

## Automated three dimensional depletion capability for the Pennsylvania State University research reactor

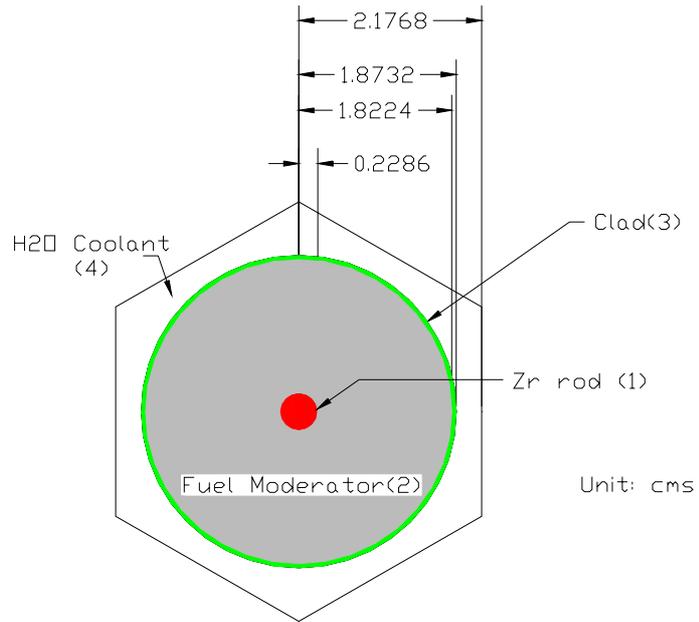
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This paper describes the new depletion calculation capability for the Pennsylvania State University research reactor (PSBR). The calculation scheme employs the general purpose Monte Carlo code MCNP4C coupled with the versatile nuclear depletion code ORIGEN2.2 via the recently developed interface code, TRIGSIM. The main functions of the TRIGSIM code are automatic generation of MCNP and ORIGEN inputs from one TRIGSIM input and interfacing the data exchange between the two codes. The PSBR core loading 1, core loading 2 and core loading 3 were modeled using TRIGSIM code. The excess reactivity results from the core calculations have shown reasonable agreement compared to the measured excess reactivity from the operational log book.

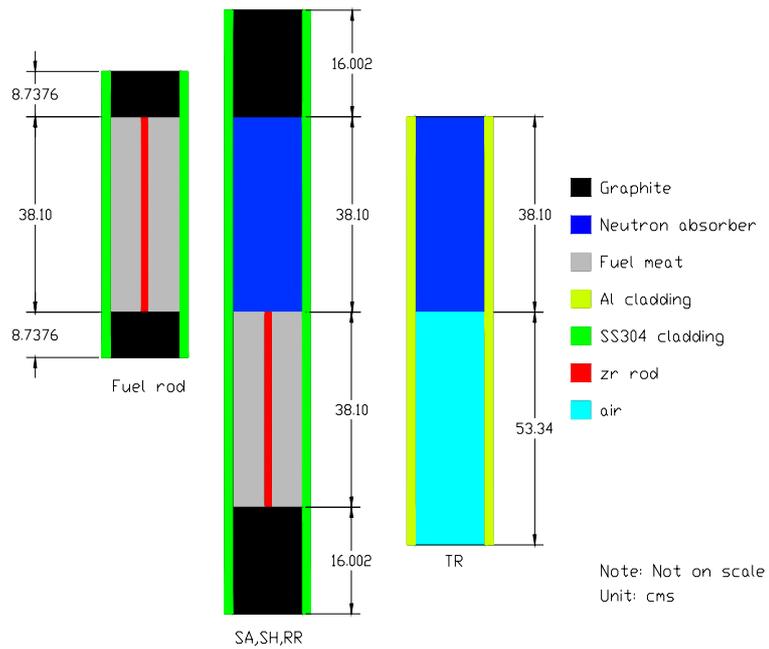
**KEYWORDS:** *MCNP, ORIGEN, Research reactor, Depletion calculation, Monte Carlo calculation, Fuel management*

