# Least Square Fitted Scaling Factor for Radioactive Waste Storage Drum

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## 1. Introduction

Scaling factor has been widely used to quantify difficultly measuring (DTM) radioactive isotopes by using the key (KEY) isotopes which are relatively easily measured. It is defined as the relative inventory ratio based on the key isotopes such as A_DTM/A_KEY and the key isotopes are frequently chosen as Co-60 Cs-137, and Ce-144.[1][2] Several isotopes including activation products(Co-58, Co-60, Fe-55, Nb-94, Ni-59, Ni-63), fission products(H-3, C-14, I-129, Ce-144, Sr-90, Tc-99, Cs-137), and actinides shall be clearly quantified before when a radioactive waste drum is stored in the storage site. In order to apply properly, it is required information about the detail production history of active isotopes and the waste treatment flows including chemical change and filtering. But it takes lots of burden and also requires additional works including simulations and experiments.

In this paper, a simplified simulation test for scaling factors is carried out by using the ORIGEN-S code[3]. Fuel depletion and decay effects are solely taken into consideration for various uranium enrichments and fuel burnups. In order to obtain explicit formula for scaling factors as a function of enrichment and burnup, the generalized least square fitting (LSF) method is applied, too.[4] After obtaining scaling factors from the LSF method, the decay effects are also implemented by multiplying exponential decay term including decay constant of each isotope. The results of scaling factors are compared with those of simulation results from the ORGIEN-S code.

## 2. Simulation Conditions for Analytic Scaling Factor

For the application of the general scaling factor, a typical fuel assembly library in the ORIGEN-S code is used such as CE16X16. The uranium enrichment varies from 3.5 wt%U-235 to 5.5 wt%U-235. And the fuel burnup is given between 30 GWD/MTU and 60 GWD/MTU. And decay time is given as 5 years. One metric ton uranium is loaded and 30 kg Stainless Steel is added for the structural material. The element composition is given in Table I.

Table I: Element Composition for Simulation of Scaling Factor

| Element | U | Fe | Cr | Ni |
|---|---|---|---|---|
| Weight (kg) | 1,000 | 20.64 | 5.7 | 2.67 |

The total number of target isotopes is 12 and a group of alpha emission isotopes including about 35 actinide isotopes described in the IAEA guide.[5] From the results of ORIGEN-S, the inventories of 47 isotopes are evaluated as a function of decay time. Figs. 1 and 2 show scaling factors of various isotopes based on the Cs-137 and Co-60, respectively, when the enrichment is 4.5 wt%U-235 and the fuel burnup is 30 GWD/MTU. Depending on the characteristics of isotopes, the trend is quite different as a function of decay time. Most of chosen isotopes decrease as decay time increases but some isotopes exhibit inversely due to different half -lives.

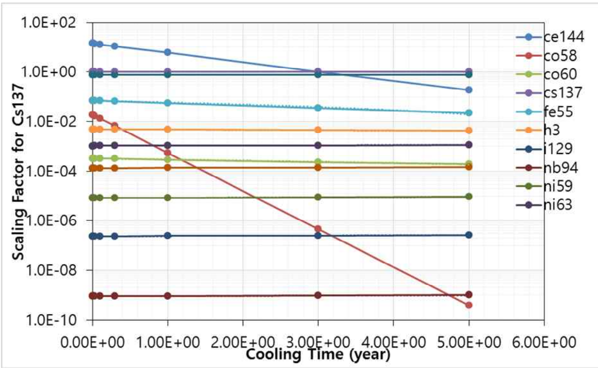


Fig. 1. Scaling factor change based on the Cs-137

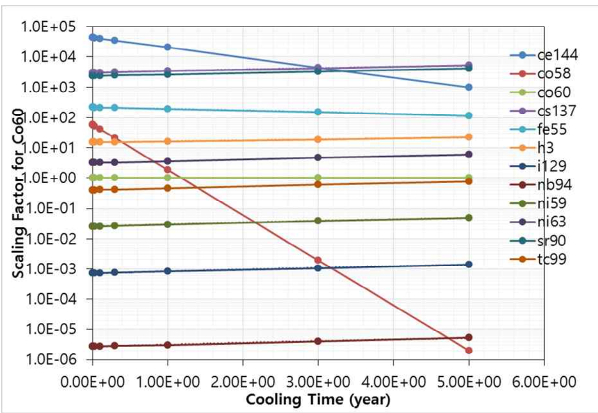


Fig. 2. Scaling factor change based on the Co-60

The simulation cases of ORIGEN-S are chosen as follows:

