A Study on Validation of MCS Criticality Calculation with Burnup Credit for TN-32 cask

Ta Duy Long, Ser Gi Hong*, [a]Ho Choel Shin, [b]Deokjung Lee
Dept. Of Nuclear Engineering, Kyung Hee University, 1732 Deogyeong-daero, Giheung-gu, Yongin
[*]*Corresponding author: sergihong@khu.ac.kr*
[a]*Core and Fuel Analysis Group, Korea Hydro & Nuclear Power Central Research Institute, Daejon*
[b]*UNIST, UNIST-gil 50, Eonyang-eup, Ulju-gun, Ulsan 689-798*

1. Introduction

The critical safety analyses with burnup credit are necessary to ensure that the spent nuclear fuel storage or transportation system meets sufficiently requirements on subcriticality with consideration of biases and bias uncertainties. The biases and biases uncertainties for criticality safety analyses with burnup credit are mainly classified into two different types: (1) Biases and bias uncertainties related to cross-sections and computational method in estimating k_{eff}, and (2) the ones related to estimation of spent fuel compositions in depletion calculation. Typically these biases and bias uncertainties were quantified by analyzing the results from experiments and code calculations.

In this work, we determine the Upper Safety Limit (USL) for MCS for the TN-32 spent fuel cask model without consideration of bias and bias uncertainty related to isotopic composition. Due to the limitation of experiment with fission product (FP) and minor actinide (MA) nuclides, we only considered a set of five critical problems with mixed oxide fuel, while the bias and bias uncertainty related to the presented FP and MA nuclides were conservatively quantified. The applicable experiments to the TN-32 cask application model were first evaluated by sensitivity calculations with TSUNAMI-3D and TSUNAMI-IP module in SCALE6.1 code system before performing criticality calculations with MCS. Additionally, these calculations were performed with MCNP6 for comparison with MCS.

2. Methods and Results

2.1. Computer Code System

MCNP6 is a general purpose, continuous-energy, generalized-geometry Monte Carlo radiation transport code developed by Los Alamos national laboratory. The MCNP6 code can be used for neutron, photon, electron transport and it includes the capability to calculate eigenvalues for critical systems. MCS is a 3D continuous energy Monte Carlo code for particle transport, which was developed at Ulsan National Institute of Science and Technology (UNIST), Korea since 2013. The MCS have two options for criticality calculations and fixed source for shielding problems. In this work, the critical calculations were performed using both the MCNP6 and MCS codes with ENDF/B-VII.1 cross-section library.

The SCALE code package is a comprehensive modeling and simulation suite for nuclear safety analysis and design that was developed by Oak Ridge National Laboratory. In this work, the TSUNAMI-3D and TSUNAMI-IP modules in SCALE have been used in sensitivity calculations to determine the similarity of the critical experiments to the applied TN-32 cask model.

2.2. The TN-32 spent nuclear fuel cask model

In this work, it was assumed that the TN-32 cask model consists of 32 PWR fuel assemblies of 17x17 lattice structure, which have an initial enrichment of 4.5 wt% ^{235}U and burnup of 48 GWd/MTU with 5 years cooling time. This TN-32 cask model has the basket for fuel assemblies surrounded by absorber plates, which have thickness of 0.1016 cm. The cask has the outer diameter of 111.44 cm with 24.13 cm of carbon steel wall in thickness, and the cask total height is 467.36 cm, as shown in Figure 1.

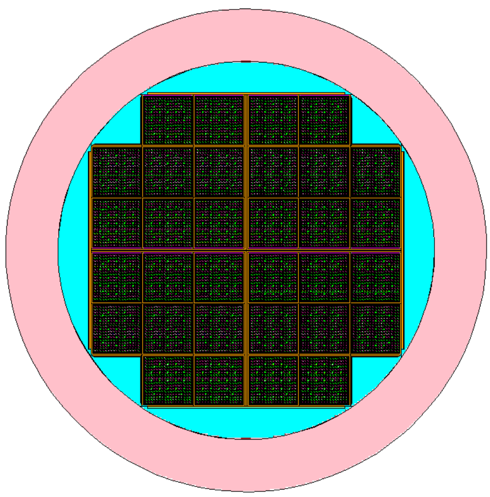

Fig 1. TN-32 cask model

2.3. Critical Benchmark Problems

To determine the bias and bias uncertainty related to nuclear data, five critical benchmark problems with a total of 80 experiment configurations were considered in this work. These experiments consist mixed plutonium-uranium oxide fuel which have the plutonium content ranged from 2.0 to 6.6 wt%. Details of these critical problems were provided in [1] with the identification numbers from MIX-COMP-THERM-002 to MIX-COMP-THERM-006. The first three problems considered square-pitched lattice fuel arrays moderated and reflected by water, while the remaining have triangular lattice fuel arrays.

