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Generating Models of the Flattop Critical Assembly for Benchmark Experiments with Python

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INTRODUCTION

Los Alamos National Laboratory has been performing nuclear criticality experiments since 1946 at the Pajarito site, starting the Los Alamos Critical Experiments Facility in 1948 [1]. A transition period occurred between 2004 and 2011 as operations moved to the National Criticality Experiments Research Center (NCERC), where criticality experiments are now performed [2]. Criticality experiments are essential for determination and verification of nuclear data used in calculations and modeling—such as radiation transport codes—throughout the industry, enhancing nuclear criticality safety [3]. In addition to nuclear data validation and benchmarking, the remotely operated critical assemblies at NCERC are used for a variety of experiments and training classes supporting criticality safety [4].

Flattop

Operations began on the Flattop critical assembly in 1958, performing fundamental reactor physics research focusing on its simple one-dimensional spherical structure [5]. Previously, Flattop's simple geometry was utilized for fast-energy benchmark critical experiments. More recently, Flattop has been primarily used for a combination of fission/activation product experiments, dosimetry testing, and training classes, on top of other criticality safety experimentation [4].

Flattop's geometry remains constant, with a central spherical core region surrounded by a thick natural uranium (NU) reflector. Two central spherical cores are currently available: an HEU core and a delta-phase WGPu core. The mass and specifics of the central spherical core can be adjusted using mass adjustment buttons, glory hole pieces, and pedestal caps. The consistency in configurations allows for comparable and repeatable experiments, even over many years. The Flattop central spherical core sits on a NU pedestal. The pedestal-core is placed into a stationary hemisphere of NU, and two quarter spheres of NU move to complete a spherical NU reflector around the core. Each of these components are shown in the disassembled view in Fig. 1.

Fig. 2 shows a schematic of Flattop with all sections assembled and in place, with a plan view and an elevation view in the upper and lower schematics, respectively. Furthermore, a cross section of the assembly is shown in Fig. 3. Additional components of the assembly are shown in these figures, notably the three control rods (the large rod "F" and small rods "G" and "E") and the glory hole that allows for additional pieces of fissile material, spacers, or samples to be irradiated.

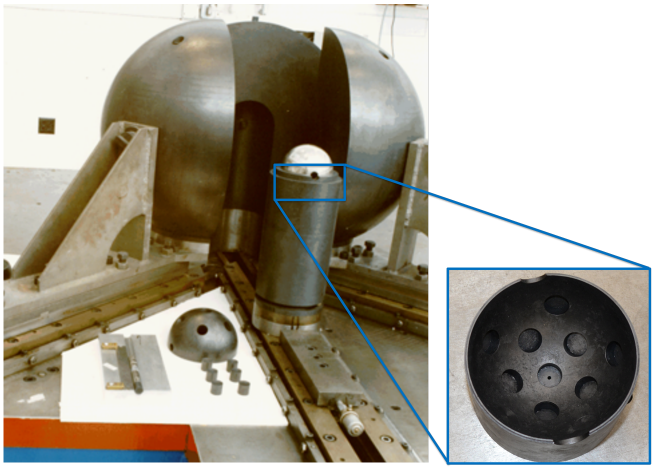

Fig. 1: The disassembled Flattop critical assembly [6]. Highlighted region of the pedestal is shown from a top-down view without the core, displaying the mass adjustment button locations.

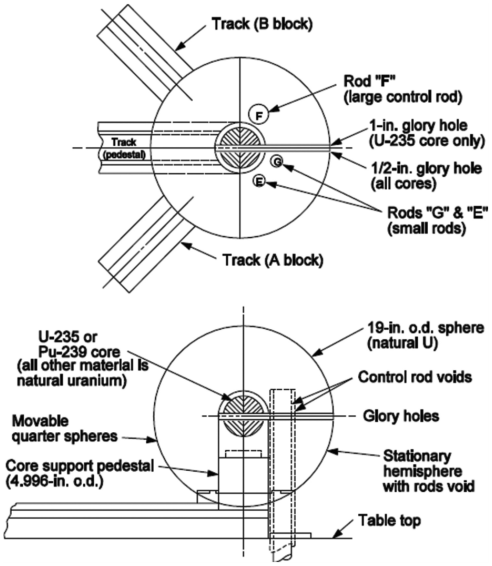

Fig. 2: Flattop critical assembly schematic [4].