### 1. Introduction

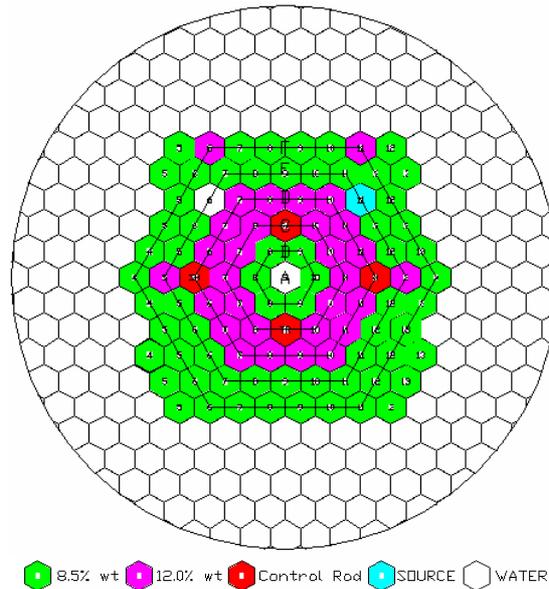
The Pennsylvania State University Breazeale Reactor (PSBR) is a TRIGA Mark III research reactor manufactured by General Atomic. TRIGA reactors are used for research throughout the world, and are preferred for their operational flexibility and their inherent safe characteristics. The PSBR has been operated since 1965, when the core was upgraded from MTR type fuel. The PSBR is a light water cooled, pool type reactor designed for 1 MW (t) steady-state power operation (up to 2000 MW when pulsing) with natural circulation cooling. It is used for experimental, training, educational and service purposes. The PSBR core system is loaded with 20% enriched U-ZrH<sub>x</sub> fuel mixture. The H in the fuel acts as a moderator while the water outside of the fuel rods acts as a coolant. The uniform lattice in PSBR is formed in hexagonal shape. The center of the core is the location of the central thimble (the water rod), which is surrounded by hexagonal rings. The rings running from the center outward are designated B, C, D, E, F and so on. The PSBR has currently two types of fuel elements: 8.5% wt. and 12% wt. fuel rods. The fuel element of the PSBR consists of three sections: the top and the lower sections being graphite bars, which act as neutron reflectors while the middle section is a fuel-moderator matrix in which a Zr rod is inserted in the center. The PSBR fuel element hexagonal lattice dimensions are shown in Fig. 1. In addition to fuel elements, there are three control rods (shim, regulating and safety) which are fuel follower control rods driven by a motor. They are composed of graphite at the top and bottom, fuel and absorber (borated graphite) sections in the middle. The fourth control rod is the transient rod (air rod), the only control rod without fuel material, which is driven by an electro-pneumatic drive during the steady state. Fig. 2 shows the PSBR fuel element and control rod dimensions. Currently, the PSBR is operated using core cycle 51 (as shown in Fig. 3) which loading is a combination of 8.5% wt. and 12% wt. fuel elements. There are 94 fuel elements; 30 of them are 12% wt. and 64 of them are 8.5% wt. The neutron source used in PSBR is a 3-Curie americium-beryllium (Am-Be) neutron source doubly encapsulated in type 304L stainless steel.



