# Hybrid Computing Technique for Nuclear Facility Design with Best Estimate Source Terms – 12313

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#### ABSTRACT

When overall source term representing a variety of spent fuels or radwastes with different irradiation and decay profile is estimated, there are some restrictions in conventional analysis tools. A hybrid computing program that employs several functional modules was developed to support R&D action plan on an advanced fuel cycle adopting a pyroprocess in connection with a sodium-cooled fast reactor in South Korea. Requirements for the advanced program were first defined, followed by development of several functional modules. With the developed modules, it was possible to carry out a source term assessment taking into account respective physical, irradiation, and aging characteristics of each spent fuel. And it was found that typical conservativeness in the design of nuclear facilities can be minimized through the hybrid technique and program proposed in this study.

#### **INTRODUCTION**

There are now twenty-one commercial nuclear power plants operating in South Korea: four CANDU and seventeen PWR reactors [1]. The total amount of spent fuel (SF) generated by the end of 2010 was revealed to be about 11,371 tons of uranium (MTU). The annual arising rate is about 700 MTU [2]. The SFs from PWRs are stored at reactor wet storage pools. The SFs from CANDU reactors are stored at reactor wet storage pools.

The Korean government and nuclear industry have sought to come up with a national policy for the long-term management of SF [3, 4]. In 2007, the 3<sup>rd</sup> Comprehensive Nuclear Energy Promotion Plan [5], passed at the 254<sup>th</sup> meeting of the Atomic Energy Commission, was announced as an R&D action plan for the development of an advanced fuel cycle adopting a sodium-cooled fast reactor (SFR) in connection with a pyroprocess for a sustainable stable energy supply and a reduction in the amount of SF. It is expected that this fuel cycle can greatly reduce the SF inventory through a recycling process in which transuranics (TRU) and long-lived nuclides are burned in the SFR and cesium and strontium are disposed of after sufficient interim storage. Additionally, the period needed for the radiological toxicity of SF to be reduced to that of natural uranium can be shortened to hundreds of years through burning of the recovered TRU in the SFR [6].

For the success of the R&D plan, there are several issues related to the source term analysis. These are related with the following: (a) generation of inflow and outflow source terms of mixed SF in each process for the design of the pyroprocess facility, (b) source terms of mixed radwaste in a canister for the design of storage and disposal systems, (c) overall inventory estimation for TRU and long-lived nuclides for the design of the SFR, and (d) grand source terms for the practical design of the interim storage facility of SFs.

A source term evaluation for a SF or radwaste with a single irradiation profile can be easily accomplished with the conventional computation technique. However, source term assessment for a batch of SFs or a mixture of radwastes generated from SFs with different irradiation profiles—a task that is

essential to support the aforementioned activities—is not possible with the conventional technique. Therefore, hybrid computing technique for source term analysis to support the advanced fuel cycle was developed and its usefulness was explained here.

# NEED OF ADVANCED SOURCE TERM ANALYSIS TOOL

## **R&D** Action Plan

Figure 1 shows the milestone of the R&D action plan for development and verification of the proliferation-resistant pyroprocess and SFR [7]. The design and construction of an engineering-scale mock-up system and equipment with an annual processing capacity of 10 tons of depleted uranium will be completed by 2011. Construction, installation of equipment for the mechanical head-end process and follow-on integrated processes for SF processing, acquisition of an operating license, and performance test of process operation using simulated fuel will be carried out by 2016 for the establishment of an engineering-scale verification facility (ESPF) with an annual processing capacity of 10 tons. Validation of the engineering-scale pyroprocess technology will be carried out using simulated fuel by 2020, including generation of design data for a pilot facility named Korea Advanced Pyroprocess Facility (KAPF) with an annual capacity of 100 tons.

The extensive research for management of a variety of radwastes generated from the abovementioned advanced fuel cycle (AFC) are also taken into consideration in the R&D action plan. Research on key technologies related to disposal system design, characterization of deep geological foundation, verification of engineered barrier, and total safety assessment has been carried out since 2007.

