

Impact of New Nuclear Data Libraries on Small Sized Long Life CANDLE HTGR Design Parameters

Peng Hong Liem¹, Donny Hartanto², Hoai Nam Tran³

¹Nippon Advanced Information Service (NAIS Co., Inc.) Scientific Computational Division, 416 Muramatsu, Tokaimura, Ibaraki, Japan

²Fast Reactor Design Division, Korea Atomic Energy Research Institute (KAERI), 111, Daedeok-daero 989, Yuseong-gu, Daejeon 34057, Korea

³Institute of Research and Development, Duy Tan University, K7/25 Quang Truong, Da Nang, Vietnam

Email: liemph@nais.ne.jp

Abstract. The impact of new evaluated nuclear data libraries (JENDL-4.0, ENDF/B-VII.0 and JEFF-3.1) on the core characteristics of small-sized long-life CANDLE High Temperature Gas-Cooled Reactors (HTGRs) with uranium and thorium fuel cycles was investigated. The most important parameters of the CANDLE core characteristics investigated here covered (1) infinite multiplication factor of the fresh fuel containing burnable poison, (2) the effective multiplication factor of the equilibrium core, (3) the moving velocity of the burning region, (4) the attained discharge burnup, and (5) the maximum power density. The reference case was taken from the current JENDL-3.3 results. For the uranium fuel cycle, the impact of the new libraries was small, while significant impact was found for thorium fuel cycle. The findings indicated the needs of more accurate nuclear data libraries for nuclides involved in thorium fuel cycle in the future.

1. Introduction

Recently pursued innovative reactor design such as CANDLE (Constant Axial shape of Neutron flux, nuclide densities and power shape During Life of Energy producing reactors) [1] requires an assessment of the accuracy of their main reactor design parameters to determine properly the design feasibility, their safety margins, and in the future their economical margins. Innovative reactor designs often adopt a novel way of fuel burning scheme and fuel compositions which result in very heterogeneous core and/or blanket regions involving complex spatial power as well as different neutron spectra distributions across the reactor. In addition, the designs are commonly aimed at a very high discharged fuel burnup which require accurate reactor physics constants for nuclear transmutation whose accuracy is naturally rooted back to the high quality of the evaluated nuclear data used.

Several new evaluated nuclear data libraries have been released, namely the JENDL-4.0 [2] (replacing the older version of JENDL-3.3), ENDF/B-VII.0 [3] and JEFF-3.1 [4] etc, which cover more number of nuclides and have better agreement with integral measurement results. The release of the new evaluated nuclear data was followed by compilation works of code-specific working libraries for productive reactor design and analysis. For example, after Japan Atomic Energy Agency (JAEA) released the JENDL-4.0, the Agency also prepared, tested, verified and validated the JENDL-4.0 based SRAC2006 library [5]. SRAC2006 [5] used in the present work is a comprehensive neutronics



calculation code system which consists of many modules from transport based cell calculation module to multidimensional diffusion based whole core neutronics calculation module.

In the present paper, the impacts of new evaluated nuclear data libraries (JENDL, ENDF/B and JEFF) on the core characteristics of the innovative CANDLE reactor design are investigated. Although the novel CANDLE burnup scheme can be applied both for fast and thermal reactors, in the present work, we consider prismatic (block) type high temperature gas-cooled reactors (HTGR) which operate under thermal neutron spectra. Two fuel cycles are considered for the CANDLE HTGRs, namely the uranium and thorium fuel cycles. Thorium fuel cycle are not commonly used presently, however in the future, the thorium potential would be utilized and investigation on the impact of the new evaluated nuclear data libraries on the thorium fuel cycle performance is of great interest. Both the CANDLE HTGRs with uranium and thorium fuel cycles may reach very high discharge burnup levels of more than 100 GWd/t.

2. CANDLE high temperature gas-cooled reactor

2.1. CANDLE Concept

The innovative CANDLE (Constant Axial shape of Neutron flux, nuclide densities and power shape During Life of Energy producing reactor) burning scheme was proposed by Sekimoto et al. [1] originally aimed for fast reactors. Under this burning scheme, the burning region (sometime it is called burning wave) moves autonomously with a constant velocity along the core axis from bottom to top (or from top to bottom) as shown in Fig. 1. As shown in the figure, the core can be roughly divided into three regions: (1) fresh fuel region ($k_{inf} < 1$), (2) burning region ($k_{inf} > 1$) and (3) spent fuel region ($k_{inf} > 1$). When the burning scheme is applied to a prismatic/block-type HTGR, burnable poison (for e.g. natural gadolinium) is used to adjust the k_{inf} of the fresh fuel to be sub-critical.