2.4. Similarity between TN-32 cask model and criticality experiments

This section presents result of similarity indices for those criticality experiments compared to the TN-32 cask model. This work was performed by two steps: (1) Perform sensitivity calculations by TSUNAMI-3D for the cask model and the experiments to generate sensitivity data files, and (2) Using those sensitivity data files to establish the similarity indices c(k) of those experiments compared to the TN-32 cask model with TSUNAMI-IP.

The spent fuel for TN-32 cask was considered with 28 actinide and fission product nuclides that are important to burnup credit criticality analyses [2]. These nuclides are provided in Table 1, and the result of the similarity indices are listed in Table 2.

Table 1. Actinide and fission product nuclides important to burnup credit criticality analyses

^{234}U	^{235}U	^{236}U	^{238}U	^{237}Np	^{238}Pu
^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu	^{241}Am	^{243}Am
^{95}Mo	^{99}Tc	^{101}Ru	^{103}Rh	^{109}Ag	^{133}Cs
^{143}Nd	^{145}Nd	^{147}Sm	^{149}Sm	^{150}Sm	^{151}Sm
^{152}Sm	^{151}Eu	^{153}Eu	^{155}Gd		

Table 2. Similarity indices of MOX experiments to TN-32 cask model

Experiment	c(k)	Experiment	c(k)	Experiment	c(k)	Experiment	c(k)
MIX-002-01	0.8474	MIX-004-09	0.8346	MIX-006-11	0.8029	MIX-006-31	0.8361
MIX-002-02	0.8787	MIX-004-10	0.8486	MIX-006-12	0.8044	MIX-006-32	0.8349
MIX-002-03	0.8108	MIX-004-11	0.8502	MIX-006-13	0.8005	MIX-006-33	0.8346
MIX-002-04	0.8952	MIX-005-01	0.8082	MIX-006-14	0.8030	MIX-006-34	0.8345
MIX-002-05	0.8170	MIX-005-02	0.7964	MIX-006-15	0.8058	MIX-006-35	0.8323
MIX-002-06	0.8957	MIX-005-03	0.7903	MIX-006-16	0.8015	MIX-006-36	0.8363
MIX-003-01	0.7903	MIX-005-04	0.7952	MIX-006-17	0.8054	MIX-006-37	0.8353
MIX-003-02	0.7765	MIX-005-05	0.8156	MIX-006-18	0.8052	MIX-006-38	0.8365
MIX-003-03	0.7887	MIX-005-06	0.8509	MIX-006-19	0.8072	MIX-006-39	0.8363
MIX-003-04	0.7429	MIX-005-07	0.8676	MIX-006-20	0.8065	MIX-006-40	0.8371
MIX-003-05	0.7463	MIX-006-01	0.8140	MIX-006-21	0.8062	MIX-006-41	0.8356
MIX-003-06	0.7719	MIX-006-02	0.8022	MIX-006-22	0.8044	MIX-006-42	0.8363
MIX-004-01	0.8167	MIX-006-03	0.7994	MIX-006-23	0.8083	MIX-006-43	0.8365
MIX-004-02	0.8223	MIX-006-04	0.8110	MIX-006-24	0.8057	MIX-006-44	0.8359
MIX-004-03	0.8242	MIX-006-05	0.8349	MIX-006-25	0.8050	MIX-006-45	0.8356
MIX-004-04	0.8165	MIX-006-06	0.8452	MIX-006-26	0.8038	MIX-006-46	0.8352
MIX-004-05	0.8199	MIX-006-07	0.8002	MIX-006-27	0.8066	MIX-006-47	0.8365
MIX-004-06	0.8236	MIX-006-08	0.7995	MIX-006-28	0.8096	MIX-006-48	0.8352
MIX-004-07	0.8287	MIX-006-09	0.8031	MIX-006-29	0.8323	MIX-006-49	0.8364
MIX-004-08	0.8314	MIX-006-10	0.8018	MIX-006-30	0.8331	MIX-006-50	0.8368

As mentioned in NUREG/CR-7109 [3], those experiments which have similarity indices less than 0.8 are not recommended to use for safety analyses with application model. From the results in Table 2, 69 experiments that meet the similarity requirement are used in criticality calculations with MCS and MCNP6.

