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Assessment of MCNP-4B Codes Using DCA Experimental Data

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ABSTRACT

In order to assess the applicability of the MCNP-4B code for the heavy water moderated, light water cooled and pressure-tube type reactor, MCNP-4B physics calculations have been carried out for the Deuterium Critical Assembly (DCA), and the results were compared with those of the experimental data. In this study, the key safety parameters such as the effective multiplication factor, void coefficient and local power peaking factor are simulated. New MCNP libraries have been generated from ENDF/B-VI release 3 to use with the cross section data consistently for the fuels to be analyzed in the future. Generally, the MCNP-4B calculation results show reasonable agreement with experimental data of the DCA core. The maximum discrepancy in the effective multiplication factor is ~6 mk. The void reactivity change agrees within 4 mk and the maximum difference of the local power peaking factor is ~2.3%.

1. INTRODUCTION

As a part of the computational benchmarking of advanced CANDU fuels, the experimental data of the Deuterium Critical Assembly (DCA)[1] were assessed using the Monte Carlo MCNP-4B code.[2] The MCNP is a general-purpose Monte Carlo transport code, which is capable of generalized geometry modeling, time-dependent calculation and coupled neutron-photon-electron calculation. In this study, the key safety parameters such as the multiplication factor, void coefficient and local power peaking factor were estimated and compared with the experimental data of DCA. The cross-section libraries of the MCNP have been consistently generated from ENDF/B-VI release 3 [Ref. 3] for future applications to various fuel types.

The DCA was originally designed in JNC (Japan Nuclear Cycle Development Institute) and a series of critical experiments were performed to study the core physics of the heavy water moderated, light water cooled and pressure-tube type reactor system. The DCA criticality experiments are performed for two lattice pitches (22.5 cm or 25.0 cm) and various fuel types (natural and enriched uranium oxide fuels and PuO_2 enriched mixed oxide fuels). In this study, the experimental data of 25.0 cm lattice pitch was chosen for the benchmark calculation to reflect the neutronic characteristics of the typical CANDU core which has the lattice pitch of 28.575 cm.

2. CHARACTERISTICS OF DCA

The DCA was used to develop the related core technologies of the Advanced Thermal Reactor (ATR) in Japan. The reactor core is geometrically highly heterogeneous : cluster-type fuel is contained in a pressure tube, together with a coolant, which is separated from the D_2O moderator by a calandria tube. In such a system, neutron behavior is not only complex but sensitively dependent on slight changes in the core geometry or material.

The DCA facility consists of a heavy water tank of 3 m diameter and 3.5 m height, which is made of 10 mm thick aluminium having removable pressure tubes and grid plates. It contains a square lattice of either 121 unit cells in 22.5 cm pitch or 97 cells in 25.0 cm pitch. The DCA core configurations for these two types of lattice pitches with 25 channels of PuO_2-UO_2 test fuel assemblies loaded in the central zone are shown in Figs. 1 and 2, respectively. The cluster type fuel is bundled with two tie plates and two intermediate aluminium spacers.

The standard DCA fuel cluster has 28 fuel rods and consists of three concentric layers of fuel pins which are shown in Figs. 3 and 4. The fuel bundle is loaded in a pressure tube and the calandria tube surrounds the pressure tube which physically separates the moderator from the coolant. The aluminium is used for both the pressure tube and caladria tube material. The pressure tube is filled with H_2O as the coolant, while the heavy water (99.5 mol% purity) is used as the moderator. The fuel clusters used for the experiment have an effective length of 2 m. Dimensions and compositions of the DCA core and fuel clusters are summarized in Tables 1 and 2, respectively.

In the DCA core, the criticality is adjusted by changing the moderator level in the core tank. In the unvoided core, the light water level in the pressure tube is made nearly equal to the critical level of the moderator during the critical search. Throughout the experiment, all the components are maintained at an ambient temperature of 22℃.

