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A Study on MCNPX-CINDER90 System for Activation Analysis

Sung-Min Kim and Myung Hyun Kim*
Department of Nuclear Engineering, Kyung Hee University, 446-701, Rep. of Korea
**Corresponding author: mhkim@khu.ac.kr*

1. Introduction

Many kinds of coupled system of MCNP [1] with ORIGEN [2] have been developed for different research applications. For the evaluation of radio-toxicity from neutron activation, this system is very effective and reliable compared with the other computational methods. Neutron fluxes for all specified regions are evaluated by MCNP and these are transferred to ORIGEN for the evaluation of one group cross section for all nuclides in interest with zero dimensional spectrum equation. After that, ORIGEN is used to calculate inventory changes of many nuclide chains, as many as 1,700 nuclides.

However, neutron spectrum at every cell is different depending on the geometrical characteristics. For the problem of neutron activation to the reactor containment wall, neutron spectra are varying from the center of core to the containment wall. Therefore, process of one group cross section library for all relevant isotopes need an extensive works for all locations [3]. On the other hand, CINDER [4] can concerns 3 dimensional geometry effects and handles up to 3,400 nuclides. It is believed that CINDER is more reliable and accurate compared to ORIGEN because it treats 63-group cross section.

In this paper, a new coupling of MCNP-CINDER was tested and compared with MCNP-ORIGEN and MCNPX 2.6.0. MCNPX is a coupled code of MCNP with CINDER90 for fuel depletion chain only.

The simple UO2 single pin was modelled in order to compare and evaluate the fission product densities for fuel depletion chains. The simple reactor pressure vessel (RPV) and concrete wall were modelled for the comparison of isotopic inventory chains for activation products simulating the RPV boundaries.

2. Calculation Codes and Methods

2.1 MCNPX 2.6.0

MCNPX 2.6.0 is an extended version of MCNP code with additional functions. MCNP is used to calculate only neutron particles. On the other hand, MCNPX can concerns all particles and all energies. Particularly, MCNPX 2.6.0 also included improvements in transmutation module and library tools through CINDER90 code. CINDER90 library file contains decay, fission yield, and 63-group cross section data not calculated by MCNPX. But, this module is suited to evaluate fuel depletion chain only because it treats some nuclides and isotopes which are related fuel depletion chain.

2.2 ORIGEN 2.1

ORIGEN 2.1 is used to evaluate nuclear material characteristics. The materials most commonly characterized include radioactive wastes, spent fuel, recovered elements, et cetera.

ORIGEN 2.1 code cannot concern geometry effects because it solves a problem as one point about reactor. Furthermore, neutron spectrum and flux level at every cell are different depending on geometrical characteristics. Additionally, ORIGEN 2.1 uses one group collapsed cross section, the cross section required to estimate through accurate MCNP simulation.

In this study, neutron spectrum and one group cross section in each specified regions are generated through MCNPX 2.6.0 and it applied to ORIGEN 2.1 code.

2.3 CINDER90

CINDER90 is used to calculate the inventory of nuclide in an irradiated material. In nuclear reactor applications, such a code is commonly called a burn up code, since it follows the temporal burn up of fissionable material and the associated production of fission products. It calculates the atom density and activity density of each and every nuclide present at a specified time.

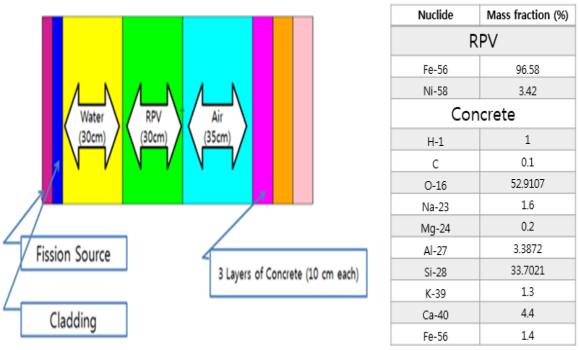
CINDER90 is a unique transmutation code having a library of 63-group cross sections and requiring no library preparation prior to execution. The library of nuclear data, constantly growing in breadth and quality with international cooperation, describes 3400 nuclides, 1325 fission products, and yield sets for over 30 actinides in the range $1 \leq Z \leq 103$. Also, CINDER90 is the automatic generation of the chain structure.

