Numerical Verification of the Theory of Coupled Reactors for a Deuterium Critical Assembly Using MCNP5

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Summary

The theory of multipoint coupled reactors developed by multi-group transport is verified by using the probabilistic transport code MCNP5. The verification was performed by calculating the multiplication factors (or criticality factors) and coupling coefficients for a two-region test reactor known as Deuterium Critical Assembly, (DCA). The variations of the criticality factors and the coupling coefficients were investigated by changing of the water levels in the inner and outer cores. The numerical results of the model developed with MCNP5 code were validated and verified against published results and the mathematical model based on coupled reactor theory.

1. Introduction

Designing a multi-spectrum CANDU reactor as a possible actinide burner requires a numerical verification of the theory of coupled reactors with the use of neutron transport codes. The multi-spectrum nuclear reactor consists of two or more distinct regions, which are operated in a coupled fashion. The term ‘coupled’ means that, in each of the regions, some of the fission neutrons are born in the other region. The current Deuterium Critical Assembly model [1] consists of a two-region reactor. The inner core is a fast region fuelled by 2.7 wt% U-235/U enriched uranium rods surrounded by light water. The outer core is the thermal region fuelled by 1.2 wt% U-235/U enriched uranium rods and moderated by heavy water. The internal region typically has a dominant fast neutron spectrum, while the external region has a dominant thermal one. Both regions would be independently subcritical on their own. The combination of the two regions is designed in such a way that the neutron leakage between them can provide sufficient reactivity to drive the combined system to criticality. The advantage of using the theory of coupled reactors consists in the fact that one can gain a better understanding in the multiplication factor for each region rather just for the whole system, which helps in improving the physical understanding of the detailed characteristics of the multiplying system used as an actinide burner.

2. The Theory of the Coupled Reactor

The theory of a coupled reactor was first pioneered by Avery [2], [3], and [4]. The theory was modified and extended by Komata [5], Kobayashi [6] and Nishihara [1]. A brief mathematical formulation of the nodal equations of the coupled reactor system was derived by Kobayashi [6]. For this two point reactor model, one can obtain easily the criticality factor k_{eff} which is related to regional criticality factors k_{11} and k_{22}, and the coupling coefficients k_{12} and k_{21} by Equation (1):

$$k_{eff} = \frac{1}{2}\left[k_{11} + k_{22} + \sqrt{(k_{11} - k_{22})^2 + 4k_{12} \cdot k_{21}}\right] \quad (1)$$

The criticality coefficients are defined by Allan [7] as

$$k_{12} = \frac{R_{f,1-2}}{(R_{f,1} + R_{f,2})} \times k_{eff} \quad (2)$$

$$k_{21} = \frac{R_{f,2-1}}{(R_{f,1} + R_{f,2})} \times k_{eff}, \quad (3)$$

Where,
$R_{f,1}$: is the fission rate in the inner region (fission cm^{-3} s^{-1}),
$R_{f,2}$: is the fission rate in the outer region (fission cm^{-3} s^{-1})),
$R_{f,1-2}$: is the fission rate in the inner region triggered by from neutrons born in the outer region (fission cm^{-3} s^{-1}),
$R_{f,2-1}$: is the fission rate in the outer core triggered by from neutrons born in the inner region (fission cm^{-3} s^{-1});
k_{11}: is the average number of next generation fission neutrons in the inner fast region resulting from a single fission neutron born in the inner fast region,
k_{22}: is the average number of next generation fission neutrons in the outer thermal region resulting from a single fission neutron born in the outer thermal region,
k_{21}: is the average number of next generation fission neutrons in the outer thermal region resulting from a single fission neutron born in the inner fast region, and
k_{12}: is the average number of next generation fission neutrons in the inner fast region resulting from a single fission neutron born in the outer thermal region.