3. BENCHMARK CALCULATION OF DCA

3.1 Calculation Model

For the MCNP calculations, the DCA core was modeled using a three-dimensional 1/4 core model in the radial direction and the specular reflection boundary condition was applied for the inner boundaries of the DCA core. The fuel rods, cladding, fuel gap, pressure tube and calandria tubes are modeled explicitly for every fuel channel. However, the guide tubes, spacer grids and the others for the safety rods are neglected. The cross-sectional view of the MCNP model of the 1/4 DCA core is shown in Fig. 5. For the upper and lower core region, the structural arrangement is simplified by uniform layers of homogenized material superposed in the axial direction along the core axis. In order to facilitate the explicit modeling of fuel bundles in the core, a repeated structure option of the MCNP was used. This option makes it possible to describe a cell and surfaces only once to model their distribution in a core, and therefore, input description and calculation memory can be saved appreciably.

Because the public MCNP cross-section libraries have a limited number of isotopes and temperature data, it is not sufficient to analyze various fuels which have complex isotopic compositions. Therefore, new cross-section libraries were generated based on ENDF/B-VI release 3 to use the cross section data consistently for the fuels to be analyzed in the future. In this study, the NJOY nuclear data processing system version 97.114 [Ref. 4] was used and the library generation was performed on a HP9000 C180EG workstation under a HP-UX 10.20 operating system. The fractional tolerance used in the NJOY input parameter is 0.001. The neutron $S(\alpha,\beta)$ thermal cross-section data was also newly generated and used for the light water and heavy water medium to take account of the thermal motion of the target molecules.

The MCNP calculations were performed for various DCA core status to predict safety parameters. The standard MCNP methods were used, i.e., the newly generated cross-section libraries based on the ENDF/B-VI release 3, no special treatment for unresolved resonances, explicit treatment of (n,2n) reaction, $S(\alpha,\beta)$ treatment of thermal neutron scattering on hydrogen and deuterium in water. Because of the statistical nature of the Monte Carlo calculation, the accuracy of the result depends not only on the simulation model, the cross-section data and the temperatures of the transport media, but also on the statistical variance of the computed k_{eff}. Therefore, each simulation was allowed to run for a sufficient number of cycles with a sufficient number of source histories per cycle. All the MCNP calculations were performed with 10,000 particles per cycle and 1,000 active cycles after 100 inactive cycles.

3.2 Effective Multiplication Factor (k_{eff})

The k_{eff} was calculated for several kinds of the DCA core configurations as follows:

- Uniform core loaded with 1.2 wt% enriched UO_2 fuel assembly,
- Two-region core loaded with 5Spu and 1.2 wt% enriched UO_2 fuel assembly,
- Two-region core loaded with 8Spu and 1.2 wt% enriched UO_2 fuel assembly,
- Two-region core loaded with 0.7 wt% and 1.2 wt% enriched UO_2 fuel assembly, and
- Two-region core loaded with 1.5 wt% and 1.2 wt% enriched UO_2 fuel assembly,

where, 5Spu and 8Spu are defined as

5Spu = $0.542\times(PuO_2 \,/\, (PuO_2 + UO_2))$ wt%, and

8Spu = $0.862\times(PuO_2 \,/\, (PuO_2 + UO_2))$ wt%.

Two kinds of coolant void fractions (0% and 100% void) are considered for all the above core configurations and the calculations are performed at 25.0 cm square lattice pitch which is close to the lattice pitch of CANDU fuel bundle. The 97 fuel bundles are arranged in the calandria tubes of the DCA core with 25.0 cm square lattice pitch. For a two-region core, the test fuel assemblies are loaded in 25 channels (0.7 wt% and 1.5 wt% enriched UO_2, 5Spu and 8 Spu) of the central zone as shown in Fig. 2.