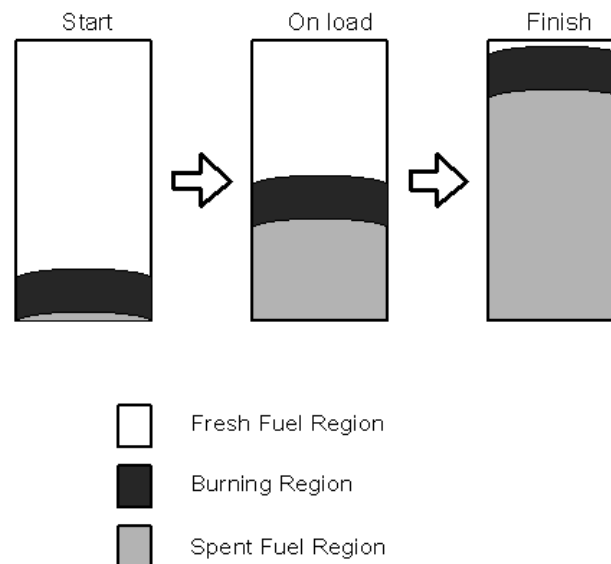


Figure 1. CANDLE burnup concept.

The CANDLE HTGR burn-up process is as follows (Fig. 2). Neutrons leaked from the burning region into the fresh fuel region will be absorbed by the burnable poison and the burning region will move slowly into the fresh fuel region with depleted burnable poison. In the burning region, depletion of fissile material for energy production is accompanied by conversion of fertile material into fissile material. The spent fuel region is the region left by the burning region which contains mainly fission products and depleted fuel. After the CANDLE HTGR is operated for a certain core life time, the

reactor can be shut down for refueling. If the core active height is design properly the CANDLE concept may feature a long life HTGR design as will be shown later.

For a unique combination of core geometry and fresh fuel composition, one can find an equilibrium critical condition where CANDLE burning scheme is realized. Under the equilibrium condition, the moving (axial) velocity of the burning region is constant. Analytical codes for obtaining either the equilibrium condition or for simulating the reactor start-up (running-in phase) have been developed. In our previous works as well as in the present work we consider small sized long life prismatic/ block-type HTGRs adopting CANDLE burning scheme which can take full advantages of CANDLE properties:

1. Constant reactor parameters (e.g. power peaking, reactivity coefficients etc.) during reactor operation. This will simplify not only the reactor design itself and its licensing process but also simplify its reactor operation and maintenance.
2. No requirement for burn-up reactivity control mechanism. Besides simplifying the reactor design, a severe control rod ejection accident during full power operation (under nominal pressure) can be avoided.
3. Proportionality of core height to reactor core life. A long life core can be easily designed by adjusting the core height.
4. Sub-criticality of fresh fuel. No criticality accident will occur during transportation and storage of fresh fuels.

In addition, application of CANDLE burning scheme to small sized long life HTGRs can be realized by the present coated fuel particle and HTGR reactor technologies. As for the fuel cycle, CANDLE HTGRs can be applied for uranium [6] and thorium [7] fuel cycles. In our previous work [7], we showed that CANDLE HTGRs with thorium fuel gave better burnup performance than the ones with uranium fuel. This fact is also true for other thorium fueled HTGRs of the pebble bed type with once-through-then-out (OTTO), multipass as well as peu-a-peu (PAP) schema as described, analyzed and reviewed comprehensively by Liem et al. [8].

