# Preliminary Derivation of the APEC Functions for 3 Dimensional CANDU Color-sets with Liquid Zone Controllers

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# 1. Introduction

Generally, CANDU-type reactor is analyzed using coarse-mesh finite difference method (FDM) instead of fine-mesh FDM for a better performance due to the usage of lattice-homogenized cross sections [1]. As FDM is not consistent in this application, a robust and consistent method is needed. In 2018 Motalab et al. successfully implemented the nodal equivalence theory for 2-Dimensional (2-D) CANDU-type reactor analysis with the aid of albedo-corrected parameterized equivalence constant (APEC) method [2], which is a new leakage correction method developed by KAIST [3]. The nodal equivalence theory guarantees an accurate nodal solution based on homogenized crosssection (XS) only if the reaction rates are preserved by introducing discontinuity factor (DF), which allows the flux discontinuity at each surfaces [4]. However, as the XS and DF are position dependent, a further correction is needed to achieve an accurate solution [5]. The APEC functions for XS and DF are implemented to correct both XS and DF simultaneously. As Motalab et al. only did the analysis in 2-D problem, in this study the APEC method is applied for 3-D LZC-loaded CANDU-type color-set model. The main purpose of this study is to show the effects of APEC method applied for 3-D LZC-loaded CANDU-type reactor analysis.

#### 2. Implementation of APEC method

The two-step procedure consists of two level analysis. First of all, the lattice-cell and super-cell calculation are performed with all reflective boundary condition to obtain the two-group volume- and flux-weighted constant (FWC) and assembly discontinuity factor (ADF) using the transport or standard Monte Carlo code. In this study, the lattice calculation has been done using Serpent 2 code with ENDF/B-VII.1 library [6]. In the second step, the condensed and homogenized XS and ADF are used to perform the nodal calculation. In this study, an in-house nodal expansion method (NEM) code with a partial-current based CMFD (p-CMFD) acceleration is utilized to perform the nodal calculation [7]. Due to the unphysical reflective boundary conditions used in the lattice calculation, it is inevitable to obtain an inherent inaccuracy from the nodal calculation using lattice-based FWC and ADF. Since homogenized group constants are position-dependent,

some corrections are required to achieve nodal equivalency [5].

The APEC method functionalizes XS and DF in terms of current to flux ratio (CFR) and surface CFRs simultaneously. During iteration, the APEC functions are activated to correct the XS and DF at each assembly according to the assembly CFR. Eventually, the corrected XS and DF by APEC functions lead to the nodal equivalence and converge to an accurate solution.

#### 2.1 Functionalization of Fuel Assembly XS

Kim et al. showed that the two-group homogenized XSs of an assembly have a strong relationship with the assembly-wise CFR [3]. CFR for fuel assembly m is defined as:

$$CFR_g^m = \frac{\sum_s J_g^{m,s}}{\sum_s \phi_g^{m,s}},\tag{1}$$

where the numerator is summation of  $g^{th}$  group outward net currents of assembly *m* and the denominator is summation of  $g^{th}$  group surface fluxes of assembly *m*.

In APEC method, XS changes due to non-zero leakage are defined as a function of CFR value. Due to the physics of CANDU reactor, a simple linear function can be applied rather than a quadratic function applied in light water reactor. Thus, the APEC functions for assembly m, reaction x and group g are defined as follows:

$$\sum_{x,g}^{m} = \sum_{x,g}^{SA} + \Delta \sum_{x,g}^{m}, \qquad (2)$$

$$\Delta \sum_{x,g}^{m} = a_{x,g} CFR_g^m + C_{x,g}, \qquad (3)$$

where  $\sum_{x,g}^{m}$  is the corrected XS,  $\sum_{x,g}^{SA}$  is the FWC XS from single lattice calculation, and  $\Delta \sum_{x,g}^{m}$  is the change of XS. Coefficients  $a_{x,g}$  and  $C_{x,g}$  are determined by least square method using various results obtained from few color-set calculations.