For the critical height given by the heavy water level, the predicted k_{eff}'s of the DCA cores show very good agreement with the experimental value. The average k_{eff} is 0.99745±0.0024. The maximum discrepancy in k_{eff} is 6 mk, which is the case of two-region core loaded with 0.7 wt% and 1.2 wt% enriched UO_2 fuel assembly. The results are summarized in Table 3.

3.3 Coolant Void Reactivity

The coolant void reactivity is an important parameter for the reactor design. Especially for the CANDU reactor, it is important to estimate the void reactivity accurately because the void reactivity is positive. In this section, MCNP prediction accuracy for the void reactivity is examined against the DCA experimental data.[5]

The coolant void reactivity was calculated for three kinds of DCA cores with 25.0 cm square lattice pitch as follows:

- Uniform core loaded with 1.2 wt% enriched UO_2 fuel assembly,
- Two-region core loaded with 5Spu and 1.2 wt% enriched UO_2 fuel assembly, and
- Two-region core loaded with 8Spu and 1.2 wt% enriched UO_2 fuel assembly.

For 1.2 wt% enriched UO_2 and 5Spu and 8Spu fueled DCA cores, the k_{eff}'s have been simulated for 0% and 100% void fractions. For all cases, the coolant is assumed to be uniformly distributed inside the pressure tube. Then, the coolant void reactivity was calculated by reducing the coolant density from the nominal value to the perturbed one such as

$$\alpha_V\,(mk) = 1000 \times \left[\frac{1}{k_{nominal}} - \frac{1}{k_{perturb}} \right]. \tag{1}$$

The k_{eff}'s obtained by perturbing coolant density from 0% to 100% void fractions, the measured void reactivity and calculated void reactivity are given in Table 4 for the different core configurations. Generally, the predictions of the void reactivity change by the MCNP agree well with those of the experimental data within 4 mk for all core states. For the cases analyzed in this study, if the enrichment of the plutonium increases in the fuel, the void reactivity decreases. This fact can be explained by a very large resonance near 0.3 eV of the fissile substances such as ^{239}Pu and ^{241}Pu in the PuO_2-UO_2 fuel.

3.4 Local Power Peaking Factor (LPF)

As mentioned in Sec. 3.3, the plutonium showed a tendency to reduce the void reactivity, and the use of the PuO_2-UO_2 fuel is advantageous in the void reactivity viewpoint of nuclear safety of the heavy water reactor. However, the plutonium fuel raises a serious power peaking problem because its large neutron absorption cross section brings about a large thermal neutron shielding effect. In order to estimate the integrity of the fuel bundle, therefore, it is very important to predict the power distribution within a plutonium fuel bundle accurately.

In this study, the LPFs were calculated in 25.0 cm square lattice pitch for the 5Spu and 8Spu clusters using MCNP code and compared with the experimental data. The LPF is defined as the ratio of the power density of individual fuel ring over the average power density of a fuel bundle such as

$$LPF = \frac{Power\ in\ Each\ Ring}{Average\ Power\ in\ Cluster}. \tag{2}$$

The calculated and measured LPF are compared as shown in Table 5. Compared with the LPF of the experimental data,[6] the maximum difference of the LPFs of MCNP calculations is ~2.3%. Considering the error of the measured LPFs, the results of MCNP agree well with those of the experiment.

As shown in Table 5, the pin power in the inner ring is lower than that in the outer ring. And, as the enrichment of the plutonium in the fuel cluster is higher, the pin power in the inner ring is lower. It is due to the self-shielding of thermal neutrons in the fuel cluster. Because the pin power distribution is closely related to the thermal neutron distribution, the power peaking appears in the outer-most circles. For the dependence of the power on the coolant void fraction, the power depression in the fuel cluster is slightly enhanced by the presence of H_2O coolant. The enhancement by the presence of H_2O coolant can be considered to be due to the shortening of average diffusion length in the fuel cluster by H_2O coolant and H_2O coolant enhances the thermal neutron self-shielding effect in the fuel cluster.