a) enrichment(wt%): 3.5, 4.5, 5.5
b) burnup(GWD/MTU): 30, 35, 40, 45, 50, 55, 60

Thus, we obtain total 21 separate cases are obtained and the results are used for the explicit functional form of scaling factors.

### 3. Least Square Fitted Scaling Factors

The scaling factors of specified isotopes are obtained as a function of burnup when the enrichment of uranium is fixed as shown in Fig. 3 which depicts the scaling factor of Ce-144 based on Cs-137. Two decay times of 9hr and 5 years are chosen and the behavior of scaling factor is quite different as shown in Fig. 3.

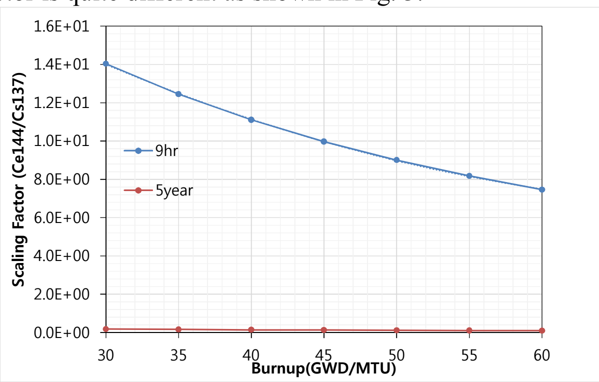


Fig. 3. Scaling factors of Ce-144 for 3.0 wt%U-235 as a function of burnup.

Then by using of a generalized least square fitting method, the scaling factor can be expressed in the quadratic form as follows.

$$y = (A_2 \pm \sigma_{A_2})x^2 + (A_1 \pm \sigma_{A_1})x + (A_0 \pm \sigma_{A_0}) \quad (1)$$
$$= A_2 x^2 + A_1 x + A_0 \pm (\sigma_{A_1} x^2 + \sigma_{A_1} x + \sigma_{A_0})$$

where x is burnup and y is scaling factor.

. From the data, a least square fitting in the second order polynomial can be applied such as

$$\begin{pmatrix} 1 & x_0 & x_0^2 \\ 1 & x_1 & x_1^2 \\ \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 \end{pmatrix} \begin{pmatrix} A_0 \\ A_1 \\ A_2 \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_n \end{pmatrix} \quad (2)$$

where $x_i$ is a i-th burnup, $A_j$ is a coefficient of $x^j$ polynomial to be determined, and $y_i$ is a scaling factor. The equation is written as in the matrix form as follows

$$XA = Y \quad (3)$$

Equation (3) is solved easily with the standard least square fitting by multiplying the transpose matrix of $X$ on both terms.

$$X^T XA = X^T Y \quad (4)$$

Then the coefficients are obtained as

$$A = \left(X^T X\right)^{-1} X^T Y \quad (5)$$

and their variances are also obtained as

$$Var(A_j) \approx \frac{R}{n-m}\left(X^T X\right)_{jj}^{-1} \quad (6)$$

In this case, the coefficients and their errors are easily obtained and are given in Table II.