Flattop has been used for a number of benchmark critical experiments presented in the International Criticality Safety Benchmark Evaluation Project (ICSBEP), including HEU-MET-FAST-028 (known as Flattop-HEU) [4, 7]. The Flattop-HEU criticality benchmark experiment was performed in the mid-1960s and used a highly enriched uranium (HEU) sphere as the core, reflected by NU [8].

Flattop-HEU was chosen to be reevaluated to better characterize the assembly [9]. Flattop's frequent use for reactivity worth measurements and criticality safety training classes ben-

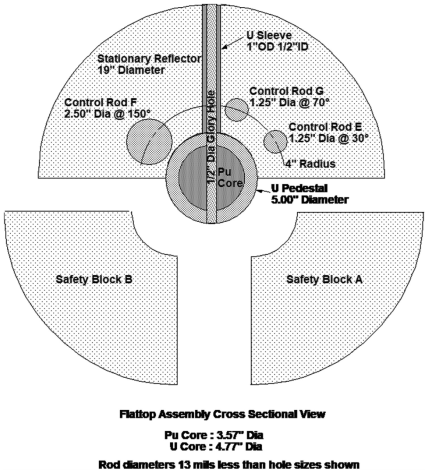

Fig. 3: Flattop critical assembly cross section [4].

efits from improved characterization. A detailed Monte Carlo N-Particle® Transport Code (MCNP®)[1] model—not currently in the ICSBEP handbook—was developed in 2016 and is shown in Fig. 4 [10]. However, there are many uncertainties associated with the physical parameters of the HEU and NU parts in particular. This leads to a discrepancy between the experimental k_{eff} of 1.00344 ± 0.00001 and the calculated k_{eff} using the detailed model (computed using MCNP6.1.1b and ENDF/B-VII.1 cross section data) of 1.00976 ± 0.00002 [9]. These uncertainties originate from a lack of reported parameters in the original Flattop-HEU benchmark as well as other available documentation.

MODEL ACCURACY AND MEASUREMENTS

Running the detailed model using MCNP6.2 and ENDF/B-VIII.0 cross section data yields a k_{eff} value of 1.00776 ± 0.00002 [10, 11]. The previously reported difference between the experimental and calculated values was 0.00632 [9]. Between the minor model adjustments made since then and the use of more recent versions of MCNP and ENDF, this difference has decreased by nearly a third to 0.00432. The use of the updated data library is likely the primary contributor, indicating an improvement in cross section data to more accurately reflect experimental realities. The use of the measurements is expected to further decrease this difference between the experimental and calculated values.

The mass and volume uncertainties associated with the HEU and NU parts preliminarily yield relative k_{eff} uncertainties of ±0.00071 and ±0.00137, respectively. It is seen that these values are the largest uncertainty contributions by comparing these values to the total estimated uncertainty in the benchmark k_{eff} of ±0.00157 (with an uncertainty of $+100\%/-0\%$) [9]. Measurements to determine the dimensions of the parts using a coordinate measuring machine and calipers have been completed [4]. If possible, mass values were measured using a scale, and volume values were determined using a pycnometer. The inclusion of accurate measurements will provide for a model with increased accuracy and a more representative k_{eff} value. The work detailed in this paper is in support of quick preliminary analysis of this modeling.

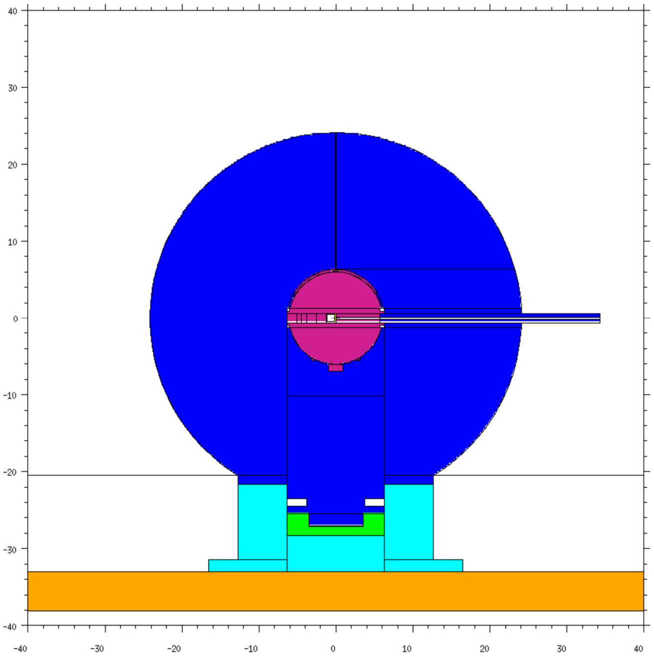

Fig. 4: Flattop critical assembly detailed MCNP model view of X-Z plane through y = 0.03 cm. Dark red is HEU, dark blue is NU, light blue and orange are steel, green is brass, yellow is aluminum, and white is void [9].