4. CONCLUSION

As a part of the computational benchmarking of the advanced CANDU fuels, the experimental data of a DCA research reactor was assessed using the Monte Carlo MCNP-4B code. New cross-section libraries were generated based on ENDF/B-VI release 3.

The benchmark calculations of the DCA core have been performed for the effective multiplication factor, coolant void reactivity and local power peaking factor. The results of the MCNP calculation have shown good agreement with the experimental data. The predicted k_{eff}'s of the DCA cores show very good agreement with the experimental value. The maximum discrepancy in k_{eff} is 6 mk, which is the case of two-region core loaded with 0.7 wt% and 1.2 wt% enriched UO_2 fuel assembly. The void reactivity change agree well within 4 mk for different core states. The maximum difference compared with the LPF of the experimental data is ~2.3%, and, the results of MCNP agree well with those of the experiment.

Consiquently, it can be concluded that the MCNP code predicts well the key safety parameters for the DCA.

ACKNOWLEDGEMENT

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Table 1. Dimensions of DCA Lattice and Core

Item	Value
Fuel Cluster Radius of each ring : middle inner outer	 13.13 mm 30.00 mm 47.58 mm
Hanger wire Diameter Material	 2.00 mm Al
Cluster length Standard fuel meat length	2223.0 mm 2000.0 mm
Pressure tube Outer diameter Inner diameter Material	 121.0 mm 116.8 mm Al
Calandria Tube Outer Diameter Inner Diameter Material	 136.5 mm 132.5 mm Al
Moderator Material Purity	 D_2O 99.4 mol%
Core tank Outer diameter Inner diameter Height Material	 3035.0 mm 3005.0 mm 3500.0 mm Al
Lattice pitch (square)	225 or 250 mm
Upper and Lower grid plates Material	 Al
Temperature	~ 22 ℃

Table 2. Experimental Fuel Clusters

Fuel Type	0.54 wt% PuO_2-UO_2	0.84 wt% PuO_2-UO_2	1.2 wt% UO_2	0.7 wt% UO_2	1.5 wt% UO_2
Fuel Pellet					
Density (g/cm^3)	10.17	10.17	10.36	10.36	10.38
Diameter (mm)	14.69	14.72	14.80	14.80	14.77
Enrichment (wt%)	5Spu*	8Spu**	1.203	0.711	1.503
Composition (wt%)					
U-235	0.6214	0.6194	1.057	0.625	1.317
U-238	86.782	86.503	86.793	87.255	86.563
Pu-238	0.000102	0.000145			
Pu-239	0.4304	0.6849			
Pu-240	0.04115	0.06584			
Pu-241	0.004359	0.006960			
Pu-242	0.000303	0.000510			
O	12.12	12.12	12.15	12.12	12.12
Fuel Pin (mm)					
Clad Material	Zircaloy-2	Zircaloy-2	Al	Al	Al
Clad Inner Dia.	15.06	15.06	15.03	15.03	15.03
Clad Outer Dia.	16.68	16.68	16.73	16.73	16.73
Gap Material	He Gas	He Gas	Air	Air	Air

*5Spu = 0.542×(PuO_2 / (PuO_2 + UO_2)) wt%

**8Spu = 0.862×(PuO_2 / (PuO_2 + UO_2)) wt%

Table 3. Comparison between Experiment and Calculation for Effective Multiplication Factor

(Lattice Pitch : 25.0 cm)

Core Type	Coolant Void Fraction (%)	D2O Critical Height (cm)	MCNP-4B	
1.2wt% UO_2(97) Uniform Core	0	107.05	0.99851	±0.00020
	100	105.59	0.99712	±0.00021
5Spu(25) and 1.2wt% UO_2(72) Two-Region Core	0	91.64	0.99432	±0.00018
	100	96.63	0.99345	±0.00021
8Spu(25) and 1.2wt% UO_2(72) Two-Region Core	0	77.96	0.99635	±0.00020
	100	87.02	0.99530	±0.00022
0.7wt% UO_2(25) and 1.2wt% UO_2(97) Two-Region Core	0	169.76	1.00070	±0.00021
	100	140.25	0.99959	±0.00023
1.5wt% UO_2(13) and 1.2wt% UO_2(84) Two-Region Core	0	94.01	1.00041	±0.00021
	100	97.72	0.99875	±0.00024