Table II: Coefficients of Least Square Fitted Scaling Factor for Ce-144 based on Cs-137

| | | | |
|---|---|---|---|
| A2 | 3.357E-03 | σ(A2) | 2.136E-04 |
| A1 | -5.175E-01 | σ(A1) | 1.932E-02 |
| A0 | 2.646E+01 | σ(A0) | 4.200E-01 |

When completing evaluation of coefficients for all specified isotopes, the general scaling factors may be expressed as the Lagrange 2nd order interpolation functions such as

$$f_{B_1}(E) \approx A_2 E^2 + A_1 E + A_0$$
$$f(B,E) = \frac{(B-B_3)(B-B_2)}{(B_1-B_3)(B_1-B_2)} f_{B_1}(E)$$
$$+ \frac{(B-B_3)(B-B_1)}{(B_2-B_3)(B_2-B_1)} f_{B_2}(E) + \frac{(B-B_1)(B-B_2)}{(B_3-B_1)(B_3-B_2)} f_{B_3}(E)$$

where E is enrichment (wt%U-235) and B is burnup (GWD/MTU).

Additionally, a decay time is corrected simply by multiplying exponential decay term as follows

$$f(B,E,t) = \frac{A_i e^{-\lambda_i t}}{A_k e^{-\lambda_k t}} = (A_i / A_k) e^{-(\lambda_i - \lambda_k)t} \approx f(B,E) e^{-(\lambda_i - \lambda_k)t}$$

where t is decay time and λ is decay constant.

Fig. 4 depicts the least square fitted scaling factor of Ce-144 for 3 wt%U-235 as a function of burnup by comparing scaling factors evaluated directly by the ORIGEN-S. The difference of two scaling factors is not significant and the fitted scaling factors predicts well enough. Table III shows fitted scaling factors of various isotopes based on the Cs-137 when the enrichment of 4.2 wt%U-235, the burnup of 52 GWD/MTU, and 10 year decay time is given.

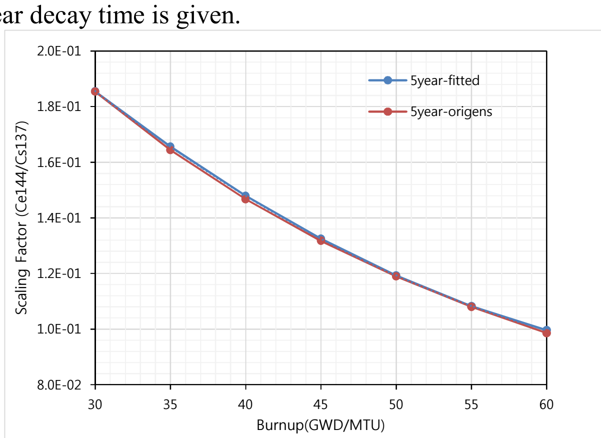


Fig. 4. Comparison of least square fitted scaling factors of Ce-144 for 3.0 wt%U-235 as a function of burnup.

Table III: Least Square Fitted Scaling Factor based on Cs-137 when 4.2 wt%, 52 GWD/MTU, and 10 year decay time.

| | Scaling Factor | Error |
|---|---|---|
| Ce144 | 1.50E-03 | 3.17E-04 |
| Co58 | 4.56E-18 | 1.84E-18 |
| Fe55 | 7.53E-03 | 1.76E-04 |
| H3 | 3.93E-03 | 5.42E-05 |
| I129 | 3.24E-07 | 9.18E-09 |
| Nb94 | 1.62E-09 | 8.61E-11 |
| Ni59 | 1.17E-05 | 4.84E-07 |
| Ni63 | 1.48E-03 | 1.53E-04 |
| Sr90 | 6.70E-01 | 8.66E-03 |
| Tc99 | 1.52E-04 | 1.98E-05 |
| alpha | 2.18E+00 | 1.64E-01 |

## 4. Conclusions

By using the ORIGEN-S code, scaling factors are evaluated with a function of enrichment, burnup, and decay time through the least square fitting method and Lagrange interpolation scheme. The fitted results are confirmed by comparing with the direct results of the ORIGEN-S. These simulations are adaptable for various initial conditions such as different fuel type and fuel burnup, too. In future, least square fitted scaling factors may be utilized to validate the measured data for the radioactive waste drum.

## REFERENCES

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