**Fig.1** PSBR fuel rod cross section (horizontal plane through fuel mixture )



**Fig.2** PSBR fuel element and control rod dimensions



**Fig.3** Present core loading configuration (core loading 51)

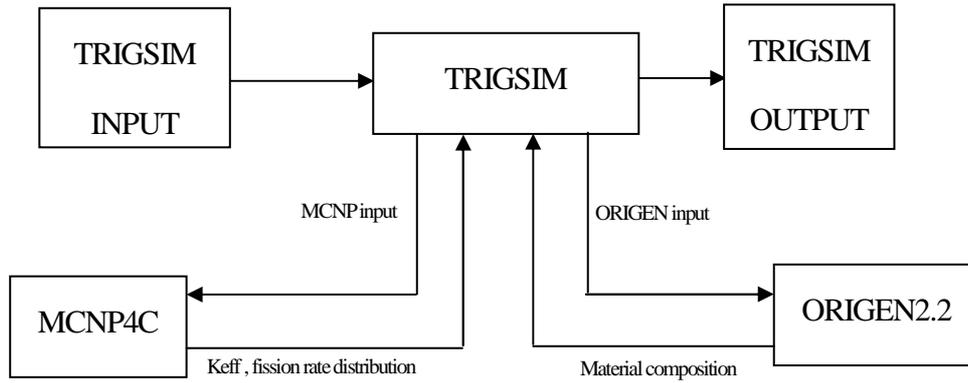
The PSBR facility has been using a core design system originally published in 1972 by W.F. Naughton in a PhD dissertation [1]. A TRIGA core management model (TRICOM) was developed, validated and applied for performing core optimization reload analysis based on the LEOPARD and EXTERMINATOR2 computer codes. In 1979 an improved version of EXTERMINATOR2 called MCRAC was developed by H.Y. Huang and adopted to the core management model [2]. The code is restricted to analyzing core with quarter core symmetry and the calculated results must always be substantially normalized to experimental data. Therefore, newer and more advanced fuel management plan for the PSBR have been established. The new efforts have been focused on using both deterministic and Monte Carlo methods. For the deterministic methods, the possibility to replace the old core system with the modern HELIOS/ADMARCH-H system has been studied [3]. Moreover, a new fuel management plan using the transport theory PENTRAN code is being investigated [4]. This paper, on the other hand, discusses the effort to use Monte Carlo method for PSBR fuel management plan.

It is a common practice nowadays to perform nuclear reactor analysis by computer calculations. Such analysis is performed by nuclear engineers to ensure safe and reliable reactor operation. With the rapid development of computer hardware, nuclear engineers have gained increasing interest in using Monte Carlo calculations for the reactor analysis. The advantages of the Monte Carlo calculation over the deterministic calculation include explicit three dimensional geometry modeling and continuous energy treatment although the results from Monte Carlo calculations are inevitably subject to statistic deviations. The well-known Monte Carlo code MCNP4C [5] is used in this study. Since the MCNP4C code has no capability to perform depletion calculation itself, a depletion module is needed to perform depletion calculation. The versatile nuclear depletion code ORIGEN2.2 [6] is employed in this study. Even though a coupled system between the MCNP and ORIGEN codes provides powerful methodology to perform reactor analysis, a great deal of data interfaces between the two codes is also required. A new and efficient coupled code, TRIGSIM (TRIGA SIMULATOR), has been developed specifically to accommodate the MCNP and ORIGEN code system for PSBR core. The PSBR core loading 1, core loading 2 and core loading 3 were then modeled by the TRIGSIM code to verify its functionality.

## 2. Methodology

To assess reactor analysis and fuel management calculation of the PSBR, a computer model requires both steady-state and depletion calculation capabilities. The computation scheme divides total operation time into sub-time steps assuming no flux distribution change during each sub-time step. For the PSBR TRIGA reactor, it is possible to use each core loading as a sub-time step since the core configuration remains unchanged during each core loading. The steady-state calculation is performed at the beginning of each sub-time step to obtain eigenvalue and fission rate distribution. With the fission rate distribution, the power for each burnup zone can be determined and burnup calculation can be performed based on the derived power. The burnup calculation is used to predict the material composition changes due to neutron exposure. Afterwards, the material composition result of the burnup calculation is updated into the subsequent steady-state calculation. The next step calculation is repeated in the same manner and so on until the end of life has reached. In this study, the general purpose Monte Carlo N-Particle code MCNP4C is employed for steady-state calculation while the versatile nuclear depletion code ORIGEN2.2 is used for the depletion calculation. The MCNP4C code is a well-established Monte Carlo code. It is selected to model the PSBR core because it can model arbitrary three dimension geometry and also because it utilizes continuous energy treatment. MCNP4C is equipped with a wide variety of continuous cross section libraries derived from ENDF/B data libraries. The newest cross section library for each isotope is selected to be used in this study. Nevertheless, the drawback of MCNP4C is that it lacks temperature dependent cross section libraries – mostly room temperature cross section libraries are available. The development and verification of the PSBR model is therefore performed at room temperature. A new plan to develop temperature dependent cross section libraries for PSBR has been established as well. The ORIGEN2.2 code is a computer code for calculating the buildup, decay and processing of radioactive material. It uses a matrix exponential method to solve a large system of coupled, linear, first-order ordinary differential equations with constant coefficients. The ORIGEN2.2 includes standard and extended-burnup PWR and BWR cross sections. However, the TRIGA burnup dependent cross section library is not available in ORIGEN2.2 code. The PWR cross section library was chosen to be used in the TRIGA core burnup with acceptable error at low burnup [7]. A TRIGA cross section library for ORIGEN2.2 code is planned to be developed using HELIOS1.7 code [8] for the TRIGSIM code system.

