Modeling the effect in of criticality from changes in key parameters for small High Temperature Nuclear Reactor (U-Battery™) using MCNP4C.

A M Pauzi
Department of Mechanical Engineering, College of Engineering, Universiti Tenaga Nasional (UNITEN), Jalan UNITEN-IKRAM, 43000 Kajang, Selangor, Malaysia
E-mail: anas@uniten.edu.my

Abstract. The neutron transport code, Monte Carlo N-Particle (MCNP) which was well known as the gold standard in predicting nuclear reaction was used to model the small nuclear reactor core called “U-battery™”, which was develop by the University of Manchester and Delft Institute of Technology. The paper introduces on the concept of modeling the small reactor core, a high temperature reactor (HTR) type with small coated TRISO fuel particle in graphite matrix using the MCNPv4C software. The criticality of the core were calculated using the software and analysed by changing key parameters such coolant type, fuel type and enrichment levels, cladding materials, and control rod type. The criticality results from the simulation were validated using the SCALE 5.1 software by [1] M Ding and J L Kloosterman, 2010. The data produced from these analyses would be used as part of the process of proposing initial core layout and a provisional list of materials for newly design reactor core. In the future, the criticality study would be continued with different core configurations and geometries.

1. Introduction
In order to meet the energy needs without harming our planet, the application of nuclear power would be highly important. One of the challenges faced in applying nuclear energy comes from the high capital cost involved in setting up large power reactors. Hence the development small nuclear reactor would be a solution. A nuclear reactor produces its energy through nuclear processes that involves an understanding of the neutron interaction at microscopic level. A model of the nuclear reactor from the perspective of reactor physics is created by using MCNP4C software that could precisely and accurately predict the neutronic behaviour, specifically, the criticality of the reactor.

U-Battery
The term U-Battery is used to refer to a small High Temperature Reactor (HTR) and emphasizes on its special characteristic of long – life core, transportability and inherent safety [1]. The basic parameters of the U – Battery are suggested as below:

| Parameters       | Value                      |
|------------------|----------------------------|
| Reactor Type     | Block Type HTR             |
| Energy conversion system | Light water cycle          |
| Fuel type        | 90% U 235                  |
| Thermal Power    | ~20 MW                     |
| inlet Helium Temperature | 490°C                     |
| outlet Helium temperature | 350°C                     |
| Core lifetime    | 3 - 10 years               |
| Number of control rod | 7                        |
| Geometric parameters: |                           |
| Core Height      | 2.7 m                      |
| Core Diameter    | 3.24 m                     |
| Coolant          | Helium gas, CO2 gas, FI      |
| Bottom reflector |                             |

Table 1. Basic parameters of the U-Battery. [1]

Figure 1. Rough layout of the U-Battery reactor core [1]
2. Review on reactor core material.

The criticality of a reactor core is closely related to the material type and composition of the core. To model the reactor inside MCNP requires research on detail materials of each section inside the core including the percentage and composition of all molecules for each material.

Parameters variation for the test

The U-Battery was simulated for different enrichment level of uranium oxide fuel, from natural uranium of 0.7204% enrichment to weapon grade of 90% enrichment. Altogether, 72 criticality calculations had been made.

| Table 2 Models of U-Battery |
|----------------------------|
| Parameters | 1 | 2 | 3 | 4 |
| TRISO coating | SiC | ZrC |
| Coolant | CO₂ | He | F-Li-Be |
| Control Rod | Void | Ag-In-Cd | B₄C | HfC₂ |

Neutron capture cross section

The criticality of a reactor core would highly depend on the value of neutron cross section of its materials. It is define as the capability to capture neutron by a nuclei. The figure below shows some materials that have very high thermal neutron capture and mostly used as material in a reactor core control rod, and wall.

![Neutron Capture Cross Section](image)

Figure 3. Thermal neutron capture of some material in reactor core [4]

3. Modelling the U-Battery using MCNPv4C software

The MCNP input files describes the problem geometry, specifies the materials and source, and defines the results you desire from the calculation. The geometry is constructed by defining cells that are bounded by one or more surfaces. Cells can be filled with a material or be void. Figure 4 shows the input file structure.

Geometry modelling - Cell card and surface card

The cell card defines the geometrical regions from all first and second degree surfaces and fields, and then combines them with Boolean operators. Next, the surface card defines the surface by with coefficients and constants of the first and second degree equations. Usually, to ease the modelling process, the first step is to write the surface cards, as this would build the outline structure of the model. Only then would be to complete the cell cards, where volume of spaces bounded by surfaces. Lastly would be to specify the materials and calculating the criticality.

![Geometry Modelling](image)

Figure 4: Hexagonal assembly lattice.

