Nuclear Engineering and Design 256 (2013) 56–66

Contents lists available at SciVerse ScienceDirect

Nuclear Engineering and Design

journal homepage: www.elsevier.com/locate/nucengdes

A code development for LLFP transmutation analysis based on the whole pin-wise calculation in PWRs

Kun Liu, Hongchun Wu, Liangzhi Cao*, Youqi Zheng, Changhui Wang

School of Nuclear Science and Technology, Xi'an Jiaotong University, Xi'an 710049, Shaanxi, China

HIGHLIGHTS

- A new computational code system for in-core transmutation calculation in PWRs is developed.
- Detailed depletion calculation is embedded for the in-core transmutation analysis.
- The numerical tests demonstrate that the code is accurate and capable of handling the in-core transmutation calculation.

ARTICLE INFO

Article history:
Received 11 January 2012
Received in revised form
18 September 2012
Accepted 22 November 2012

ABSTRACT

Most of these conventional transmutation analyses were performed either on a single assembly scope or by macro-depletion calculations. This might not indicate the real transmutation capacities of these reactor systems. A numerical code system designed for in-core transmutation analysis, evaluation and optimization is integrant and indispensable. An in-core transmutation analysis code system, named CATE, considering pin-wise flux calculation and fine depletion processes is developed. The code is designed to implement in-core transmutation calculation for PWRs by combining an in-core fuel management code with the micro depletion calculation code ORIGEN2. The in-core transmutation constants, such as transmutation rate and nuclides inventories can be computed and evaluated by the code. The verifications and validations of the code are presented in the paper by calculating some benchmarks and a preliminary LLFP transmutation loading pattern. Numerical results indicate that CATE can be used for the transmutation evaluation for PWRs.

1. Introduction

The global electricity demand is expected to have increased by about a factor 2.5 by 2050 (OECD/NEA, 2008). Therefore, a strongly increasing demand for nuclear power can be expected. However, Fission Products (FP) and some transuranic isotopes (TRU) are inevitably generated and accumulated with the operation of nuclear power plants. FPs are one of the most limiting factor in designing the repository facilities due to the decay heat emission that increases proportionally to the spent fuel burnup (Setiawan and Kitamoto, 2001). Especially, some long lived fission products (LLFP), such as ^{99}Tc, ^{129}I, ^{93}Zr and ^{135}Cs, whose half-lives are in the order of 10^5–10^6 years, may contribute to the radiotoxicity and hazard in the geologic repository. Based on the systematic researches and investigations on the LLFP transmutation, ^{99}Tc and ^{129}I are among the most important nuclides that dominate the beta activity of discharged fuel after one hundred years. Since their solubility in underground water is high, they are easily migrated to the environment once they are released from the geological repository. To reduce the dose risk and with the consideration of transmutability, ^{99}Tc and ^{129}I should be partitioned from the discharged fuel and transmuted separately (Setiawan and Kitamoto, 2001; Yang et al., 2004; Artisyuk et al., 2005).

For transmuting the LLFP, thermal reactors and accelerator driven transmutation facilities might be the possible choices (Baetslé, 1996). Specific transmutation system, such as accelerator driven system (ADS), needs a longer technological development. Thus, evaluations are performed to be done on the existing technologies which are more exactly approached at present time. Setiawan and Kitamoto investigated the multi-recycle transmutation of LLFP both in PWRs and BWRs based on the mass balance of nuclides in the core by the cell depletion calculation for the homogeneous core model (Setiawan and Kitamoto, 2001). Yang utilized assembly calculation with reflective boundary conditions to estimate the LLFP transmutation performance of PWRs through various LLFPs target designs and loading optimization studies based on the assumption that good agreement between assembly-level and full core analyses (Yang et al., 2004). Scoping-type studies of various

* Corresponding author. Tel.: +86 2982663285; fax: +86 2982668916.
E-mail addresses: caolz@mail.xjtu.edu.cn, caoliangzhi@gmail.com (L. Cao).

0029-5493/$ – see front matter © 2012 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.nucengdes.2012.11.014

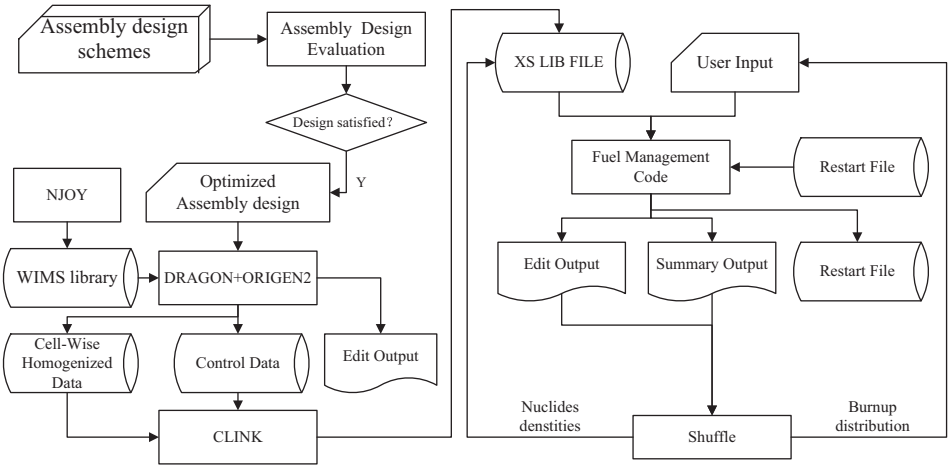

Fig. 1. Flowchart for CATE.

target design and loading optimization have been performed to determine the best transmutation capabilities. However, almost all these previous studies focus on analyses to estimate the potential transmutation rates in LWR with limited consideration of design and safety constraints. It is difficult or practically impossible to extrapolate certain neutronic values obtained from the assembly calculations to the behavior of the whole core. To devise an optimal strategy for LLFP transmutation in the thermal reactors, the whole core irradiation capacities, operation history, and their impacts on the geological repository should be carefully considered. Therefore, the LLFP transmutation analyses based on whole-core calculation needs to be performed.

Neutronics tools used for the modeling of current LWR reactor designs and whole-core analysis capabilities are thoroughly assessed. Coupled Monte Carlo and depletion code systems such as MOCUP (Moore et al., 1995), MONTEBURNS (Poston and Trellue, 1999), and MCODE (Xu and Hejzlar, 2008) have been developed for the analysis of advanced systems. However, the method is particularly useful for analysis of specified designs but not sufficiently efficient for use in parametric and trade studies required for developing an optimized design (Yang and Taiwo, 2004). Direct heterogeneous whole core calculation with depletion computation procedure might perform the core calculation directly without generating homogenized few-group constants in advance. Kochuna et al. investigated that the time required to perform the 3-D cycle depletion by DeCART code system was 1936 CPU hours (Kochuna et al., 2012). This might indicate this method, by heterogeneous whole core pin-by-pin transport depletion calculation, is particularly useful for analysis of specified designs but not sufficiently efficient for use in parametric and trade studies required for developing an optimized design. Therefore, practical LWR core analyses and fuel management calculation are performed with two steps at present: assembly calculations are first performed to generate the few-group homogenized group constants, and then full core neutronics and depletion calculation using these few-group data follow. Most of the current and practical fuel management code systems for the analysis of LWRs core design and fuel management calculation, such as CASMO-4/SIMULATE-3 (Knott et al., 1995; Cronin et al., 1995) and WIMS/PANTHER (Hutton et al., 2000), are based on this calculation strategy. Due to high efficiency, two-step fuel management codes are widely used in fuel loading optimization programs and core monitoring systems.