2.4 Activation analysis procedure and methods

The UO2 single pin was modelled in order to compare and evaluate the fission product densities for fuel depletion chains using the MCNPX 2.6.0. Also, the simple RPV and concrete wall were modelled for comparison of isotopic inventory chains for activation products using the MCNPX 2.6.0. Fig. 1 shows the UO2 single pin structure and composition. UO2 single pin radius is 2.5cm and the height is 100cm. Fig. 2 shows the simple RPV and concrete wall. The volume of RPV is 300,000 cm^3 and concrete wall is 100,000 cm^3.

Nuclide	Mass fraction (%)
U-235	35
U-238	55
H-1	1.1
O-16	8.9

Fig. 1. Structure and composition of the UO2 single pin



Nuclide	Mass fraction (%)
RPV	
Fe-56	96.58
Ni-58	3.42
Concrete	
H-1	1
C	0.1
O-16	52.9107
Na-23	1.6
Mg-24	0.2
Al-27	3.3872
Si-28	33.7021
K-39	1.3
Ca-40	4.4
Fe-56	1.4

Fig. 2. Structure and composition of the RPV and concrete wall

Neutron fluxes for all each cell are estimated by MCNP 2.6.0 and these are transferred to ORIGEN 2.1 and CINDER90. ORIGEN 2.1 and CINDER90 require neutron fluxes of the average / total specified regions, material composition, source term characterization, and irradiation / cooling time. Fig. 3 shows the calculation procedure of MCNPX 2.6.0, ORIGEN 2.1, and CINDER90 codes.

U-238 in UO2 single pin was selected in order to compare and evaluate the fission product density for fuel depletion chains. Fe-56 and Co-58 in simple RPV were selected for the comparison of isotopic inventory chains for activation products. O-16 in concrete wall was also selected for the same reason of isotopes in RPV. The results of calculation were compared by MCNPX 2.6.0, ORIGEN 2.1, and CINDER90.

The irradiation time of each model is 30 * 9 days and the cooling time of each model is 30 * 3 days. The thermal power of the model assumed as 10MW.

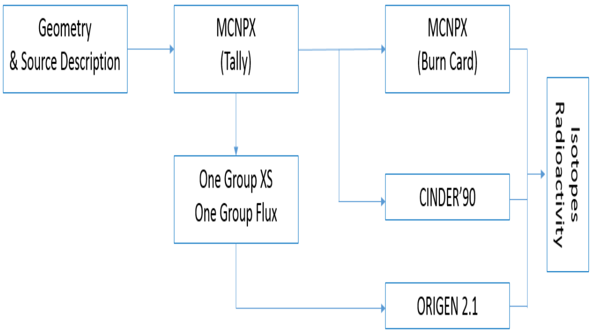


Fig. 3. Calculation procedure of MCNPX, ORLGEN 2.1, and CINDER90

3. Calculation results

The results of inventory change of nuclide chains and the radioactivity were compared with MCNPX 2.6.0, ORIGEN 2.1, and CINDER90. Table I and Table II show the inventory change and radioactivity for the U-238 in the UO2 single pin model. In the case of the inventory change of the U-238, the average relative error was compared based on MCNPX 2.6.0. In the case of ORIGEN 2.1, the average relative error was 3.32% for the irradiation time and 1.76% for the cooling time. On the other hand, in the case of CINDER90, the average relative error was -2.25% for the irradiation time and -3.38% for the cooling time. The result of radioactivity shows that the average relative error was 1.54% for irradiation time and 3.35% for cooling time in the case of ORIGEN 2.1. And the average relative error was -2.50% for irradiation time and -3.88% for cooling time in the case of CINDER90. Fig. 4 and Fig. 5 show the relative error between the codes for the U-238. Table III shows the inventory change for the Fe-56 in RPV and Table IV shows the inventory change of the O-16 in concrete wall. The difference for Fe-56 and O-16 were negligible among three codes. Fig.6 and Fig. 7 show the relative error between the codes in the Fe-56 and O-16. The Table V shows inventory change of the Co-58, and Table VI shows radioactivity in RPV. The result of inventory change of the Co-58 shows the average relative error of -45.23% for irradiation time and -55.72% for cooling time in the case of ORIGEN 2.1, the average relative error of 9.49% for irradiation time and 10.44% for cooling time in the case of CINDER90. Fig. 8 and Fig. 9 show the relative error between the codes for Co-58.