Table 4. Comparison between Experiment and Calculation for Coolant Void Reactivity

(Lattice Pitch : 25.0 cm)

Core Type	Coolant Void Fraction (%)	MCNP-4B	Experimental Value (%K)	MCNP-4B
1.2wt% UO_2(97) Uniform Core	0 100	0.99851±0.00020 1.00094±0.00021	-0.044±0.015	0.243±0.029
5Spu(25) and 1.2wt% UO_2(72) Two-Region Core	0 100	1.00005±0.00021 0.97998±0.00023	-2.406±0.307	-2.048±0.032
8Spu(25) and 1.2wt% UO_2(72) Two-Region Core	0 100	1.00041±0.00021 0.95277±0.00025	-4.980±0.500	-4.998±0.035

Table 5. Comparison between Experiment and Calculation for Local Power Peaking Factor

(Lattice Pitch : 25.0 cm)

	Fuel Enrichment	Coolant Void Fraction (%)	Experiment (E)	MCNP-4B (C)	C/E-1 (%)
Fuel Pin Position 1	5Spu	0	0.64±0.01	0.643±0.002	0.52
		100	0.76±0.01	0.770±0.001	1.32
	8Spu	0	0.61±0.01	0.613±0.002	0.48
		100	0.71±0.01	0.726±0.001	2.27
Fuel Pin Position 2	5Spu	0	0.82±0.01	0.813±0.001	-0.82
		100	0.86±0.01	0.856±0.001	-0.43
	8Spu	0	0.79±0.01	0.791±0.001	0.11
		100	0.81±0.01	0.823±0.001	1.57
Fuel Pin Position 3	5Spu	0	1.18±0.01	1.183±0.001	0.22
		100	1.13±0.01	1.129±0.001	-0.06
	8Spu	0	1.20±0.01	1.201±0.001	0.11
		100	1.17±0.01	1.157±0.001	-1.10