There are three limitations if the conventional two-steps fuel management code systems were employed directly for the in-core transmutation calculation. The first limitation is that the conventional multi-group nuclear data library applied to an assembly depletion code, without the consideration of LLFP resonance absorption effects in the assembly computation, is not appropriate for transmutation study. The second limitation is the nodal method applied to reactor neutron diffusion calculation in the most of commercial in-core calculation code, which cannot give the fine flux distribution of the transmutation target. The third limitation is in-core depletion chain description is too simple to get accurate transmutation results.

To devise an optimal strategy for LLFP transmutation in the thermal reactors, considering the whole core irradiation capacities and operation history, and to evaluate its impacts on the geologic repository, a systematic code for LLFP in-core transmutation evaluation is needed. In present paper, a modular in-core transmutation code system named computational analyses for transmutation evaluation (CATE) is developed, implementing the fine neutronic calculation and the fine depletion analysis for the thermal reactors.

This paper reviews calculation models in Section 2, addresses validations and applications of the code in Section 3 and Section 4, respectively, and summarizes some conclusions in Section 5.

2. Methods and code development

To break through these limitations for the conventional and practical core analyses code system, a new code for PWR transmutation evaluation is developed as in Fig. 1.

2.1. The multi-group nuclear data library

To characterize the LLFP transmutation evaluation, the resonance effect of transmutation nuclides should be considered. Fig. 2 gives the capture cross section of ^{99}Tc (Revol, 2001) and ^{129}I (Ingelbrecht et al., 2002). It can be found that ^{99}Tc has severe neutron absorption resonance peaks between 1 eV and 3000 eV and ^{129}I has a lot of resonance peaks around 100 eV. In conventional multi-group nuclear data library, the resonance effect for LLFP nuclide is neglected because of the low fission yields. However, it might have significant influences in LLFP transmutation study for the large initial inventories. Based on this point, a new specific nuclear data library in WIMS format is generated from ENDF/B-VII by Liu (2011).

2.2. Assembly depletion calculation code

The DRAGON code (Marleau et al., 2000), based on collision probability techniques, is used to perform the 2D assembly

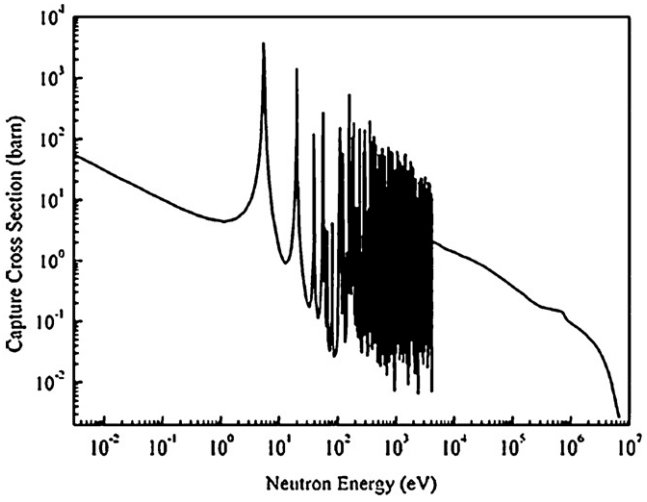

Fig. 2. Capture cross section of ^{99}Tc and ^{129}I.

transport calculation and generates the few group constants for subsequent core calculations.

Different from conventional assembly depletion calculation process, the calculation process for transmutation requires detailed and reliable depletion chain description. Based on this, development of a validated and detailed assembly depletion code is the prerequisite for transmutation study. The generic coupled assembly neutronic-burnup code, by means of combing the lattice physics code DRAGON and the fine depletion code ORIGEN2 (Croff, 1980) is developed, as shown in Fig. 3. It executes DRAGON for assembly transport computation. The neutron flux and effective microscopic cross sections in each depletion region are calculated and transformed into ORIGEN2 input format. Spectra in depletion regions are employed for condensing the multi-group cross sections to one group cross sections for updating the library of ORIGEN2. With the updated library, ORIGEN2 is executed to perform the depletion calculation. The nuclides vectors are extracted from ORIGEN2 output file and prepared for next step transport calculation. The feedback criteria for certain nuclides are selected with the consideration of significant inventories and other characteristics such as radiotoxicity.

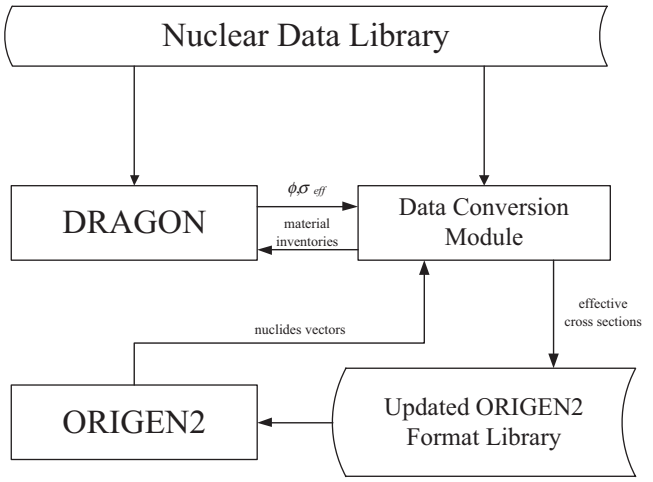

Fig. 3. Coupling of DRAGON and ORIGEN2.

2.3. Cross sections fitting

The assembly constants, such as homogenized few group cross sections and fission products yields, are calculated by assembly depletion code only in the limited conditions. However, the operation of PWR is a continuous progress. It is necessary to fit the few-group constants by least-square method and to apply the polynomials for subsequent in-core calculation.

A fitting code named CLINK is developed to process few group constants generated by assembly depletion code into a data library for in-core calculation in CATE. The data from assembly depletion calculation are fitted into the following form:

$$\Sigma_x = f_1(BU, C_B)\cdot f_2(P_r) + f_3(C_B, U) + f_4(BU, C_B)\cdot \delta(Cr) + N_{Xe}\cdot \sigma_{Xe}(BU, C_B, P_r, U, Cr) + N_{Sm}\cdot \sigma_{Sm}(BU, C_B, P_r, U, Cr) \quad (1)$$

where $f_i(x)$, (i = 1,2,3,4) is a polynomial of variable x, $\delta(Cr)$ the Dirac function which equals to 1 or 0 when control rod clusters exist or not, BU the burnup (GWd/tHM); U the relative moderator density and Pr the relative power. The microscopic capture cross section of fission poisons σ_{Xe} and σ_{Sm} are fitted in the following form:

$$\sigma_{Xe,Sm} = f_1(BU, C_B)\cdot f_2(P_r) + f_3(C_B, U) + f_4(BU, C_B)\cdot \delta(Cr) \quad (2)$$

which have the similar polynomials as those of pin cells macroscopic cross sections.

Since cell normalized spectrum is considered as the functions of burnup, relative power, moderator density and critical soluble boron concentration and so on, microscopic cross sections condensed by spectrum might be influenced by all these factors and consequently are fitted into the following form presented in Eq. (3). Thus, CLINK is also applied to the fine depletion process, as shown in Fig. 4.

$$\sigma_x = f_1(BU, C_B)\cdot f_2(P_r) + f_3(C_B, U) \quad (3)$$

2.4. In-core calculation code

In the present reactor analysis code system, such as SIMULATE-3 (Cronin et al., 1995) and SMART (Greg and Richard, 1994), advanced nodal method is employed for neutron diffusion equation calculation. These codes work well in the static core analysis and reactor designs but are not appropriate for the in-core transmutation studies. The first limitation is that the heterogeneous effect induced by transmutation targets is homogenized in nodal diffusion methods. Fig. 5 shows the procedure of an assembly homogenization. Based on this method, it is not possible to obtain the real flux for the target pins due to the homogenization.

