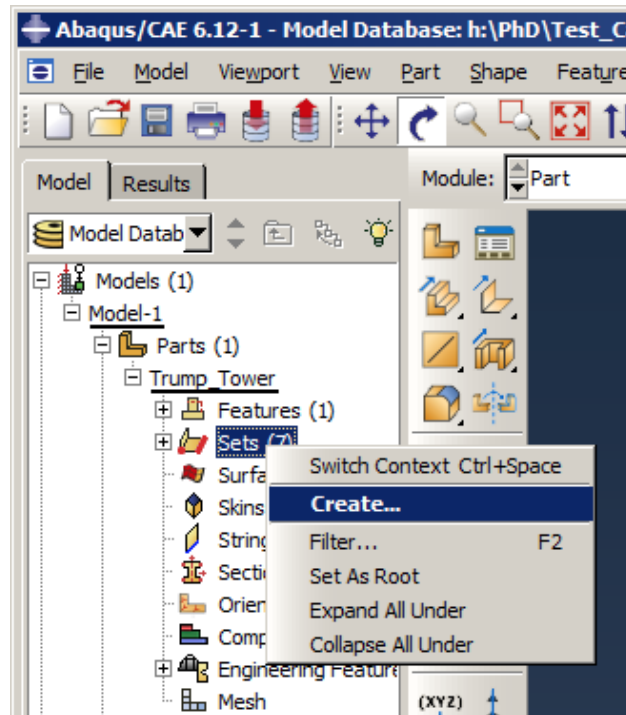


Figure 9: Creating a set in Abaqus/CAE® 6.12-1

Materials are created by right clicking “Materials” in the model tree and selecting “Create” as is the same for creating element sets. Name the material with the following naming convention: “material_name_###” where material_name can be anything and the ### is the number corresponding to the MCNP6 material card and set number. Figure 10 shows the “Edit Material” window that displays when creating a material. With the “Edit Material” window open, set the density by selecting **General** >> **Density** and entering the density of the material following the MCNP sign conventions ((-) for g/cc (+) for atoms/barn-cm) and click “OK”.

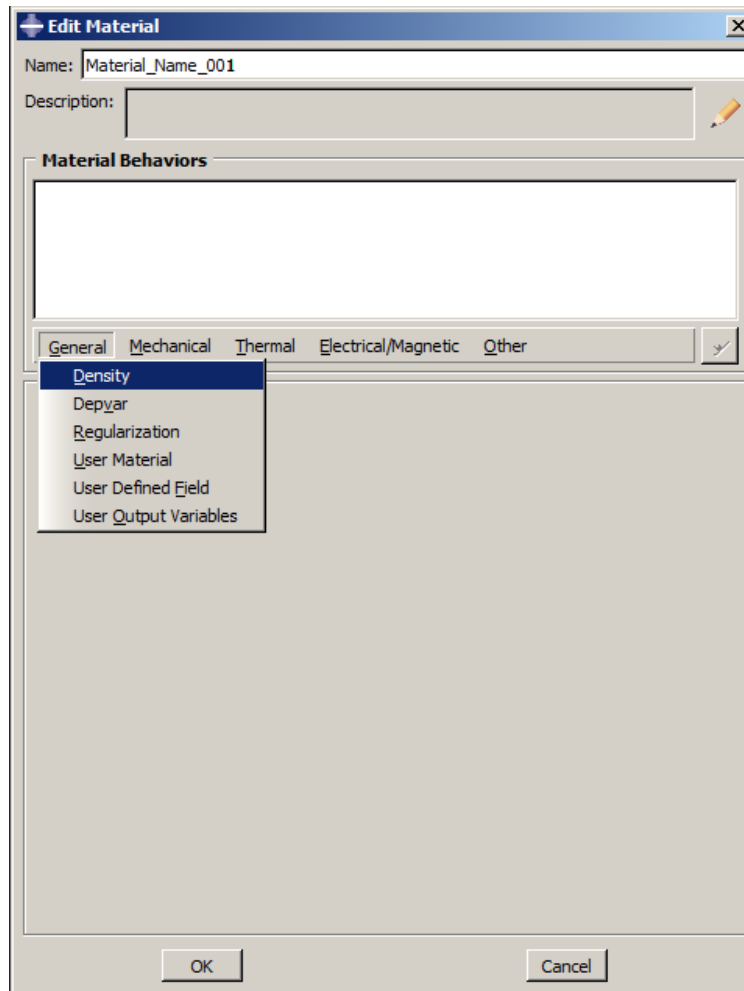


Figure 10: Creating a material in Abaqus/CAE® 6.12-1

After making the element sets and creating materials, the mesh needs to be generated. Navigate to the “Mesh” module shown in Figure 11 and select  to seed the mesh.

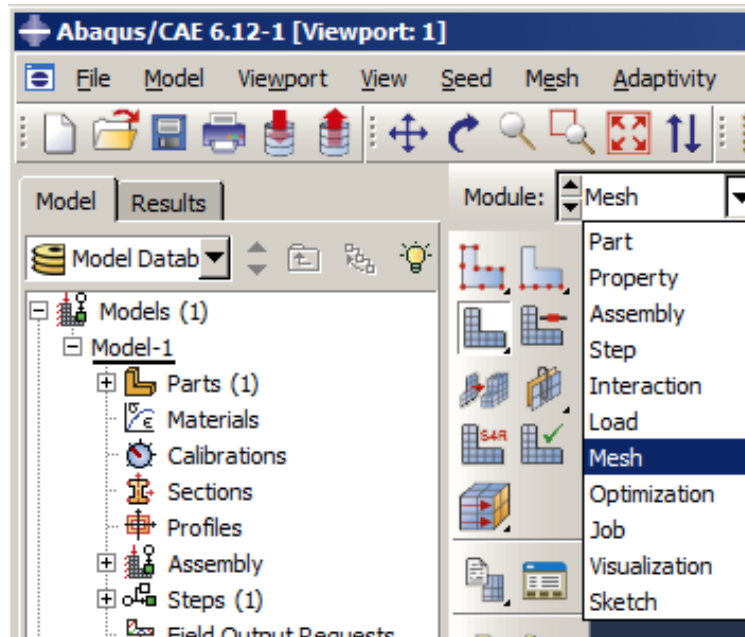


Figure 11: Navigating to the “Mesh” module in Abaqus/CAE® 6.12-1

In the “Global Seeds” window displayed, accept the default values by clicking “Apply” and “Ok.” Select the “Assign Mesh Controls” icon , select the entire region of the city model, select “Tet” under the “Element Shape” banner in the “Mesh Controls” window, click “Ok”, and “Done” to finish the mesh control assignments. Figure 12 shows the final view of setting mesh controls for the city model. Generate the mesh by clicking the “Mesh Part” icon  and selecting “Yes” in the “Ok to mesh part?” prompt.

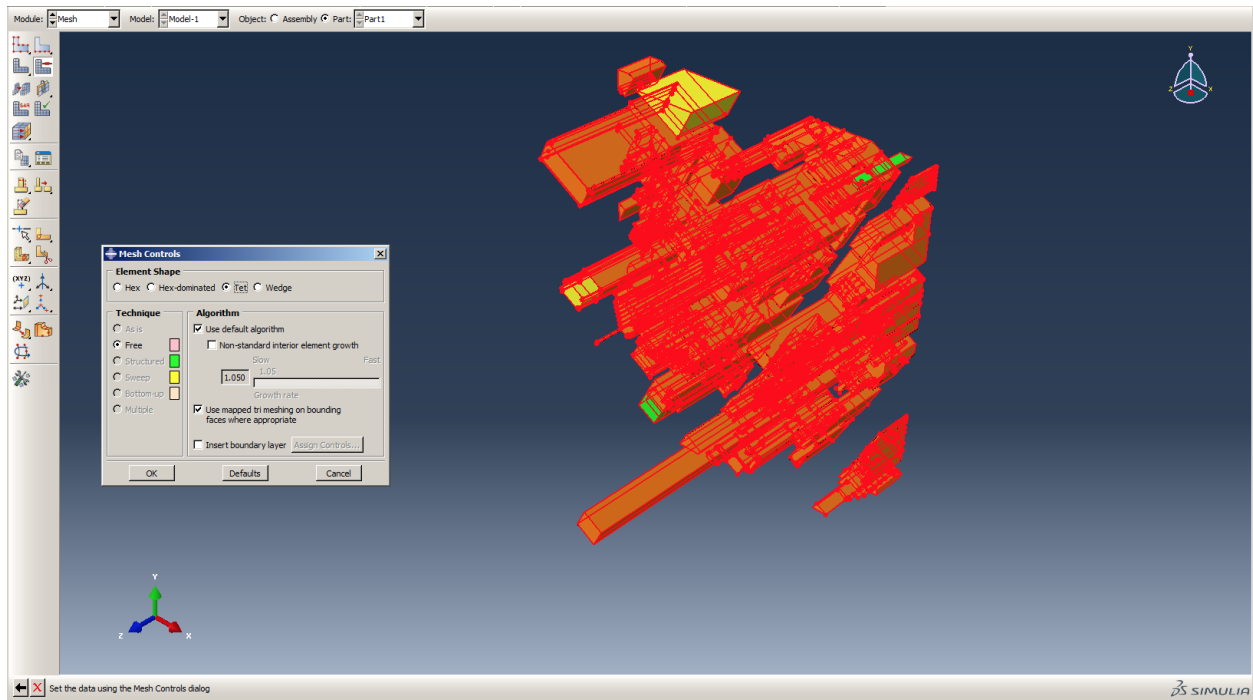


Figure 12: Final view of setting mesh controls in Abaqus/CAE® 6.12-1

Now, add the part to the assembly by selecting “Assembly” in the Module drop-down menu, selecting the “Create Instance” icon , selecting the part in the “Create Instance” window and clicking “OK” as shown in Figure 13.