3. The Research Approach

In the present work, the probabilistic computer code MCNP5 (Monte Carlo N-Particle) [8] is used to simulate the DCA experiment. The nuclear data library used with MCNP5 is ENDF/B-VI.5 which is the same library used by TWOTRAN [9] code in Nishihara's work [1] . The materials temperatures were set at room temperature at (293.6 K). The criticality factors k_{eff}, k_{11} and k_{22} were computed with MCNP5 along with the coupling coefficients k_{12} and k_{21} from Equations (1) and (2). The coupling between the two DCA regions is validated by comparing k_{eff} calculated by Equations (1), (2) and (3) with that computed directly by MCNP5 and that computed by Nishihara [1] by using the TWOTRAN [9]code.

3.1. Heavy Water Critical Assembly (DCA)

The DCA has a cylindrical geometry shape with an outer radius of 150.25 cm. It consists of two reactor core regions. The inner and outer regions are separated by air gap of thickness 9.2 cm as shown in Figure 1. The inner region is loaded with 2.7 wt.% U-235/U enriched metallic uranium fuel rods in aluminum clad surrounded by light water coolant. The outer region is loaded with 1.2 wt.% U-235/U enriched uranium rods in aluminum clad surrounded by heavy water. The inner region consists of 140 fuel rods distributed within a square lattice with lattice pitch 1.9 cm. The middle cell of the inner region is an air tube of inner radius 1.5 cm and aluminum wall of thickness 0.2 cm. The inner core consists in an aluminum cylinder of inner radius 16.8 and outer radius 17.5 cm. The inner radius of the outer core is 33.851 cm and the outer radius is 133.875 cm. The outer core is surrounded by two heavy water reflectors. The outer reflector thickness is 16.375 cm and the inner reflector thickness is 4.351 cm. In both cores the fuel rod diameter is 1.45 cm and its length is 200 cm. The fuel rods are cladded in aluminum tubes. More details and dimensions are shown in Figure 1(A). The inner region or the fast core is designated as Core 1 and the outer region or thermal core is referred to as Core 2.

3.2. Design and Simulation of the Two Regions DCA with Exact Dimensions and Optimal Components using MCNP5

There are some data that were not included in the Nishihara's published work [1]. These unknown data values are used as degrees of freedom of the DCA optimization. These degrees of freedom are: 1) The number of fuel pins in the thermal region, 2) the lattice pitch of the thermal region and, 3) The thickness of aluminum clad of fuel in the whole DCA reactor. An MCNP5 model is created with the exact dimensions and structures with only these three degrees of freedom. The constraints used to optimize these values are: 1) the two regions should be subcritical on their own and, 2) the published values of criticality factors by Nishihara [1] when the water (LW and HW) in the two regions at are 100 cm high. The lattice pitch and number of fuel pins per lattice in the thermal region were optimised. The optimum values of the thermal lattice pitch is 9.66 cm and the number of fuel pins is 4 pins per lattice cell. The last degree of freedom (or the remaining unknown value) is the thickness of aluminum cladding. The aluminum cladding thickness was changed from 0.5 mm up to 1.5 mm. Then, the criticality factors k_{eff}, k_{11} and k_{22} were compared using the same values under the same conditions as Nishihara's results [1] as shown in Table (1).

Table (1) Determination of the Optimum Value of the Aluminum Cladding Thickness

	Al-Clad thickness (cm)	k_{eff} at F100-T100*	k_{22} at F100-T100*	k_{11} at F100-T100*
Reference data [1]	not included	1.020	0.988	0.810
Current calculations	0.1300	1.0234	0.9983	0.7424