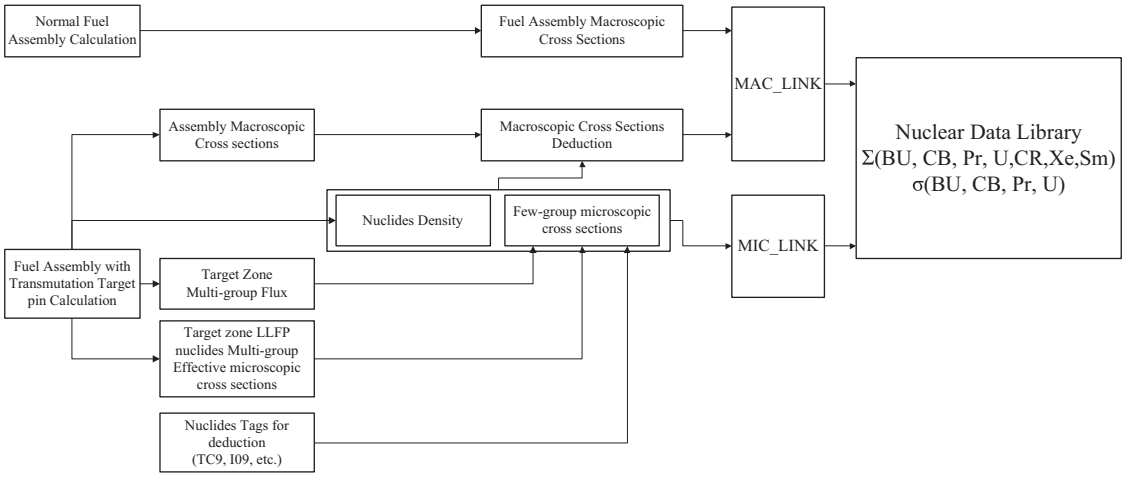

Fig. 4. Calculation flowchart of CLINK.

The second limitation is that most of core analysis codes utilize macro depletion calculation. In-core micro depletion calculation is limited to the poisons and related precursors. It is not satisfied in the transmutation calculation.

To break through the limitations of conventional core analysis program, a new reactor analysis code CATE is developed. The fine mesh differential calculation code CITATION (Fowler et al., 1969) is applied to pin-wise flux calculation and the micro depletion calculation code ORIGEN2 is utilized for fine depletion analyses for important nuclides. To enhance the reliability and accuracy of micro depletion calculation, local few group fluxes obtained by CITATION are employed for one-group microscopic cross sections updating. Meanwhile, the macro depletion calculation is also kept for non-transmutation lattices. Fig. 6 gives the computational flow for in-core fuel management calculation and transmutation evaluation.

3. Validation of CATE

The code CATE is developed based on the modules mentioned above. The OECD/NEA PWR cell benchmark for actinides transmutation is employed for validation of assembly depletion code. OECD-L336 (C5) benchmark problem and infinite homogenized plate depletion problem are utilized for validation of in-core pin-wise neutronic calculation and micro depletion calculation, respectively. Based on these, a fuel management problem for commercial PWR reactors is calculated and the results are compared with that of conventional analysis program for the code CATE validation.

3.1. The OECD/NEA PWR cell benchmark

This is a PWR cell benchmark of actinides transmutation published by OECD/NEA. It describes a PWR cell with light water moderation, containing uranium, plutonium and minor actinides (MA). Four desirable plutonium and MA compositions are originally considered in the benchmark specification. These are denoted as MOX11, MOX21, MOX12 and MOX22. Here, results of the MOX22 lattice with normal moderation, MA 2.5% are analyzed in presented paper. The results are compared with the references given by OECD/NEA (OECD/NEA, 2000). The k-infinity and concentrations of isotopes are compared as given in Tables 1 and 2. Since no experimental value or a reference value exists to compare the performance of the different codes, an average value among the results of the benchmark participants is selected as the reference result, to estimate the difference of the results of each participant respect to this value. It can be seen from Tables 1 and 2 that the average difference of k-infinity and ^{237}Np atomic density

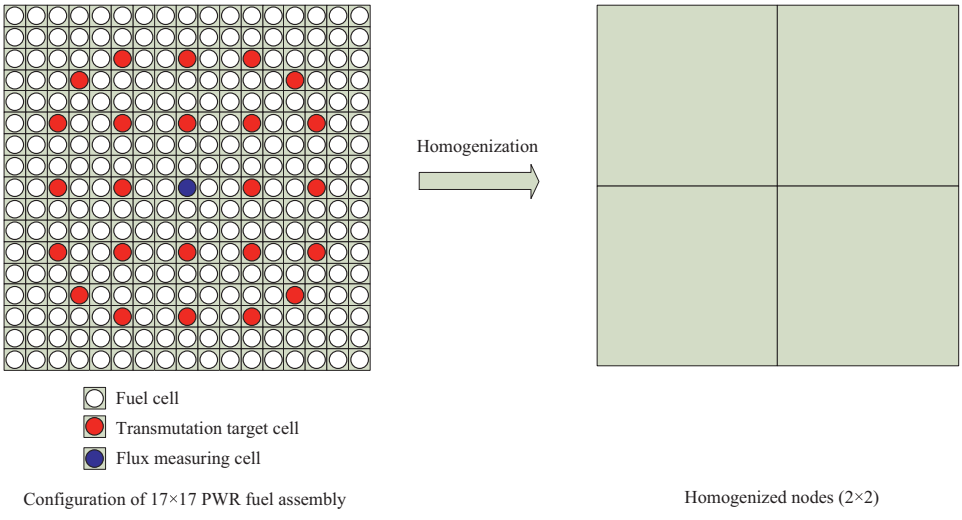

Fig. 5. Assembly homogenization.

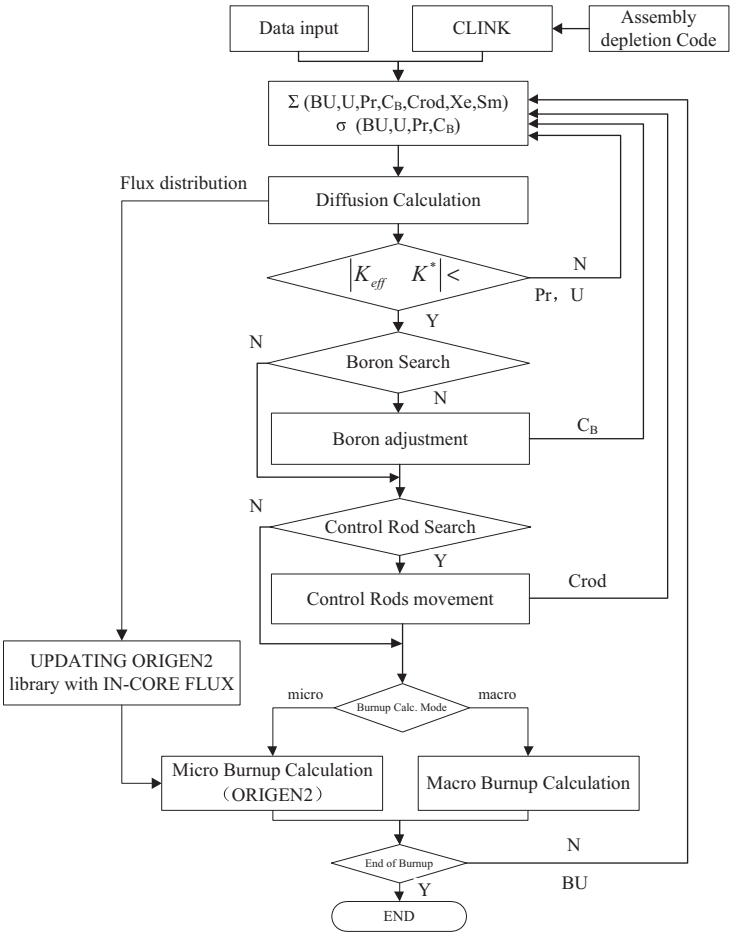

Fig. 6. Flowchart of CATE.