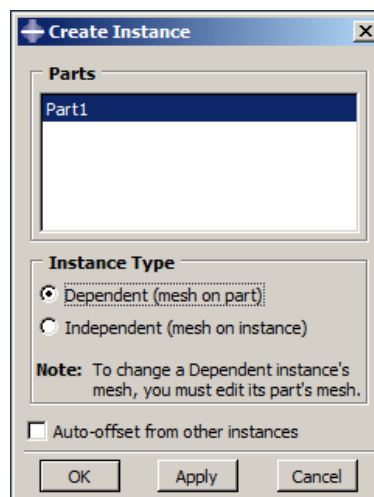


Figure 13: “Create Instance” window in Abaqus/CAE® 6.12-1

In order to generate the Abaqus/CAE[®] input file as required by MCNP6, a Job needs to be created in Abaqus/CAE[®] by navigating to the “Job” module in the Module drop-down menu, selecting the “Create Job” icon , clicking “Continue” in the next prompt, and “OK” in the following prompt. Click the “Job Manager” icon  and select “Write Input” in the column on the right of the window. The Message Area at the bottom of the Abaqus/CAE[®] displays the name of the newly generated input file, and the file will be located in the working directory.

A.5 MCNP6 Operations

MCNP6 comes with a set of utilities that aid in working with unstructured meshes. **um_pre_op** is one of the mentioned utilities that can perform a number of functions including creating a MCNP input file from a Abaqus .inp file by executing the following command:

```
um_pre_op -m abaqus_input_file.inp -b 0 -o mcnp_input_file.in
```

where the -m indicates that **um_pre_op** should create a MCNP6 input file, abaqus_input_file.inp is the name of the Abaqus input file, -b 0 is setting the background material to void, -o mcnp_input_file.in is setting the name of the MCNP6 input file to mcnp_input_file.in. An example of the mcnp_input_file.in is shown below:

```
No description for this unstructured mesh file
c
c Created from file      : example_for_doc_abaqus.inp
c Created on            : 10-16-2018 @ 13:42:32
c
c
c PSEUDO CELLS
01      1      -1.00000      0  u=1
02      2      -1.00000      0  u=1
03      3      -1.00000      0  u=1
04      4       0.00000      0  u=1
05      5       0.00000      0  u=1
```

```

06      6      0.00000      0   u=1
07      7      0.00000      0   u=1
08      0              0   u=1
c
c  LEGACY CELLS
09      0              -99   fill=1
10      0              99
c
c  SURFACES
99  sph    2.19869E+04    2.19139E+04    2.13152E+04    4.51704E+04
c
c  DATA CARDS
embed1  meshgeo=abaqus
        mgeoin=example_for_doc_abaqus.inp
        meeout=example_for_doc_abaqus.eeout
        length= 1.00000E+00
        background=      8
        matcell=  1   1   2   2   3   3   4   4   5   5   6   6   7   7
c
c
c

```

Add the source term, materials, other tallies, etc. to the skeleton MCNP6 input file above to calculate desired results and run input file like a normal run of MCNP6. Section [A.6](#) has a complete input file demonstrating how the user can add sources and materials to the skeleton input file above. Note that in order to score the volume averaged flux in each mesh element volume, the **eembee** card must be used. Details on how to score volume averaged flux in each mesh element volume is discussed in detail in the MCNP6 manual.

When a run has completed with the flux scored in each mesh element volume, the flux data along with the mesh construction data is stored in an elemental edit file with the filename given to the **meeout** parameter in the **embed** card. One of the ways to view the flux profile on the mesh is to convert the elemental edit file to a VTK and use a program such as VisIT or ParaView to view the graphics. However, there is a bug in the **um_post_op** utility that creates a corrupt VTK file. To fix the bug, copy the file located in Section [A.7](#) to the **UM-Utilities** directory in the MCNP6 distribution, name the patch file *patch_file* and execute the following set of commands while in the **UM-Utilities** directory:

```
cd UM-post-op
patch < ../patch_file
make clean
make build
```

Copy the newly created **um_post_op** utility to a folder in your PATH. In order to create the VTK file from the elemental edit file, execute the following command:

```
um_post_op -vtk elemental_edit_file.eeout -ex vtk
```

where -vtk tells **um_post_op** to create a VTK file, *elemental_edit_file.eeout* is the elemental edit filename, and -ex vtk adds the “.vtk” to the elemental edit filename. To view the file, open the file in VisIT or ParaView. Figures [14](#), [15](#), & [16](#) show an example of the visualization of a model of Trump Tower and the surrounding city blocks using the methods described in this tutorial. Figure [14](#) shows how seven different materials were assigned to specific regions of the model and Figures [15](#) & [16](#) show the energy integrated volume averaged neutron flux as scored in the unstructured mesh elements at different views.