Table I: Activation Analysis result of U-238(Mass)

Unit : Kg

Code	Irradiation Time (Days)									Relative Error (%)
	30	60	90	120	150	180	210	240	270	
MCNPX	2.06E+01	2.05E+01	2.04E+01	2.03E+01	2.02E+01	2.01E+01	2.01E+01	2.00E+01	1.99E+01	Reference
ORIGEN 2.1	2.06E+01	2.06E+01	2.06E+01	2.06E+01	2.06E+01	2.06E+01	2.05E+01	2.05E+01	2.05E+01	1.76
CINDER'90	2.04E+01	2.03E+01	2.01E+01	1.99E+01	1.98E+01	1.96E+01	1.94E+01	1.93E+01	1.91E+01	-2.25

Code	Cooling Time(Days)			Relative Error (%)
	30	60	90	
MCNPX	1.99E+01	1.99E+01	1.99E+01	Reference
ORIGEN 2.1	2.05E+01	2.05E+01	2.05E+01	3.32
CINDER'90	1.91E+01	1.91E+01	1.91E+01	-3.38

Table II: Activation Analysis result of U-238(Activity)

Unit : Ci

Code	Irradiation Time (Days)									Relative Error (%)
	30	60	90	120	150	180	210	240	270	
MCNPX	6.91E-03	6.88E-03	6.88E-03	6.85E-03	6.82E-03	6.80E-03	6.77E-03	6.74E-03	6.68E-03	Reference
ORIGEN 2.1	6.93E-03	6.93E-03	6.93E-03	6.92E-03	6.92E-03	6.91E-03	6.91E-03	6.91E-03	6.90E-03	1.54
CINDER'90	6.87E-03	6.81E-03	6.76E-03	6.70E-03	6.64E-03	6.59E-03	6.53E-03	6.47E-03	6.42E-03	-2.50

Code	Cooling Time(Days)			Relative Error (%)
	30	60	90	
MCNPX	6.68E-03	6.68E-03	6.68E-03	Reference
ORIGEN 2.1	6.90E-03	6.90E-03	6.90E-03	3.35
CINDER'90	6.42E-03	6.42E-03	6.42E-03	-3.88

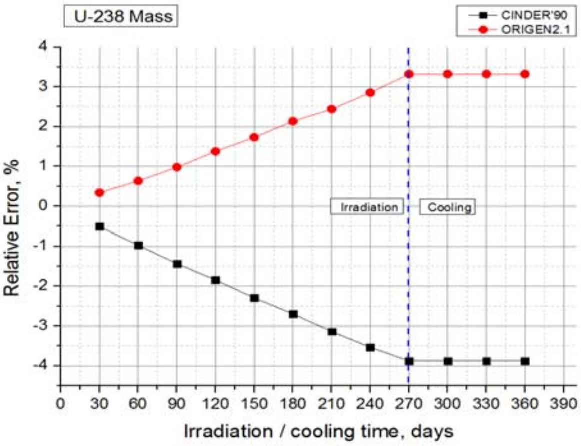


Fig. 4. The relative error of the inventory change in U-238

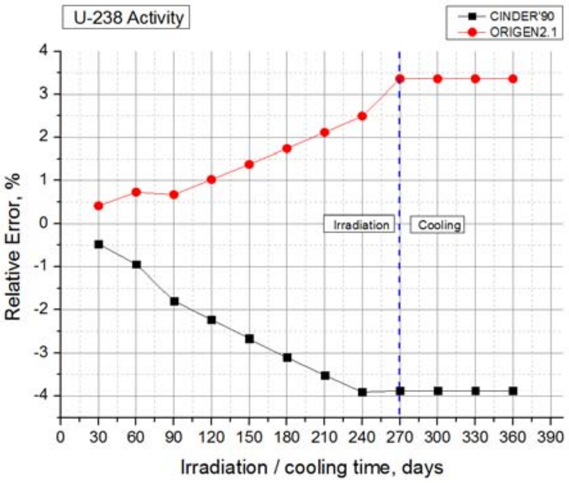


Fig. 5. The relative error of the radioactivity in U-238

Table III: Activation Analysis result of Fe-56

Unit : Kg

Code	Irradiation Time (Days)									Relative Error (%)
	30	60	90	120	150	180	210	240	270	
MCNPX	2.29E+03	2.29E+03	2.29E+03	2.29E+03	2.29E+03	2.29E+03	2.29E+03	2.29E+03	2.29E+03	Reference
ORIGEN 2.1	2.29E+03	2.29E+03	2.29E+03	2.29E+03	2.29E+03	2.29E+03	2.29E+03	2.29E+03	2.29E+03	0
CINDER'90	2.29E+03	2.29E+03	2.29E+03	2.29E+03	2.29E+03	2.29E+03	2.29E+03	2.29E+03	2.29E+03	0