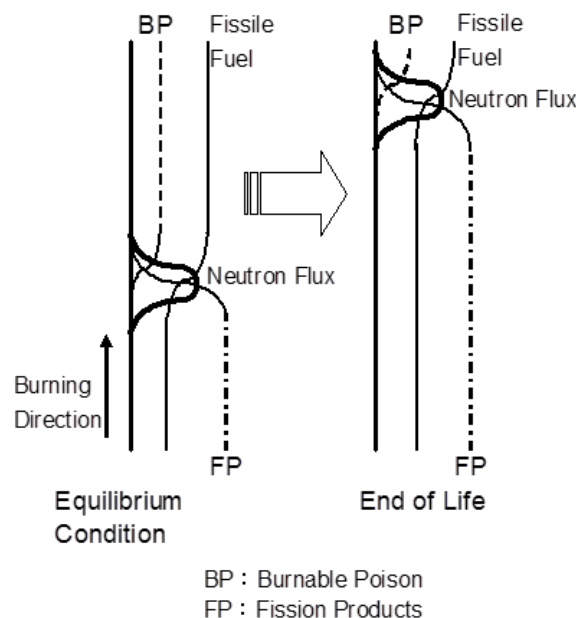


Figure 2. CANDLE burnup application to HTGR.

2.2. CANDLE Analytical Code and Group Constants

An in-house analytical tool for obtaining the CANDLE burnup equilibrium condition has long been developed in our previous works for both fast and thermal reactors. The code takes into account the

burning region movement, nuclides burnup and criticality equations simultaneously. The details of the computational procedures are given in the references by Ohoka and Sekimoto [6] and Ismail et al. [7]. In this section the group-constants preparation, CANDLER burnup equilibrium and critical search procedure as well as the calculation conditions are discussed since they are directly affected by the evaluated nuclear data library used.

The analytical tool used for obtaining the CANDLER burnup equilibrium condition, in principal, needs (1) effective microscopic cross sections and (2) burnup related data such as fission product yields, decay constants, branching ratios and a depletion chain. The effective microscopic cross sections are prepared using the collision probability (PIJ) module of SRAC2006 code system with a SRAC library based on a particular evaluated nuclear data. For the present version of SRAC2006, the available SRAC libraries are based on JENDL-3.3 [11], JENDL-4.0, ENDF/B-VII.0 and JEFF-3.1 evaluated nuclear data libraries. The burnup related data are taken directly from the SRAC library.

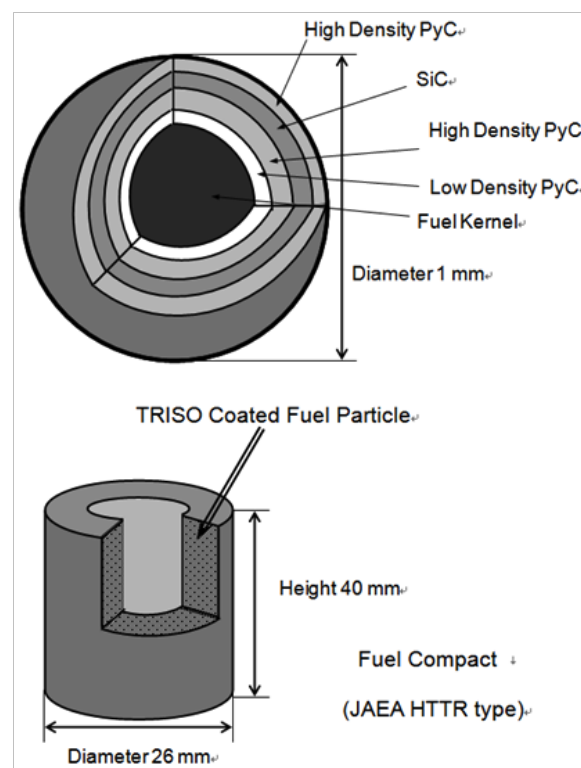


Figure 3. TRISO coated fuel particle and HTTR type fuel compact.

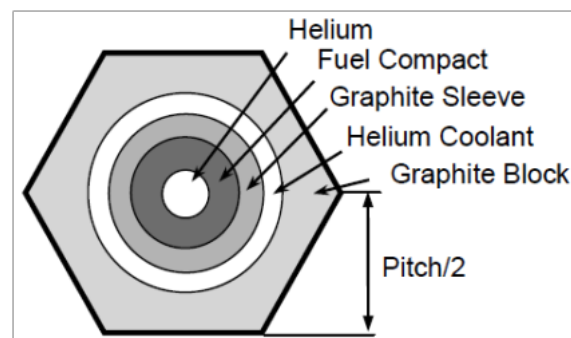


Figure 4. Cell calculation model by SRAC2006 code system.

Table 1. Neutron energy group structure for CANDLE calculations (4-group).