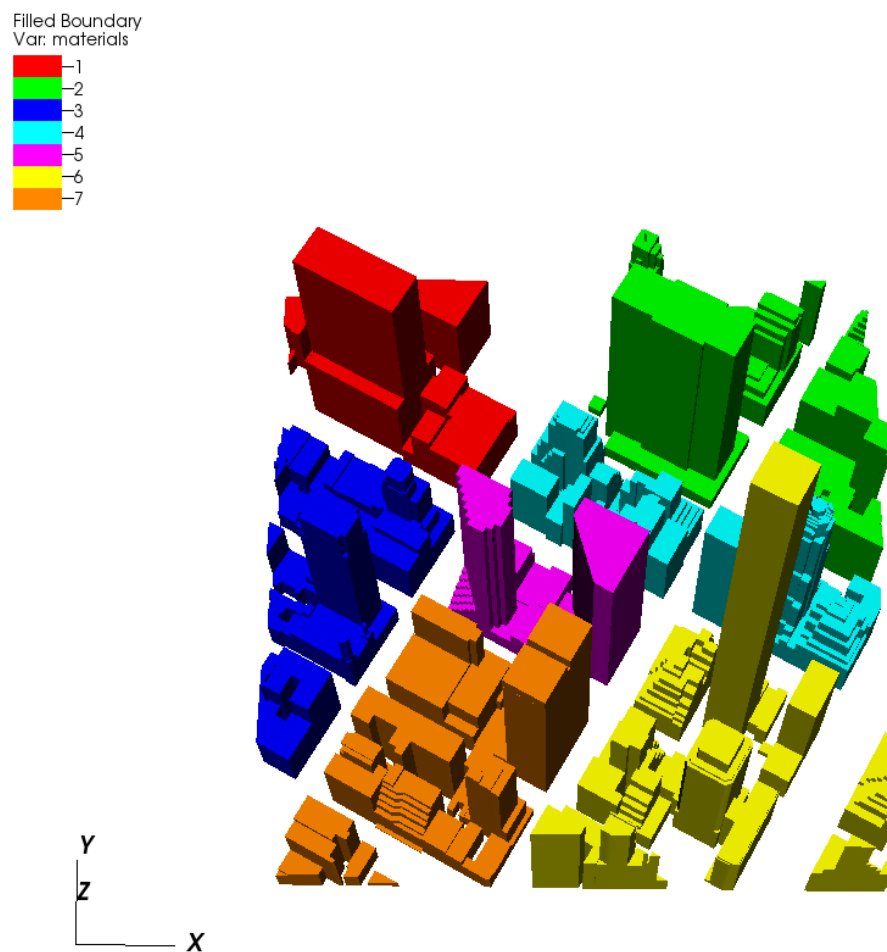


Figure 14: Materials in the Trump Tower model

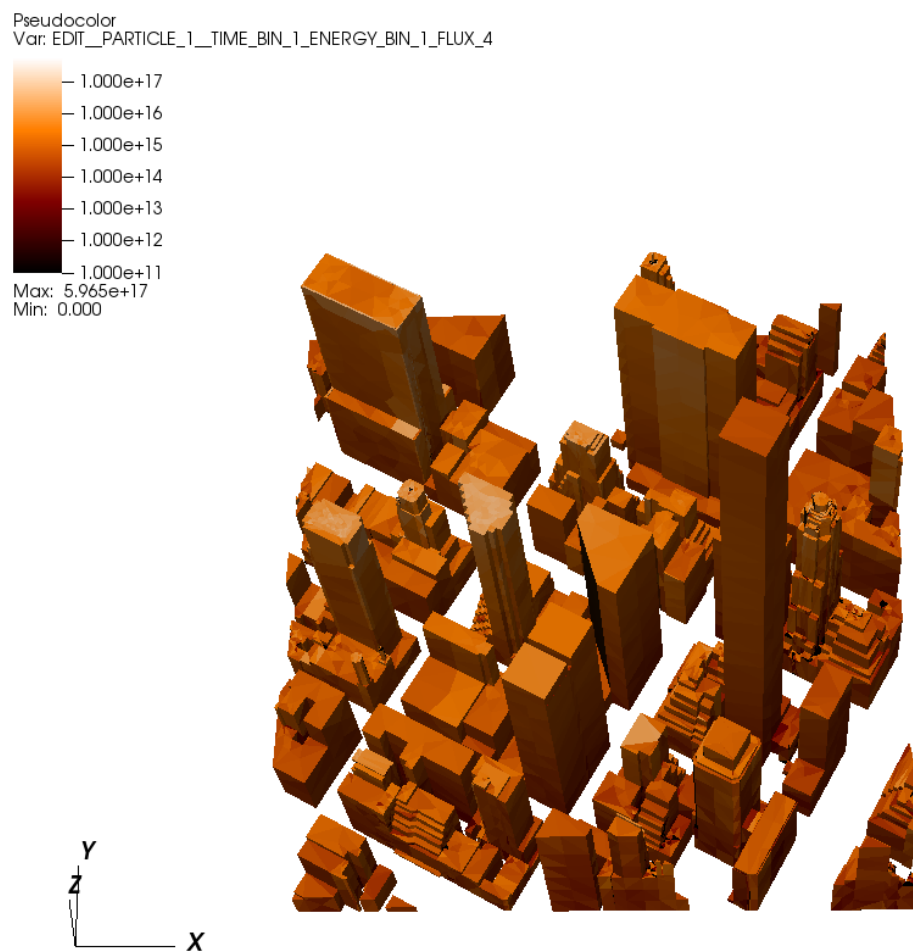


Figure 15: Energy Integrated Neutron Flux (n/cm²) over Trump Tower

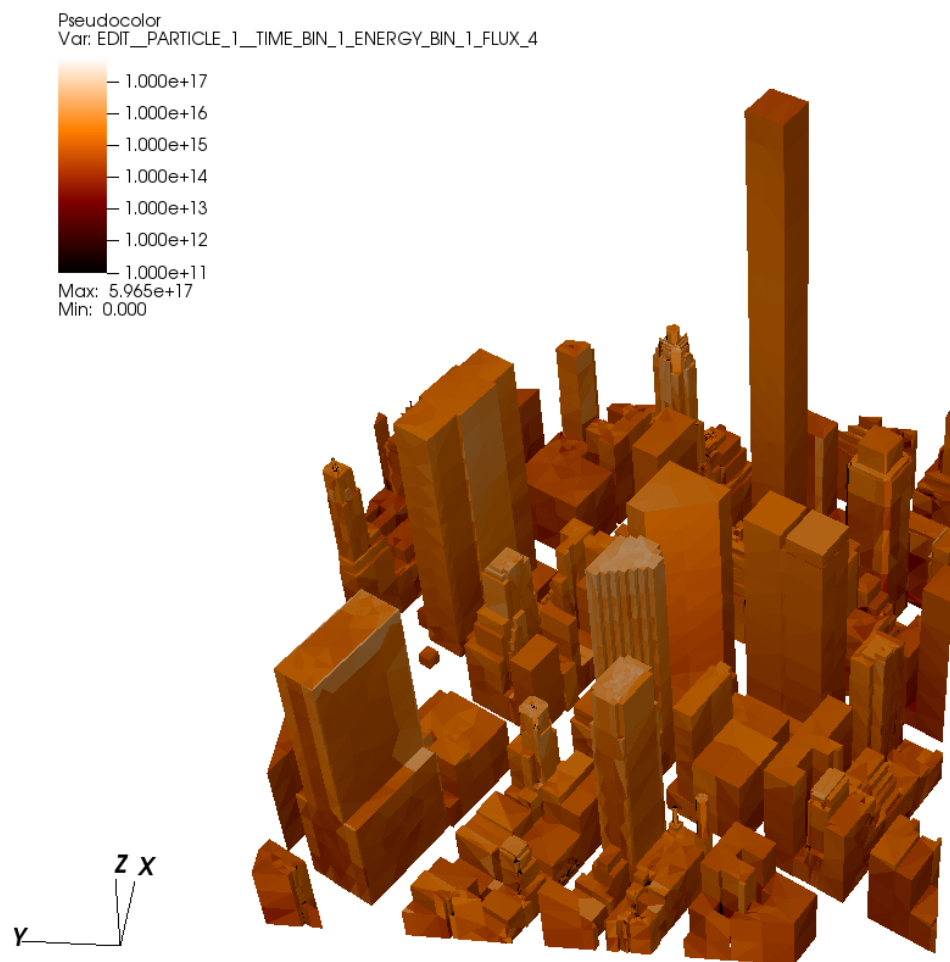


Figure 16: Energy Integrated Neutron Flux (n/cm²) over Trump Tower

A.6 Example MCNP Input File

```
No description for this unstructured mesh file
c
c   Created from file      : One_More_Time.inp
c   Created on            : 10- 2-2018 @ 14:48: 5
c
c
c PSEUDO CELLS
01      1      -2.35      0   u=1
02      2      -2.36      0   u=1
03      3      -2.37      0   u=1
04      4      -2.38      0   u=1
05      5      -2.39      0   u=1
06      6      -2.40      0   u=1
07      7      -2.41      0   u=1
08      8      -0.001205  0   u=1
c
c LEGACY CELLS
09      0              -99   fill=1
10      0              99
c
c SURFACES
99   sph    2.19869E+04   2.19139E+04   2.13152E+04   4.51704E+04
c
c DATA CARDS
embed1 meshgeo=abaqus
      mgeoin=example_for_doc_abaqus.inp
```

```

meeout=example_for_doc.eeout
length= 1.00000E+00
background=      8
matcell=  1  1  2  2  3  3  4  4  5  5  6  6  7  7
c
embee4:n embed=1
c Ordinary Concrete PNNL
c rho = 2.35 g/cc
M1 1001 -0.008485
      6000 -0.050064
      8016 -0.473483
      12000 -0.024183
      13027 -0.036063
      14000 -0.145100
      16000 -0.002970
      19000 -0.001697
      20000 -0.246924
      26000 -0.011031
M2 1001 -0.008485
      6000 -0.050064
      8016 -0.473483
      12000 -0.024183
      13027 -0.036063
      14000 -0.145100
      16000 -0.002970
      19000 -0.001697
      20000 -0.246924
      26000 -0.011031
M3 1001 -0.008485
      6000 -0.050064

```

	8016	−0.473483
	12000	−0.024183
	13027	−0.036063
	14000	−0.145100
	16000	−0.002970
	19000	−0.001697
	20000	−0.246924
	26000	−0.011031
M4	1001	−0.008485
	6000	−0.050064
	8016	−0.473483
	12000	−0.024183
	13027	−0.036063
	14000	−0.145100
	16000	−0.002970
	19000	−0.001697
	20000	−0.246924
	26000	−0.011031
M5	1001	−0.008485
	6000	−0.050064
	8016	−0.473483
	12000	−0.024183
	13027	−0.036063
	14000	−0.145100
	16000	−0.002970
	19000	−0.001697
	20000	−0.246924
	26000	−0.011031
M6	1001	−0.008485
	6000	−0.050064

```

      8016  -0.473483
      12000 -0.024183
      13027 -0.036063
      14000 -0.145100
      16000 -0.002970
      19000 -0.001697
      20000 -0.246924
      26000 -0.011031
M7 1001  -0.008485
      6000  -0.050064
      8016  -0.473483
      12000 -0.024183
      13027 -0.036063
      14000 -0.145100
      16000 -0.002970
      19000 -0.001697
      20000 -0.246924
      26000 -0.011031
m8 6000  -0.000124
      7014  -0.755268
      8016  -0.231781
      18000 -0.012827
c
c
nps 1E6
imp:n 1 8R 0
c Source location is 100 m above Trump Tower
sdef pos 16.379905E3 22.19021E3 30.36501E3 erg 2.0
print

```

A.7 Patch for um_post_op

```
— um_post_op_vtk_mod.F90          2018-10-17 08:15:17.023909759 -0400
+++ um_post_op_vtk_mod_fixed.F90    2018-10-17 08:20:52.903898114 -0400
@@ -173,7 +173,7 @@
      write(nfout, '(A,I20,A)') "POINTS ", nNodes, " float"

      do i = 1, nNodes
-         write(nfout, '(3(1X,F12.6))') xyzNodes(i,1:3)
+         write(nfout, '(3(1X,F12.6))') xyzNodes(1:3,i)
      end do

      ! Find the total connectivity data.
```

B ACTIUM Manual

UM Activation Documentation

Release 0

Tucker McClanahan

Nov 12, 2019

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ACTIVATION

This class sets up and runs activation calculation.

Developer: Tucker McClanahan (tmcclan@lanl.gov or tmcclana@vols.utk.edu)

class `um_activation.activation.Activation`

Bases: `object`

This class method that sets up the activation run.

...

run_options

Run_Options class object that contains the run options

Type `object`

cinder_options

Cinder_Options class object that contains the cinder options

Type `object`

files

Files class object that contains the details of the outp, bigza, and eeout files

Type `object`

timesteps

TimeSteps class object that contains the details of the timesteps that are used in the activation calculation

Type `object`

worker_database

Worker_Database class object that contains the results for each worker

Type `object`

G

continue_run

Set option to True if this is a continue run

Type `bool` (default: False)

run_activation()

Run the activation calculation.

set_cinder_working_directory (*cinderwd*)

Set the cinder working directory.

set_num_mesh_elements (*number*)

Set the number of mesh elements to run through.

FILE PARSERS

2.1 bigza_file

Contains BIGZA file data

Developer: Tucker McClanahan (tmcclan@lanl.gov or tmcclana@vols.utk.edu)

class `um_activation.file_parsers.bigza_file.BIGZA_File` (*filename*)

Bases: `object`

Class that contains the data for one BIGZA File

...

Parameters `filename` (*str*) – Name of the BIGZA File

filename

Name of the BIGZA File

Type `str`

nuclides

Array of Nuclide class objects

Type `ndarray`

elements

Array of Natural Element class objects

Type `ndarray`

Nuclide

Class containing information on a nuclide

Type `class(object)`

parse_input ()

Reads and assigns the data to proper variables

get_natural_abundance (*nuclide_number*)

Returns the natural abundance fraction of a nuclide corresponding to the *nuclide_number* in the BIGZA File

get_atomic_weight (*nuclide_number*)

Returns the atomic weight of the nuclide in amu corresponding to the *nuclide_number* in the BIGZA File

get_natural_isotopics (*element_number*)

Returns a dictionary of key-value pairs: Keys -> Nuclide numbers Values -> Nuclide class object corresponding to nuclide number

```

get_elemental_weight (element_number)
    Returns a float of the elemental weight

get_elemental_nuclides (element_number)
    Returns ndarray(int) of the nuclide numbers corresponding to the element number

is_element (zam)
    Returns whether or not the zam is an element in the BIGZA file

is_nuclide (zam)
    Returns whether or not the zam is a nuclide in the BIGZA file

class Element (number)
    Bases: object

    Class that stores the data for one element

    ...

    Parameters number (int) – Element number (Z0000)

number
    Element number (Z0000)
    Type int

elemental_weight
    Elemental weight of the nuclide
    Type float

nuclides
    Array of nuclides that make up the natural isotopics of the element
    Type ndarray(float)

set_elemental_weight (elemental_weight)
    Assigns the elemental_weight input to the elemental weight of the class

add_nuclide (number)
    Adds a nuclide to the nuclides list

get_nuclides ()
    Returns a ndarray of nuclides that make up the natural element

get_elemental_weight ()
    Returns the elemental weight in amu

get_number ()
    Returns the element number Z000

add_nuclide (number)
    Adds the number to the list of nuclide numbers in self.nuclides

get_elemental_weight ()
    Returns the elemental weight of the element

get_nuclides ()
    Returns a ndarray(int) of the nuclides

get_number ()
    Returns the Z000 number of the element

set_elemental_weight (weight)
    Assigns the weight to self.elemental_weight