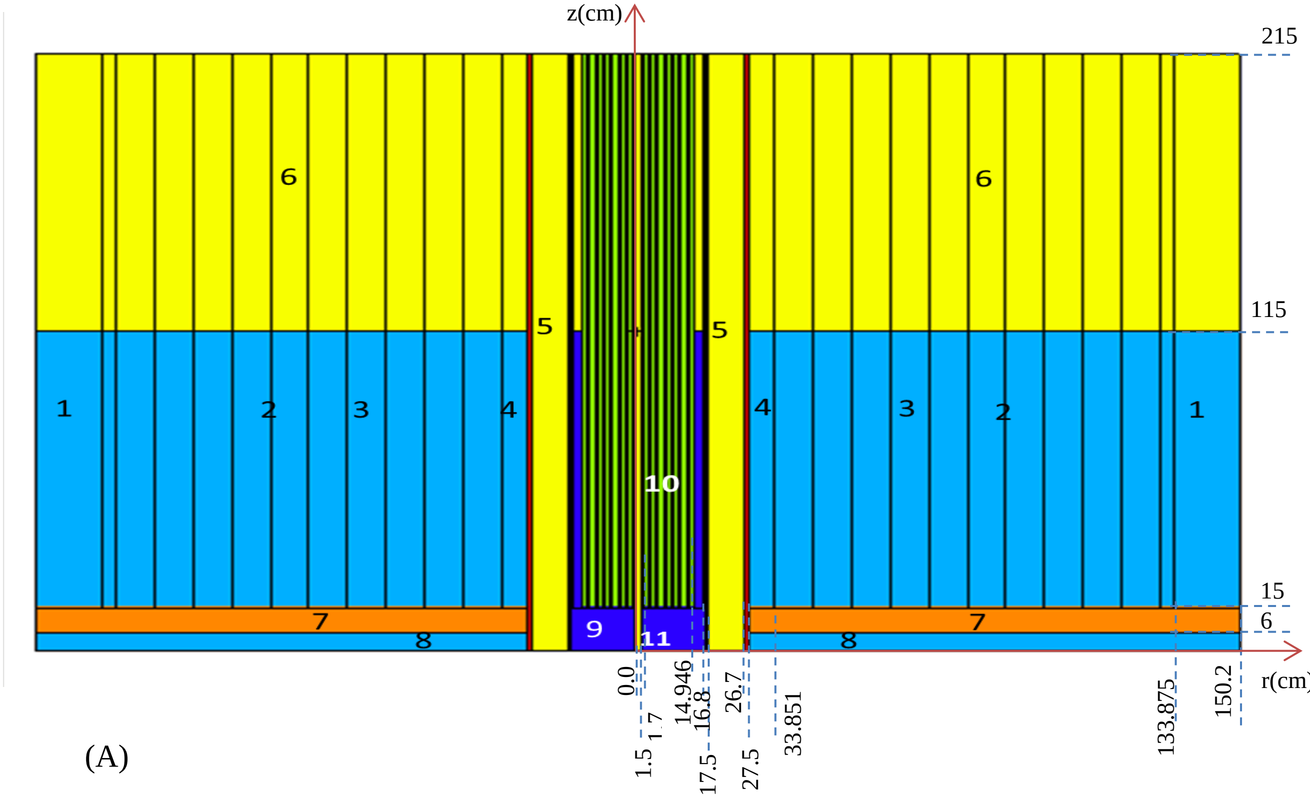
*F100-T100 = Light water level at 100 cm and Heavy water level at 100 cm

The thermal core lattice was optimized to a 474 fuel clusters in a square lattice cells. The thermal lattice pitch is 9.66 cm. Each cluster has four fuel rods for total of 1896 fuel rod. The aluminum clad thickness of the fuel rod is optimized to 1.3 mm. This optimum values is the regarding to the closest values of criticality factors produced by Nishihara [1] as shown in Table (1).

Figure 1 (A) and (B) show the vertical and horizontal cross sections of the DCA model for levels the heavy water and light water in the thermal and fast regions set at 100 cm. Figure 1 (C) and (D) show close-up views of the lattice pitch of the thermal and fast cores respectively. Figure 1 (E) shows the fast core lattice.

3.3. Methodology

As the DCA model was optimized, the coupling theory was verified by driving the system to criticality. Different values of criticality factors k_{eff}, k_{11} and k_{22} and corresponding values of coefficients k_{12} and k_{21} were calculated by changing the level of heavy water in the thermal region and setting the light water level at 100 cm in the fast region, and vice versa. The simulation steps can be summarized as follows:



(1) Heavy water external reflector.
(2) Thermal core fuel lattice.
(3) Heavy water moderator.
(4) Internal heavy water reflector.
(5) Air gap
(6) Air upper the thermal core
(7) Steel (SUS340)
(8) Heavy water.
(9) Light water in the fast core
(10) Fast core fuel lattes.
(11) Aluminum tube in the middle of the fast core of wall thickness 0.2 mm . it contains air .