The diagram illustrates the nuclear reaction network for the synthesis of superheavy elements. It shows a series of isotopes from Th to Cn, with various decay and reaction pathways. A legend at the bottom left defines the symbols: α decay (dashed arrow), EC (solid arrow), $(n, 2n)$ (solid arrow), (n, γ) (solid arrow), IT (solid arrow), and β^- decay (solid arrow).

After obtaining the effective microscopic cross sections in 107 energy group (the largest number for SRAC code and library) then the cross sections are collapsed into 4 energy group (Table 1) to be used

for the CANDLE burnup calculations. The depletion chain which consists of 29 heavy metal, 66 important fission product (including one pseudo fission product) nuclides and 16 burnable poison nuclides is based on SRAC's THCM66FP chain [5] shown in Fig. 5.

2.3. CANDLE Burnup Equilibrium and Critical Search Procedure

In order to obtain a CANDLE burnup equilibrium and critical condition, in the first stage, one has to determine the fresh fuel kernel composition, i.e. the fissile U-235 or U-233 enrichment, natural Gd burnable poison, and search the CANDLE burnup equilibrium condition.

In this stage, the obtained equilibrium condition may give an effective neutron multiplication factor (k_{eff}) which is not critical. In the second stage, only the natural gadolinium burnable poison concentration is adjusted to obtain a critical ($k_{eff}=1.0$) and equilibrium condition of CANDLE burnup. This two-stage iterative procedure is terminated if the k_{eff} is near 1.0 within 1 % convergence criterion. There is a possibility that a certain composition of U-235 or U-233 enrichment and Gd burnable poison weight fraction will not give a critical and equilibrium condition of CANDLE burnup.

Table 2. Design parameters of small sized long life thorium CANDLE high temperature gas-cooled reactor.

Thermal power (MWth)	30
Core	
Diameter (cm)	230
Active height (cm)	800
Radial reflector (graphite)	
Thickness (cm)	100
Coated fuel particle	
Fuel	(U-235/U-238)O ₂ or (U-233/Th-232)O ₂
Uranium enrichment (w/o)	< 20%
Burnable poison material	Natural gadolinium
Type	TRISO
Kernel diameter (mm)	0.608
Particle diameter (mm)	0.940
Coating material	PyC / PyC / SiC / PyC
Thickness (mm)	0.060 / 0.030 / 0.030 / 0.046
Density (g/cm ³)	1.143 / 1.878 / 3.201 / 1.869
Packing fraction (v/o)	30.0
Fuel compact	JAEA HTTR type
Inner diameter (cm)	1.00
Outer diameter (cm)	2.60
Graphite sleeve	
Inner diameter (cm)	2.60
Outer diameter (cm)	3.40
Coolant annulus channel	
Inner diameter (cm)	3.40
Outer diameter (cm)	4.10
Fuel pitch	
Flat to flat distance (cm)	6.60

2.4. Main Design Parameters and Calculation Conditions

In order to investigate the impact of the new evaluated nuclear data libraries on the core characteristics of the CANDLE HTGRs we selected our previous small sized, long-life CANDLE HTGR design as a reference where the design adopted both uranium and thorium fuel cycles. The reactor main design

parameters are shown in Table 2. This reference design, up to now, was calculated by using JENDL-3.3 based SRAC library. To investigate the impact of the new libraries, we selected the available SRAC libraries, namely the JENDL-4.0, ENDF/B-VII.0 and JEFF-3.1 based ones.

The most important parameters of critical CANDLE core characteristics are (1) infinite multiplication factor (k_{inf}) of the fresh fuel containing burnable poison, (2) the effective multiplication factor (k_{eff}) of the equilibrium core, (3) the moving velocity of the burning region (Vel), (4) the attained discharge burnup (BU), and (5) the maximum power density (Q_{max}). In order to clearly observe the impact of the new libraries on these parameters, we adopted the fresh fuel composition of the reference case (calculated with JENDL-3.3 library) and used the fresh fuel composition for other libraries and keeping other calculation conditions unaltered.