The described computation scheme is automated via the recently developed interface code, TRIGSIM. The main purpose of the TRIGSIM code is to integrate the coupling between MCNP and ORIGEN codes particularly for PSBR TRIGA reactor. The PSBR core modeling is more convenient and effective by the TRIGSIM code since the code will automatically perform all calculation steps from one TRIGSIM input. MCNP input generation, MCNP calculation execution, MCNP output extraction, ORIGEN input generation, ORIGEN calculation execution and ORIGEN output extraction are parts of TRIGSIM modules. The TRIGSIM function flow diagram is shown in Fig. 4. The TRIGSIM input requires rod type and geometry description, rod locations, control rod positions, initial fuel material compositions and operating conditions for each core loading. The fuel elements can be shuffled by specifying different rod locations to analyze different core loading patterns. Also, control rod movement can be modeled easily by specifying different control rod positions. The TRIGSIM code is entirely written in C language. It is developed and compiled by Microsoft Visual C++ version 6.0. The code was written in several modules for the ease of debugging and future development.

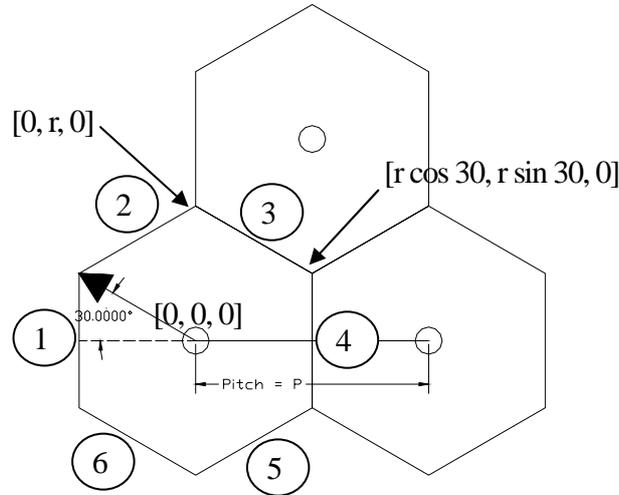


**Fig.4** TRIGSIM function diagram

The TRIGSIM code utilizes the repeated capability of MCNP to define infinite array of hexagonal lattice. For hexagonal lattice (LAT =2), the six bounded surfaces must be supplied. These surfaces are generally represented in the equation form of

$$Ax + By + Cz - D = 0 \quad (1)$$

where A, B, C, D are coefficients referenced to the center of the hexagon. Those coefficients have to be input by P card. The TRIGSIM code automatically determines the coefficients by considering the fuel rod pitch (P in cm.) in a TRIGA reactor as in Fig. 5.



**Fig.5** Hexagonal lattice surfaces

$$r \cos 30 = \frac{p}{2} \Rightarrow r = \frac{\frac{p}{2}}{\left(\frac{\sqrt{3}}{2}\right)} = \frac{P}{\sqrt{3}} \quad (2)$$

Surfaces 2, 3, 5 and 6 are general planes while surfaces 1 and 4 are simple planes normal to x axis. For example, the coefficients of the surface 3 are determined by knowing that the plane will pass through point  $[0, r, 0]$  and point  $[r \cos 30, r \sin 30, 0]$ . Then the slope is given by

$$m = \frac{(r - r \sin 30)}{(0 - r \cos 30)} = \frac{\left(\frac{r - r}{2}\right)}{\left(0 - \frac{\sqrt{3}}{2}r\right)} = \frac{\left(\frac{r}{2}\right)}{\left(-\frac{\sqrt{3}}{2}r\right)} = -\frac{1}{\sqrt{3}} \quad (3)$$