2.5. Results of Criticality calculations

In this section, the criticality calculations for these criticality experiments were performed by MCS and MCNP6 using ENDF/B-VII.1 cross-section library. Those calculations are performed with 500 active cycles and 20,000 histories per cycle. The standard deviation of the calculated k_{eff} is about less than 30 pcm, while the experimental uncertainties are varied about few hundreds pcm. The criticality results presented in Table 3 showed a good agreement between MCS and MCNP6 with the discrepancies less than 50 pcm for most of the experiments, except for several cases having the discrepancies about 100 pcm. These criticality results then are used to establish the USL for the TN-32 cask model based on the single-sided tolerance limit method, which is presented in next section.

Table 3. Results of criticality experiments

Experiment	Exp. Result	MCS result	MCNP6 result	Diff. MCS vs MCNP6	Experiment	Exp. Result	MCS result	MCNP6 result	Diff. MCS vs MCNP6
MIX-002-01	1.0010	1.00060	1.00053	7.0	MIX-006-17	1.0023	0.99042	0.99042	-21.3
MIX-002-02	1.0009	1.00181	1.00184	-3.0	MIX-006-18	1.0032	0.99179	0.99167	-0.5
MIX-002-03	1.0024	1.00212	1.00218	-6.0	MIX-006-19	1.0033	0.99093	0.99103	12.3
MIX-002-04	1.0024	1.00633	1.00613	20.0	MIX-006-20	1.0030	0.99064	0.99053	-9.7
MIX-002-05	1.0038	1.00359	1.00357	2.0	MIX-006-21	1.0024	0.99035	0.99037	11.0
MIX-002-06	1.0029	1.00572	1.00585	-13.0	MIX-006-22	1.0030	0.99092	0.99098	-1.8
MIX-004-01	1.0000	0.99647	0.99620	27.2	MIX-006-23	1.0030	0.99037	0.99141	-5.7
MIX-004-02	1.0000	0.99696	0.99704	-8.0	MIX-006-24	1.0024	0.99091	0.99095	-104.1
MIX-004-03	1.0000	0.99716	0.99703	13.3	MIX-006-25	1.0021	0.99037	0.99021	-3.6
MIX-004-04	1.0000	0.99697	0.99687	10.0	MIX-006-26	1.0033	0.99116	0.99160	15.9
MIX-004-05	1.0000	0.99782	0.99780	1.6	MIX-006-27	1.0033	0.99191	0.99142	-43.9
MIX-004-06	1.0000	0.99783	0.99760	22.6	MIX-006-28	1.0040	0.99827	0.99898	49.2
MIX-004-07	1.0000	0.99779	0.99771	8.1	MIX-006-29	1.0043	0.99768	0.99810	-71.4
MIX-004-08	1.0000	0.99829	0.99818	10.9	MIX-006-30	1.0045	0.99746	0.99736	-41.7
MIX-004-09	1.0000	0.99867	0.99874	-7.1	MIX-006-31	1.0037	0.99557	0.99633	10.2
MIX-004-10	1.0000	0.99831	0.99843	-12.5	MIX-006-32	1.0043	0.99523	0.99568	-76.2
MIX-004-11	1.0000	0.99842	0.99841	1.1	MIX-006-33	1.0037	0.99451	0.99462	-45.0
MIX-005-01	1.0008	1.00298	1.00293	5.0	MIX-006-34	1.0044	0.99768	0.99750	-10.9
MIX-005-05	1.0026	1.00645	1.0065	-5.0	MIX-006-35	1.0036	0.99615	0.99621	18.0
MIX-005-06	1.0033	1.00620	1.0063	-10.0	MIX-006-36	1.0041	0.99547	0.99583	-6.5
MIX-005-07	1.0035	1.00765	1.00797	-32.0	MIX-006-37	1.0044	0.99433	0.99480	-36.3
MIX-006-01	1.0016	0.99880	0.99872	7.8	MIX-006-38	1.0042	0.99297	0.99340	-47.1
MIX-006-02	1.0017	1.00210	1.00224	-14.0	MIX-006-39	1.0038	0.99244	0.99243	-43.2
MIX-006-04	1.0051	1.00408	1.00407	1.0	MIX-006-40	1.0038	0.99236	0.99267	1.4
MIX-006-05	1.0040	1.00430	1.00419	11.0	MIX-006-41	1.0036	0.99193	0.99254	-30.7
MIX-006-06	1.0055	1.00209	1.00211	-2.0	MIX-006-42	1.0044	0.99281	0.99355	-61.0
MIX-006-07	1.0024	0.99544	0.99530	13.8	MIX-006-43	1.0044	0.99287	0.99316	-73.6
MIX-006-09	1.0035	0.99395	0.99410	-14.8	MIX-006-44	1.0040	0.99319	0.99369	-29.4
MIX-006-10	1.0021	0.99247	0.99248	-1.3	MIX-006-45	1.0040	0.99274	0.99369	-50.5
MIX-006-11	1.0032	0.99242	0.99255	-13.2	MIX-006-46	1.0040	0.99260	0.99300	-94.7
MIX-006-12	1.0032	0.99187	0.99215	-27.8	MIX-006-47	1.0038	0.99290	0.99291	-39.6
MIX-006-13	1.0021	0.99444	0.99430	14.1	MIX-006-48	1.0039	0.99300	0.99303	-0.8
MIX-006-14	1.0026	0.99314	0.99338	-23.6	MIX-006-49	1.0044	0.99352	0.99365	-3.3
MIX-006-15	1.0033	0.99295	0.99297	-2.3	MIX-006-50	1.0023	0.99042	0.99042	-13.1
MIX-006-16	1.0035	0.99237	0.99239	-2.4					