3. Impact of new evaluated nuclear data libraries

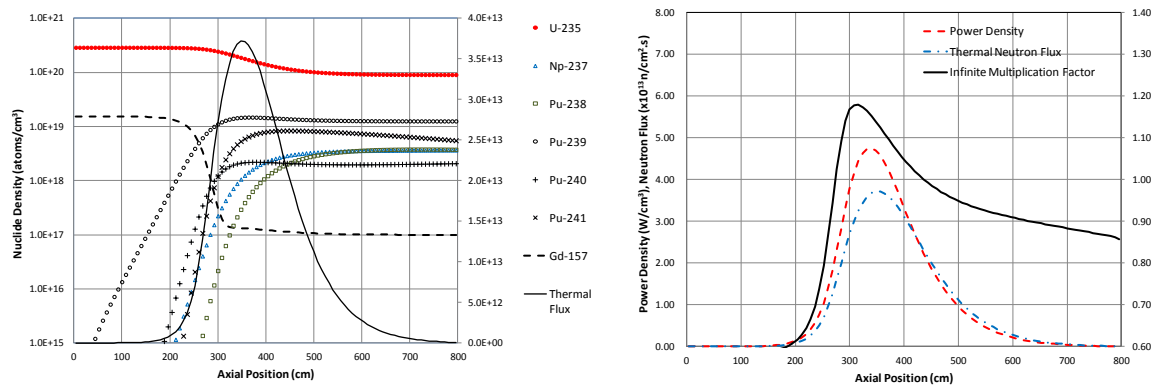
Firstly, the core characteristics of the CANDLE HTGR for the reference case i.e. the ones calculated by using the JENDL-3.3 library is shown in Table 3. For both uranium and thorium fuel cycles, four values of fissile (U-235 or U-233) enrichment were evaluated. The smallest enrichment (6.5 w/o) was determined from the criticality requirement of the design, while the highest enrichment (19.75 w/o) was attributed to the non-proliferation issue that is the use of LEU. In the table, for a particular fissile enrichment the unique value of burnable poison (natural Gd) concentration needed to establish an equilibrium and critical CANDLE HTGR is also shown. Since a higher fissile enrichment will result in a higher initial k_{inf} (without Gd) then the required Gd concentration increases with higher fissile enrichment. Compared to uranium fuel cycle, the same fissile enrichment of U-233 provides more reactive composition than the U-235 does so that higher fuel burnup can be expected.

Calculation results of representative example of CANDLE HTGR with uranium fuel cycle and thorium fuel cycle are shown in Figs. 6 and 7, respectively (fissile enrichment of 15 w/o). In Fig. 6, the burning region (wave) is moving from right to left approximately 30 cm/year, and the depleted fuel in the right side of the figure has the average burnup of approximately 100 GWd/t. The maximum power density is less than 5 W/cm³ which assures the safety of the reactor during normal and accident conditions.

Table 3. Calculated main parameters of CANDLE HTGR core characteristics with uranium and thorium fuel cycles (reference case, JENDL-3.3).

Fuel Cycle	Enrichment (w/o)	Gd (w/o)	k_{inf}	k_{eff}	BU (GWd/t)	Vel. (cm/year)	Q_{max} (W/cm ³)
Uranium	19.75	3.80	0.66223	1.00970	121.8	24.2	4.75
	15	2.90	0.58728	1.00146	98.6	29.7	4.75
	10	1.70	0.50888	1.00394	65.5	44.1	4.61
	6.5	0.90	0.45136	1.00253	42.5	67.4	4.09
Thorium	19.75	11.70	0.87426	1.00187	175.1	18.5	5.37
	15	8.75	0.79043	1.00164	138.4	22.7	5.93
	10	5.40	0.66629	1.00300	95.5	31.8	6.10
	6.5	2.90	0.54432	1.00249	57.7	51.1	6.04