FLATTOP MODEL GENERATION

In anticipation of these measurements, a Python script was written to edit the detailed Flattop model input file. It is expected that the use of Python will allow for quick, complete, and precise adjustments to the Flattop model. The purpose of this script is twofold: to simplify creation of MCNP models for various Flattop configurations (using the mass adjustment buttons, glory hole pieces, and pedestal caps) and to develop a script structure that may be utilized moving forward to generate a full, standalone model with interdependent parameters.

Regarding the first goal, a base MCNP input file has been adapted from the previous detailed Flattop model. Since the majority of the Flattop geometry remains constant for each configuration, the base file will remain mostly identical while the script "inserts" pieces from an inventory list in the desired arrangement. Updates were made to remove the included configuration, adjust some values with those measured, and to include the proper ASTM-A7-46 bridge steel composition for the table [12]. Fig. 5 shows two 3D views of this updated model, which is seen to be similar to the previous model aside from the configurational components.

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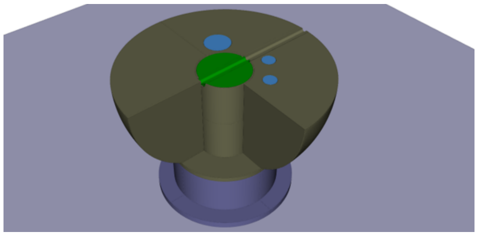
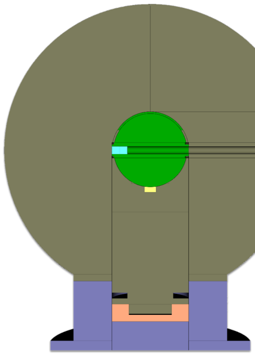
[1] MCNP® and Monte Carlo N-Particle® are registered trademarks owned by Triad National Security, LLC, manager and operator of Los Alamos National Laboratory. Any third party use of such registered marks should be properly attributed to Triad National Security, LLC, including the use of the designation as appropriate. For the purposes of visual clarity, the registered trademark symbol is assumed for all references to MCNP within the remainder of this paper.



(a) Base model, cut by X-Y plane through z = 0 (safety block A hidden).



(b) Generated model, cut by X-Z plane through y = 0.

Fig. 5: Two 3D cross-sectional views of the Flattop model (using gxsview). The HEU core and glory hole adapter are shown in green, the NU reflector and pedestal are shown in gold, the NU control rods are shown in light blue, the brass pedestal adapter is orange, the carbon steel support base is dark gray, and the bridge steel table is light gray. The glory hole pieces are shown in light blue and the mass adjustment buttons are yellow.

A "Part" class was defined containing instance attributes associated with part parameters, methods to perform volume and density calculations, and methods to create strings for surface cards, cell cards, and material cards. The below pseudocode gives an overview of this class definition.

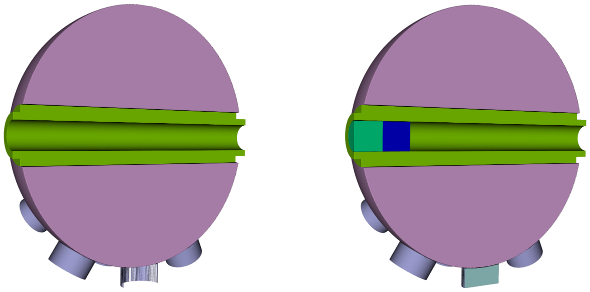
Part Class Pseudocode

```
initialize instance attributes for part name, ID #, shape,
dimensions, mass, material name, material card number,
isotopic breakdown and fractions, and ENDF library to use;
calculate extra dimensions (e.g., radius from diameter);
and combine isotopic breakdown and fractions into 1 array
- vol_calc method:
    if shape is XYZ -> calculate volume from formula
    if shape has other shapes within -> calculate volume
        & subtract other shape
- den_calc method:
    calculate mass density with rho = m/V
    calculate atomic density with N = (rho x Na)/M
- mat_card method:
    create material card (code adapted from N. Thompson)
- surf_card method:
    if shape is XYZ -> use surface/macrobody type XYZ,
        start at given coordinates,
        bound at coordinates calculated from dimensions
- cell_card method:
    format cell card string with part attributes, index
    #, den_calc method, and given surfaces
```