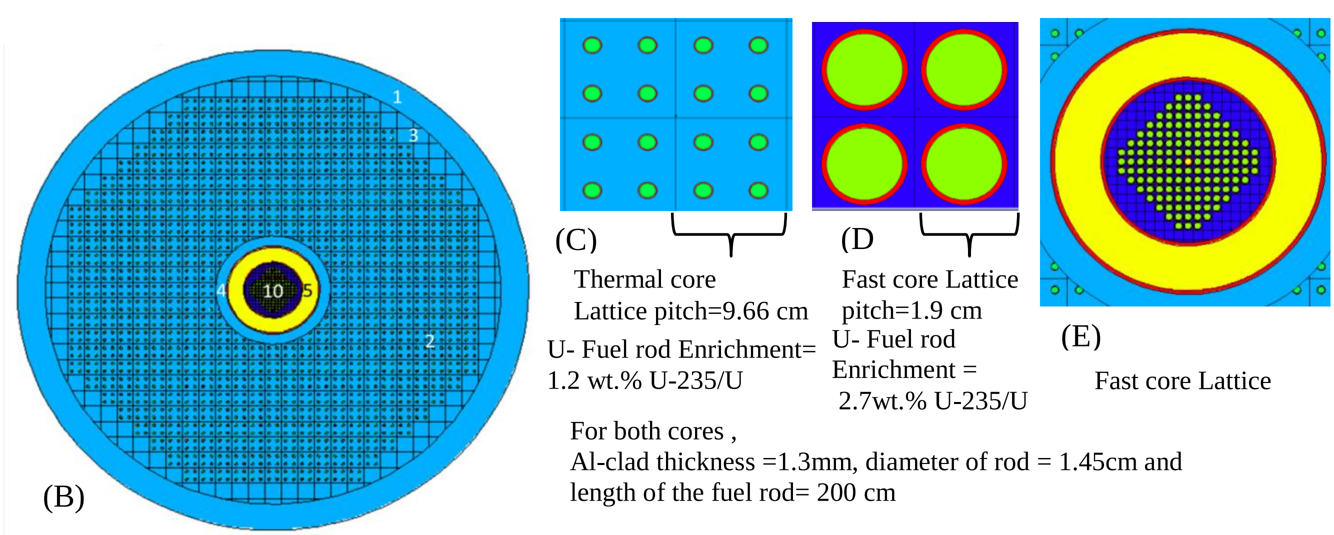


Figure 1 MCNP Model of the Deuterium Critical Assembly

1) The criticality factor k_{11} was calculated by setting the importance of neutrons in the thermal part at a zero value and calculating the k_{eff} of the system, which represents only the criticality coefficient k_{11} of the fast region. Similarly, the coefficient k_{22} was calculated by setting the importance of the neutrons in the fast region to a value of zero.
1) The two regions of the DCA model were simulated, using the probabilistic code MCNP5, at different levels of heavy water and light water, and the criticality factors k_{eff}, k_{11} and k_{22} were calculated. The fission reaction rates $R_{f,1-2}$ and $R_{f,2-1}$ were calculated, therefore the coupling coefficients k_{12} and k_{21} could be found from Equations (2) and (3) respectively.
2) The criticality factor k_{11} was calculated by setting the importance of neutrons in the thermal part at a zero value and calculating the k_{eff} of the system, which represents only the criticality factor k_{11} of the fast region. Similarly, the factor k_{22} was calculated by setting the importance of the neutrons in the fast region to a value of zero.
3) Both k_{11}, k_{22} were calculated for various the levels of water in the fast and thermal regions, respectively.
4) By using the flagged cell tally CF4 in the MCNP5 [8] code, the neutron flux for three energy groups that diffuse from the thermal region to the fast region and vice versa could be calculated.
5) The average cross sections were calculated for each neutron energy group (thermal, epithermal and fast) corresponding to energy ranges 10^{-11} eV to 0.625 eV, 0.625 eV to 0.1 MeV and 0.1 MeV to 14 MeV respectively. The fission reaction rates R_{1-2} and R_{2-1} were also calculated consequently, the coupling coefficients k_{21} and k_{12} could be calculated from Equation (2) and (3) respectively.
6) The criticality factors (multiplication factor) k_{eff} calculated from coupling Equation (1) were compared with the criticality factors (multiplication factor) k_{eff} that were calculated numerically by MCNP5 for the system as a whole for different levels of heavy and light water in the two regions.