```

```

class Nuclide(number)
    Bases: object

    Class that stores the data for one nuclide

    ...

    Parameters number (int) – Nuclide number ( $ZAM = Z*10000+A*10+M$ )

number
    Nuclide number ( $ZAM = Z*10000+A*10+M$ )
    Type int

atomic_weight
    Atomic weight of the nuclide
    Type float

natural_abundance
    Natural abundance of the nuclide
    Type float

set_atomic_weight (atomic_weight)
    Assigns the atomic_weight input to the atomic weight of the class

set_natural_abundance (natural_abundance)
    Assigns the natural_abundance input to the natural abundance of the class

get_atomic_weight ()
    Returns the atomic weight in amu

get_natural_abundance ()
    Returns the natural abundance in fraction

get_number ()
    Returns the ZAM number of the nuclide

get_atomic_weight ()
    Returns the atomic weight of the nuclide

get_natural_abundance ()
    Returns the natural abundance of the nuclide

get_number ()
    Returns the ZAM number of the nuclide

set_atomic_weight (atomic_weight)
    Assigns the atomic_weight to self.atomic_weight

set_natural_abundance (nat_abun)
    Assigns the nat_abun to self.natural_abundance

get_atomic_weight (nuclide)
    Returns the atomic weight of nuclide

get_elemental_nuclides (element_number)
    Returns a ndarray(int) of the nuclides of a specific element

get_elemental_weight (element_number)
    Returns the elemental weight in amu of the element

get_natural_abundance (nuclide)
    Returns the natural abundance fraction of a nuclide

```

get_natural_isotopics (*element_number*)

Returns the dictionary of Nuclide classes that make up the natural isotopics of the element (nuclides that have natural abundances)

is_element (*zam*)

Determine if zam is a element.

is_nuclide (*zam*)

Determine if zam is a element.

parse_input ()

Reads in the data from the BIGZA file

2.2 eeout_file

Contains class for reading the eeout file from a MCNP6.2 run.

Developer: Tucker McClanahan (tmcclan@lanl.gov or tmcclana@vols.utk.edu)

class um_activation.file_parsers.eeout_file.EEOUT_File (*filename*)

Bases: `object`

Class for one eeout file's contents.

...

Parameters *filename* (*str*) – Path and name of the eeout file

filename

Name of the original eeout file

Type `str`

File_Type

Parameter that tells if file is in ASCII or Binary format

Type `str`

Mesh_Source

Source of what produced the mesh file (example: ABAQUS)

Type `str`

Version

Version number of the EEOUT file

Type `int`

Prob_ID

MCNP6 user supplied problem description

Type `str`

Calling_Code

Code using the library

Type `str`

Code_Version

Code using the library version

Type `str`

Date_Time

Date and time the EEOUT file was generated

Type `str`

Inp_File

MCNP6 input file used to generate the EEOUT file

Type `str`

Outp_File

MCNP6 output file used to generate the EEOUT file

Type `str`

Runtpe_File

MCNP6 runtpe file used to generate the EEOUT file

Type `str`

Geom_Inp_File

Abaqus input file that contains the mesh description

Type `str`

Num_Particles

Number of particles in the calculation

Type `int`

Num_Nodes

Number of nodes in mesh

Type `int`

Num_Mats

Number of materials in calculation

Type `int`

Num_Instances

Number of instances in mesh

Type `int`

Num_First_Tets

Number of first order tetrahedral elements in mesh

Type `int`

Num_First_Pents

Number of first order pentagonal elements in mesh

Type `int`

Num_First_Hexs

Number of first order hexagonal elements in mesh

Type `int`

Num_Second_Tets

Number of second order tetrahedral elements in mesh

Type `int`

Num_Second_Pents

Type int Number of second order pentagonal elements in mesh

Num_Second_Hexs

Number of second order hexagonal elements in mesh

Type int

Num_Histories

Number of histories from the Monte Carlo calculation upon which the edit results are based

Type int

Num_Edits

Number of edits or embee cards that were specified in the input

Type int

Length_Conversion

Multiplier needed to convert from the units of the original mesh model to centimeters. This value has already been applied to all coordinates appearing in the EEOUT file.

Type float

Norm_Factor

Normalization factor that has been applied to all results in the file

Type float

Particle_List

Particle numbers from the calling code. These numbers correspond to the numbers used to identify MCNP6 particle types. Example: 1 is neutron, 2 is photon

Type ndarray(int)

Particle_Edit_List

2D array mapping particles to the edits where the first index is for the edit number and the second index is for the particle type. The value stored in the array is the internal edit number to which the particle contributes.

Type ndarray(int)

Edit_Description

A set of 6 integers that describe the edits in the EEOUT file. Index 0: number of different particles Index 1: number of elemental edits Index 2: number of elemental edits Index 3: maximum number of problem energy bins Index 4: maximum number of problem time bins Index 5: maximum number of problem response bins

Type ndarray(int)

Edit_Data_Groups

Variable number of data-sets which describe details of the elemental edits.

Keys: Particle numbers from Particle_List Value: Edit_Data_Group_Data_Structure class object

Type dict

Edit_Data_Group_Data_Structure

Data Structure for the Edit_Data_Groups dictionary

Type class(object)

Materials

Alphanumeric names of the materials

Type ndarray(str)

Cumulative_Instance_Element_Totals

The cumulative value of elements added to instances as the instances are added to the part.

Type ndarray(int)

Instance_Element_Names

Alphanumeric names of the pseudo-cells. One record for each pseudo-cell.

Type ndarray(str)

Instance_Element_Type_Totals

2D array of one record of 12 integers per pseudo-cell in the model in the same order as the Instance_Element_Names. Using the following notation for the indexes [i,j] where i is the index of the pseudo-cells:

Index j=0: First element number of first-order tetrahedra type Index j=1: Last element number of first-order tetrahedra type Index j=2: First element number of first-order pentahedra type Index j=3: Last element number of first-order pentahedra type Index j=4: First element number of first-order hexahedra type Index j=5: Last element number of first-order hexahedra type Index j=6: First element number of second-order tetrahedra type Index j=7: Last element number of second-order tetrahedra type Index j=8: First element number of second-order pentahedra type Index j=9: Last element number of second-order pentahedra type Index j=10: First element number of second-order hexahedra type Index j=11: Last element number of second-order hexahedra type

Type ndarray(int)

Nodes

Class containing the details on the X, Y, and Z nodes

Type class(object)

Element_Type

Element type for each of the global element starting at 1 and proceeding to the maximum number of elements in the mesh model where each element type is as follows:

4 = First-order tetrahedra 5 = First-order pentahedra 6 = First-order hexahedra 14 = Second-order tetrahedra 15 = Second-order pentahedra 16 = Second-order hexahedra

Type ndarray(int)

Element_Material

Material number assigned to each element starting at 1 to the maximum number of elements in the mesh model

Type ndarray(int)

Connectivity_Data

Nodes for each element of a specific type of meshal element. Keys:

‘first-order_tet’ ‘first-order_pent’ ‘first-order_hex’ ‘second-order_tet’ ‘second-order_pent’
‘second-order_hex’

Values (for each key): ndarray(int) – 2D array of node numbers with indexes [i,j] where i is the index corresponding to element number and j is the index corresponding to the connectivity of a side of the element

Type dict

Nearest_Neighbor

Element numbers for each element of the neighboring element ordered by face number. Keys:

‘first-order_tet’ ‘first-order_pent’ ‘first-order_hex’ ‘second-order_tet’ ‘second-order_pent’
‘second-order_hex’

Values (for each key): ndarray(int) – 2D array of node numbers with indexs [i,j] where i is the index corresponding to element number and j is the index corresponding to the nearest neighbor face of the element

Type dict

Data_Results

Edit set results stored in Data_Results_Structure class objects

Type ndarray(class(object))

Data_Set_Groups_Data_Structure

Data strcture for the Data_Results array

Type class(object)

Centroids

Class object of the centroid data in x,y,z.

Type class(object)

Density_Data

Densities for each element in mesh

Type ndarray(float)

Volume_Data

Volumes for each element in mesh

Type ndarray(float)

parse_input ()

Reads in the EEOU file and assigns the appropriate values to the variables above.

get_data_results (particle_number, edit_list_number)

Returns the Data Results Structure class for the particle number and edit list number supplied

class Centroid_Data_Structure

Bases: object

Centroids in mesh

...

X

x-locations of nodes 1 through max number of centroids in (cm)

Type ndarray(float)

Y

y-locations of nodes 1 through max number of centroids in (cm)

Type ndarray(float)

Z

z-locations of nodes 1 through max number of centroids in (cm)

Type ndarray(float)

```

set_as_ndarray()
    Convert the lists to numpy arrays

class Data_Results_Structure (meb, mtb)
    Bases: object
    Data Structure for the Data Set Groups objects
    ...

    Parameters
    • meb (int) – Maximum number of energy bins from the Edit Description array (index 3)
    • mtb (int) – Maximum number of time bins from the Edit Description array (index 4)

particle_number
    MCNP6 particle number
    Type int

edit_list_number
    Edit number
    Type int

comment
    User-added comment
    Type str

data_set
    Data results in a 3D array where the indexes are [e,t,en] where e is the energy bin number, t is the time
    bin number, and en is the element number.
    Type ndarray(float)

time_bins
    Time upper bin edge values
    Type ndarray(float)

time_mult_bins
    Time mulitplier bin values
    Type ndarray(float)

energy_bins
    Energy upper bin edge values
    Type ndarray(float)

energy_mult_bins
    Energy multiplier bin values
    Type ndarray(float)

total_time_data
    Total time data broken up into energy bins
    Type ndarray(float)

total_energy_data
    Total energy data broken into time bins
    Type ndarray(float)

set_as_ndarray()
    Convert the lists to numpy arrays and slice the data_set array down to applicable size

set_as_ndarray (leb, ltb)
    Convert the lists to ndarrays and slice the data_set array