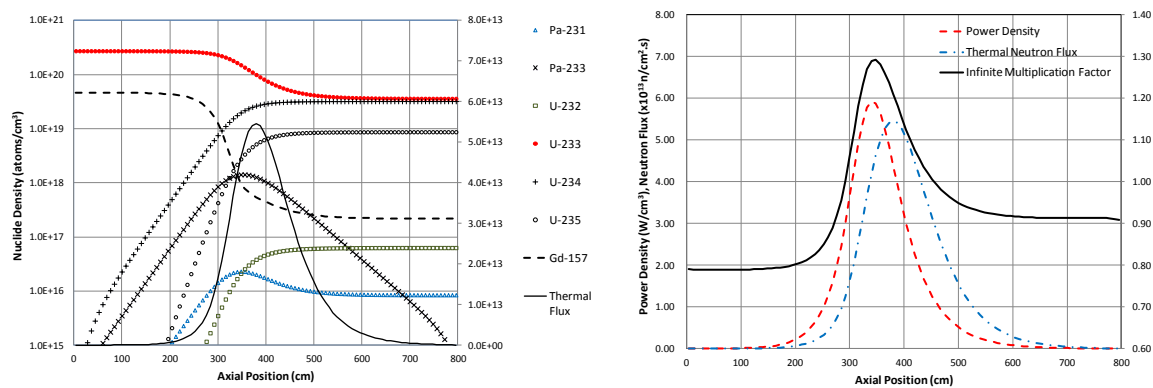
As discussed above, the thorium fuel cycle (cf. Fig. 7) shows better core characteristics in term of achievable fuel burnup and much slower burning region (wave) moving velocity. Slower velocity allows the reactor designer to produce longer core life time for the same effective core height. The downside of thorium fuel cycle compared with the uranium one is a higher maximum power density. Although in the present small long life CANDLE HTGR design, the absolute values are low, the maximum power density would be problematic for large power CANDLE HTGRs.



[Left] Nuclide densities (left axis) and thermal group neutron flux (right axis)

[Right] Power density, thermal group neutron flux (left axis) and kinf (right axis)

Figure 6. Critical and equilibrium condition of CANDLE HTGR with U-235 enrichment of 15 w/o and burnable poison Gd concentration of 2.90 w/o (reference case, JENDL-3.3).



[Left] Nuclide densities (left axis) and thermal group neutron flux (right axis)

[Right] Power density, thermal group neutron flux (left axis) and kinf (right axis)

Figure 7. Critical and equilibrium condition of CANDLE HTGR with U-233 enrichment of 15 w/o and burnable poison Gd concentration of 8.75 w/o (reference case, JENDL-3.3).

Secondly, the impact of new libraries on the core characteristics of CANDLE HTGR are shown in Figs. 8 and 9, for uranium and thorium fuel cycles, respectively. The impact of the new libraries was shown in term of the ratio of the evaluated parameter (by a new library) divided by the one of the reference case (by JENDL-3.3 library).

The impact on the uranium fuel cycle case (shown in Fig. 8) is discussed first. For a particular fissile enrichment, the initial fuel composition (including Gd burnable poison) is identical however as can be observed in the Fig. 8, the kinf values show differences which systematically decrease as the fissile enrichment increases. For the kinf parameter, comparing with other new libraries, JENDL-4.0 based parameters are relatively closer to the reference case (JENDL-3.3). The equilibrium CANDLE HTGR effective multiplication factors (keff) of the new libraries show much better agreement with the reference keff (JENDL-3.3).

In a CANDLE reactor, a slower burning region velocity will result in a higher fuel burnup. These particular core characteristics can be observed from Fig. 8. Among the four values of fissile enrichment investigated in the present work, the fissile enrichment of 10 w/o shows the largest differences in the burning region velocity (approximately -2%) and consequently the achievable fuel burnup (approximately +2%). No clear systematic dependency of the velocity (and burnup) on the fissile enrichment. In addition, for this fissile enrichment (10 w/o), the maximum power density

calculated by the new libraries shows also largest differences (approximately -3%) than other fissile enrichment does. Except for the initial fuel k_{inf} , no significant differences are found among the new libraries for all parameters considered, i.e. their variations are less than $\pm 1\%$.

Next, the impact on the thorium fuel cycle case (shown in Fig. 9) is discussed. In general, compared with the previous impact on the uranium fuel cycle case, except for the initial k_{inf} , all parameters evaluated show much larger differences against the reference case as well as among the new libraries themselves.

Although the initial k_{inf} differences against the reference case are smaller compared to the uranium case, the k_{eff} values at the equilibrium condition show relatively much larger differences for all fissile enrichment values considered (approximately +4%). Large differences against the reference case in the burning region velocity (and consequently the achievable fuel burnup) are also found for all fissile enrichment values considered, however, the ones of 6.5 w/o fissile enrichment show significantly large differences (approximately $\pm 14\%$). For larger fissile enrichment values the differences are smaller, i.e. less than $\pm 8\%$. The maximum power density differences of the new libraries against the reference case show a consistent dependency on the fissile enrichment, where the differences move from negative values (-8%) to positive values (+8%) as the fissile enrichment increases. The differences at most $\pm 2\%$ are found among the new libraries for all core parameters considered here.