as a function of burnup obtained by DRAGON + ORIGEN2 present good agreements: 0.67% $\delta k/k$ and 0.20% $\delta n/n$. Table 3 illustrates the FP production at 33 GWd/tHM burnup in the case of MOX22 with normal moderation, MA 2.5%. The concentrations of specific fission products, ^{99}Tc, ^{129}I and ^{135}Cs, calculated by DRAGON + ORIGEN2 are in good agreement with the reference results.

3.2. OECD-L336 (C5) benchmark problem

The OECD-L336 problem (Lefebvre et al., 1991) was issued by OECD-NEA Nuclear Science Committee to test the applicability of various core analysis methods to a core loaded with mixed-oxide (MOX) fuel assemblies. The C5 configuration that we used consists of two types of fuel assemblies (i.e., uranium oxide (UO_2) and

Table 1
Comparison of k-infinity as a function of burnup for MOX22 and MA 2.5%.

Burnup	$k_{average}$	(%) $\delta k/k$[a]					
MWd/tHM		FZK	IPPE	JAERI	ITEP	UNAM[c]	CATE
0	1.0884	0.38	1.06	−0.24	−0.97	−0.23	−0.71
150	1.0828	0.44	1.15	−0.04	−0.85	−0.70	−0.61
500	1.0812	0.44	1.16	0.00	−0.84	−0.75	−0.64
1000	1.0796	0.49	1.14	−0.03	−0.83	−0.77	−0.64
2000	1.0767	0.45	1.21	0.00	−0.84	−0.81	−0.64
4000	1.0715	0.54	1.26	−0.07	−0.83	−0.91	−0.66
6000	1.0671	0.63	1.24	−0.02	−0.86	-0.99	−0.68
10,000	1.0604	0.66	1.35	−0.03	−0.92	−1.06	−0.64
15,000	1.0520	0.89	1.43	−0.21	−0.90	−1.21	−0.69
20,000	1.0448	0.87	1.57	−0.23	−0.93	−1.28	−0.66
22,000	1.0418	0.89	1.56	−0.21	−0.91	−1.33	−0.67
26,000	1.0357	1.07	1.54	−0.36	−0.86	−1.39	−0.70
30,000	1.0298	1.21	1.61	−0.39	−0.97	−1.46	−0.71
33,000	1.0255	1.16	1.60	−0.41	−0.87	−1.49	−0.71
Average[b]		0.78	1.35	−0.16	−0.88	−1.03	−0.67
S.D.		0.28	0.19	0.15	0.05	0.35	0.03

[a] $\frac{\delta k}{k} = \frac{k_{average} - k_{code}}{k_{average}} \times 100\%$.
[b] Average of absolute values.
[c] Calculated by HELIOS (Guzmán and Francois, 2007).

Table 2
Comparison of the ^{237}Np density as a function of burnup for MOX22 and MA 2.5%.

Burnup	$n_{average}$ 10^{24} n/cm^3	(%) $\delta n/n$[a]					
MWd/tHM		FZK	IPPE	JAERI	ITEP	UNAM[c]	CATE
0	2.54E−05	−0.33	−0.11	0.32	−0.01	−0.02	0.14
150	2.53E−05	−0.19	−0.19	0.24	0.13	0.02	−0.12
500	2.53E−05	−0.29	−0.29	0.14	0.25	0.18	0.09
1000	2.53E−05	−0.44	−0.01	−0.01	0.10	0.36	0.34
2000	2.52E−05	−0.43	−0.43	0.00	0.32	0.55	0.42
4000	2.49E−05	−0.89	−0.02	−0.24	0.30	0.85	0.16
6000	2.46E−05	−1.49	−0.39	0.49	0.60	0.79	−0.14
10,000	2.42E−05	−2.61	−0.36	0.76	0.87	1.34	0.00
15,000	2.37E−05	−4.13	−0.69	1.14	1.48	2.20	0.05
20,000	2.33E−05	−5.38	−0.72	1.38	1.73	2.98	0.38
22,000	2.31E−05	−5.48	−0.78	1.33	1.68	3.25	0.31
26,000	2.27E−05	−6.83	−1.09	2.25	2.13	3.53	0.10
30,000	2.24E−05	−7.78	−0.76	1.91	2.51	4.12	0.24
33,000	2.23E−05	−8.41	−1.08	2.09	2.70	4.70	0.86
Average[b]		−3.19	−0.49	0.84	1.06	1.78	0.20
S.D.		2.95	0.35	0.81	0.92	1.59	0.25

[a] $\frac{\delta n}{n} = \frac{n_{average} - n_{code}}{n_{average}} \times 100\%$.
[b] Average of absolute values.
[c] Calculated by HELIOS (Guzmán and Francois, 2007).

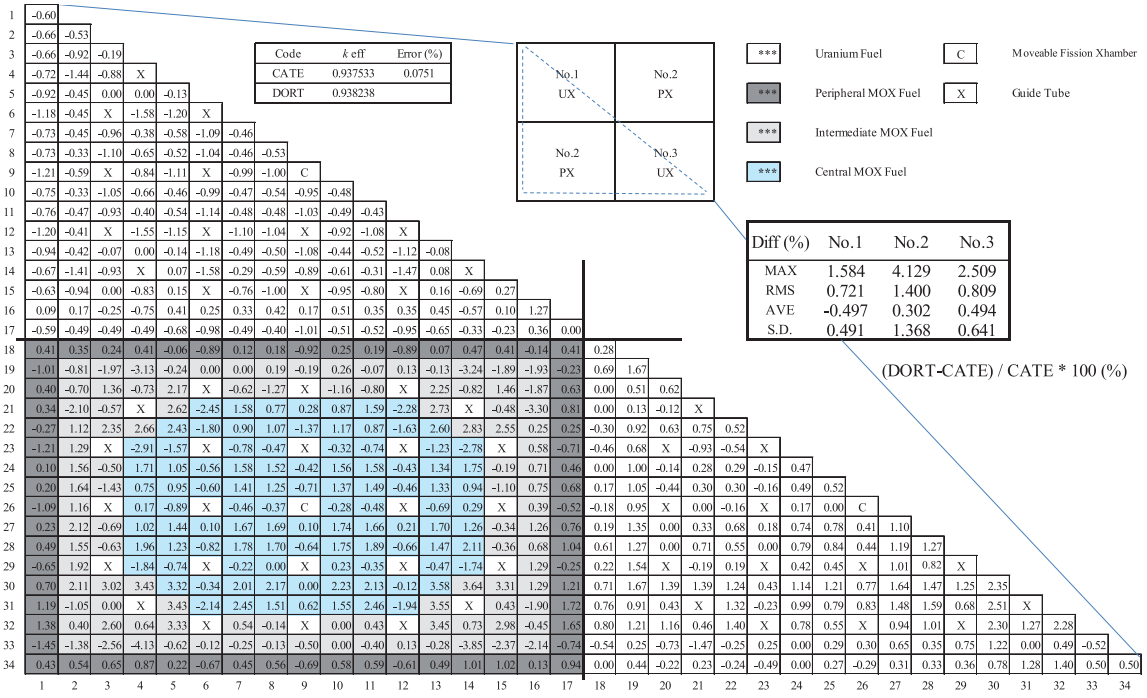

Fig. 7. Comparison of normalized power distribution between CATE and DORT.

