Design and Implementation of a Radiation Transport Code Input Generation Interface

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ABSTRACT

Accurate modeling of radiation transport is essential for ensuring the safety and reliability of nuclear reactors. To achieve precision and safety, Monte Carlo N-Particle Transport Code (MCNP) and modeling software under the SCALE code system simulate the behavior of radiation transport. The Workbench Analysis Sequence Processor (WASP) project provides the necessary tools to efficiently enable data access and processing. Our project utilizes WASP in an interface design that produces problem-specific radiation transport code inputs. Each database is JSON-formatted, thus utilizing a universal format and WASP components in structuring the material composition data. The implementation includes methods for building, checking, and translating information into an acceptable format. Furthermore, the code structure can be integrated into a graphical user interface, offering enhanced accessibility and alleviating the effort of manual input generation. Thus, our project's products provide an accessible, accurate, and error-free approach to generating material descriptions for radiation transport simulations.

Project Statement

The interface designed during the duration of this research aims to provide a means of generating efficient, accurate radiation transport code inputs for use in SCALE and MCNP.

INTRODUCTION

This project focuses on the development of a tool to interpret information about materials composition and radioactive materials from national laboratory databases. The WASP project enables the data access and processing to parse and interpret the databases. The tool's functionality hinges around a series of methods that build, prepare, and display the data to be transformed into a radiation transport code input. To ensure quality assurance, the interface undergoes extensive testing before becoming an available interface. The developed interface will handle radiation transport input generation.

Table 1. Variation of radiation transport code inputs for Acetone.

SCALE MAVRIC/Keno

```
'  PNNL-15870Rev2
'  Acetone, C3H6O, 0.7899
g/cm^3
'  The above density is
estimated to be accurate to 4
significant digits.
Uncertainties are not
addressed.
'  The following data was
calculated from the input
formula.
     wtptAcetone  1  0.7899  3
          1000   10.4131
          6000   62.0392
          8000   27.5476   end
```

MCNP

```
c  PNNL-15870Rev2
c  Acetone, 0.7899 g/cm3
c  The above density
is estimated to be accurate
to 4 significant digits.
Uncertainties
are not addressed.
c  The following data was
calculated from the input
formula.
   m1 1000  -0.104131
      6000  -0.620392
      8000  -0.275476
```

SCALE ORIGEN

```
% 1 gram of acetone using
Weight Fractions
mat {
    iso= [ H=0.104131
           C=0.620392
           O=0.275476 ]
    units=grams
}
```

Generic

```
#  PNNL-15870Rev2
#  Acetone, 0.7899 g/cm^3
       1   H   0    0.104131
       6   C   0    0.620392
       8   O   0    0.275476
c  Generic Weight Fractions
```

METHODS AND MATERIALS

- Two types of database files, material composition and mass database, were used during this project.
  - ❖ It employs 15 different sources of material data with 9,590 materials that have both composition and density.
- Materials composition information from the various databases are read using data structures and algorithms provided by WASP.
- Three primary classes were developed to define databases, their materials, and their compositions. Likewise, three classes were constructed to read in data from a masses database, defining the database, the materials, and the isotopes.
- The "Database" and "Masses" classes have functions to "build" objects by assigning read-in values to their data members. Objects can also be displayed, converted to several composition types, and formatted for SCALE and MCNP code systems.

Quality Assurance

- Ninja, ctest, and tools from WASP were instrumental in building environments and running tests on the interface.
- Checks internal to the interface and tests run by ctest allow developers to measure accuracy and provide quality assurance of the project.

```
{ "Name": "Water",
  "Density": 1.0,
  "Type": "Chemical Formula",
  "Formula": "H2O",
  "Contains": [
     {"Element": "H", "Atoms": 2.0 },
     {"Element": "O", "Atoms": 1.0 }
]
}
```

Figure 1. Water Chemical Formula Material from ARH-600

RESULTS

➢The interface prepares radiation transport inputs using composition conversions and formatting standards. Five conversions transform object compositions among weight fractions, atomic fractions, and atoms per molecule.
➢A program was written to simulate the functionality of a graphical user interface (GUI). The stand-in GUI linked each material to its index and each specified command to an integer. The commands were as follows.

0) Display Masses
1) Display Material
2) Search
3) Advanced Search
4) Change Material
5) Check Components
6) Create a Nuclear Code

Future Work

By making available an intuitive and widely accessible input generation tool, this project strives to tackle the challenges associated with input generation in radiation transport simulations. The future progress of this project will see a visual representation of this interface built into popular code systems (SCALE or MCNP). Accordingly, errors recorded in databases should be easier to catch by the time the code is integrated.

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