```

```

...
Parameters
  • leb (int) – Last energy bin
  • ltb (int) – Last time bin

class Edit_Data_Group_Data_Structure
  Bases: object

  Data structure for the Edit Data Groups

  ...

  internal_edit_number
    Internal edit number
    Type int

  user_edit_number
    User edit number; negative if errors requested
    Type int

  combined_energy_deposition
    Special combined energy deposition indicator; 9 if a combined edit; 0 otherwise
    Type int

  REGL_particle_number
    Particle number in REGL
    Type int

  MCNP6_particle_number
    Particle number from MCNP6
    Type int

  num_energy_bins
    Number of energy bins
    Type int

  num_time_bins
    Number of time bins
    Type int

  num_response_bins
    Number of response bins
    Type int

  energy_unit_conv_factor
    Energy unit conversion factor
    Type float

  time_unit_conv_factor
    Time unit conversion factor
    Type float

  upper_energies
    upper energy cut points for the energy bins
    Type ndarray(float)

  energy_mult
    energy multipliers
    Type ndarray(float)

```

```

upper_times
    upper time cut points for the time bins
    Type ndarray(float)

time_mult
    time multipliers
    Type ndarray(float)

upper_responses
    upper response cut points for the response bins
    Type ndarray(float)

response_mult
    response multipliers
    Type ndarray(float)

class Nodes_Data_Structure
    Bases: object
    Nodes in the mesh
    ...
    x
        x-locations of nodes 1 through max number of nodes in (cm)
        Type ndarray(float)
    y
        y-locations of nodes 1 through max number of nodes in (cm)
        Type ndarray(float)
    z
        z-locations of nodes 1 through max number of nodes in (cm)
        Type ndarray(float)
    set_as_ndarray()
        Convert the lists to numpy arrays

get_data_results(particle_number, edit_list_number)
    Return the Data Results Structure class.

    This method returns the Data Results Structure class corresponding to the particle_number and
    edit_list_number.

parse_input()
    Parses input from the eeout file.

```

2.3 mcnp6_outp_file

Contains MCNP6 outp file data

Developer: Tucker McClanahan (tmcclan@lanl.gov or tmcclana@vols.utk.edu)

```

class um_activation.file_parsers.mcnp6_outp_file.MCNP6_Outp(filename)
    Bases: object

```

Class that contains the data for one MCNP6 output file using unstructured mesh

...

Parameters *filename* (*str*) – Name of the MCNP6.2 output file

filename

Name of the MCNP6.2 output file

Type `str`**materials****Dictionary of materials in the file where:** Keys -> material numbers (int) Values -> Material class objects**Type** `dict`**Material**

Data structure for one material

Type `class(object)`**parse_input ()**

Reads and assigns the data to proper variables

get_atom_fraction (material_number)**Returns the atom fraction dictionary where:** Keys -> zam ($Z*10000+A*100+M$) of the nuclide Values -> atom fraction**get_mass_fraction (material_number)****Returns the mass fraction dictionary for the material number where:** Keys -> zam ($Z*10000+A*100+M$) of the nuclide Values -> mass fraction**class Material**Bases: `object`

Material Class that contains the information for a material in the MCNP output file

...

number

Material number

Type `int`**atom_fraction**Keys-> ZAM ($Z*10000+A*100+M$) Values-> atom fraction for the ZAM**Type** `dict`**mass_fraction**Keys-> ZAM ($Z*10000+A*100+M$) Values-> mass fraction for the ZAM**Type** `dict`**atom_density**

Atom density of the material in atoms/b-cm

Type `float`**gram_density**

Density of the material in g/cc

Type `float`**add_atom_fraction (zam, fraction)**

Add atom fraction data

add_mass_fraction (zam, fraction)

Add mass fraction data

```

get_atom_density()
    Return the atom density variable.

get_atom_fraction()
    Retrieves atom fraction dict

get_gram_density()
    Return the gram density variable.

get_mass_fraction()
    Retrieves mass fraction dict

get_number()
    Retrieves material number

set_atom_density(number)
    Set atom density.

set_gram_density(number)
    Set gram density.

get_atom_fraction(material_number)
    Returns the atom_fraction dictionary for a specific material_number

get_mass_fraction(material_number)
    Returns the mass fraction dictionary for a specific material_number

get_materials()
    Return the materials dictionary.

parse_mcnp_output()
    Reads in the data from the MCNP6.2 output file

```

2.4 spectra_file

Contains class for processing the spectra files from a CINDER 08 run

Developer: Tucker McClanahan (tmccclan@lanl.gov or tmccclana@vols.utk.edu)

```

class um_activation.file_parsers.spectra_file.Spectra(sp_file)
    Bases: object

    Class for one spectra_ts_decay, spectra_l, or spectra_h file's contents.

    ...

    Parameters sp_file (str) – spectra_ts_decay, spectra_l, or spectra_h filename

filename
    Filename of the spectra_ts_decay, spectra_l or spectra_h file

    Type str

energies
    Energies of the gamma spectrum

    Type ndarray(float)

timesteps
    Timestep Class objects

    Type ndarray(object)

```

times

Timesteps (sec) from the CINDER2008 activation run

Type ndarray(float)

total_gammas

Total gammas for each timestep

Type ndarray(float)

Timestep

Class containing information pertaining to a specific timestep

Type class(object)

parse_input (*sp_file*)

Reads in the file and assigns values to the energies and timesteps arrays.

Examples

```
>>> from AARE.spectra_file_tools import Spectra
>>> spectra_file_data = Spectra('spectra_h')
```

```
>>> spectra_file_data.energies
array([ 0.00000000e+00,  1.00000000e-02,  3.00000000e-02,  6.00000000e-02,  1.
↪00000000e-01,  2.00000000e-01,  3.00000000e-01,  5.00000000e-01,  5.25000000e-
↪01])
```

```
>>> spectra_file_data.times
10.0
```

```
>>> spectra_file_data.timesteps[5].gamma_data
array([ 7.25300000e-06,  0.00000000e+00,  0.00000000e+00,  1.74200000e-04,  2.
↪58800000e-04,  0.00000000e+00,  5.70100000e-03,  9.71600000e-01,  2.55300000e-
↪03])
```

class Timestep (*line*)

Bases: object

Class containing information for one timestep.

...

Parameters *line* (*str*) – One line from the filename file

source_on

Source on (True) or off (False)

Type bool

time

Time of the timestep in seconds

Type float

total_gammas

Normalization value of the gamma spectrum

Type float

gamma_data

Gamma spectrum intensities in gammas/sec/energy_bin

Type ndarray(floats)

add_data (*line*)

Add another value of gamma data from the line.

Keyword arguments: line – String value of one line from the spectra_ts_decay_file

parse_input ()

Read the sp_file and populate the energies and timesteps numpy arrays.

2.5 tables_by_nuclide_file

Contains class for reading the tables_by_nuclide file from a CINDER08 run

Developer: Tucker McClanahan (tmcclan@lanl.gov or tmcclana@vols.utk.edu)

class um_activation.file_parsers.tables_by_nuclide_file.TBN (*tables_file*)

Bases: `object`

Class for one tables_by_nuclide file's contents.

...

Parameters **tables_file** (*str*) – Path and name of the tables_by_nuclide file

filename

Filename of the tables_by_nuclide file

Type `str`

timesteps

Timestep structure of the file

Type `ndarray(float)`

times

Cumulative time structure of the file

Type `ndarray(float)`

nuclides

Keys: zam of nuclide ($z*10000+a*10+m$) Values: Nuclide class objects

Type `dict`

total_mass

Total mass in each timestep

Type `ndarray(float)`

total_activity

Total activity in each timestep

Type `ndarray(float)`

total_atom_density

Total atom density in each timestep

Type `ndarray(float)`

total_activity_density

Total activity density in each timestep

Type `ndarray(float)`

total_decay_power_density
Total decay power density for each timestep
Type ndarray(float)

total_decay_power
Total decay power for each timestep
Type ndarray(float)

total_macroscopic_particle_absorption
Total macroscopic particle absorption for each timestep
Type ndarray(float)

total_radionuclide_hazard_air_dilution_factor
Total radionuclide hazard air dilution factor for each timestep
Type ndarray(float)

total_radionuclide_hazard_water_dilution_factor
Total radionuclide hazard water dilution factor for each timestep
Type ndarray(float)

total_spontaneous_fission_density
Total spontaneous fission density for each timestep
Type ndarray(float)

total_spontaneous_fission_power_density
Total spontaneous fission power density for each timestep
Type ndarray(float)

total_spontaneous_fission_power
Total spontaneous fission power for each timestep
Type ndarray(float)

total_n_fission_density
Total (N,Fission) density for each timestep
Type ndarray(float)

total_n_fission_power_density
Total (N, Fission) power density for each timestep
Type ndarray(float)

total_n_fission_power
Total (N, Fission) power for each timestep
Type ndarray(float)

total_total_fission_density
Total bin of the total fission density for each timestep
Type ndarray(float)

total_total_fission_power_density
Total bin of the total fission power density for each timestep
Type ndarray(float)

total_total_fission_power
Total bin of the total fission power for each timestep

Type ndarray(float)

total_multigroup_gamma_spectra_low

Total multigroup gamma spectra low for each timestep

Type ndarray(float)

total_multigroup_gamma_spectra_high

Total multigroup gamma spectra high for each timestep

Type ndarray(float)

total_total_air_dilution_volume

Total bin of the total air dilution volume for each timestep

Type ndarray(float)

total_total_water_dilution_volume

Total bin of the total water dilution volume for each timestep

Type ndarray(float)

total_fraction_CAT3_threshold

Total fraction CAT3 threshold for each timestep

Type ndarray(float)

total_dose

Total dose for each timestep

Type ndarray(float)

total_threshold_ratio

Total threshold ratio for each timestep

Type ndarray(float)

Nuclide

Object that contains the data for one nuclide

Type class(object)

parse_input ()

Reads the tables_by_nuclide file and builds the nuclides dictionary and timesteps array

write_mcnp_mat_card (filename, tsn, mat_num)