5Spu : 5Spu(25) and 1.2wt% UO_2(72) Two-Region Core

8Spu : 8Spu(25) and 1.2wt% UO_2(72) Two-Region Core

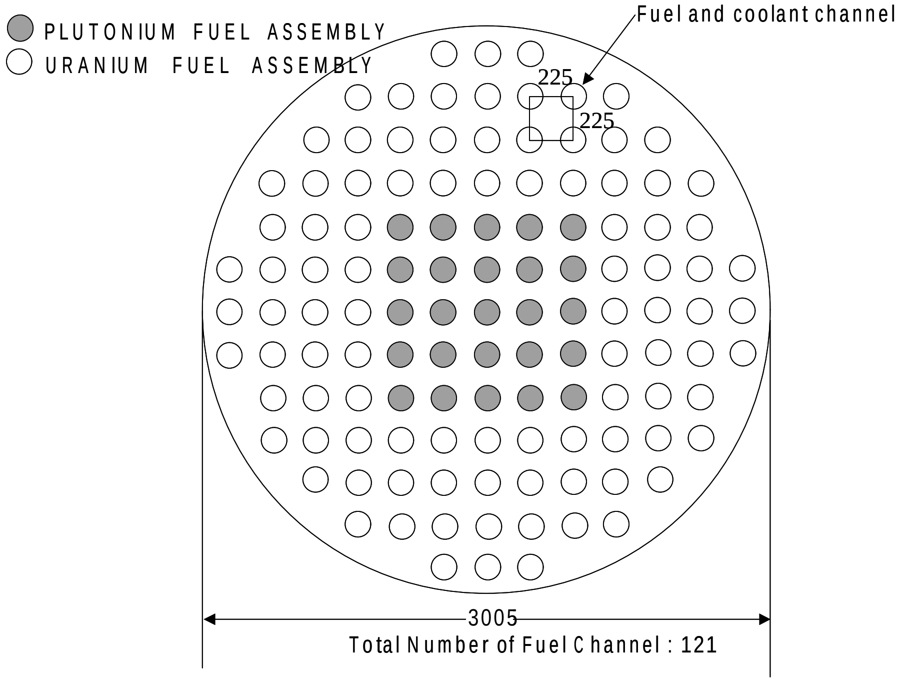

Fig. 1 Configuration of DCA Core Having 22.5 cm pitch lattice and 25 Channels PuO_2-UO_2 Test Fuel Assemblies

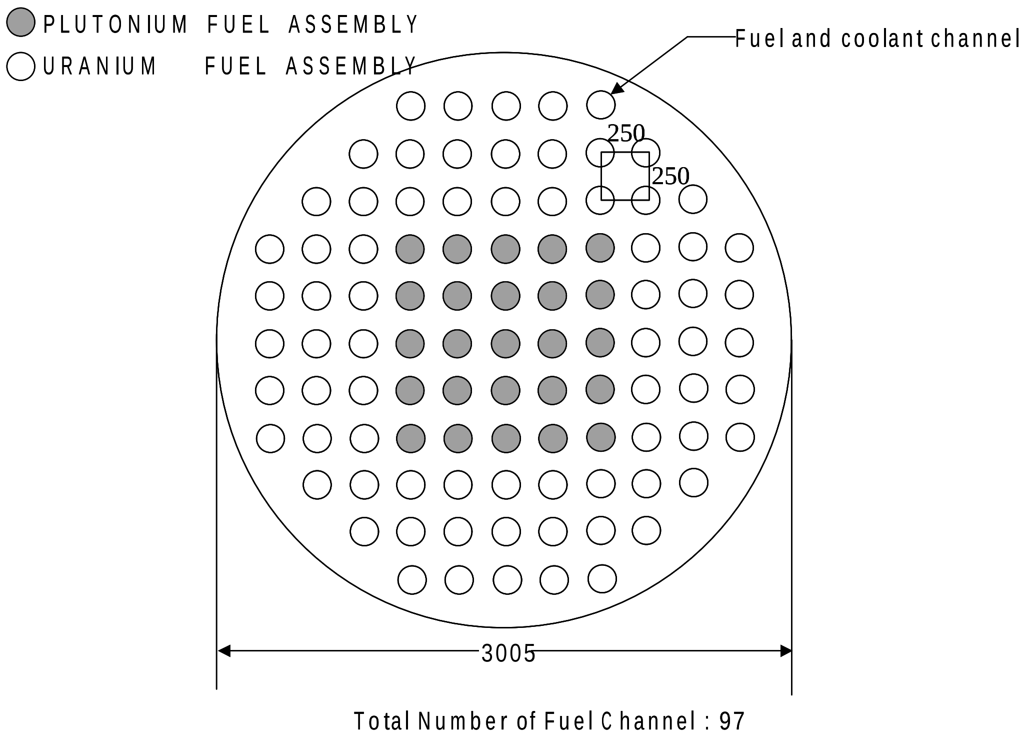

Fig. 2 Configuration of DCA Core Having 25.0 cm pitch lattice and 25 Channels PuO_2-UO_2 Test Fuel Assemblies