Code	Cooling Time(Days)			Relative Error (%)
	30	60	90	
MCNPX	2.29E+03	2.29E+03	2.29E+03	Reference
ORIGEN 2.1	2.29E+03	2.29E+03	2.29E+03	0
CINDER'90	2.29E+03	2.29E+03	2.29E+03	0

Table IV: Activation Analysis result of O-16

Unit : Kg

Code	Irradiation Time (Days)									Relative Error (%)
	30	60	90	120	150	180	210	240	270	
MCNPX	1.22E+02	1.22E+02	1.22E+02	1.22E+02	1.22E+02	1.22E+02	1.22E+02	1.22E+02	1.22E+02	Reference
ORIGEN 2.1	1.22E+02	1.22E+02	1.22E+02	1.22E+02	1.22E+02	1.22E+02	1.22E+02	1.22E+02	1.22E+02	0
CINDER'90	1.22E+02	1.22E+02	1.22E+02	1.22E+02	1.22E+02	1.22E+02	1.22E+02	1.22E+02	1.22E+02	0

Code	Cooling Time(Days)			Relative Error (%)
	30	60	90	
MCNPX	1.22E+02	1.22E+02	1.22E+02	Reference
ORIGEN 2.1	1.22E+02	1.22E+02	1.22E+02	0
CINDER'90	1.22E+02	1.22E+02	1.22E+02	0

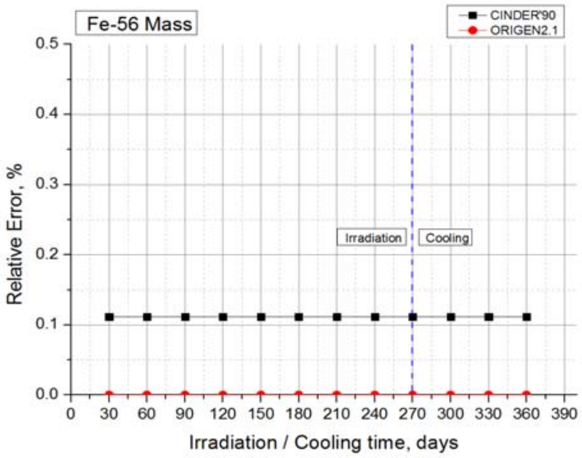


Fig. 6. The relative error of the inventory change in Fe-56

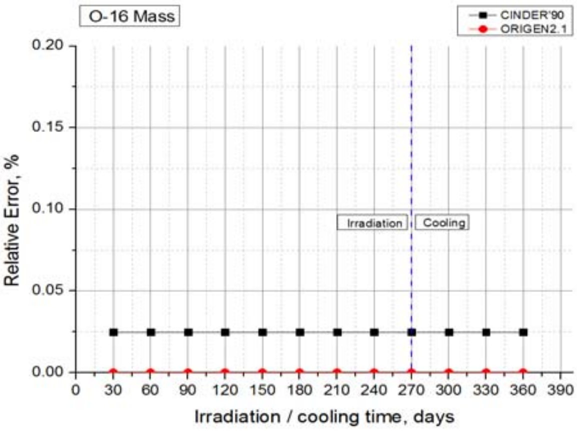


Fig. 7. The relative error of the inventory change in O-16

Table V: Activation Analysis result of Co-58(Mass)

Unit : Kg

Code	Irradiation Time (Days)									Relative Error (%)
	30	60	90	120	150	180	210	240	270	
MCNPX	3.03E-07	5.78E-07	7.30E-07	8.74E-07	9.11E-07	9.85E-07	1.07E-06	1.23E-06	1.30E-06	Reference
ORIGEN 2.1	2.34E-07	3.66E-07	4.39E-07	4.79E-07	5.01E-07	5.11E-07	5.16E-07	5.18E-07	1.22E+02	-45.23
CINDER'90	3.47E-07	6.10E-07	8.06E-07	9.52E-07	1.06E-06	1.14E-06	1.20E-06	1.25E-06	1.28E-06	9.49

Code	Cooling Time(Days)			Relative Error (%)
	30	60	90	
MCNPX	9.69E-07	7.23E-07	5.39E-07	Reference
ORIGEN 2.1	3.86E-07	2.87E-07	2.87E-07	-55.72
CINDER'90	9.61E-07	7.17E-07	7.17E-07	10.44

Table VI: Activation Analysis result of Co-58(Activity)

