CANDU6 PCR Evaluation with a Detailed 3-D Monte Carlo Analysis

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Abstract

In the original CANDU6 design, the PCR was evaluated to be clearly negative. However, the latest physics design tool predicts that PCR is slightly positive for a wide range of reactor power. In this work, the CANDU6 PCR is re-evaluated by a detailed 3-D CANDU6 core model using Monte Carlo code Serpent2 with considering two thermal hydraulic models, at design and operating condition. The Doppler broadening rejection correction method was implemented in the Serpent2 code to take into account thermal motion of uranium nucleus. It is found that the CANDU6 PCR can be clearly negative at low power range for both design and operating conditions.

1. Introduction

Heavy water is used in CANDU6 reactor as coolant and moderator simultaneously and they are arranged in such a way that allow the natural-U as fuel. Due to a bulky moderator, a highly thermalized neutron spectrum is obtained that provide a good neutron economy. The complicated neutron interaction in the coolant and moderator make the CANDU6 reactor exceptional in terms of the safety parameters such as coolant temperature coefficient (CTC) and fuel temperature coefficient (FTC), and the resulting power coefficient of reactivity (PCR).

Because of the unique fuel design and core configuration characteristics, there is less resonance absorption of neutrons in the fuel which leads to a relatively small negative FTC[1][2]. A recent deterministic study [2]reveals that the FTC of CANDU6 is undoubtedly negative for a fresh fuel and it can be even positive for a highly-burned fuel, FTC becomes less negative or more positive with the fuel temperature. Roh et al.[2] showed that the positive FTC in CANDU6 is largely attributed to the up-scattering by oxygen in fuel and the large thermal fission resonance of Pu-239. Unlike the pressurized light water reactor, CANDU6 has a positive coolant void reactivity (CVR) and coolant temperature coefficient (CTC). The positive CVR is a long-standing safety concern of CANDU6 [1][2].

In nuclear reactors, PCR is the collective effect of FTC and CTC, and a negative PCR is important to extend inherent safety and stability. The small negative FTC and positive CTC make the CANDU6 PCR slightly negative or close to zero either positive or negative for full power conditions. For a negative PCR in CANDU6, a negative FTC is necessary condition since CTC is permanently positive for the operational conditions [1][2]. But for an equilibrium CANDU6 core, the PCR as well as FTC was estimated to be noticeably positive when a new reactor physics codes were used [3]. This indicates that the PCR and FTC evaluation in CANDU6 is subjected to non-

trivial uncertainties and the evaluation method should be improved for better understanding of the CANDU6 safety characteristics.

Since the FTC is rather small and the PCR is very close to zero in CANDU reactors, high-fidelity physics approaches are essential for the accurate evaluation of the safety parameters. During the typical reactor analysis, the asymptotic scattering kernel is generally used and the thermal motion of target nuclides such as U-238 is overlooked. It is well established that in the scattering reaction, the thermal movement of the target nuclides can affect the scattering reaction noticeably in the vicinity of the scattering resonance and heighten neutron capture. Some recent works have revealed that the thermal motion of U-238 affects the scattering reaction and the resulting Doppler broadening of the scattering resonance enhances the FTC of thermal reactors including PWRs by 10-15% [4][5][6][7].

In order to recognize the impacts of the Doppler broadening of the scattering resonances on the criticality and FTC, a recent investigation [8] was performed for a clean and fresh CANDU fuel lattice using a revised version of MCNPX [9] for the analysis. In Ref. 6, the DBRC (Doppler Broadened Rejection Correction) method [5][6][8] was employed to consider the thermal movement of U-238. It has been shown in earlier studies that the FTC is slightly improved due to the consideration of U-238. Kim et. al. [10][11] also completed a preliminary investigation of the FTC and PCR of CANDU6 at near equilibrium conditions by using the Monte Carlo method for a standard 2-D CANDU6 lattice model and established that the CANDU FTC can be improved considerably by taking into account the U-238 thermal motion.

In this study, the PCR of CANDU6 is re-evaluated by using the continuous energy Monte Carlo code Serpent2 [12] which adopts the DBRC method to simulate the thermal vibration of U-238. The analysis is performed for a full 3-D detailed CANDU6 core and the PCR is evaluated at near equilibrium burnup. For a high-fidelity Monte Carlo calculation, 15 billion neutron histories are considered in this investigation.

2. 3-D CANDU Model[13]

In order to evaluate the safety parameters of the CANDU6 reactor, a 3-D full core is modeled in detailed in the current work. The rated power of CANDU6 is 2061.4 MWth. In the CANDU6 reactor, there are 380 fuel channels and each channel contains 12 fuel bundles. The standard fuel bundle consists of 37 fuel rods and two end caps at the end of the bundle. The fuel bundles are loaded into the pressure tube bi-directionally and a calandria tube surrounds the pressure tube that physically separates the moderator from the coolant. The air gap between the pressure tube and the calandria tubes allows the moderator to be at low temperature and close to atmospheric pressure.