Dictionaries and arrays containing the part information were defined and used to create the Part objects. A configuration is made using a dictionary containing a list of Part objects for the glory hole piece order (and a list of floats to adjust offsets between pieces), a list of Part objects for the mass adjustment button positions, and several strings stating if specific parts are in use. A function is called using a name for the input file and the specified configuration dictionary. The code excerpt below shows how the configuration in Fig. 5b was generated. Fig. 6 shows a side-by-side comparison of the base input file and the generated configuration, focused on the core to highlight the glory hole pieces and mass adjustment buttons.

Configuration Specification Code

```
flattop_config = {
     ’core’ : ’HEU’,
     ’GH config’ : [GH_8283B, GH_8287],
     ’GH air offset’ : [0., 0., 0., 0., 0.],
     ’MA config’ : [’MT’, ’MT’, ’MT’, MA_8494, ’MT’,
        ’MT’, ’MT’, ’MT’, ’MT’, ’MT’, MA_8491],
     ’Cap’ : ’10913’,
     ’adapter’ : ’yes’,
     ’sleeve’ : ’yes’}
# call input file generation function
input_gen(’flattop_gen’, flattop_config)
```



(a) Base (b) Generated

Fig. 6: 3D closeup views (using gxsview), cut by the X-Z plane through y = 0, of the Flattop HEU core with glory hole reducer and mass adjustment holes in the pedestal. Fig. 6a shows the base input file geometry, and Fig. 6b shows the modified configuration input file geometry including two glory hole pieces and two mass adjustment buttons (center button visible).

A header is generated for the new file, the text from the base input file is copied into the new file, and surface, cell, and material cards are created using information from one another and those from other parts. These input files are then run using MCNP to determine the k_{eff} value and the corresponding reactivity worth of the piece configuration.

FULL GENERATION & UNCERTAINTY ANALYSIS

While this has only been used so far to develop configurations, generation of the base model could also be easily incorporated into this, inherent to the script’s second purpose. Certain script capabilities would need to be further developed for this, and these sections have been marked by raising

"NotImplementedError." Completing model updates manually leads to several potential issues due to its complexity. The Flattop model contains geometry defined by multiple surfaces that are dependent upon a single part dimension. This is best dealt with by adjusting the surfaces simultaneously to ensure completeness. Additionally, these values will need to be changed several times for each dimension due to the measurement uncertainties. Calculating volumes and updating densities corresponding to the dimensional changes is also necessary. Keeping track of these edits would prove to be time-consuming and error-prone by hand whereas coding allows for the focus to be maintained on determining the interconnected parameters. The code itself then performs the value adjustments both quickly and simultaneously. From the interdependence of the configuration pieces it is seen that this approach works, and the methodology would work as well for full model generation using the new measurements and any potential measurement updates moving forward.

In this case, the script will also be expanded to include uncertainty analysis, which the code is uniquely suited for. Three input files will then be generated for each dimension with associated uncertainty: one using the measured values for all dimensions, one incorporating the negative uncertainty of the specified dimension and all other measured values, and one incorporating the positive uncertainty in the same manner. These parametric perturbations will detail how significant the effect of the corresponding uncertainties of each measurement is on k_{eff} by running the input files using MCNP. These uncertainty considerations specifically may be well-addressed using the MCNP parameter study tool (pstudy) [13]. This option, instead of that previously detailed, would allow for a single input file to be generated for each dimension rather than three while still examining the effect of the measurement uncertainties.

CONCLUSION

This work is being performed to assist the modeling efforts of the Flattop critical assembly, specifically for the Flattop-HEU critical benchmark experiment reevaluation. This updated Flattop model will be informed by precise measurements of the assembly to yield a high-fidelity model. Accurate model development for this reevaluation may help validation of available nuclear data.

The development of this Python script will also lead to the more efficient use of the Flattop critical assembly moving forward, past the Flattop-HEU benchmark reevaluation. Generating input files will be useful to grant precise k_{eff} values to determine the reactivity worth of a given configuration, making the process easier and more meticulous. Overall, this will lead to a more informed experimental design where a large number of configurations are easily computed prior to experimentation, illuminating the most desirable options.

ACKNOWLEDGMENTS

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