4. Results and Discussion

The dependence of the criticality factors k_{eff}, k_{11} and k_{22} and coupling coefficients k_{12} and k_{21} for different levels of heavy water in the thermal region, with the level of light water in the fast region set at 100 cm is shown in Figure 2 and Figure 3. The criticality factors k_{eff}, k_{11} and k_{22} and coupling coefficients k_{12} and k_{21} at different levels of light water in the fast region with the level of heavy water in the thermal region set at 100 cm are shown in Figure 4 and Figure 5.

1) In Figure 2, as the heavy water level increased in the thermal region, the criticality coefficients of this region k_{22} increased gradually. Consequently, the criticality factor k_{12} increased because more neutrons diffuse from the thermal region to the fast one resulting in more fission interactions. There is a small increase in the criticality coefficient k_{21} due to an increase in the fission rate in the fast core as there are a small number of neutrons diffusing from the fast to the thermal region. All of these values affect the total values of k_{eff} at each heavy water level. The value of k_{11} is not changed because it is calculated independently at a fixed level of light water in the thermal core.
2) Figure 3 represents the detailed behaviour of the change of the criticality factors k_{eff} from the MCNP5 calculations, the coupling equation calculations and those calculated by Nishihara [1] using the TWOTRAN [9] code as the heavy water level increases from 0 to 200 cm. One can find very good agreement between the k_{eff} value calculated directly by MCNP5 and that

calculated from coupling theory. The overall percentage difference between these results is 1.6%. Therefore; the coupling theory could be verified with the MCNP5 code.

3) From Figure 4, as the light water level is increased in the fast region, the criticality factor of this region, k_{11} increases sharply until the light water level is around 25 cm. Then, it increased gradually until the light water level comes to 100 cm. This is because of the effect of the light water moderation in the fast core. But, as the level of light water increases, the rate of neutron absorption also increases and gives the result of a flattening of the criticality factor k_{11} to become similar to the value of the fast core when it works independently.

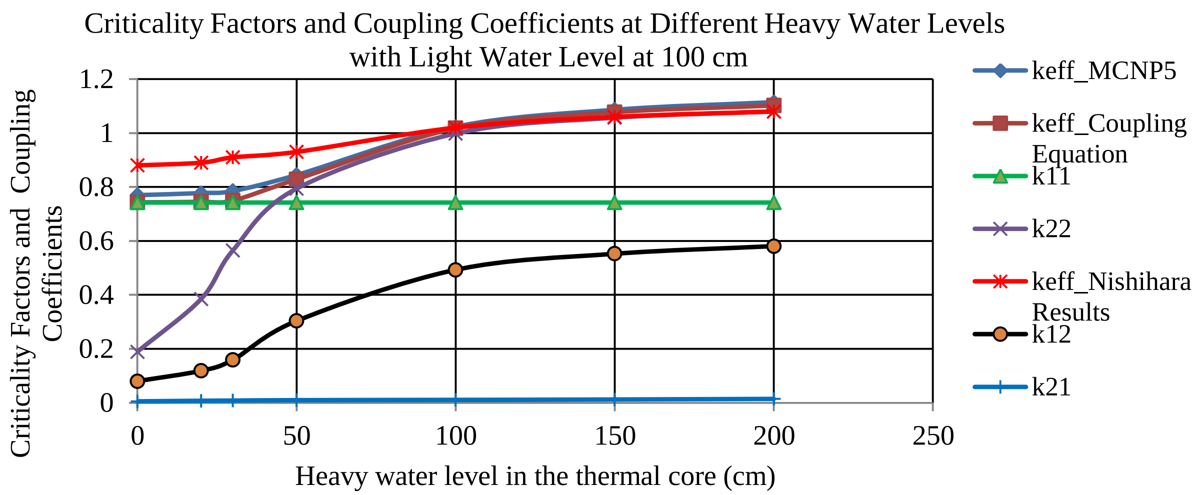


Figure 2: Criticality Factor and Coupling Coefficients at Different Heavy Water Levels in the Thermal Core With Light Water at 100 cm in the Fast Core.