The basic lattice cell has dimension of 1 lattice pitch (28.575 cm) by 1 lattice pitch (28.575 cm) by 1 fuel-bundle length (49.53 cm). The design data of the CANDU6 lattice are given in Tables I. Figure1 describes the Serpent2 model of CANDU6 lattice in the x-y plane. Due to the large pitch-to-diameter ratio of the fuel bundle, almost 99% of the neutrons are thermalized in the bulky moderator. Serpent2 model of CANDU6 core configuration is shown in Figure 2.

Fuel pin	
- Number of pin	37
- Fuel pin radius	0.608 cm
- Cladding radius	0.648 cm
Pressure tube	
- Inner radius	5.179 cm
- Outer radius	5.613 cm
Calandria tube	
- Inner radius	6.450 cm
- Outer radius	6.590 cm
Fuel density	10.492 g/cc
Clad density	6.520 g/cc
Pressure tube density	6.515 g/cc
Calandria tube density	6.544 g/cc
Coolant D ₂ O purity	99.10 wt%
Moderator D ₂ O purity	99.85 wt%

Table I. Design data of the CANDU6 lattice



Figure 1: CANDU6 lattice Configuration

The CANDU6 reactor includes several types of reactivity devices for different kinds of reactivity controls. All reactivity devices are introduced into guide tubes which are permanently located in the low-pressure moderator region. These guide tubes are situated interstitially in between calandria tubes, as shown in Figure 2. For accurate analysis of the CANDU6 reactor, it is important to take into account the complicated geometry of the reactivity control devices. The locations of the various reactivity devices are shown in Figure 3. The detector systems in the CANDU6 core are modelled as guide tubes in the Serpent2 simulation. The whole core is extended up to the principal calandria tube in radial direction and two end reflector to the axial direction, as shown in Figure 2 and 3.

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Figure 2: Cross-sectional view of the CANDU6 reactor

It is worthwhile to note that the end reflector region is also modeled in detail in the 3-D whole CANDU6 core model. In modelling each fuel bundle, the end cap is also explicitly considered in this work.





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Due to the on-power refueling features in CANDU6 core, the actual fuel management is typically executed with a core-tracking model taking into account the refueling history of the core. Meanwhile, it is necessary to outline a typical core model for the design and analysis of a CANDU6 core. For this purpose, a time-independent time-average core model has been developed. It is well known that the time-average equilibrium model well characterizes the real daily-fluctuating CANDU6 core in terms of the core characteristics.

As the CANDU6 reactor allow on-line refueling so the equilibrium core holds fuel with a distribution of irradiations, ranging from zero to discharge values. The neutronic parameters of an equilibrium CANDU6 core can be demonstrated by using the time-average model method[13]. In the standard CANDU6 design, the neutronic analysis is performed by the RFSP-IST [14] code. In the CANDU6 design, the time-average core model is actually determined by a coupled iterative calculation of the RFSP-IST neutronic analysis and the thermal-hydraulic analysis with the NUCIRC [15] code. It is worthwhile to note that the time-average core model provides a detailed bundle-wise burnup distribution. In the time-average calculation, the core power distribution is determined by the RFSP-IST code and the corresponding temperature profiles of the coolant and fuel are calculated by NUCIRC and the core power profile is updated again by RFSP-IST until convergence. In this study, a generic time-average model [15] of the CANDU6 reactor has been adopted as the equilibrium core model for the PCR evaluation.

As described previously, each fuel bundle is explicitly modeled in the detailed 3-D core model but due to the memory limitation in this work, the whole core is divided into 14 zones corresponding to the 14 LZCs, as shown in Figure 4, and 14 zone-wise fuel compositions are used in the core model. The zone-wise fuel composition is determined by taking a zone average burnup distribution. It is expected that the zone-average model will be a good approximation to the detailed bundle-wise burnup model since the actual bundle burnups are rather similar in each 14 LZC zones in the time-average model.



Figure 4: Zone numbers for LZC regions in CANDU6

To get the zone-wise fuel composition, a standard 3-D CANDU6 lattice has been depleted by using the Serpent2 code up to the corresponding zone average burnup. These zone-wise fuel compositions were used to model the equilibrium CANDU6 core for the PCR analysis.

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In the time-average model, coolant temperature and density distributions for a whole core are obtained by the NUCIRC [15][16] code for different power levels with the power distributions determined by the RFSP code. Due to the big impact of the coolant temperature on the PCR, the bundle average coolant properties have been modeled very explicitly in this study.