2.6. Determination of Upper Safety Limit for the TN-32 cask

In this part, we presented the calculations for determining USL for the TN-32 cask using single-sided tolerance limit method [4]. With the assumption that the criticality results for the experiments follow normal statistical distribution, the USL can be calculated by

$$USL = K_L - \Delta_{SM} - \Delta_{AOA}, \qquad (1)$$

where K_L is the one-sided lower tolerance limit, Δ_{SM} is the margin of sub-criticality and Δ_{AOA} is the additional margin of sub-criticality resulted from the extension to the area of applicability. The one-sided lower tolerance limit is defined by

$$K_L = \bar{k}_{eff} - US_p, \qquad (2)$$

where U is the single-sided lower tolerance factor, and the pooled variance S_p is calculated using

$$S_p = \sqrt{s^2 + \bar{\sigma}^2}. \qquad (3)$$

In Eq. (3), $\bar{\sigma}$ represents the average total uncertainty, which is given by

$$\bar{\sigma}^2 = \frac{n}{\sum_{i=1}^{n} \frac{1}{\sigma_i^2}} \quad , \tag{4}$$

The variance about the mean (s^2) in Eq. (3) is calculated by using Eq. (5), with the index i represents each critical experiment, and σ_i is the combination error of the experimental and calculation uncertainty for each experiment.

$$s^2 = \frac{(\frac{1}{n-1}) \sum_{i=1}^{n} \frac{1}{\sigma_i^2} (k_{eff,i} - \bar{k}_{eff})^2}{\frac{1}{n} \sum_{i=1}^{n} \frac{1}{\sigma_i^2}}. \tag{5}$$

In Eq. (2) and Eq. (5), the weight mean k_{eff} calculated by

$$\bar{k}_{eff} = \frac{\sum_{i=1}^{n} \frac{1}{\sigma_i^2} k_{eff,i}}{\sum_{i=1}^{n} \frac{1}{\sigma_i^2}}. \tag{6}$$

As shown in Table 3, there are number of experiments having experimental k_{eff} slightly larger than 1.0, so that the value of k_{eff} in the above equations are replaced by the normalized values as follows:

$$k_{norm} = {k_{cal}}/{k_{exp}}. \tag{7}$$

The values of weight mean k_{eff}, variance about the mean, average total uncertainty and pooled variance calculated using MCS and MCNP6 criticality results are presented in Table 4. The single-sided tolerance factor (U) is 2.065 which corresponds to the case having number of experiments larger than 50 [4]. With these results, the one-sided lower tolerance limits K_L are estimated to be 0.99596 and 0.996 for MCS and MCNP6, respectively.