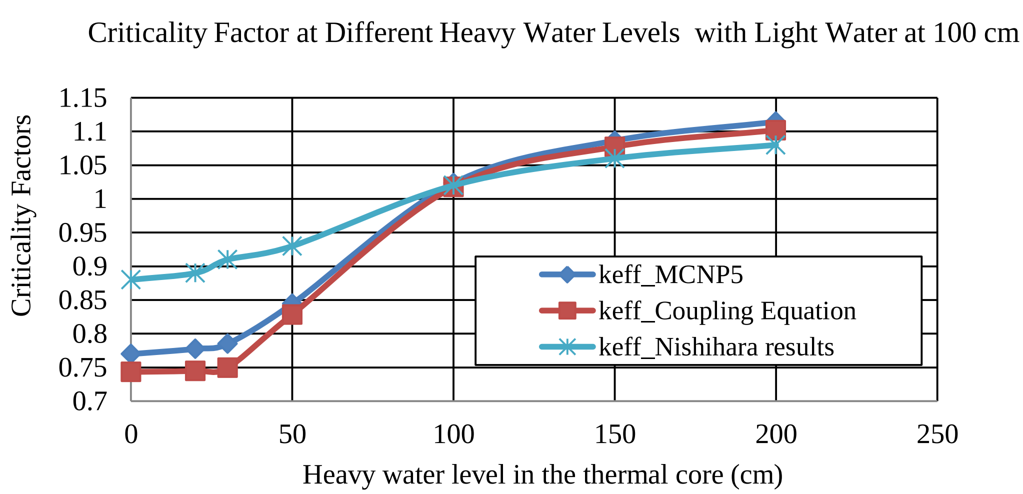


Figure 3: Criticality Factors at Different Heavy Water Levels in the Thermal Core with Light Water at 100 cm in the Fast Core.

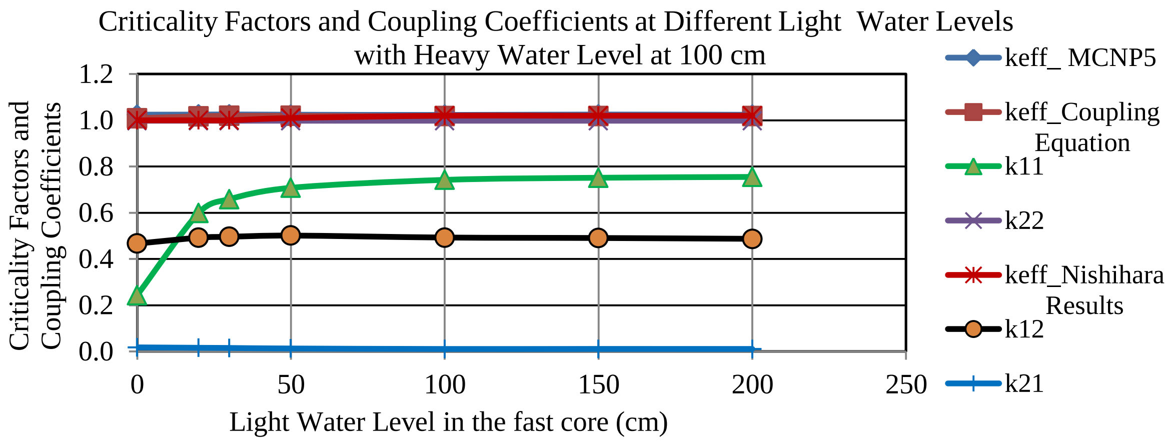


Figure 4: Criticality Factor and Coupling Coefficients at Different Light Water Levels in the Fast Core With Heavy Water at 100 cm in the Thermal Core