MOX fuel assemblies) and water reflector. Each fuel assembly is 21.42 cm wide and contains 17 × 17 homogenized pin cells of different types. The problem is characterized by the presence of large thermal flux gradients near the interfaces between the UO_2 and MOX fuel assemblies, because of very different neutronic properties of the two types of fuel assemblies. The cross sections specified in the benchmark are fitted by CLINK and the benchmark is calculated by CATE. The numerical results are shown in Fig. 7. Compared to DORT (Rhoades, 1993), it can be seen that the relative deviation of *k*-infinity is 0.00751%. A good agreement for normalized power distribution in UO_2 assemblies can be observed, while discrepancies for pin-wise power in MOX assemblies for diffusion theory is inferior to the transport theory in modeling the local steep thermal flux gradients due to strong discontinuity of the materials.

Table 3
Fission products weight (kg) of ^{99}Tc, ^{129}I and ^{135}Cs generated at the burn-up 33 GWd/tHM normalized to 1 t fuel.

	Nuclides		
	^{99}Tc	^{129}I	^{135}Cs
Reference	0.800	0.200	1.170
CATE	0.798	0.205	1.194

3.3. Infinite homogenized plate depletion problem

The purpose for this problem is to validate the fidelity of in-core depletion calculation. To avoid additional difference induced by deterministic neutronics calculation theory, the infinite homogeneous depletion problem is designed. Table 4 summarizes

Table 4
Infinite homogenized plate specification.

Parameters	Values
Linear power (MW/cm)	0.01344
Specific power (MW/tHM)	12.233
Discharge burnup (GWd/tHM)	33.0
Material temperature (K)	300.0
Plate width (cm)	11.0
Material specification (nuclide density 10^{24} n/cm^3)	
^{235}U	1.51220E−03
^{238}U	2.14770E−02
^{1}H	4.70130E−02
^{16}O	6.94515E−02

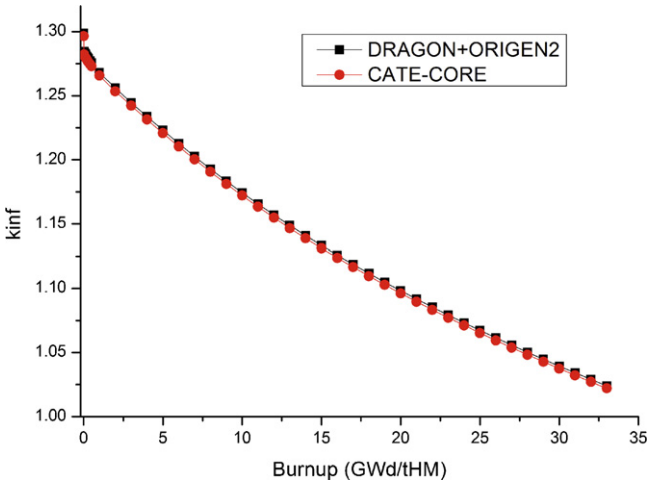

Fig. 8. *k*-Infinity versus burnup for infinite homogenized plate.

the parameters of the problem. Macroscopic and microscopic cross sections and other few-group constants calculated by DRAGON + ORIGEN2 are fitted by CLINK and applied by in-core pin-wise diffusion and detailed depletion calculation, to verify the numerical accuracy of in-core detailed depletion computation. The results obtained by CATE in-core calculation are denoted as CATE-CORE. Since the few-group constants are generated by assembly depletion code DRAGON + ORIGEN2, it is reasonable to compare the results of DRAGON + ORIGEN2 and CATE-CORE.

Table 5
Comparisons of *k*-infinity and nuclide densities for infinite homogenized plate depletion problem (33.0 GWd/tHM).

	k-Infinity (%) $\delta k/k$	^{238}U atomic density (%) $\delta n/n$	^{239}Pu atomic density (%) $\delta n/ns$
Average	0.1906	0.0226	0.1019
S.D.	0.0034	0.0097	0.1450

The variation of *k*-infinity values and nuclide densities in the depletion process are shown in Figs. 8 and 9, respectively. The average relative deviations are summarized in Table 5. From these two figures, the *k*-infinity and nuclide densities calculated by CATE-CORE agree well with the reference result, the average differences are 0.1906%, 0.0226% and 0.1019%, respectively.

3.4. Fuel cycle simulation

In this section, to validate the ability of three-dimensional steady reactor core analysis, a fuel cycle is simulated. The calculation is based on the 13th fuel cycle for Unit 1 reactor of Daya Bay Nuclear Power Plant, considering the ARO condition. The reference results are calculated by CSIM-3B (Liao and Xie, 2003), which uses the nonlinear iterative semi-analytic nodal method (NLSANM) for neutron diffusion calculation. The loading pattern is shown in Fig. 10.

The critical concentrations of boric solution at hot zero power (HZP) mode, hot full power (HFP) mode and the normalized power distributions at different burnup are compared. From the results presented in Table 6, it can be figured out that discrepancies of soluble boron concentrations at HZP mode and HFP mode between the two codes are relatively small. Meanwhile, the critical concentrations of boric solution as a function of burnup for different fuel

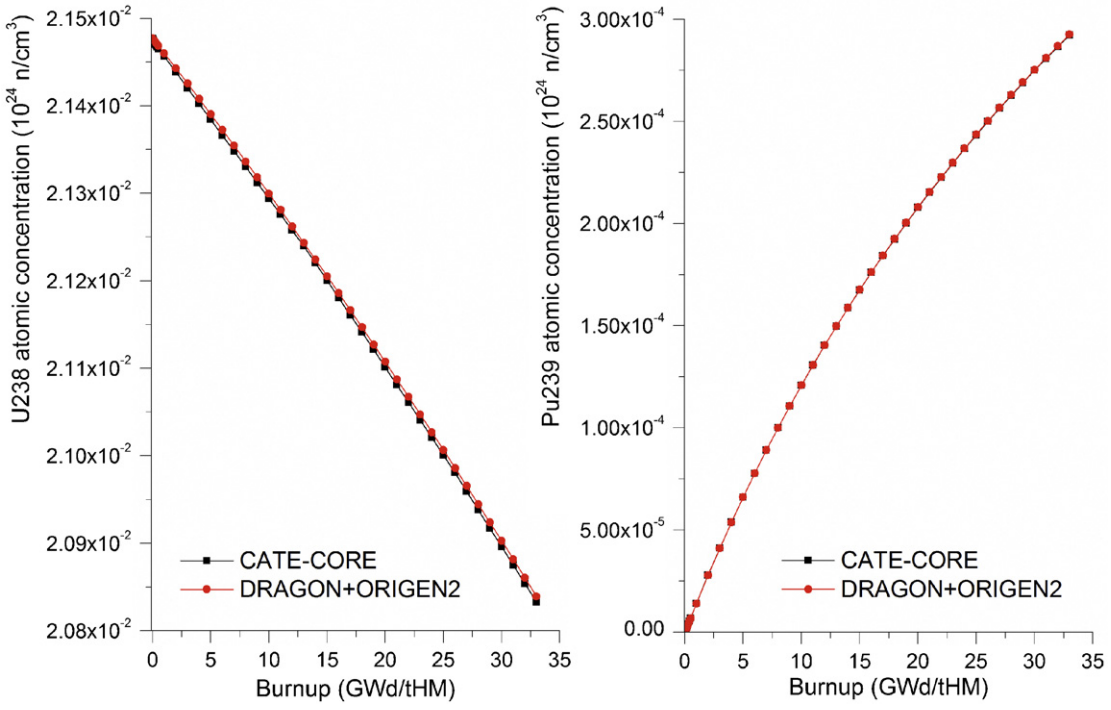

Fig. 9. Nuclide density versus burnup for infinite homogenized plate.