Creates a mcnp material card using the material details for a specific timestep

Examples

```
>>> from AARE.tables_by_nuclide_file_tools import TBN
>>> file_data = TBN('tables_by_nuclide')
```

```
>>> file_data.nuclides[130261].name
'Al26m1'
```

```
>>> file_data.nuclides[130261].halflife
6.3452
```

```
>>> file_data.timesteps
array([ 1.00000000e-08,  1.00000000e-06,  1.00000000e+00,
        5.00000000e+00,  1.00000000e+01,  3.00000000e+01])
```

```
>>> file_data.total_activity
array([ 0.00000000e+00,  3.52000000e-08,  1.55700000e-12,
        9.60200000e-13,  5.65000000e-13,  8.37900000e-14])
```

```
>>> file_data.nuclides[130261].mass
array([ 0.00000000e+000,  2.18300000e+001,
        1.95700000e+001,  1.26400000e+001,
        7.32200000e+000,  8.23700000e-001])
```

class Nuclide

Bases: `object`

Class that contains the data for one nuclide

...

name

Elemental name of the nuclide

Type `str`

z

Atomic number of the nuclide

Type `int`

a

Atomic mass of the nuclide

Type `int`

m

Metastable state of the nuclide

Type `int`

zam

Identifier of the nuclide $z*10000+a*10+m$

Type `int`

halflife

Halflife of the nuclide in seconds

Type `int`

mass

Masses in kg over each timestep

Type `ndarray(floats)`

activity

Activities in Ci over each timestep

Type `ndarray(floats)`

atom_density

Atom densities in a/barn-cm over each timestep

Type `ndarray(floats)`

activity_density

Activity density in Ci/cm3 over each timestep

Type `ndarray(floats)`

decay_power_density
Decay power density in (watts/cc) for each timestep
Type ndarray(float)

decay_power
Decay power (watts) for each timestep
Type ndarray(float)

macroscopic_particle_absorption
Macroscopic particle absorption in (/cm) for each timestep
Type ndarray(float)

radionuclide_hazard_air_dilution_factor
Radionuclide hazard air dilution factor for each timestep
Type ndarray(float)

radionuclide_hazard_water_dilution_factor
Radionuclide hazard water dilution factor for each timestep
Type ndarray(float)

spontaneous_fission_density
Spontaneous fission density in (#/cc-s) for each timestep
Type ndarray(float)

spontaneous_fission_power_density
Spontaneous fission power density in (watts/cc) for each timestep
Type ndarray(float)

spontaneous_fission_power
Spontaneous fission power in (watts) for each timestep
Type ndarray(float)

n_fission_density
(N,Fission) density in (#/cc-s) for each timestep
Type ndarray(float)

n_fission_power_density
(N, Fission) power density in (watts/cc) for each timestep
Type ndarray(float)

n_fission_power
(N, Fission) power in (watts) for each timestep
Type ndarray(float)

total_fission_density
Total fission density (#/cc-s) for each timestep
Type ndarray(float)

total_fission_power_density
Total fission power density (watts/cc) for each timestep
Type ndarray(float)

total_fission_power
Total fission power (watts) for each timestep
Type ndarray(float)

multigroup_gamma_spectra_low
Multigroup gamma spectra low in (#/bin-s-cc) for each timestep
Type ndarray(float)

multigroup_gamma_spectra_high

Multigroup gamma spectra high in (#/bin-s-cc) for each timestep

Type ndarray(float)**total_air_dilution_volume**

Total air dilution volume for each timestep

Type ndarray(float)**total_water_dilution_volume**

Total water dilution volume for each timestep

Type ndarray(float)**fraction_CAT3_threshold**

Fraction CAT3 threshold for each timestep

Type ndarray(float)**dose**

Dose for each timestep

Type ndarray(float)**threshold_ratio**

Threshold ratio for each timestep

Type ndarray(float)**get_zam** (*line*)

Assigns name, z, a, m, and zam of the nuclide

Parameters **line** (*str*) – Line from the tables_by_nuclide file**Notes**Primarily used in the `parse_input()` function**parse_input** ()

Parses the data in the tables_by_nuclide file

Notes`parse_input()` populates the following attributes of the TBN class:

timesteps

nuclides

total_mass

total_activity

total_atom_density

total_activity_density

write_mcnp_mat_card (*filename*, *tsn*, *mat_num*)

Creates a mcnp material card using the material details for a specific timestep

...

Parameters

- **filename** (*str*) – Filename that is to be created and the material card written to
- **tsn** (*int*) – Index of timestep

- `mat_num` (*int*) – Material number that is to be written in the material card.

Example

```
>>> TBN.write_mcnp_mat_card('test_mat_card.txt', 2, 3)
(within 'test_mat_card.txt' data for Al-28 for timestep number 2 )
m3 13028 -1.0
```

METHODS

3.1 process_materials

This method processes a given material object.

Developer: Tucker McClanahan (tmcclan@lanl.gov or tmcclana@vols.utk.edu)

class `um_activation.methods.process_materials.Process_Materials` (*materials*,
bigza_file)

Bases: `object`

This method processes a given material.

...

Parameters

- **materials** (*list*) – list of Material class objects
- **bigza_file** (*object*) – BIGZA_File class

materials

Materials class object from the parameters

Type `class`

bigza_file

BIGZA_File class object from the parameters

Type `class`

cinder_materials

List of Cinder Material class objects

Type `list`

get_cinder_materials ()

Returns ndarray of Cinder Material class objects

get_cinder_material_numbers ()

Returns ndarray of cinder material numbers: float

class Cinder_Material

Bases: `object`

Class that contains the details a Cinder Material.

...

number

Material number

Type `int`

atom_fraction
 Keys: `int` -> ZAM ($Z*10000+A*10+M$) Values: `float` -> Atom fraction
Type `dict`

mass_fraction
 Keys: `int` -> ZAM ($Z*10000+A*10+M$) Values: `float` -> Mass fraction
Type `dict`

atom_density
 Atomic density in atoms/b-cm
Type `float`

gram_density
 Density in g/cc
Type `float`

set_atom_density (*number*)
 Assigns the atom_density to number

get_atom_density ()
 Returns the atom_density value

set_gram_density (*number*)
 Assigns number to gram_density

get_gram_density ()
 Returns the gram_density value

get_number ()
 Returns the material number

get_atom_fractions ()
 Returns dict of atom fractions

get_atom_fraction (*zam*)
 Returns atom fraction value for the zam

add_atom_fraction (*zam*, *fraction*):
 Adds a dict entry to atom_fraction with: Key -> zam Value -> fraction

add_atom_fraction (*zam*, *fraction*)
 Add atom fraction data.

get_atom_density ()
 Return the atom density variable.

get_atom_fraction (*zam*)
 Return the atom fraction for zam.

get_atom_fractions ()
 Retrieve atom fraction dict.

get_gram_density ()
 Return the gram density variable.

get_number ()
 Retrieve material number.

set_atom_density (*number*)
 Set atom density.

```

set_gram_density (number)
    Set gram density.

set_number (number)
    Set material number.

get_cinder_material (material_number)
    Return Cinder Material class object of material number.

get_cinder_material_numbers ()
    Return ndarray of cinder material numbers.

get_cinder_materials ()
    Return ndarray of cinder materials classes.

```

3.2 process_fluxes

This method processes a given flux.

Developer: Tucker McClanahan (tmcclan@lanl.gov or tmcclana@vols.utk.edu)

```

class um_activation.methods.process_fluxes.Process_Fluxes (energies, flux, cin-
                                                         der_library)

```

Bases: `object`

This method processes a given flux.

This method takes in a energy ndarray and flux ndarray and rebins it to match the CINDER library energy group structure.

...

Parameters

- **energies** (*ndarray*) – Upper bin edges in MeV
- **flux** (*ndarray*) – Flux value for each energy bin
- **cinder_library** (*str*) – Path to cinder library

energies

Upper bin edges in MeV of the incoming energies

Type `list`

flux

Flux values in units n/E_bin/s

Type `list`

cinder_energies

Upper bin edges in MeV of the cinder library energy group structure

Type `list`

cinder_library

Path to the cinder library

Type `str`

rebinned_fluxes

Rebinned flux values with the cinder library energy group structure with units of n/E_bin/s

Type `ndarray`

get_rebinned_fluxes ()
Returns the rebinned fluxes ndarray

get_rebinned_fluxes ()
Return the rebinned fluxes.

3.3 write_input_file

This method writes the CINDER2008 input file.

Developer: Tucker McClanahan (tmcclan@lanl.gov or tmcclana@vols.utk.edu)

class um_activation.methods.write_input_file.**Write_Input_File**(*cinder_options*,
timesteps,
file_location)

Bases: `object`

This method writes the input file.

This class takes in the *file_location*, cinder options and timesteps class objects and writes an CINDER2008 input file to the path specified in the *file_location* variable.

...

co

Cinder Options class object

Type `object`

ts

TimeSteps class object

Type `object`

file_location

Path to the working directory for CINDER

Type `str`

3.4 write_material_file

This method writes the CINDER2008 material file.

Developer: Tucker McClanahan (tmcclan@lanl.gov or tmcclana@vols.utk.edu)

class um_activation.methods.write_material_file.**Write_Material_File**(*cinder_material*,
mesh_element_number,
file_location)

Bases: `object`

This method writes the material file.

...

Parameters

- **cinder_material** (*obj*) – Cinder Material Class
- **mesh_element_number** (*int*) – Mesh element number
- **file_location** (*str*) – Full path to where the material file should be located

3.5 write_locate_file

This method writes the CINDER2008 locate file.

Developer: Tucker McClanahan (tmcclan@lanl.gov or tmcclana@vols.utk.edu)

```
class um_activation.methods.write_locate_file.Write_Locate_File(library_path,
                                                             cindergl_path,
                                                             file_location)
```

Bases: `object`

This method writes the locate file.

...

This method takes in the `cinder_options` class object and writes the locate file in the `file_location` directory, which includes the full paths to the CINDER data library, `cindergl.dat` file, etc.