The y intercept is found by choosing a point, in this case (0, r, 0). Then the equation representing the surface 3 is

$$y = -\frac{1}{\sqrt{3}}x + r \quad (4)$$

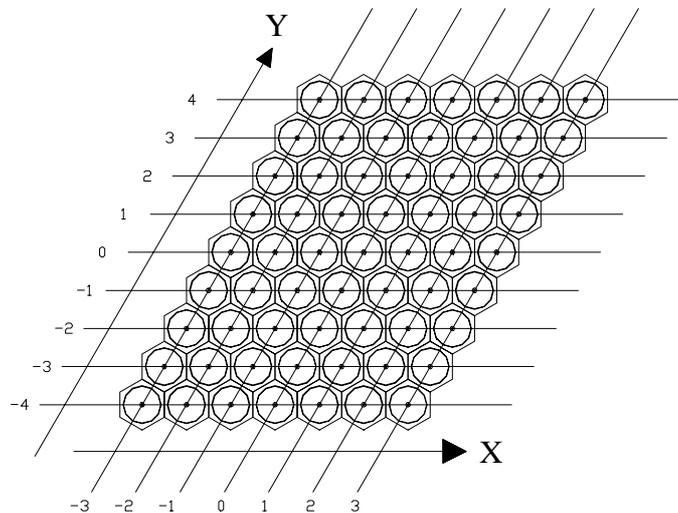
Since MCNP wants the equation in the form  $Ax + By + Cz - D = 0$ , the above equation is written as

$$\frac{1}{\sqrt{3}}x + y + 0z - \frac{P}{\sqrt{3}} = 0 \quad (5)$$

Therefore  $A = \frac{1}{\sqrt{3}}$ ,  $B = 1$ ,  $C = 0$ ,  $D = \frac{P}{\sqrt{3}}$ .

When the user inputs the fuel rod pitch P to the TRIGSIM code, the surface 3 is then modeled by MCNP. In the same manner, the surfaces 2, 5 and 6 can be determined by the TRIGSIM code.

In the next step, the PSBR rod models are constructed using the input or default dimensions. The PSBR rods can be categorized into three types: fuel element, fuel follower control rod and air follower control rod. For the fuel element type, six cells including Zr rod, fuel meat, SS304 clad, top graphite bar, bottom graphite bar and coolant water are defined in the MCNP model. For the fuel follower control rod model, seven cells including Zr rod, fuel meat, B<sub>4</sub>C absorber, SS304 clad, top graphite bar, bottom graphite bar and coolant water are defined. Lastly, for the air follower type, four cells including air, B<sub>4</sub>C absorber, Aluminum clad and coolant water are defined. The TRIGSIM code assigns a unique universe (u card) for each fuel element and control rod to fill in one of the hexagonal lattice cells according to their positions in the PSBR core. A universe in MCNP is defined as either a lattice or an arbitrary collection of cells. The fuel element position (X,Y) is defined consistently with MCNP lattice position where (0,0) is the central thimble rod position. Fig. 6 displays the MCNP lattice cell position in X and Y



**Fig.6** Lattice cell position used by TRIGSIM code

One issue of generating MCNP input for criticality calculations is to provide the initial fission sources (ksrc card). In order to ensure fast convergence of the fission sources, the fission source should be provided for every cell which has fissile material. The TRIGSIM code specifies the location of the fission source automatically by determining the dimensions of the fuel element. To guarantee that the location (X,Y,Z) of the fission source is within fuel meat cell, TRIGSIM calculates certain radial and axial offsets from the center point of the fuel element. The radial offset is equal to the average distance of Zr rod radius and fuel meat radius. Furthermore, the axial offset from the center of the fuel element is equal to zero, while that of the fuel follower type control rod is determined from the control rod position where control rod position is defined as the length of fuel follower which overlaps the fuel elements. In this case, the axial offset is equal to the difference between the control rod position and the fuel element part length. A proper neutron cross section for each isotope is looked up from the MCNP cross section file (xsdir). The newest neutron cross section libraries processed at the temperature within 10% deviation from the specified reactor temperature are selected. In TRIGSIM model, each fuel element is regarded as burnup zone. Initial fuel material composition of each fuel element specified in TRIGSIM input is transferred to MCNP input. Also, TRIGSIM code adds tally cards (f7 card) for each fuel element to calculate fission rate distribution. The criticality card (kcode card) can be also specified from TRIGSIM input. Finally, the reactor model calculation boundary is determined. The PSBR core is automatically modeled in cylindrical shape. Since most of the fuel elements in the reactor core have graphite reflectors on top and bottom, eight centimeters of water layers are sufficient to add on the top of the highest element in the core and below the bottom of the lowest rod in the core to represent neutron reflection from water. In addition, the radial reactor model boundary must provide sufficient water reflector. It has been studied by Young-su Kim [9] that the radial water layer of 14 cms. (about 3.2 times of PSBR fuel element pitch) is sufficient for the PSBR to represent the neutron reflection from water. For the TRIGSIM code, the thickness of the water layer is equal to four times the fuel element pitch. The water layer is automatically added to the farthest core peripheral.