4) The criticality factor k_{21} increases by very small values due to more diffusion from the fast region to the thermal region where there is a minor increase of the fission neutrons sources in the thermal region. The values of k_{eff} are not affected as much as for the change of the light water level in the fast core due to the volume and amount of fuel in the thermal region, which are much higher than those of the fast region.
5) The contribution of the thermal region to the values of k_{eff} is more important than that of the fast one due to its larger volume and the amount of fuel in the thermal region in addition to the contribution of the heavy water moderation and reflectors in the thermal fission.
6) There is an excellent agreement between the values of k_{eff} as calculated by MCNP5 directly and those calculated by Nishihara [1] using the TWOTRAN code [9] when the level of heavy water is fixed at 100 cm in the thermal region, while changing the level of light water in the fast region as shown in Figure 5. The percentage difference is about 2.7%.

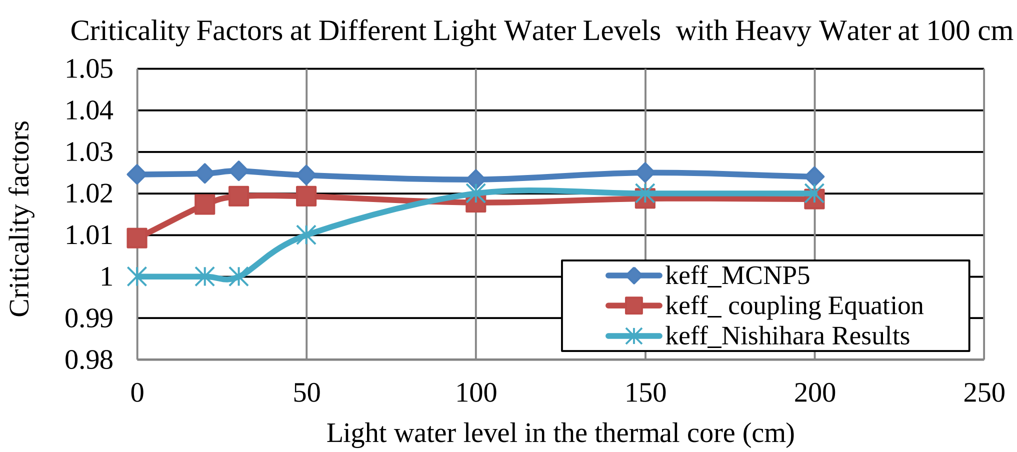


Figure 5: Criticality Factors at Different Light Water Levels in the Fast Core with Heavy Water at 100 cm in the Thermal Core

7) In the case of a changing level of heavy water in the thermal region while fixing the light water level at 100 cm in the fast region, the agreement is very good when the heavy water level is at

100 cm and above with percentage difference 1.2%. But, when the heavy water level was changed between 0 and 100 cm, a reasonable agreement with a percentage difference of 8% was obtained. For both cases the average percentage difference is 4.6%.

8) The values of k_{eff} calculated directly have an excellent agreement with those calculated from the coupling Equation (1). The minor difference in the results from the MCNP5 code and those calculated by Nishihara [1] may due to: (a) Using a three energy group in the present work rather than 4 energy groups as in the Nishihara's work [1], (b) Using a different cross section library, and (c) inaccuracy of the TWOTRAN code [9] at this energy range for fast reactor criticality calculations.

5. Conclusion

The criticality factors calculated by the coupling coefficients and regional criticality factors using the coupled reactor theory agree well with those obtained directly from the MCNP5 based model. There is a very good agreement between the result obtained numerically from the MCNP5 Code and those from the TWOTRAN code. Therefore, it is numerically confirmed that the coupling coefficients can be calculated with sufficient accuracy. Thus, the validity of the coupled reactor theory has been verified. The coupled reactor theory using the MCNP5 transport code could be applicable for designing a multipoint or multi-spectrum CANDU reactor.

6. Future Work

From here, the work is presently in progress aiming to expand the coupled reactor theory as applicable to two, three or greater region reactor and applying this theory to a multi-spectrum reactor based on CANDU reactor design for the design of an actinide burner reactor.

7. References

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