Concerning R&D for the establishment of a SFR, an advanced concept for a commercial Generation IV SFR will be developed by the end of 2011, followed by construction of an integral test loop for demonstration of key technologies. Standard design for the demonstration reactor will be completed by 2017. Reactor system performance will be demonstrated and standard design approval will be released by 2020. After obtaining a construction permit for the demonstration reactor by 2023, construction will be completed by 2028.



Fig. 1. R&D Action Plan for Safe Management of Spent Fuel

## **Essential Functions for Advanced Source Term Analysis**

For source term analysis to support R&D action plan noted above, an advanced computation tool should meet the following requirements:

- perform irradiation and decay calculation for the fuel itself and hardware comprising the fuel assembly.
- estimate source terms for radwastes considering material flow of the pyroprocess when a single fuel assembly is processed.
- estimate source terms for radwastes considering the material flow of the pyroprocess when a variety of fuel assemblies with different fuel design, initial enrichment, irradiation history, discharge burnup, and cooling time are processed.
- estimate source terms for mixed radwastes generated at different times.
- estimate source terms of hardware taking into account contamination; furthermore, estimate source terms for top-end and bottom-end pieces reflecting rapidly varying neutron spectrum.
- prepare a database of SF to take into account realistic data when the grand source terms such as nuclide inventory, radioactivity, decay heat, and hazard index are evaluated.

## **DEVELOPMENT OF HYBRID COMPUTING TOOL**

#### **Functional Module**

Currently, there is no available tool that has functions to fully support the aforementioned requirements. It is not efficient to develop an entire program, as much time is needed to prepare a variety of peripheral parameters such as nuclear data and cross-section values, and to verify the developed module. Therefore, a hybrid method that adopts many functional modules to perform a user-defined job was proposed. Within this approach, ORIGEN-S [8] in SCALE code package [9] was chosen as a depletion and decay chain solver.

#### - Screening

This module extracts SFs, to which calculations are to be performed, from a SF database. The SF database prepared through this study includes physical characteristics such as assembly design, an array, <sup>235</sup>U enrichment, uranium loading, and information on structural materials. It also provides irradiation characteristics such as the loading date, discharge burnup, discharge date, and the residence period of a fuel in a core, and storage characteristics such as the cooling time at a storage facility. These data are recorded for each fuel assembly identification (ID). The major function of this module is to provide information needed for the depletion and decay calculation, including physics parameters.

## - DeplDec

The role of this module is to irradiate and decay SF for specified irradiation and cooling time considering appropriate physics parameters. As noted earlier, it uses ORIGEN-S for the depletion and decay calculation. The main function of this module is to supply parameters such as the specific power, effective full power day, the number of cycles, initial loading of uranium, and index designating cross-section library, which are needed for ORIGEN-S to solve Eq. (1).

$$\frac{d\mathbf{N}_i}{dt} = \sum_j \delta_{ij} \lambda_j \mathbf{N}_j + \sum_k f_{ik} \sigma_k \phi \mathbf{N}_k - (\lambda_i + \sigma_i \phi) \mathbf{N}_i, \qquad (1)$$

where  $\sigma_i$  = the absorption cross section of nuclide *i*,

 $\delta_{ii}$  = the fraction of radioactive decay from nuclide *j* to *i*,

 $f_{ik}$  = the fraction of neutron absorption by nuclide k and transmuted to isotope i; other terms have conventional meanings.

The neutron flux to solve Eq. (1) for the depletion calculation of the fuel itself is always retrieved by Eq. (2). However, the neutron flux for the activation calculation of the assembly hardware is retrieved by multiplying the flux scaling factor by the average neutron flux of the fuel, as delineated in Eq. (3).

$$\overline{\phi}_{fuel} = \frac{6.242 \times 10^{18} (\overline{P})}{\sum_{i} N_i^f \sigma_i^f R_i},\tag{2}$$

where  $\overline{P}$  and  $R_i$  represent the average specific power and recoverable energy of fission of nuclide *i*, respectively.

$$\overline{\phi}_{hardware} = \omega \overline{\phi}_{fuel} \tag{3}$$

where  $\omega$  is the pre-generated or user-supplied flux scaling factor to represent the neutron flux of the structural component.