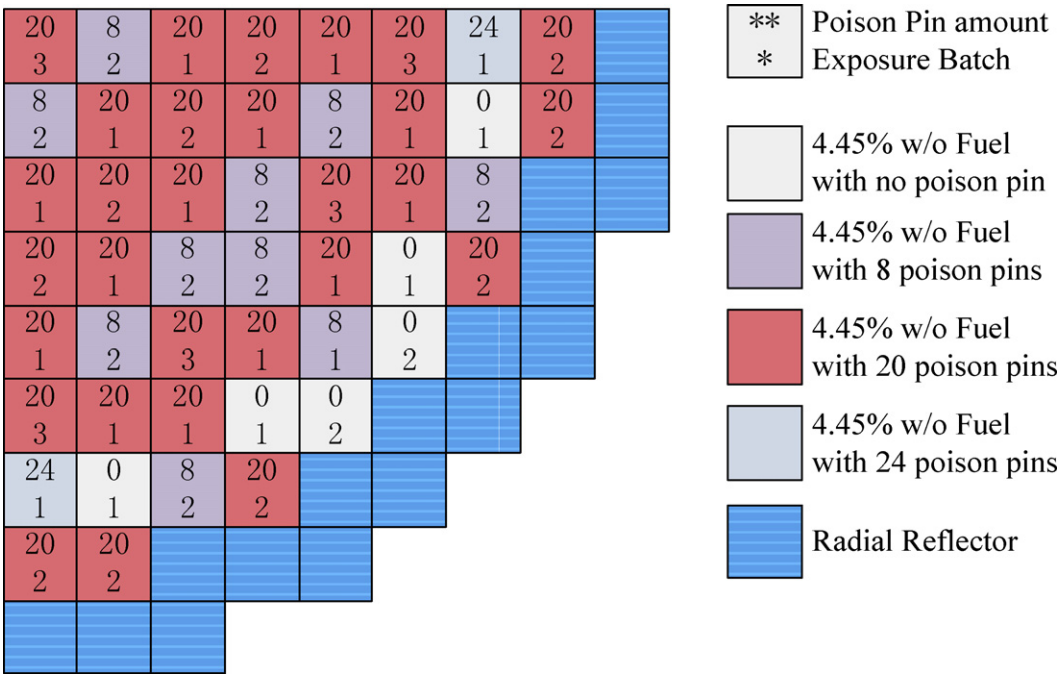

Fig. 10. In-core assembly loading pattern.

Table 6
Comparison of *k*-effective and soluble boron concentration search in HZP and HFP.

Mode	CSIM-3B		CATE	
	k-Effective	C_B (ppm)	*k*-Effective	C_B (ppm)
HZP	1.000006	1943.050	1.000059	1941.486
HFP	0.999697	1862.434	0.999692	1859.026

management codes are illustrated in Fig. 11. A good agreement can be observed between CSIM-3B and CATE.

The absolute deviations of normalized power distribution in specific burnup points are shown in Fig. 12. It can be observed in the figures that the absolute deviation of normalized power distribution as a function of burnup is small and acceptable.

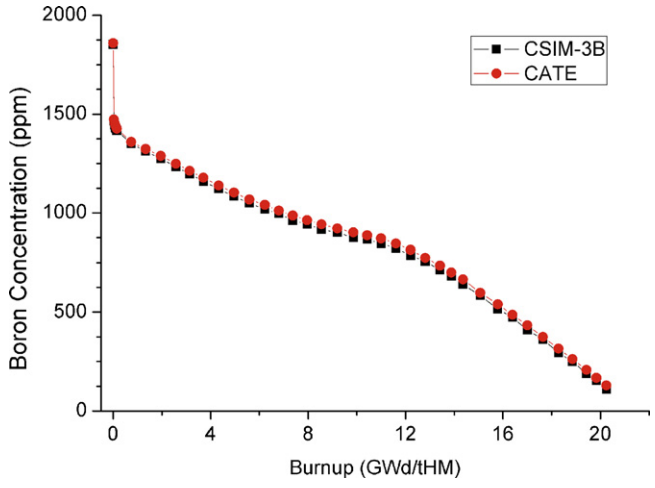

Fig. 11. Critical concentration of boric solution as a function of burnup.

4. Application of CATE

A preliminary transmutation target loading pattern is designed for LLFP in-core transmutation evaluation and the code CATE is employed for transmutation analysis. The loading pattern is based on previous fuel assembly loading scheme, with eight transmutation assembly loaded in the core. The loading pattern is shown in Fig. 13. To obtain higher flux level, the assemblies with transmutation target are loaded in the center of the core. The initial target inventory is given in Table 7 and the target in-assembly loading pattern is shown in Fig. 14.

Since both ^{99}Tc and ^{129}I have relatively large capture cross sections in the thermal and epithermal energy, the cylindrical target form reduces the effective capture cross sections, because of the spatial self-shielding effects. This is especially true for ^{99}Tc since it has a large capture resonance at 5.6 eV. In order to enhance the capture reactions by reducing the spatial self-shielding effects, the LLFP target materials need to be loaded as dilutely as possible. A homogeneous mixture of target and the inert matrix is utilized in this study. The inert matrix applied in this study is a 50–50 mix of magnesia–zirconia ($MgO–ZrO_2$). The metallic forms of Technetium-99 and sodium iodide (Iodine-129) are mixed in the inert matrix.

The length of lifetime is 510.0 EFPD, and the discharge burnup is 20.245 GWd/tHM. The transmutation rate of LLFP nuclides is illustrated in Table 8.

It denotes that transmutation rate for ^{99}Tc and ^{129}I in Table 8 are low. For nuclides transmutation in a neutron facility, the transmutation rate is influenced by both effective cross sections and in-core

Table 7
Material specification of transmutation target pin.

Nuclides/components	Nuclides density (10^{24} n/cm^3)
Zr-nat.	8.63725E−03
Mg-nat.	1.60478E−02
Na-nat.	5.89884E−03
^{129}I	5.89884E−03
^{99}Tc	3.03725E−02
^{16}O	3.33223E−02