Assume all channel form a hexagonal lattice with one coolant in centre and six fuel channels.
3.1.1. Assembly. Consist of hexagonal graphite block which have multiple holes where coolant channels, fuel rods and poison channels are placed. The assembly would then be repeated to form the reactor core and limited by cylindrical surface. Graphite reflectors are placed at assemblies at the edge that were cut by the cylindrical surface and the upper and bottom part.

3.1.2. TRISO particles. The TRISO particle contains uranium dioxide surrounded by different layers of graphite. It is placed in the fuel rod. In real situation, TRISO particles are random among the graphite matrix. Since it would be really difficult to place randomly in MCNP, the TRISO are placed in regular lattice where each coated particle take up one cell.

3.1.3. Burnable poison channel. Consume neutron to maintain the reactivity constant above one. At the beginning life of the reactor, the reactivity is needed to reduce. Hence, the capacity to consume neutron are reduce and eventually, near the end on reactor life, they do not absorb neutron and allow the remaining reactivity in the fuel to drive the reactor.

3.1.1. Control rod. Consists of boron or neutron absorber that would control the reactivity during shutdown, or to increase in reactivity when overpower. Control rod is located in the middle of the fuel assembly; hence, a new type of assembly with control rod is defined. The fuel rod and coolant channel that were cut by the control rod were replaced with graphite.

**Figure 6:** Illustration of TRISO particle with dimension.  
**Figure 7:** Illustration of assembly with poison channels  
**Figure 8:** Illustration of assembly with control rod

Data card
Would usually the lengthiest is the source card which consists of the source descriptions, tally instructions, cross sections and material composition.

3.1.2. Material. Based on the geometry defined, the materials were filled and research on the criticality of the U-Battery is done by varying the materials. In order to generate model of the materials in MCNP, the three basic information needed to be calculated are:

a) All the fraction atoms available in the material including different isotopes and fragment nuclide. This need to be calculated

b) ZAID – Atomic number followed by atomic mass and the extension based on ENDF/B-VI data library of MCNPv4C

c) Nuclide atom fraction (atom/b-cm)

| Table 3: Description of the MCNP input code |
|--------------------------------------------|
| Code | Description |
|-----------------|-------------|
| m1 | 92238.61c | 1.692-4 | 92235.61c | 2.30-02 | 8016.60c | 4.64-02 | 0.7204% |

The procedure to produce material card shown above is applied for all other material of the core

3.1.3. Criticality. The data is submitted to MCNP using the “kcode” where information the Number of cycles and number of particles per cycle to be started in eigen-mode calculations. Then the “ksrc” would specify the initial spatial fission distribution. A fission source point will be placed at each point with coordinates, X, Y, and Z.
4. Results and discussions

A few criticality output from the simulation were validated using the SCALE 5.1 software by [1] M Ding and J.L. Kloosterman, 2010. The results for the criticality on U-Batteri with the same core configuration with same enrichment level were compared. Since SCALE produces results of the criticality of the full life cycle of the burnable fuel, the result from the MCNPv4C are compared with the results of year 0 of the effective full power year (EFPY).

| U235 Enrichment | 20% |
|-----------------|-----|
| $K_{\text{eff}}$ MCNPv4C | 1.1162 |
| $K_{\text{eff}}$ SCALE 5.1 | 1.162 |
| Dev (%) | 3.774 |

Table 4: Comparison result from SCALE5.1 and MCNPv4C

From the results above, the deviation are acceptably high. The results of $K_{\text{eff}}$ from varying material are shown in figure 10 – 12.

**Figure 10.** Graph of $K_{\text{eff}}$ against enrichment level for different coating material  
**Figure 11.** Graph of $K_{\text{eff}}$ against enrichment level for different coolant  
**Figure 12.** Graph of $K_{\text{eff}}$ against U235 enrichment for different control rod material at closer view

**Conclusion**

TRISO coating material should have the characteristic of low thermal neutron cross section in order not to waste the neutron produce hence reduces the efficiency. The test results that shows little difference when varying the commonly SiC to ZrC show a positive results for the criticality, besides its physical advantages.

All three coolants would be good options in terms of neutronic properties where there are insignificant effects on criticality. Both gas type and even liquid salt have little effect on criticality, hence, in order to optimise the design of the reactor, only parameters regarding the heat transfer and other physical properties needed to be considered.

Finally, by applying control rods to the reactor core would significantly lower the criticality. With different type of control rods, the magnitudes of neutron control are very similar. A good control rod material should have the ability to decrease as much $K_{\text{eff}}$ value as possible. From the model, B4C control rod is the best neutron absorber as proven by [4]

**References**

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