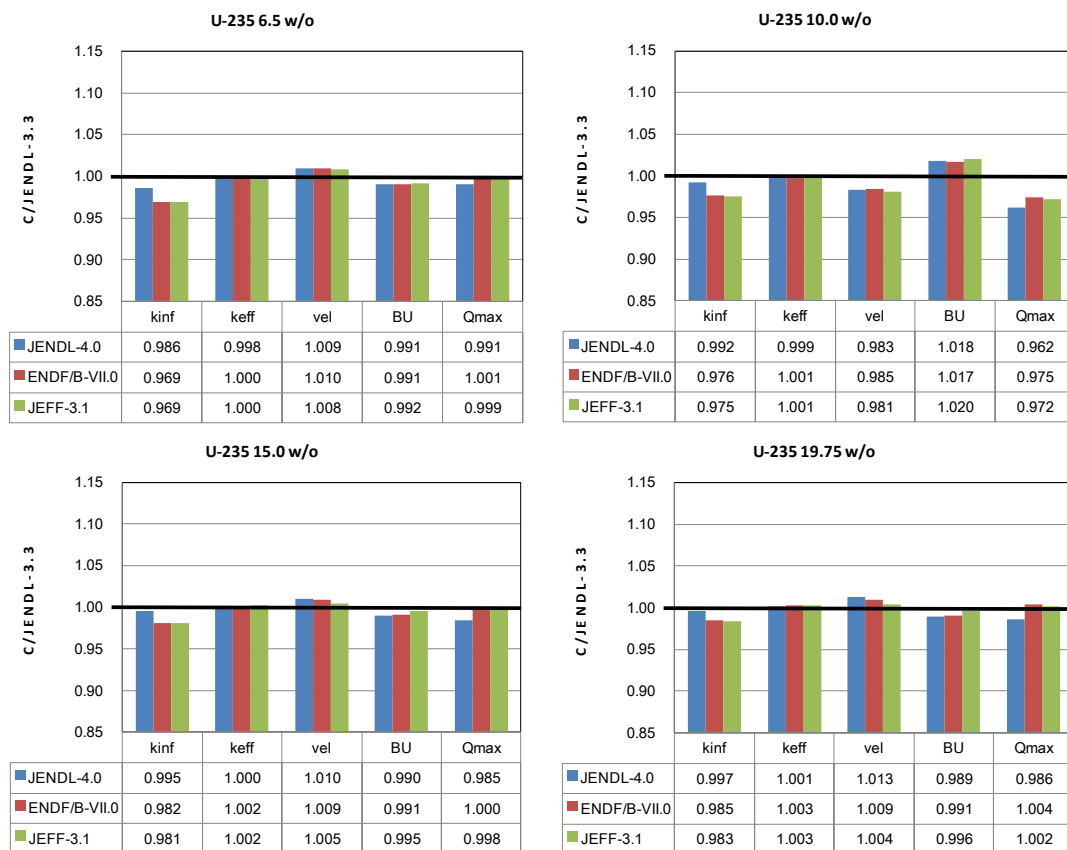


Figure 8. Impact of new libraries on the main parameters of the CANDLE HTGR core characteristics with uranium fuel cycle (ratio of a parameter calculated by new library and the one by JENDL-3.3).