Operational experiences of CANDU6 reactors indicate [17] that the coolant temperature of the conventional CANDU6 reactor tends to increase by ~3°C from the design value with the operation period due to the deposition of corrosion materials in the steam generator tubes. Such an increase in the coolant inlet temperature can change the CTC considerably. Therefore, two types of thermal hydraulic models are considered in this work, one is based on the design inlet coolant temperature and the other is based on the actual operating inlet coolant temperature. The inlet coolant temperature for each case is 534.6 K and 537.6 K, respectively. The NUCIRC calculations were done using these two coolant inlet temperatures in the determination of the time-average CANDU6 model.

Once the coolant temperature of a fuel bundle is determined, the associated average fuel temperature in the fuel bundle can be obtained by using a simple relation in the standard CANDU6 core analysis. In the time-average CANDU6 core model, for a coolant temperature and a fuel bundle power, the bundle-average fuel temperature can be determined by using the following Eq. 1[18]. The bundle-average fuel temperatures have been used to calculate the zone-average fuel temperature in the simplified equilibrium CANDU6 core model in this work.

$$T_{fuel} = T_{coolant} + A \times P_{bundle} + B \times P_{bundle}^2 , \qquad (1)$$

where T_{fuel} is the bundle-average fuel temperature in *K*, $T_{coolant}$ is the bundle-average coolant temperature in *K*, P_{bundle} is the bundle power in kW, and *A* and *B* are the burnup-dependent coefficients, which were determined to be A=0.4956 and B=0.000166, respectively.

3. **Results and Discussions**

In this work, the Monte Carlo method is used to analyze the 3-D CANDU6 model without any additional approximations and simplifications. For continuous energy Monte Carlo calculation of the sophisticated CANDU6 core model, a high-performance parallel computer is essential. All the results presented here were calculated with Serpent2 on a Linux cluster system of Intel Xeon CPU with a clock-speed of ~3.0 GHz. In this cluster, there are 18 nodes and each node has 20 CPUs.

To calculate the PCR of the CANDU6 reactor, the effective neutron multiplication factor (k-eff) was calculated for 8 power levels, i.e., 60%, 70%, 80%, 90%, 100%, 105%, 110%, and 120% power by using the Serpent2 code. Since the magnitude of the PCR is very small, the estimated PCR is quite sensitive to the statistical uncertainty of the Monte Carlo results. Therefore, the standard deviation of k-eff for the PCR evaluation should be small enough for accurate evaluation of the CANDU6 PCRs. In this study, the targeted standard deviation of k-eff is set to 1 pcm though it is very time consuming. In order to achieve the small statistical uncertainty, in the Serpent2 Monte Carlo calculations, a total of 5000 cycles with 500 inactive cycles are used with 3,000,000

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particles per cycle. The number of inactive cycles was heuristically determined by taking into account the relatively slow Monte Carlo convergence in the loosely-coupled CANDU6 core.

The evaluated nuclear data library ENDF-B/VII.0 is used throughout the evaluation. On-the-fly Doppler broadening has also been considered for a specific temperature cross section data. Thermal scattering law $S(\alpha, \beta)$ data has been taken from MCNP data libraries and a constant temperature $S(\alpha, \beta)$ data has been considered through the whole evaluation.

For the equilibrium CANDU6 core, the k-effvalues for the 8 different power levels are plotted for the design inlet temperature in Figure 5.



Figure 5: Reactivity change as function of power level for the design coolant inlet condition (ENDF-B/VII.0)

As shown in Figure 5, it is observed that the DBRC method provides a slightly lower neutron multiplication factor compared to the non-DBRC method. This is simply because of enhanced neutron capture by U-238 by taking into account the thermal motion of U-238 nuclides in the DBRC case. From the non-DBRC curve in Figure 5, it is observed that there is insignificant reactivity change during the power change from 60% to 100%, while, in the DBRC case, reactivity is clearly decreasing with power increasing up to 100% power. This is due to the enhanced neutron capture reaction of U-238 resulting from the Doppler broadening of the scattering resonances with growing fuel temperature in the DBRC case. From the fundamental physics of CANDU6 core, reactivity is clearly observed to increase rather fast in both cases when the power is over 100%. This is because local coolant boiling begins to take place near coolant exit in many coolant channels and the resulting reactivity increase due to the positive CTC supersedes the negative FTC feedback in the CANDU6 core.

Figure 6 shows the PCR results for both the DBRC and non-DBRC cases in the design coolant inlet condition. In this work, the PCR is directly approximated by using two neighboring discrete k-eff

values for either 10% or 5% power interval. It is clearly observed that PCR becomes more negative or less positive when the DBRC method is introduced. This is again mainly because of the enhanced Doppler effect of U-238, i.e., enhanced FTC due to the DBRC method. It should be mentioned that the statistical uncertainty of the estimated PCRs is still rather significant even though such a huge number of neutron histories were considered in the Monte Carlo calculations. Nevertheless, Figure 6 clearly shows that PCR of CANDU6 is negative up to about 95% power level if the coolant inlet temperature remains near the design value. From Figure 6, it is expected that the CANDU6 PCR is rather constant, about -0.5 pcm/%P, in the low power range. The results establish again that the coolant boiling phenomenon can seriously weaken the reactor stability and safety in CANDU6.