Parameters

- **library_path** (*str*) – Full path to the CINDER library
- **cindergl_path** (*str*) – Full path to the `cindergl` file
- **file_location** (*str*) – Full path to the CINDER working directory

library_path

Full path to the CINDER library

Type `str`

cindergl_path

Full path to the `cindergl` file

Type `str`

file_location

Full path to the CINDER working directory

Type `str`

3.6 calculate_tet_dose

This method calculates the dose from boundary tets

Developer: Tucker McClanahan (tmcclan@lanl.gov or tmcclana@vols.utk.edu)

```
class um_activation.methods.calculate_tet_dose.Calculate_Tet_Dose(database,
                                                                parts_of_interest=None,
                                                                write_to_database=True)
```

Bases: `object`

This method calculates the dose on tetrahedral boundary elements.

This method uses the dose factors from: D. C. Kocher and K. F. Eckerman, “External Dose-Rate Conversion Factors for Calculation of Dose to the Public,” ORNL, DOE/EH-0070, Jul. 1988. to calculate the dose on the boundary tetrahedral elements by calculating the surface area and applying the dose factors per isotope activity in each boundary mesh element. The dose results are in units of mrem/hr when they are written to the existing HDF5 final database.

...

Parameters

- **database_filename** (*str*) – Path to the HDF5 database
- **parts_of_interest** (*list*, *optional*) – List of names of parts as strings of the parts where dose will be calculated (Default: Calculate dose for all parts)
- **write_to_database** (*bool*) – Whether or not to write the calculated dose to the HDF5 database (Default: True)

database_filename

Path to the HDF5 database

Type *str***database**

h5py File class object of the HDF5 database defined by database_filename

Type *object***dose_factors****Keys:** *str* Isotope name**Values:** *float* Dose coefficient in units of mrem/yr per uCi/(square meter)Type *dict***surface_areas****Keys:** *str* Part names**Values:** *ndarray* Surface area values for each mesh element as the average of the boundary faces in units of (square cm)Type *dict***dose****Keys:** *str* Isotope dataset path**Values:** *dict***Keys:** *str* Isotope names**Values:** *ndarray* Dose from the Isotope for each mesh element in units of (mrem/hr)Type *dict***total_dose****Keys:** *str* Timestep group paths**Values:** *ndarray* Total Dose for each mesh element in units of (mrem/hr)Type *dict***load_effective_dose_coeffs ()**

Assigns the dose_factors dictionary

calculate_surface_areas ()

Assigns the surface_areas dictionary

calculate_dose ()

Assigns the dose dictionary

add_dose_datasets ()

Add dose datasets to the HDF5 database.

calculate_dose ()

Calculate the dose of the boundary mesh elements.

This module calculates the dose from the boundary mesh elements using the dose_factors, activity, and surface_areas data to calculate the dose at 1 meter away from the surface in air.

calculate_surface_areas ()

Calculate the surface areas boundary mesh elements.

This module calculates the boundary mesh elements and their average boundary face surface area to combine with the dose factors.

load_effective_dose_coeffs ()

Read in the dose coefficients.

3.7 write_hdf5_database

This method creates the HDF5 database.

Developer: Tucker McClanahan (tmcclan@lanl.gov or tmclana@vols.utk.edu)

class `um_activation.methods.write_hdf5_database.Worker_Database` (*rank*)

Bases: `object`

This method provides the data structure to store the worker's results.

This method creates an in-memory database that will later be merged into one large hdf5 database.

...

Parameters

- **mesh_element_number** (*int*) – Current mesh element number
- **tbn** (*TBN class object*) – The data from the table by nuclides file
- **timesteps** (*list*) – List of upper bin edge timesteps
- **instances** (*dict*) – Keys: Instance name Values: dicts

These are dictionaries of the first and last elements of a specific instance Keys: 'first', 'last' Values: first element, last element

database

Keys: HDF5 path to dataset Values: np.array

These are arrays of values for each dataset with the length of these datasets equal to the number of mesh elements in the specific part

Type `dict`

name

Name of the worker

Type `str`

worker_database_directory

Path of the worker database directory

Type `str`

Write_To_Database()

Writes the bulk information to the database

Get_Worker_Database()

Returns the database of the worker

Set_Worker_Directory(*worker_directory*)

Set the worker directory variable with worker_directory

Write_Backup_File()

Set_Worker_Directory(*workerwd*)

Set and create worker directory.

Write_Backup_File()

Write the backup file of the worker database.

Write_To_Database(*mesh_element_number, tbn, timesteps, instances*)

Write the database.

Writes the data from a single cinder run to the worker database. This data includes the following: - Mass Data - Activity Data - Atom Density Data - Totals of all the data types

```
class um_activation.methods.write_hdf5_database.Write_HDF5_Database(hdf5_filename,
                                                                    ee-
                                                                    out_file,
                                                                    timesteps)
```

Bases: `object`

This method creates the HDF5 database.

This method creates the HDF5 database that contains the details of the unstructured mesh and the results from the cinder calculations.

...

Parameters

- **hdf5_filename** (*str*) – Path and filename of the HDF5 database
- **eeout_file** (*object*) – EEOUT_FILE class object
- **timesteps** (*object*) – Timesteps class object

Write_to_database()

Writes the bulk information to the final HDF5 database

Write_to_database()

Write the HDF5 database.

This definition writes the bulk information about the mesh to the main HDF5 database. This bulk information is for every mesh element for each instance and it includes:

- Node Data
- Connectivity Data
- Material Number
- Mass Density
- Volume
- Centroid Data

```
class um_activation.methods.write_hdf5_database.Write_Worker_HDF5_Database(h5_file,
                                                                           mesh_element_number,
                                                                           tbn,
                                                                           timesteps,
                                                                           in-
                                                                           stances)
```

Bases: `object`

This method creates a worker HDF5 database.

This method creates the temporary worker hdf5 database that will later be merged into one large hdf5 database.

...

Parameters

- **h5_file** (*hdf5.File object*) – File object of the worker hdf5 database
- **mesh_element_number** (*int*) – Current mesh element number
- **tbn** (*TBN class object*) – The data from the table by nuclides file
- **timesteps** (*list*) – List of upper bin edge timesteps
- **instances** (*dict*) – Keys: Instance name Values: dicts

These are dictionaries of the first and last elements of a specific instance Keys: 'first', 'last' Values: first element, last element

Write_to_database()

Writes the bulk information to the final HDF5 database

Write_to_database()

Write the HDF5 database.

Writes the data from a single cinder run to the worker database. This data includes the following: - Mass Data - Activity Data - Atom Density Data - Totals of all the data types

3.8 write_xdmf_file

This method writes the XDMF file to accompany the HDF5 database.

Developer: Tucker McClanahan (tcmclan@lanl.gov or tmclana@vols.utk.edu)

```
class um_activation.methods.write_xdmf_file.Write_XDMF_File(hdf5_database_filepath,
                                                             nu-
                                                             clides_of_interest=[],
                                                             at-
                                                             tributes_of_interest=[])
```

Bases: `object`

This method writes the XDMF file to accompany the HDF5 database. ...

hdf5_database_filename

Filename for the hdf5 database

Type `str`

nuclides_of_interest

List of ZAMs that will be included in the XDF5 file

Type `list`

CALCULATION PROPERTIES

4.1 cinder_options

This class sets up the cinder options.

Developer: Tucker McClanahan (tmcclan@lanl.gov or tmcclana@vols.utk.edu)

class `um_activation.calculation_properties.cinder_options.Cinder_Options`

Bases: `object`

This class contains cinder options.

...

title

Title of the run

Type `str`

norm

Normalization value used to scale results

Type `float`

volume

Volume of the cell in cc

Type `float`

tst

Chain cut off with regard to nuclide density fraction of the previous time step (default is 0.0, which implies no cut off)

Type `float`

signif

Chain cut off with regard to initial nuclide density fraction or activity of initial time step (default is 0.0, which implies no cut off)

Type `float`

epsm

$\exp(-arg) = 1$ for $arg < epsm$ $1 - \exp(-arg) = arg$ for $arg < epsm$ (default is 0.0)

Type `float`

epsn

Reciprocal of a power of 10 having exponent not exceeding the significant digits of the computer stored word (default is 0.0)

Type float

exponmax

Maximum exponent guaranteed (default 0.0)

Type float

fine

Fine group structure using gamma discrete line decay library (default is 1E4)

Type int

coarse

Coarse group structure using gamma discrete line decay library (default is 1E3)

Type int

kchn

Request of chains file (default 0, meaning no chain file is produced in the run)

Type int, {0, 1}

klib

Request of libcheck file (default 0, meaning no libcheck file is produced in the run)

Type int, {0, 1}

nfe

0 is 'none', 1 is 'thermal', 2 is 'fast', 3 is 'high-energy' Fission product flag (default is 3 meaning 'high-energy')

Type int, {0, 1, 2, 3}

nlintl

Number of titles (default is 1)

Type int

nosame

Chain loops allowed (default is 0 meaning False)

Type int, {0, 1}

library_path

Path to CINDER cross section library (default is '/usr/local/aare/data/C08lib_flat')

Type str

cxupdate

Path to Cross section library update (default is '')

Type str

cindergl

Path to cindergl.dat file (default is '/usr/local/aare/data/cindergl.dat')

Type str

tabcode

Run tabcode (default is 0 meaning False)

Type int, {0, 1}

post

Run post (default is 0 meaning False)

Type int, {0, 1}

itsord

Time step number used for ordering the tables by nuclide (default is -1 meaning the last time step will be used)

Type `int`

wspect

0 is 'flat', 1 is 'spallation', 2 is 'fission', 3 is 'fusion' Weighting spectrum used for re-binning the neutron fluxes (default is 0 meaning flat)

Type `int`, {0, 1, 2, 3}

set_volume(volume) :

Set volume with the float volume

get_volume() :

Return the volume value

set_title(title) :

Set title with the string title

get_title() :

Return the title string

set_norm(number)

Sets the normalization value to number

get_norm()

Returns the normalization value

check_environmental_variables()

Checks to see if the relevant environmental variables have been set and then assigns them to the appropriate variables if they have been set

set_tst(number)

Sets the tst with number

set_signif(number)

Sets the signif with number

set_epsm(number)

Sets the epsm with number

set_epsn(number)

Sets the epsn with number

set_exponmax(number)

Sets exponmax with number

set_fine(number)

Sets fine as number

set_coarse(number)

Sets coarse as number

set_kchn(option)