### 2.2 Functionalization of fuel assembly DF

Motalab et al. showed that DF is strongly related to surface-wise CFR (CFRs) [2]. CFRs are defined as follows:

$$CFR_g^s = \frac{J_g^s}{\phi_g^s}.$$
 (4)

The APEC method for CANDU DF is also a simple linear function as follows:

$$DF_g^s = ADF_g + \Delta DF_g^s, \qquad (5)$$

$$\Delta DF_g^s = a_g^s CFR_g^s + C_g^s, \tag{6}$$

where  $ADF_g$  is the g<sup>th</sup> group ADF, which evaluated as the ratio of heterogeneous surface flux to node average flux in single lattice calculation. CFR<sup>s</sup> is the surface-dependent CFR for g<sup>th</sup> energy group.



#### 2.3 Lattice and color-set calculation for APEC function

Although there are several reactivity devices in CANDU-type reactor, only LZC is considered as shown in Fig.1. In Fig.2, the x-z cross-section of 3-D LZC-loaded CANDU color-set is described to generate the APEC functions for XS and DF. For the lattice calculation, the standard and LZC-loaded 3-D CANDU lattice models are described in Fig.3. The color-set model consists of fuel bundles, which are comprised of various burnup from 0 GWd/tU (fresh fuel) to 12 GWd/tU, to generate the burnup-wise APEC function. Therefore, a standard 3-D CANDU lattice depletion calculation from 0 GWd/tU to 12 GWd/tU is needed to obtain burnup-wise XS and DF. Depletion and color-set calculation are performed by Serpent 2 code.

Fig. 2. The x-z cross-section of 3-D LZC loaded CANDU



color-set



Fig. 3. The x-z cross-section of 3-D fuel bundle with LZC

Particularly to treat the asymmetric LZC-loaded fuel bundle as shown in Fig.1.b, the APEC functions for XS and DF correction are defined to be position- and burnup-dependent. For XS correction, the burnup-wise fuel assemblies are categorized into five sections as shown in Fig.2, which are regular assembly, burnupwise full LZC-loaded inner and outer fuel bundle, burnup-wise empty LZC-loaded inner and outer fuel bundle. Although the basic idea of APEC functions for DF correction totally depends on their surface-wise CFR, only three surface-wise CFRs, which are facing LZC surface, opposite to LZC surface, and perpendicular to LZC surface as shown in Fig. 3.b, are considered in case of 3-D LZC loaded fuel assembly. However, for the outer empty LZC-loaded fuel bundle adjacent to reflector, specific APEC functions are considered based on two surface-wise CFRs adjacent to the reflector, respectively.

The DF-APEC functions for fuel bundle adjacent to reflector and corner fuel bundle are generated assembly-wise as shown in Fig.2. Because the DF-APEC functions are not strongly dependent to the burnup, four color-set problems with different burnup have been solved to generate the DF-APEC functions.

In this study, the nodal calculation of 3-D LZCloaded CANDU color-set is performed by in-house 2-D NEM code with 1x1 NEM equivalent DF. The 1x1 NEM equivalent DFs are generated by solving the fixed source problem with net current boundary conditions tallied by Serpent 2 code. The color-set problems are varied with different burnup to obtain enough points for APEC function generation. In this study, four color-set problems have been used to generate the APEC functions for XS and DF corrections. One of the obtained APEC functions for inner full LZC-loaded fuel bundle XS and DF are plotted respectively, as shown in Fig.5 and 6.



Fig. 5. APEC function for fast absorption XS of inner full LZC-loaded fuel bundle with various burnup points.



Fig. 6. APEC function for fast DF of inner full opposite LZC-loaded fuel bundle side with various burnup points.

In Figure 6, it is observed that the APEC functions are not well fitted. However, the fitted functions are enough to correct the DFs of the inner full LZC-loaded fuel bundle as the fuel bundle is not neighboring with quite different assembly in terms of CFR such as reflector.

2.4 Implementation of 3-D Serpent CX and heterogeneous flux to 2-D NEM nodal code.

Although serpent 2 calculation is done in 3-D, the inhouse NEM code is limited only for 2-D problem. Therefore, a few adjustments are needed. 3-D XSs generated from Serpent 2 are homogenized assemblywise and directly used for the nodal code input. In Serpent 2, heterogeneous flux, which is used to generate 1x1 NEM equivalent DF, is tallied for each surfaces of assembly. The tallied heterogeneous fluxes are simply normalized to the respective assembly axial height.

## 3. Numerical Results

To evaluate the applicability of the pre-generated APEC functions based on the previous four color-set

problems to the different problem, another color-set problem with a different burnup distribution is considered as shown in Fig. 7.