Figure 6: PCR as a function of power level for the design inlet coolant condition (ENDF_B/VII.0)

For the operating coolant inlet condition, the estimated PCR is plotted in Figure 7 together with the PCR for the design inlet temperature. 3-D RFSP-IST code results [13] have also been presented as a reference in Figure 7. In addition, Figure 7 compares the current PCR values with those from a simple 2-D lattice Monte Carlo calculation [19].

From Figure 7, it is clearly observed that the PCR values of the current detailed Monte Carlo analysis are significantly less positive than the reference in official design document. The large change in PCR between the current evaluation and the official RFSP-IST results is largely ascribed to the old cross section library (ENDF-B/VI) used in the RFSP-IST analysis and the approximate analysis methods in the RFSP-IST case. It should be mentioned that the thermal motion of U-238 was not taken into account in the RFSP-IST analysis. In other words, due to the DBRC scheme in Serpent2 and the latest nuclear data library and the high-fidelity Monte Carlo reactor modeling, the PCR becomes much less positive in this evaluation for both design and operating coolant inlet conditions than in the standard deterministic analysis.

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It is well-known that the CTC in CANDU6 is clearly positive over the whole power range of interest. Therefore, a negative FTC is essential for a negative PCR in CANDU6. In Figure 7, one can note that the PCR is quite comparable for both design and operating coolant inlet conditions when the reactor power is relatively low, e.g., less than 70%. The low-power PCR behavior indicates that positive CTC is well balanced by a negative FTC feedback effect in the CANDU6 reactor if the coolant is in a sub-cooled state.



Figure 7: PCR comparison as a function of power level (ENDF-B/VII.0)

It is worthwhile to note in Figure 7 that PCR remains negative up to about 90% power level and it begins to rise quickly above 95% power due to the coolant boiling. The impact of the slightly elevated inlet coolant temperature on the PCR is clearly observed after 95% power. The rapid increase of the PCR at the high power range is due to the coolant outlet temperature which is quite close to the saturation temperature at full power condition and also due to the subcooled boiling at the exit region of the high power channels.

In Figure 7, it is interesting to observe that a simple 2-D lattice results are very similar to those of the current detailed 3-D analysis. It should be mentioned that the good agreement between 2-D and 3-D models is possible only when the average temperatures of coolant and fuel in the 2-D lattice model are appropriately obtained from a detailed 3-D temperature profiles by accounting for the 3-D power distribution.

In this 3-D model, the whole core is divided into two zones axially, which then deviates our model from the actual state. It is necessary to consider more zones axially and determine a more dependable quasi equilibrium CANDU6 core for better results. It should be mentioned here that in the whole evaluation process a constant temperature thermal scattering $S(\alpha, \beta)$ data has been used

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where as a temperature-dependent $S(\alpha, \beta)$ is required for the accurate evaluation. It is also required to see the sensitivity of the CANDU6 PCR to the nuclear data. So JENDL-4.0 data library and temperature-dependent $S(\alpha, \beta)$ data and more accurate quasi equilibrium CANDU6 core will be used for further study.

4. Conclusion

The PCR of CANDU6 has been evaluated with a detailed 3-D reactor core model. The continuous energy Monte Carlo code Serpent2 has been used with the ENDF-B/VII.0 library to determine the temperature-dependent reactivity change in CANDU6. In particular, the thermal motion of the target nuclide was accounted for by using the DBRC (Doppler Broadened Rejection Correction) method in the neutron scattering reaction. An equilibrium CANDU6 core was developed using a zone-average burnup data from a generic time-average CANDU6 reactor model. Both DBRC and non-DBRC options were used for comparison in the evaluation of PCR. Additionally, in order to take into account the coolant inlet temperature variation during operation, two inlet coolant temperatures (design and operating conditions) were considered for the PCR evaluation for a wide range of power, 65~115% power.

In this study, the PCR of CANDU6 is found to be slightly negative up to 90% power level for operating condition, whereas in design condition it is negative up to ~95% power. PCR values begin to increase due to the enhanced coolant boiling at exits of coolant channels. The current results indicate that the standard core design tools for CANDU should be upgraded for a more accurate evaluation of physics parameters. One of the important conclusion of this study is that Doppler broadening of scattering resonance should be accurately considered for accurate FTC and a negative PCR of CANDU6. For the validation of the current study, the analysis results need to be compared with measured PCR values of CANDU6.

5. References

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