After obtaining the parameters, this module provides input for ORIGEN-S, runs ORIGEN-S, and calculates source terms as a function of time. Because this module has a pre-generated cross-section library for each fuel design in Korea, it makes ORIGEN-S choose the appropriate library by giving an indicator nominating the specific fuel design.

#### - DecRes

The function of this module is to decay SF or radwaste through a restart calculation with pre-calculated information. It makes input for ORIGEN-S to restart the decay calculation. It supplies information such as the composition for the restart calculation and additional decay period, runs ORIGEN-S, and calculates source terms as a function of time.

#### - ReproRun

This module was developed to separate radwastes generated from the pyroprocess by running ORIGEN-S, which solves Eq. (4) considering the removal ratio of nuclide *i* for each unit process specified in the user-interface. It has flexibility to address alteration of the number of unit processes and material flows to flexibly accommodate technology development.

$$\frac{d\mathbf{N}_i}{dt} = \sum_j \delta_{ij} \lambda_j \mathbf{N}_j - (\lambda_i + r_i) \mathbf{N}_i, \qquad (4)$$

where  $r_i$  represents the removal ratio of nuclide *i*.

#### - Batch

This module was introduced to calculate mixture composition when many kinds of SFs are processed or combined at the same time t. The mixture composition of nuclides is calculated through multiplication of the processing fraction by the mass of the nuclide, as shown in Eq. (5).

$$\mathbf{N}_i = \sum_j \omega^j \mathbf{N}_i^j \,, \tag{5}$$

where  $\omega^{j}$  and  $N_{i}^{j}$  represent the mixing ratio of the SF *j* and the mass of nuclide *i* originated from the SF *j*, respectively. The default value of the mixing fraction is 1.0, which means 100 percent of the irradiated pellets composing the SF is processed and mixed together.

#### **Capability and Usefulness**

This section explains the sequence of the developed program and its usefulness by introducing two pseudo problems.

## - Source Term Evaluation of Pyroprocess

This sequence has the capability to automatically characterize source terms of residual material in each unit process and discharged radwaste by taking into account the material flow of the process. This sequence uses the Screening, DeplDec, Batch, and RproRun modules.

For the fuel itself, the Screening module extracts SFs corresponding to the user-defined bin of <sup>235</sup>U enrichment, discharge burunup, and cooling time, followed by respective depletion and decay calculation by the DeplDec module for the selected assemblies up to the time of pyroprocessing. The Batch module then generates the mixture composition taking into consideration the mixing ratio, initial uranium loading, and nuclide composition vector. The default value of the mixing ratio is 1.0, and this value can be changed by the user. Finally, RproRun generates source terms as a function of time after applying the material flow of the pyroprocess. The contents extracted from the SF database are <sup>235</sup>U enrichment, initial uranium loading, index implying fuel design, discharge burnup, uranium loading date, residence period and number of cycles residing in a core, final discharge date, etc. The decay time up to the pyroprocess is determined on the basis of the final discharge date. The specific power essential to set up ORIGEN-S input are calculated by dividing discharge burnup in unit of MWd/MTU by effective full power days.

For the structural components comprising the fuel assembly, the analysis procedure is the same except that information on the flux scaling factor and the initial composition of each structural component is read from the built-in database to set up the ORIGEN-S input, prior to the irradiation and decay calculation. Built-in cross-section libraries for all fuel designs and each structural component are established, and therefore the appropriate library is utilized for each depletion calculation.

Pseudo problem for a pyroprocessing radwaste characterization problem was proposed and analyzed to demonstrate the usefulness of the previously described sequence. In the problem, four assemblies with different <sup>235</sup>U enrichment, uranium loading, burnup, irradiation period, and cooling time, listed in Table 1, were fed to the pyroprocess facility simultaneously, mixed together, and processed following material flow, resulting in different kinds of radwastes from three unit processes. The respective radwaste was assumed to contain the corresponding elements listed in Table 2. Figure 2 shows window including plot view of the radioactivity of fission product in radwaste discharged from Process #2 of the pyroprocess.