Unit : Ci

Code	Irradiation Time (Days)									Relative Error (%)
	30	60	90	120	150	180	210	240	270	
MCNPX	9.63E+00	1.84E+01	2.32E+01	2.78E+01	2.89E+01	3.13E+01	3.40E+01	3.90E+01	4.12E+01	Reference
ORIGEN 2.1	7.46E+00	1.16E+01	1.40E+01	1.53E+01	1.59E+01	1.63E+01	1.64E+01	1.65E+01	1.65E+01	-45.16
CINDER'90	1.10E+01	1.94E+01	2.56E+01	3.02E+01	3.37E+01	3.63E+01	3.82E+01	3.97E+01	4.07E+01	9.37

Code	Cooling Time(Days)			Relative Error (%)
	30	60	90	
MCNPX	3.08E+01	2.30E+01	1.71E+01	Reference
ORIGEN 2.1	1.23E+01	9.15E+00	9.15E+00	-55.65
CINDER'90	3.05E+01	2.28E+01	1.70E+01	-0.93

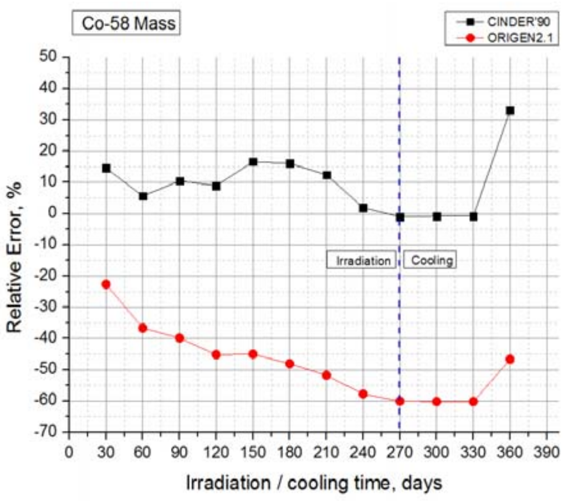


Fig. 8. The relative error of the inventory change in Co-58

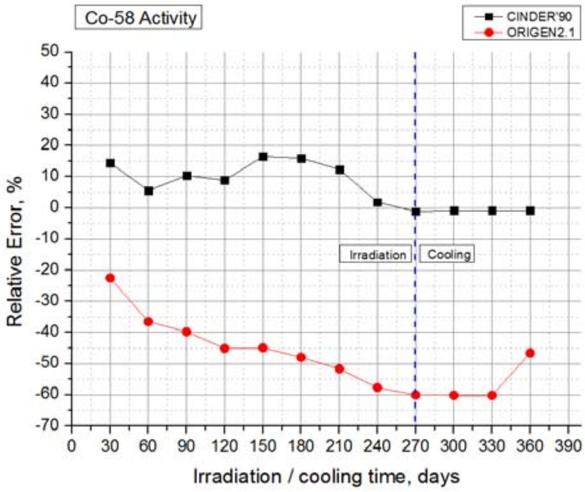


Fig. 9. The relative error of the radioactivity in Co-58

3. Conclusions

The UO2 single pin, simple RPV, and concrete wall model were modeled in order to compare inventory change and radioactivity with MCNPX 2.6.0, ORIGEN 2.1, and CINDER90. And by using three codes, the inventory change of the U-238 and radioactivity, inventory change of the Fe-56 and O-16, and inventory change of the Co-58 and radioactivity were calculated. Each result was compared and evaluated on MCNPX 2.6.0 value. Consequently, the difference for Fe-56 and O-16 were negligible among three codes and the inventory change of the nuclide and radioactivity calculation showed little difference except Fe-56 and O-16. In addition, the relative errors of three codes were similar with respect to inventory change of the U-238 and radioactivity in U-238. On the other hand, in case of inventory change and radioactivity in Co-58, the relative error of CINDER90 less than ORIGEN 2.1 for the result in comparison with MCNPX 2.6.0 value. It is regarded that CINDER90 is more reliable and accurate compared to ORIGEN 2.1 because it has 63-group multi cross section library. In addition, several error by the approximation of model description and the difference of the cross section library, fission yield data, and et cetera in each code result in the relative error between each code. Also as the decay chain is the simple nuclide, the difference of the result is little between the code and it is the complicated nuclide, the difference of the result is large between the codes. So the error by the difference of the decay chain has to be considered between each code. In conclusion, MCNP-CINDER system is more convenient and more accurate than MCNP-ORIGEN system because MCNP-CINDER system describes 3 dimensional geometry and uses 63-group cross section library and require no library preparation prior to calculation. On the other hand, in order to use MCNP-ORIGEN system, the collapsing of the one cross section is necessary and it cannot describes geometrical model. As a result of this, the practicality of MCNP-CINDER system was verified and it is expected to be used for the study on the activation analysis using MCNP-CINDER system as basic data.

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