With all these steps and some addition of other functional MCNP cards, the MCNP input for a PSBR core loading is complete. The MCNP calculation is called to execute by the TRIGSIM code. With the completion of MCNP calculation, the TRIGSIM code reads the MCNP tally file. The fission rate tally result for each fuel element and core  $K_{\text{eff}}$  are read. The normalized power for each element is determined by

$$NP_k = \frac{V_k \left( \int_0^{\infty} \sum_f (E) \phi(E) dE \right)_k}{\sum_{i=1}^N V_i \left( \int_0^{\infty} \sum_f (E) \phi(E) dE \right)_i} \quad (6)$$

where  $\int_0^{\infty} \sum_f (E) \phi(E) dE$  is fission rate tally for fuel element k (read from tally file).

Subsequently, the ORIGEN2.2 input of each individual element with burnable fuel is prepared for burnup calculation by the TRIGSIM code. The power specified in the ORIGEN2.2 input is equal to the product between the fuel element normalized power and total core operating power. The material composition before depletion is explicitly specified in the ORIGEN2.2 input. Finally, after the input preparation is finished, the ORIGEN calculation for each fuel element is called to execute. The TRIGSIM code then reads back the material composition after depletion and updates it into memories. With the same sequence,

the next time step calculation is performed until it finishes the last time step defined in the TRIGSIM input.

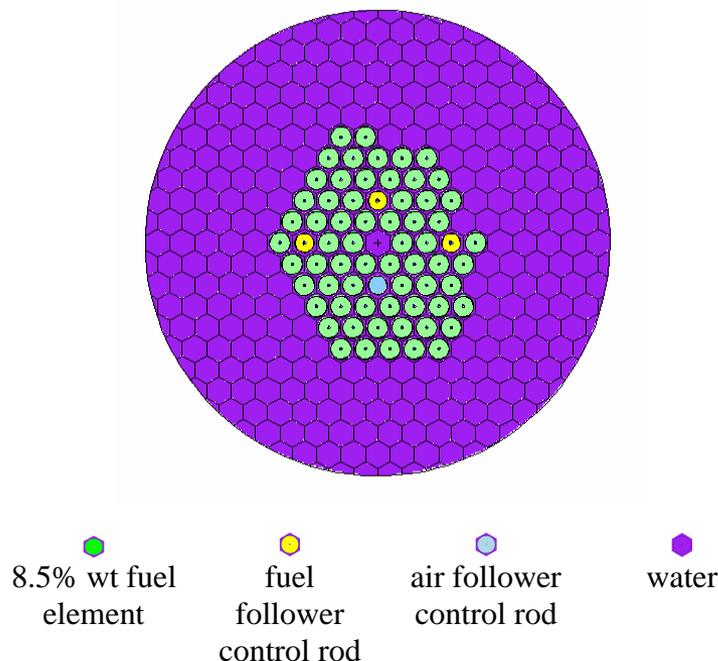
Finally, the TRIGSIM code generates three types of output files namely;

1. Output file: the output file includes input echo and the output result.
2. Run file: the run file is used to restart a problem that was earlier terminated by the user since the run file contains problem geometry and other information needed for calculation
3. Composition file: the composition file contains material composition of each fuel element of each burnup cycle. This file is also needed to restart the earlier terminated problem.

The input echo in output file is useful for the user to verify the correctness of the TRIGSIM code input. The user can utilize the MCNP input file and ORIGEN input files generated by the TRIGSIM code later since they are kept in a directory, which has the same name as the cycle name.