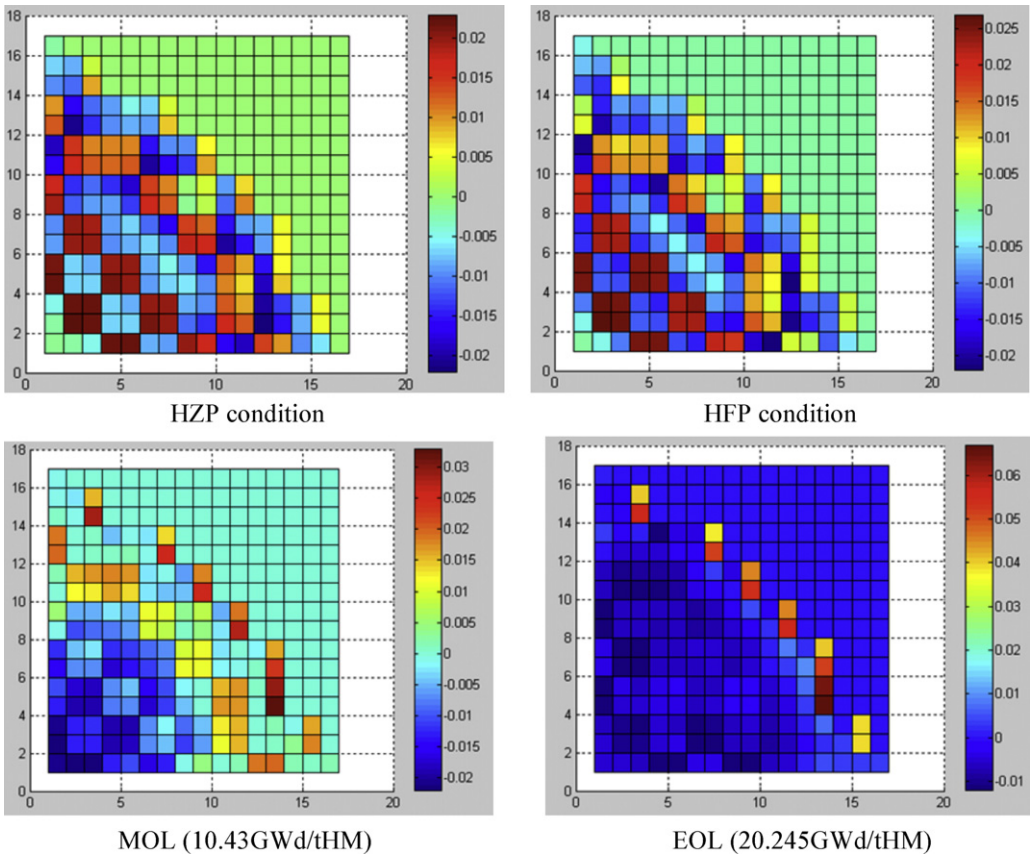

Fig. 12. Absolute deviations for normalized power distribution at different burnup between CSIM-3B and CATE.

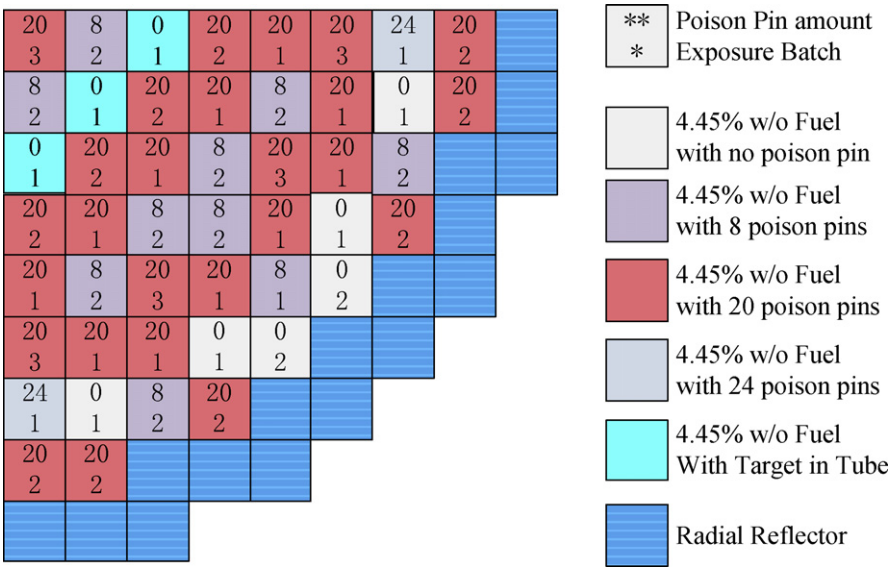

Fig. 13. In-core assembly loading pattern (with transmutation assemblies loaded).

Table 8
Transmutation rates of LLFP nuclides.

	^{99}Tc	^{129}I
Transmutation rate (%/year)	4.6286	2.6410

flux level. For the assembly depletion calculation, the multi-group fluxes in transmutation target cell and those in a fuel cell are calculated and presented in Fig. 15. Comparing with the flux distribution of a normal fuel cell, it can be observed that the spectrum of the target cell is harder, which might leads to a lower absorption rates for LLFP nuclides. Table 9 gives the one-group effective microscopic capture cross sections of different LLFP nuclides. The capture cross

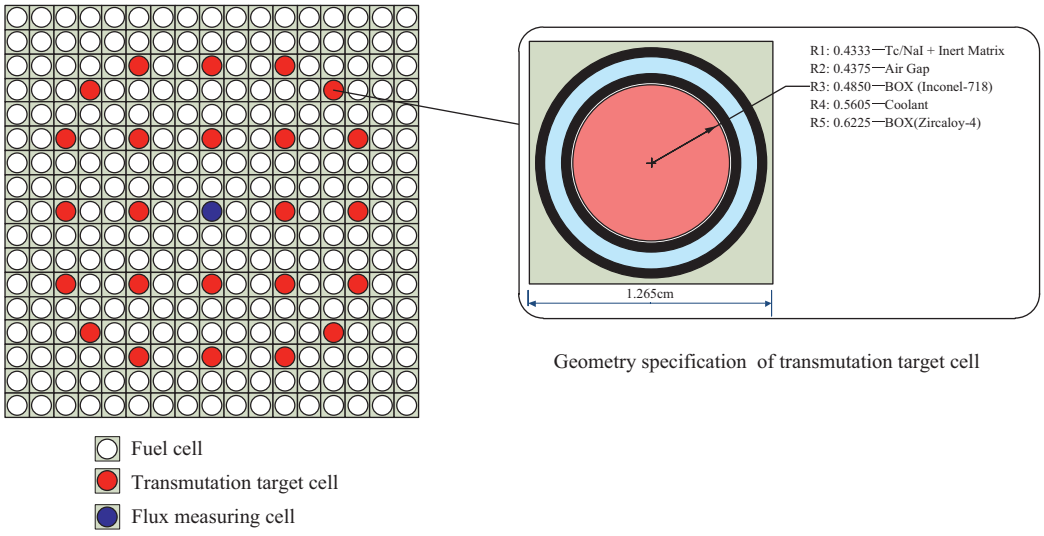

Fig. 14. Transmutation target pin in-assembly loading pattern and target design.

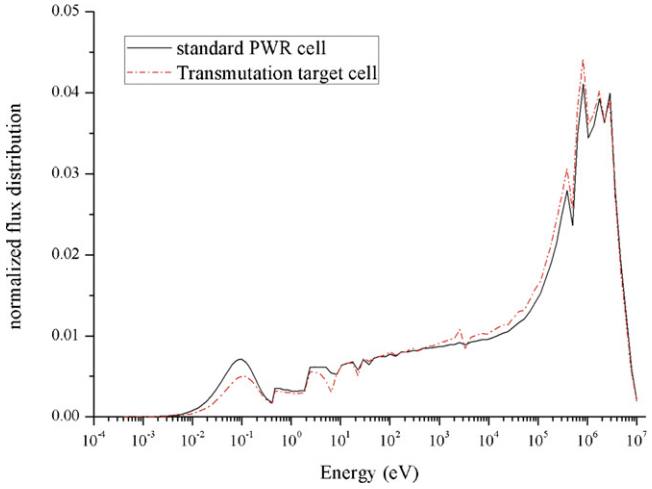

Fig. 15. Comparison of cell flux distributions in different lattices.

Table 9
Comparison of one-group microscopic capture cross sections.