Assembly ID	Enrichment (wt.%)	Urainum Loading (kg)	Discharge Burnup (MWd/MTU)	Irradiation Period (days)	Discharge Date
KK1E36	3.40	409	30,201	1,198	1988.11.15
KK2S35	3.80	413	37,613	1,206	2003.10.20
KK3F11	3.20	425	41,182	1,091	1991.12.15
KK4H42	3.44	441	34,371	1,288	1994.12.08

Table 1. Specifications, Irradiation, and Cooling History for each Fuel

Table 2.	Iransfer	Rate of	Each	Element	to	Kadwaste	tor	Each	Process

Element	Process #1	Process #2	Process #3
Sr	0.900	0.090	0.001
Cs	0.900	0.090	0.001
U	0.002	0.001	0.003
Np	0.002	0.001	0.003
Pu	0.002	0.001	0.003
Am	0.002	0.001	0.003

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Fig. 2. Window Including Plot View of Radioactivity

The usefulness to use the advanced computing system on the basis of former problem is summarized in Table 3. In the comparison, it was assumed that commonly used 4 source terms such as nuclide concentration, radioactivity, decay heat, and hazard index for 3 kinds of wastes (ws) generated from pyroprocess of simultaneous 4 PWR fuel assemblies (ass in Table 3) were calculated by ORIGEN-ARP [10] and currently developed program, named in ASOURCE in Table 3.

As shown in the table, the number of inputs user should prepare is 48 and 1 for ORIGEN-ARP and ASOURCE, respectively, because ASOURCE makes one input considering designated source terms and material flow for each process defined by the user. Computing time was compared by running those two programs. Because entire data processing except final output report activity is carried out by software in ASOURCE, data processing time for combining isotopic composition for respective stream is below 0.1 seconds. Note that all activity for data combination from respective stream should be done by the user in conventional tool. Elimination of human error in the data processing is also advantage of using the advanced computing program.

Item	ORIGEN-ARP <sup>a</sup>	ASOURCE <sup>b</sup>	Ratio (b/a)
Number of input	$4(st) \ge 3(ws) \ge 4(ass) = 48$	1	1/48
Computing time (second)	4.85 sec/case x 48 case = 232.8 sec	16.43 sec	0.071
Data processing time for averaging calculation	$\sim 10 \text{ min/output x}$ 60 sec/min x 48 = 28,800 sec	< 0.1 sec	3.5E-6
Data processing error	Possible by user	not possible	N/A

Table 3. Comparison of Computing Efficiency for Pyoroprocessing Problem

st: source terms, ws: wastes, ass: assemblies

#### - Grand Source Term Evaluation

This sequence can estimate grand source terms for the group of SFs corresponding to the user-specified bin by calling the Screening, DeplDec, Batch, and DecRes modules. The scheme to evaluate the grand source terms is as follows.

In the first step, the Screening module extracts SFs corresponding to the user-defined bin of <sup>235</sup>U enrichment, discharge burunup, and discharge year from  $t_0$  to  $t_1$ , resulting in group 1, followed by respective depletion and decay calculation by the DeplDec module for the selected assemblies up to the final date of the calendar year of  $t_1$ . The Batch module then generates the mixture composition, resulting in *mixture 1*, taking into consideration the mixing ratio, initial uranium loading, and nuclide composition vector at the final date of calendar year of  $t_1$ . Finally, the *mixture 1* is decayed by the DecRes module up to the final date of the calendar year of  $t_2$ .