### 3. Results and Discussion

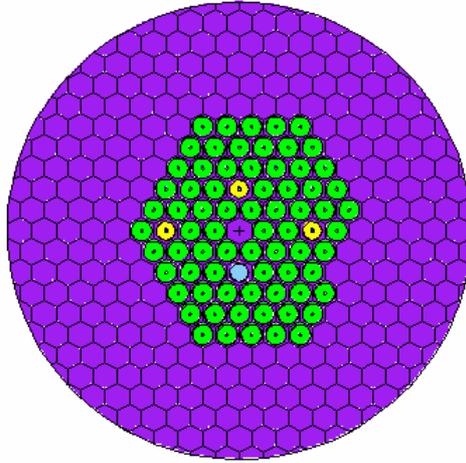
The verification of the TRIGSIM code was performed using measurements from the actual core loadings. The PSBR core loading 1 (loaded on December 31, 1965) was modeled as shown in Fig. 7. There were 64 fuel elements, three fuel follower control rods and one air follower control rod in the core. All of the fuel elements in this core were 8.5% wt type. The PSBR core loading 1 was shutdown right after the core was completely loaded; hence, there was no reactor operation between PSBR core loading 1 and PSBR core loading 2.



**Fig.7** PSBR core loading 1

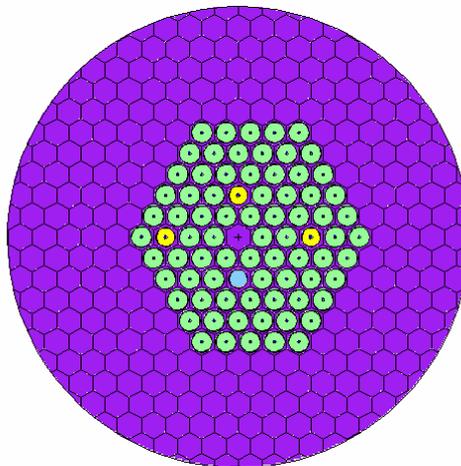
The PSBR core loading 2 (loaded on Jan 5, 1967) was subsequently modeled as shown in

Fig. 8. An additional eight fuel elements were added to core loading 1 to become core loading 2. The total burnup from core loading 2 to core loading 3 was 15.658 MWH. The burnup calculation from core loading 2 to core loading 3 is performed at the reactor power of 1 MW for 15.658 hrs.



**Fig.8** PSBR core loading 2

The PSBR core loading 3 (loaded on Jan 27, 1967) is shown in Fig. 9. A further three fuel elements were added to core loading 2 to become core loading 3.



**Fig.9** PSBR core loading 3

All PSBR core loadings were calculated at all control rods out (ARO) using 3000 neutrons/cycle with 950 active cycles and 50 inactive cycles. The excess reactivity of each core loading is calculated by the relation  $\frac{\Delta k}{k\beta}$  (\$). The comparison of excess reactivity predictions for each core loading against the measured data recorded in the operational log book is shown in Table 1.

**Table 1** Excess reactivity calculated by TRIGSIM code compared to measured excess reactivity of PSBR core loading 1, 2 and 3

Core loading	Calculated excess reactivity (\$)	Measured excess reactivity (\$)
1	$0.36 \pm 0.18 (3\sigma)$	$0.15 \pm 0.02$
2	$3.29 \pm 0.18 (3\sigma)$	$3.34 \pm 0.33$
3	$4.48 \pm 0.18 (3\sigma)$	$4.60 \pm 0.46$

It is also estimated, based on the measurement methodology in 1965, that the measured value could be associated with as high as 10% standard deviation. It is seen therefore that the result from the TRIGSIM code and the measured excess reactivity agree quite well. Further verification from the next core loading up to the current core loading (core loading 51) is being performed in order to derive the current core loading.

#### 4. Conclusion

A new Monte Carlo based fuel management methodology for PSBR has been developed. The methodology utilizes the integration between Monte Carlo calculations performed by MCNP4C2 and depletion calculations performed by ORIGEN2.2. The interface TRIGSIM code has been successfully applied to perform fuel management of the PSBR. The accuracy of the MCNP models has been validated by the measured data from operation log book. The result of excess reactivity from TRIGSIM code and the measured values agree quite well. Further testing from core loading 3 up to current core loading is being performed. In addition, a further new development for the Monte Carlo based fuel management methodology is being investigated. The new contribution will include temperature dependent cross section libraries and coupling algorithms with nodal diffusion method to provide more spatial detail in three dimensions.

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