Sets kchn with option

set_klib(option)

Sets klib with option

set_nfe(option)

Sets nfe with option

set_nlintl (*number*)
Sets nlintl with number

set_nosame (*option*)
Sets nosame with option

set_library_path (*path*)
Sets library_path with path

set_cxupdate (*path*)
Sets cxupdate with path

set_cindergl (*path*)
Sets cindergl with path

set_tabcode (*option*)
Sets tabcode with option

set_itsord (*number*)
Sets itsord with number

set_wspect (*option*)
Sets wspect with option

get_tst ()
Gets the tst

get_signif ()
Gets the signif

get_epsm ()
Gets the epsm

get_epsn ()
Gets the epsn

get_exponmax ()
Gets exponmax

get_fine ()
Gets fine

get_coarse ()
Gets coarse

get_kchn ()
Gets kchn

get_klib ()
Gets klib

get_nfe ()
Gets nfe

get_nlintl ()
Gets nlintl

get_nosame ()
Gets nosame

get_library_path ()
Gets library_path

get_cxupdate()
Gets cxupdate

get_cindergl() 76
Gets cindergl

get_tabcode()
Gets tabcode

get_itsord()
Gets itsord

get_wspect()
Gets wspect

check_environmental_variables()
Check for environmental variables.

get_cindergl()
Get the cindergl path.

get_coarse()
Get the coarse number.

get_cxupdate()
Get the cxupdate path.

get_epsm()
Get the epsm number.

get_epsn()
Get the epsn number.

get_exponmax()
Get the exponmax number.

get_fine()
Get the fine number.

get_itsord()
Get the itsord number.

get_kchn()
Get the kchn option.

get_klib()
Get the klib option.

get_library_path()
Get the library_path path.

get_nfe()
Get the nfe option.

get_nlintl()
Get the nlintl number.

get_norm()
Return the normalization value.

get_nosame()
Get the nosame option.

get_post()
Get the post option.

get_signif()
Get the signif number.

get_tabcode()
Get the tabcode option.

get_title()
Return the title string.

get_tst()
Get the tst number.

get_volume()
Return the volume value.

get_wspect()
Get the wspect option.

set_cindergl(*path*)
Set the cindergl path.

set_coarse(*number*)
Set the coarse number.

set_cxupdate(*path*)
Set the cxupdate path.

set_epsm(*number*)
Set the epsm number.

set_epsn(*number*)
Set the epsn number.

set_exponmax(*number*)
Set the exponmax number.

set_fine(*number*)
Set the fine number.

set_itsord(*number*)
Set the itsord number.

set_kchn(*option*)
Set the kchn option.

set_klib(*option*)
Set the klib option.

set_library_path(*path*)
Set the library_path path.

set_nfe(*option*)
Set the nfe option.

set_nlintl(*number*)
Set the nlintl number.

set_norm(*number*)
Set norm value with number.

set_nosame (*option*)
Set the nosame option.

set_post (*option*)
Set the post option.

set_signif (*number*)
Set the signif number.

set_tabcode (*option*)
Set the tabcode option.

set_title (*title*)
Set title with the string title.

set_tst (*number*)
Set the tst number.

set_volume (*volume*)
Set volume with the float volume.

set_wspect (*option*)
Set the wspect option.

4.2 files

This class sets up and runs activation calculation.

Developer: Tucker McClanahan (tcmcclan@lanl.gov or tmclana@vols.utk.edu)

class `um_activation.calculation_properties.files.Files`

Bases: `object`

Class contains the file paths needed for activation run.

...

mcnp6_outp_file

Path to the mcnp6 outp file

Type `str`

bigza_file

Path to the bigza file

Type `str`

eeout_file

Path to the eeout file

Type `str`

set_mcnp6_outp_file_path (*path*)

Sets the mcnp6 outp file path

set_bigza_file_path (*path*)

Sets the bigz file path

set_eeout_file_path (*path*)

Sets the eeout file path

load_mcnp6_outp_file (*mcnp6_outp_file*)

Returns mcnp6_outp_file class object containing mcnp6 output contents

```

load_bigza_file (bigza_file)
    Returns bigza_file class object

load_eeout_file (eeout_file)
    Returns eeout_file class object

check_environmental_variables ()
    Check for environmental variables.

load_bigza_file (file=None)
    Return the BIGZA_File class object.

load_eeout_file (file=None)
    Return the EEOUT_File class object.

load_mcnp6_outp_file (file=None)
    Return the MCNP6_Outp file class object.

set_bigza_file_path (path)
    Set the bigza_file with path.

set_eeout_file_path (path)
    Set the eeout_file with path.

set_mcnp6_outp_file_path (path)
    Set the mcnp6_outp_file with path.

```

4.3 run_options

This class sets up the run options.

Developer: Tucker McClanahan (tcmcclan@lanl.gov or tmclana@vols.utk.edu)

```

class um_activation.calculation_properties.run_options.Run_Options
    Bases: object

    Class to contain the run options.

    ... .. attribute:: code_name
        Name of the CINDER2008 executable

        type str

    number_of_cores
        Number of cores the activation calculation can occupy

        Type int (default 1)

    elemental_edit_number
        Elemental Edit Number

        Type int (default 1)

    particle_number
        Particle number corresponding to the same particle numbers in MCNP

        Type int (default 1)

    directory_name
        Used to form a directory name for saving the activation code input and output files Default: 'run'

        Type str

```

directory_counter

Value to be appended to the directory name Default: 1

Type `int`

use_spallation_products

Whether or not to use spallation products Default: False

Type `bool`

use_tabular

Whether or not to use neutron activation Default: True

Type `bool`

use_verbose

Whether or not to save intermediate files Default: False

Type `bool`

set_particle_number (*number*)

Sets the particle_edit_number with number

get_particle_number ()

Returns the particle_number

set_elemental_edit_number (*number*)

Sets the element_edit_number with number

get_elemental_edit_number ()

Returns the elemental_edit_number

set_code_name (*name*)

Sets the code name to name if it can find name in the path

get_code_name ()

Returns the code_name

set_number_of_cores (*number*)

Sets the number of cores used by the activation calculation

get_number_of_cores ()

Returns the number_of_cores

set_directory_name (*name*)

Sets the directory_name variable with name

set_directory_counter (*number*)

Sets the directory_counter variable with number

set_use_spallation_products (*option*)

Sets the use_spallation_products variable with option

set_use_tabular (*option*)

Sets the use_tabular variable with option

set_use_verbose (*option*)

Sets the use_verbose variable with option

get_directory_name ()

Gets the directory_name variable with name

get_directory_counter ()

Returns the directory_counter variable

get_use_spallation_products ()
Returns the use_spallation_products variable

get_use_tabular ()
Returns the use_tabular variable

get_use_verbose ()
Returns the use_verbose variable

set_use_mpi (option)
Sets the use_mpi variable to option

get_use_mpi ()
Returns the use_mpi variable

get_code_name ()
Return the code_name variable.

get_directory_counter ()
Get the directory_counter int.

get_directory_name ()
Get the directory_name str.

get_elemental_edit_number ()
Return the elemental_edit_number.

get_number_of_cores ()
Return the number of cores.

get_particle_number ()
Return the particle_number.

get_use_mpi ()
Get use_mpi variable.

get_use_spallation_products ()
Get the use_spallation_products bool.

get_use_tabular ()
Get the use_tabular bool.

get_use_verbose ()
Get the use_verbose bool.

set_code_name (name)
Set the code_name.

set_directory_counter (number)
Set the directory counting number.

set_directory_name (name)
Set directory_name to name.

set_elemental_edit_number (number)
Set elemental_edit_number with number.

set_number_of_cores (number)
Set number_of_cores value with number.

set_particle_number (number)
Set particle_number with number.

set_use_mpi (*option*)
Set use_mpi with option.

set_use_spallation_products (*option*)
Set whether or not to use spallation products.

set_use_tabular (*option*)
Set whether or not to use tabular.

set_use_verbose (*option*)
Set whether or not to use verbose.

4.4 time_steps

This class contains the details of the time_steps.

Developer: Tucker McClanahan (tmcclan@lanl.gov or tmcclana@vols.utk.edu)

class um_activation.calculation_properties.time_steps.TimeSteps

Bases: `object`

Class to contain time_steps data.

...

times

Array of upper time edges of the timesteps in seconds (Each timestep is from the beginning of time to the timestep value)

Type ndarray

powers

Array of powers (for each timestep)

Type ndarray

add_timestep (*time*, *time_unit*='s', *power*=1.0)

Adds a single timestep to the data

add_timesteps (*times*, *time_units*=None, *power*=None)

Adds the times array to the data assuming the 's' as the time units and 1.0 as the powers

get_timesteps ()

Returns the times and powers numpy arrays sorted by increasing times

add_timestep (*time*, *time_unit*='s', *power*=1.0)

Add timestep.

...

Parameters

- **time** (*number*) – Upper bound of the timestep
- **time_unit** ({'s', 'm', 'h', 'd', 'w', 'y'}, *optional*) – Unit of time
- **power** (*number*, *optional*) – Power associated with the time

add_timesteps (*times*, *time_units*=None, *powers*=None)

Add multiple timesteps.

get_timesteps()

Return timesteps and powers numpy arrays.

class timestep (*time, power*)

Bases: `object`

Single timestep data.

Vita

Tucker McClanahan was born in Knoxville, TN and graduated from Powell High School in 2011. He completed his bachelor's degree from the University of Tennessee, Knoxville (UTK) in 2015 with Magna Cum Laude standing. In August of 2015, Tucker began his graduate studies at UTK and received a Master of Science Degree in Nuclear Engineering in May 2017. Tucker's undergraduate and master's research was done at Oak Ridge National Laboratory at the Spallation Neutron Source where he was a part of experimental campaigns and neutronic support teams. Tucker was accepted into the UTK Department of Nuclear Engineering PhD program in January 2017, and began research at the Institute for Nuclear Security. In the summer of 2017, Tucker began a graduate research assistant position at Los Alamos National Laboratory (LANL) in the Intelligence and Space Research Division and is now in the Radiation Transport Applications Group. He completed his PhD in May 2020 and is planning on working at LANL.