In the second step, the Screening module extracts SFs corresponding to the identical user-defined bin for discharge year from  $t_1$  to  $t_2$ , resulting in group 2, followed by respective depletion and decay calculation for the selected assemblies up to the final date of the calendar year of  $t_2$ . The Batch module then generates the mixture composition of *mixture 2* by combining the nuclide composition of *mixture 1* at the final date of the calendar year of  $t_2$  and the nuclide composition of each assembly in group 2 at the final date of the calendar year of  $t_2$ . Finally, the *mixture 2* is decayed by DecRes module up to the final date of the calendar year of  $t_3$ .

By repeating this procedure, the grand source terms as a function of calendar year from  $t_1$  to  $t_n$  are obtained. If the information on SFs to be generated in the future on the basis of a national plan is added to the SF database, the grand source terms can be estimated as a function of the uptime time.

By using this module, the inventory of Pu, TRU, long-lived fission product, etc can be estimated as a function of calendar year for domestic SFs in Korea. These calculated composition vector of SF or TRU can be utilized for both the SFR core design and determination of the number of SFRs required.

This sequence can be used for exact estimation of decay heat or radioactivity for SFs stored at a reactor's temporary pool. Recently, an unexpected nuclear accident occurred accompanying possible core damage and SF pool dry-out at the Fukushima-daiichi nuclear power plants. In this case, primary and essential information could include overall decay heat and radioactivity for the SFs stored in the temporary pool and irradiated fuels residing in the core. Exact information rather than conservative values is needed for application of an appropriate method to prevent propagation of the accident.

When the Korean Reference Disposal System accommodating domestic SFs was developed, all SFs were assumed to be the reference SF with  $17 \times 17$  Westinghouse fuel design, initial enrichment of 4.0 wt.%, discharge burnup of 45 GWd/MTU, and cooling time of 40 years<sup>8)</sup>.

Figure 3 shows the comparison result for the predicted value of decay heat for the reference SF with exact information- based value for SFs stored at Kori unit 4. Because the reference fuel was determined by analyzing spent fuel information stockpiled by 2005, it is almost equivalent to compare decay heat from the reference fuel with that from all SFs stockpiled at Kori unit 4 by the end of 2007. These SFs revealed initial enrichment distribution of  $1.6 \sim 4.5$  wt.%, discharge burnup of  $12,000 \sim 54,000$  MWd/MTU, yielding 946 assemblies. In the figure, the dotted line represents decay heat from the reference spent fuel calculated by ORIGEN-ARP, and solid line means average decay heat calculated by ASOURCE considering respective irradiation and decay profile for 946 assemblies. As shown in the figure, it was indicated that about 1.5 times higher decay heat was applied for the Korean Reference Disposal System accommodating SFs discharged from Kori unit 4.



Fig. 3. Decay Heat as a Function of Time for Kori Unit 4

This sequence can estimate not only the grand decay heat and radioactivity for the entire SFs, but also the individual decay heat and radioactivity for each nuclide in SFs. It is expected that grand source terms evaluated by this sequence will also be useful for the design of transport casks and interim storage facilities of SFs.

#### - Other Applications

The developed program has also a sequence that can estimate source terms taking into account axial burnup profile, by calling the DeplDec, Batch, and DecRes modules. Other capability such as automatic source term characterization for assembly hardware is one of the remarkable features of the developed program.

## CONCLUSIONS

There are some restrictions with the conventional analysis tool when overall source term representing a variety of SFs or radwastes with different physical characteristics, irradiation profile, and decay history is evaluated. In this paper, a hybrid computing program that uses many functional modules to perform user-defined tasks was developed to overcome existing barriers to support the R&D action plan for an advanced fuel cycle employing a pyroprocess in connection with a sodium-cooled fast reactor in South Korea. Requirements for the advanced program were first defined, followed by development of several functional modules to perform a depletion and decay calculation, mixture composition calculation, decay only calculation, and reprocessing simulation. The ORIGEN-S was utilized as a depletion and decay chain solver. With the advanced program, it was possible to carry out a source term assessment taking into consideration respective physical, irradiation, and aging characteristics of each SF. And it was found that conservativeness in the design of nuclear facilities can be minimized through the hybrid technique and program proposed in this study.

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