Nuclides	ORIGEN2 Library[a]	Daya bay fuel cell	Target cell
^{99}Tc	9.136	8.192	6.450
^{129}I	3.225	3.010	2.198

[a] Cross sections are originated form ORIGEN2 pwru.lib.

section is smaller than that of standard ORIGEN2 library, which might lead to a lower absorption rates for LLFP nuclides and affect transmutation rate. Besides, the target assembly loading might needs to be investigated to obtain higher flux level for the transmutation. Further study, including LLFP transmutation material forms and inert matrix material from investigation, LLFP target pin design, and target assembly in-core loading pattern and refueling strategy should be performed to achieve better LLFP in-core transmutation performance.

5. Conclusion

In this paper, to meet the requirements for transmutation evaluation using the PWR cores, following studies and researches are performed and accomplished:

1. Considering the neutron resonance absorption effects of LLFP isotopes, a specific multi-group nuclear data library are generated for the assembly depletion calculation.
2. A validated fine depletion code for assembly depletion calculation is developed. The lattice physics code DRAGON is utilized to perform assembly transport calculation and the depletion code ORIGEN2 is employed for detailed depletion calculation.
3. To avoid the inappropriateness of homogenization and the simple in-core depletion chain description, the code CITATION for in-core fine flux calculation and the depletion code ORIGEN2 for in-core micro depletion calculation are applied to the LLFP in-core transmutation calculation.
4. A code system CATE, involving the modules above, is developed. This work extends the PWR transmutation analysis from assembly design to in-core irradiation simulation, with the consideration of whole core irradiation capacities and operation history.

OECD/NEA PWR cell benchmark for transmutation was computed to validate the reliability and accuracy of the assembly depletion code in CATE. The results presented in the paper allowed us to conclude that CATE can be employed for lattice physics computation and suitable for generating the few group constants for subsequent in-core transmutation calculation.

Several problems are calculated to verify and validate the accuracy and reliability of CATE, including the IAEA PWR benchmark, infinite homogenized plate problem and PWR fuel cycle simulation. The results demonstrate that the code system CATE is reliable and competent for the fuel management, core follow, reload physics calculations and in-core transmutation evaluation and optimization as well.

Using CATE, a preliminary transmutation pattern in a commercial PWR reactor is proposed. The code is capable of giving the results of transmutation rates and LLFP discharge inventory in the target pins.

From the view of application of in-core transmutation study, more developments of CATE might be accomplished, such as super-homogenization (SPH) factors in pin-wise calculation, acceleration techniques for the in-core diffusion calculation to improve the efficiency and Chebyshev rational approximation method (CRAM) for depletion calculation to improve the numerical precision. With these developments and more detailed validations, it is benefit to improve the reliability, stability, accuracy and efficiency of the code.

From the view of optimization for the in-core transmutation study, the systemic researches, such as target form design, in-core loading pattern study and refueling scheme optimization will be performed and addressed.

Acknowledgements

This research was carried out under the financial support of the National High Technology Research and Development Program of China ("863" program) (Approved number: 2009AA050705) and the National Natural Science Foundation of China (Approved number: 91126005).

References

Artisyuk, V., Satio, M., Stankovsky, A., 2005. Challenge of transmutation of long-lived nuclides. Prog. Nucl. Energy 47, 327–338.
Baetslé, J.H., 1996. A comparative systems-analysis approach on fuel cycles with partitioning and transmutation. In: The Fourth International Information Exchange Meeting on Actinide and Fission Product Partitioning and Transmutation, Mito City, Japan, September 11–13.
Croff, A.G., 1980. A User's manual for the ORIGEN2 computer code, ORNL/TM-7175. Oak Ridge National Laboratory.
Cronin, J.T. et al., 1995. SIMULATE-3. Advanced three-dimensional two-group reactor analysis code, Studsvik/SOA-95/, p. 18.
Fowler, T.B., Vondy, D.R., Cummingham, G.W., 1969. Nuclear Reactor Analysis Code: CITAITION, ORNL-TM-2496. Oak Ridge National Laboratory.
Greg, H.H., Richard, C.A., 1994. Nodal code developments at FRAMATOME/BWFC. In: Proceedings of Topical Meeting on Advances in Reactor Physics, Knoxville, TN.
Guzmán, R., Francois, J., 2007. Comparison between HELIOS calculation and a PWR cell benchmark for actinides transmutation. Ann. Nucl. Energy 34, 22–27.
Hutton, J.L., et al., 2000. Comoparison of WIMS/PANTHER calculations with measurement on a Range of operating PWR. In: Proceedings of PHYSOR 2000, Pittsburgh, USA.
Ingelbrecht, C., Lupo, J., Raptis, K., et al., 2002. ^{129}I targets for studies of nuclear waste transmutation. Nucl. Instrum. Methods Phys. Res. A 480, 204–208.
Knott, D. et al., 1995. CASMO-4: a fuel assembly burn-up program, Studsvik/SOA-95/, p. 2.
Kochuna, B., Downar, T., Taiwo, T., 2012. Equilibrium cycle pin by pin transport depletion calculations with DeCART. In: Proceedings of PHYSOR 2012, Knoxville, USA.
Liao, C., Xie, Z., 2003. Application of nonlinear iteration semi-analytical nodal method in the PWR fuel management. Chinese J. Nucl. Sci. Eng. 23, 15–21.
Liu, Z., 2011. Development of continuous energy nuclear data library and multi-group nuclear data library for neutronics calculation, M.D. Thesis (in Chinese), Xi'an Jiaotong University.
Lefebvre, LC., Mondot, J., West, JP., 1991. Benchmark Calculations of Power Distribution within Assemblies, OECD/NEACRP-L-336, http://www.nea.fr/html/science/docs/1991/
Marleau, G., Hebert, A., Roy, R., 2000. A User Guide for Dragon. Ecole Polytechnique de Montreal, Montreal.
Moore, R.L., Schnitzler, B.G., Wemple, C.A., Babcork, R.S., Wessol, D.E., 1995. MOCUP: MCNP-ORIGEN2 Coupled Utility Program, INEL-95/, p. 0523.
OECD/NEA, 2000. Calculations of Different Transmutation Concepts, an International Benchmark Exercise. Nuclear Energy Agency, Organization for Economic and Co-operation Development, Paris, France, ISBN 92-64-17638-1.
OECD/NEA, 2008. 2008. Nuclear Energy Outlook, Nuclear Energy Agency. Organization for Economic and Co-operation Development, Paris, France.
Poston, D.L., Trellue, H.R., 1999. User's Manual, Version 2.0 for MONTEBURNS Version 1.0, LA-UR-99-4999. Los Alamos National Laboratory.
Revol, J.P., 2001. An accelerator-driven system for the destruction of nuclear waste. Process Nucl. Energy 38, 153–166.
Rhoades, C., 1993. TORT-DORT: Two and Three-Dimensional Discrete-Ordinates Transport, Radiation Shielding Information Center, Oak Ridge National Laboratory, CCC-543.
Setiawan, M.B., Kitamoto, A., 2001. Study on multi-recycle transmutation of LLFP in light water reactor. Ann. Nucl. Energy 28, 1789–1797.
Xu, Z., Hejzlar, P., 2008. MCODE, Version 2.2: an MCNP-ORIGEN, DEpletion Program. MIT-NFC-TR-104, MIT.
Yang, S.W., Taiwo, T.A., 2004. Status of reactor analysis methods and codes in the U.S.A. In: PHYSOR 2004, Chicago, USA.
Yang, S.W., Kim, Y., Hill, R., et al., 2004. Long-lived fission product transmutation studies. Nucl. Sci. Eng. 146, 291–318.