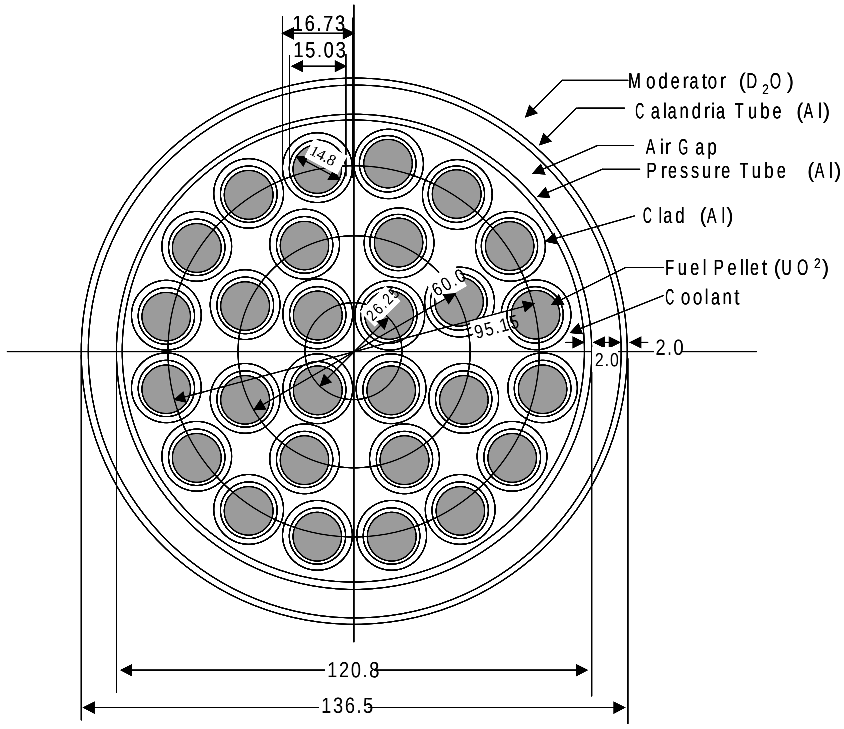

Fig. 3 Cross-sectional View of 28 Rod UO_2 Fuel Assembly

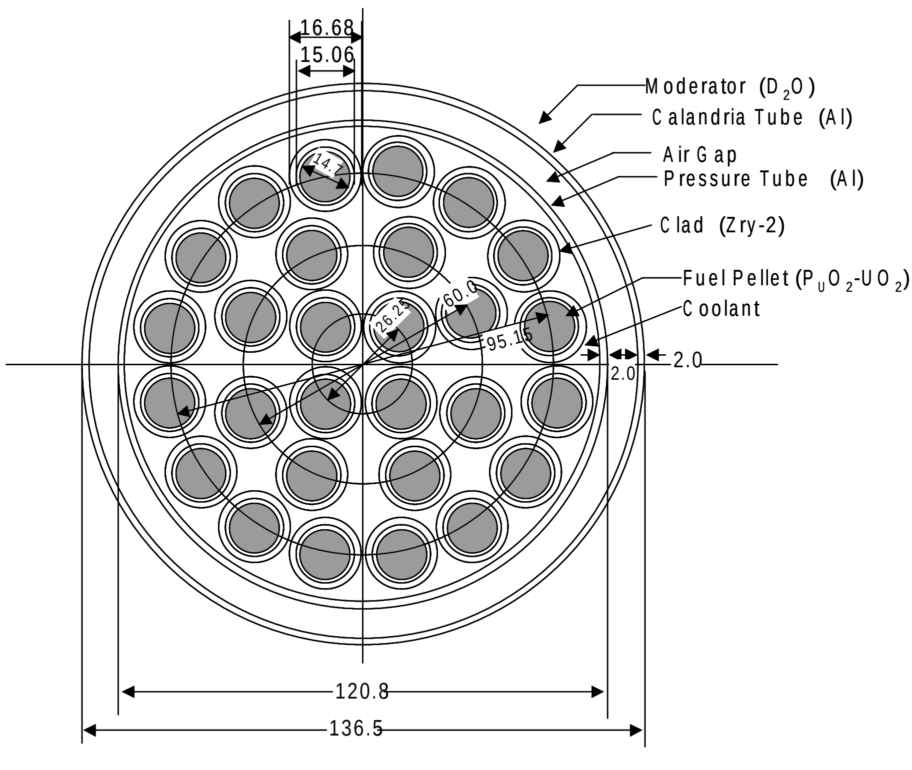