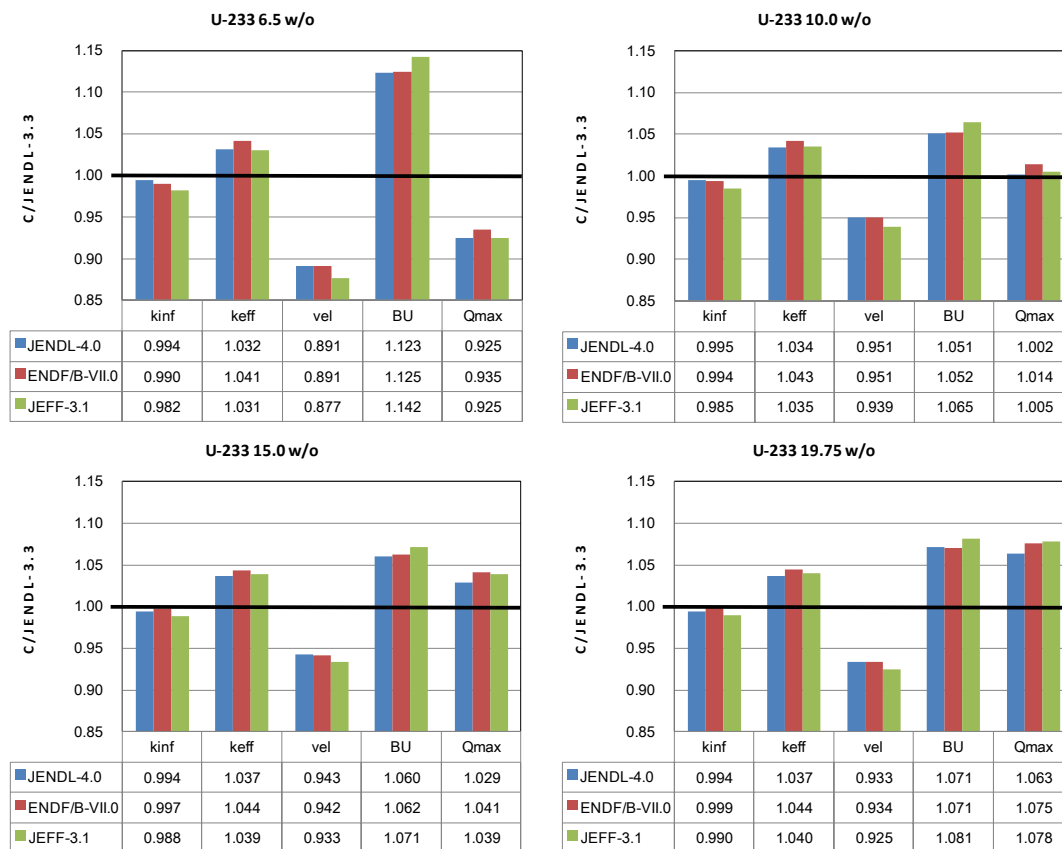


Figure 9. Impact of new libraries on the main parameters of the CANDLE HTGR core characteristics with thorium fuel cycle (ratio of a parameter calculated by new library and the one by JENDL-3.3).

4. Conclusion

The investigation on the impact of new evaluated nuclear data libraries against the core characteristics of small-sized, long-life CANDLE HTGRs shows that the new libraries have small impact on the uranium fuel cycle but have significant one on the thorium fuel cycle. In the future, more detail sensitivity analyses on the dominant nuclides and nuclear reaction types are needed to provide further feedback to the nuclear data community.

Acknowledgment

Some figures related to CANDLE burnup and cell calculation model used in the manuscript were provided by Drs. Ohoka Y. and Ismail.

References

- [1] Sekimoto H, Ryu K and Yoshimura Y 2001 *Nucl. Sci. Eng.* **139** 306
- [2] Shibata K, Iwamoto K, Nakagawa T, et al. 2011 *J. Nucl. Sci. Technol.* **48** 1
- [3] Chadwick M B, Oblozinsky P, Herman M, et al. 2006 *Nucl. Data Sheets* **107** 2931
- [4] Koning A, Forrest R, Kellet M, et al. 2006 *JEFF Report 21: The JEFF-3.0 Nuclear Data Library* OECD/NEA No. 6190
- [5] Okumura K, Kugo T, Kaneko K and Tsuchihashi K 2007 *SRAC2006: A Comprehensive Neutronics Calculation Code System* JAEA-Data/Code 2007-004
- [6] Ohoka Y and Sekimoto H 2004 *Nucl. Eng. Des.* **229** 15
- [7] Ismail, Ohoka Y, Liem P H and Sekimoto H 2007 *Ann. Nucl. Energy* **34** 120
- [8] Liem P H, Ismail and Sekimoto H 2008 *Prog. Nucl. Energy* **50** 251

- [9] Saito S, Tanaka T, Sudo Y et al. 1994 *Design of High Temperature Engineering Test Reactor (HTTR)* JAERI 1332
- [10] Yamashita K, Shindo R, Murata I et al. 1996 *Nuc. Sci. Eng.* **22** 212
- [11] Shibata K, Kawano T, Nakagawa T et al., 2002 *J. Nucl. Sci. Technol.* **39** 1125