For the spent fuel cask model, we used a recommend value of 0.05 for subcritical margin Δ_{SM}. In this work, the additional margin Δ_{AOA} was considered as: (1) The bias and bias uncertainty in determining spent fuel compositions in depletion code, and (2) The bias and bias uncertainty in determining k_{eff} related to MA and FP nuclides. As mentioned in [2], the calculated nuclide concentrations results a slight over-prediction of k_{eff} leading to a positive bias, which typically is not credited in criticality safety analyses. So, the bias in the first component of Δ_{AOA} was assumed to be zero. The bias uncertainty in determining spent fuel compositions should be considered, which is planned in the future work. In this calculation, the bias and bias uncertainty in determining k_{eff} related to MA and FP nuclides need to be considered as the second term in Δ_{AOA} due to the lack of these nuclides in the critical experiments. The bias and bias uncertainty for k_{eff} prediction related to FP and MA nuclides can be conservatively quantified by using a value of 3% of the total worth cause by these nuclides [5]. This worth is obtained by subtracting k_{eff} calculated without FP and MA nuclides from k_{eff} calculated with all FP and MA nuclides presented for the TN-32 cask model.

With the TN-32 cask information provided in section 2.2, the total worth of FP and MA nuclides were estimated to be 11059 and 11080 pcm in MCS and MCNP6, respectively. Finally, using a value of 3% of the total FPs and MAs worth for Δ_{AOA}, the USLs determined with MCS and MCNP6 are 0.94264 and 0.94268, respectively.

Table 4. Critical analysis results for the TN-32 cask model with MCS and MCNP6

	Computer code used	
	MCS	MCNP6
$\bar{k}_{eff}$	0.99604	0.99609
$\bar{\sigma}$	2.045×10^{-5}	2.044×10^{-5}
s^2	3.434×10^{-5}	3.360×10^{-5}
S_p	3.997×10^{-5}	3.933×10^{-5}
U	2.065	2.065
K_L	0.99596	0.99600
Δ_{SM}	0.05	0.05
FP and MA worth	-0.11059	-0.11080
$\Delta_{AOA}(pcm)$	331.8	332.4
USL	0.94264	0.94268

3. Conclusions

In this work, we performed criticality calculations to validate the computational method using MCS for the TN-32 spent fuel cask with burnup credit. A total of 69 mix-oxide fuel configurations have been considered in criticality calculations with MCS to determine the USL for the TN-32 cask model with burnup credit. The consistency of MCS compared to MCNP6 in criticality results demonstrates the capability of MCS in critical safety analyses for the TN-32 cask. The USL for TN-32 cask has been determined with value of 0.94264 in MCS when neglecting the bias uncertainty caused by isotopic compositions determination in depletion code. In future work, we will consider the bias uncertainty in determining spent fuel compositions, along with the bias and bias uncertainty related to FP and MA nuclides in determining k_{eff} of TN-32 cask model.

REFERENCES

[1]. Nuclear Energy Agency, "International Handbook of Evaluated Criticality Safety Benchmark Experiments", 2011

[2]. U.S.NRC, "An Approach for Validating Actinide and Fission Product Burnup Credit Criticality Safety Analyses – Isotopic Composition Predictions", NUREG/CR-7108, ORNL/TM-2011/509

[3]. U.S.NRC, "An Approach for Validating Actinide and Fission Product Burnup Credit Critical Safety Analyses – Criticality (keff) Predictions", NUREG/CR-7109, ORNL/TM-2011/514

[4]. U.S.NRC, "Guide for Validation of Nuclear Criticality Safety Calculational Methodology", NUREG/CR-6698

[5]. U.S.NRC, "Bias Estimates Used in Lieu of Validation of Fission Products and Minor Actinides in MCNP6 k-eff Calculations for PWR Burnup Credit casks", NUREG/CR-7205, ORNL/TM-2012/544
NUREG/CR-7205

[6] Los Alamos National Laboratory, "MCNP6 User's Manual" LA-CP-13-00634, (2013).

[7] H. Lee, C. Kong, D. Lee, "Status of Monte Carlo Code Development at UNIST: Proceedings of PHYSOR2014, September 28 – October 3, Kyoto, Japan.