Fig. 4 Cross-sectional View of 28 Rod 1.2 wt% PuO_2-UO_2 Fuel Assembly

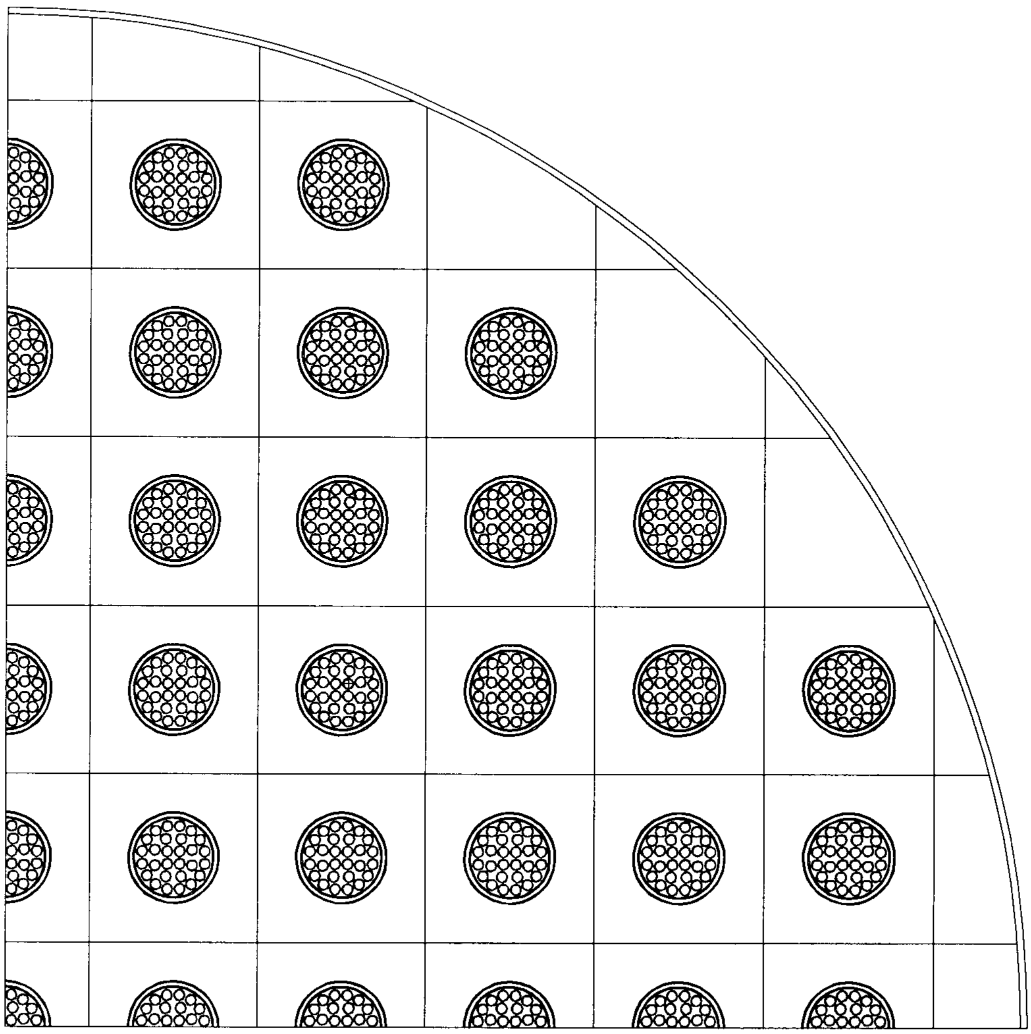

Fig. 5 Cross-sectional View of MCNP Calculational Model of 1/4 DCA Core