Fig. 7. The fuel burnup (in GWd/tU) configuration for 3-D LZC loaded CANDU color-set problem.

To investigate the effects of APEC functions, the nodal calculation is done in three ways which are the nodal calculation with reference XS and DF, FWC and ADF, and APEC corrected XS and DF as shown in Table 1.

Table I: Nodal calculation results

VO	DF	l.	Δρ	Power error (%)	
72	(1x1)	Keff	(pcm)	RMS	Max
3-D Se	rpent 2	0.991132	-	-	-
Ref	Ref	0.991137	0.47	0.03	0.08
FWC	ADF	0.990459	68.57	5.01	10.87
APEC	APEC	0.991085	4.82	0.45	1.28

In Table I, it is obvious that the in-house NEM code reproduces the reference solution because the reactivity difference, power RMS and maximum power error are small enough when the reference XS and DF calculated by Serpent 2 are used. Thus, the in-house nodal code can be utilized for 3-D LZC loaded CANDU color-set analysis. In case of FWC and ADF as a conventional 2step method, it shows a noticeable error compared to the reference in terms of reactivity difference, power RMS and maximum power error. These noticeable errors may occur due to the unphysical lattice calculation with all reflective boundary condition for XSs generation. The uncorrected ADF also contributes to those errors. In case of APEC corrected XS and DF, a significant improvement is observed compared to the FWC and ADF case. The APEC-corrected peak power error is less than 1.3% with 4.8 pcm keff error. In Fig. 8 and 9, the power error (%) distribution of FWC-ADF and APEC-APEC are plotted, respectively.

								Empt	y LZC
								Full	lzc
4.44	4.52	4.15						Refl	ector
3.67	3.90	-6.67	-8.01				_		5
3.63	4.22	-6.35	-5.82	4.29					0
3.78	4.27	-5.22	-6.55	3.81	4.29				-11
3.91	3.75	-7.21	-6.37	3.26	3.67				
3.62	3.48	-7.15	-7.15	3.33	2.87	4.70			
2.95	2.77	-9.48	-6.85	2.62	2.38	3.55			
2.55	2.13	-9.80	-8.22	2.39	2.57	3.11	4.18		
2.20	1.87	-10.99	-7.73	2.16	2.49	2.53	4.23		
1.82	1.51	-10.68	-8.35	2.11	2.27	2.61	3.80		

Fig. 8. Power error (%) of FWC-ADF nodal calculation



Fig. 9. Power error (%) of APEC-APEC nodal calculation

Table II:	Color-Set XS RMS errors (	(%)

Domenter	RMS error (%)			
Parameter	FWC	APEC		
$D_1$	0.978	0.028		
$D_2$	0.635	0.051		
$\Sigma_{a1}$	7.795	0.045		
$\Sigma_{a2}$	6.427	0.051		
$v\Sigma_{f1}$	11.344	0.148		
$v\Sigma_{f2}$	7.240	0.037		
$\Sigma_{S1 \rightarrow 2}$	4.835	0.344		
$\Sigma_{S2 \rightarrow 1}$	10.857	0.400		

In Fig. 8, it is clear that the fuel assembly power is predominantly underestimated in the LZC-loaded lattices with the conventional approach. Meanwhile, it is clearly observed that the APEC-corrected XS and DF reduce power error substantially as shown in Fig. 9. It is also observed that two fuel bundles adjacent to reflector have a power error around 1%. These are because the DF-APEC functions for those locations are not generated burn-up wise. Although the DF-APEC functions are not strongly dependent to burn-up, to get an error less than 1% for those location the burn-up wise APEC functions are needed. The results in Table II show that the RMS errors of APEC-corrected XSs are quite improved compared to the conventional FWC XSs.

#### 4. Conclusions

The APEC method has been successfully applied to a 3-D LZC-loaded CANDU color-set analysis. Burnup and position-dependent APEC functions well correct XS and DF simultaneously and reduce RMS power error to 0.45%, leading to substantially improved accuracy of CANDU nodal calculation. It is concluded that the implementation of the nodal equivalence theory for 3-D LZC-loaded CANDU-type reactor analysis is successfully done by applying burnup- and positiondependent APEC functions to correct the XS and DF. For further study, the APEC method will be extended to 3-D whole core CANDU problem.

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