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Nuclear Fuel Cycle Simulation System: Improvements and Applications

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NUCLEAR FUEL CYCLE SIMULATION SYSTEM: IMPROVEMENTS AND APPLICATIONS

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INTERNATIONAL ATOMIC ENERGY AGENCY
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FOREWORD

The Nuclear Fuel Cycle Simulation System (NFCSS) is a scenario based computer simulation tool that can model various nuclear fuel cycle options in various types of nuclear reactors. The NFCSS allows users to efficiently and accurately identify the nuclear mineral resources and technical infrastructure needed for the front end of the nuclear fuel cycle; the amounts of used fuel, actinide nuclides and high level waste generated for a given reactor fleet size; and the impact of introducing recycling of used fuel on mineral resource savings and waste minimization.

Development of the NFCSS began in the 1990s, and in 2005 the tool was made freely available to Member States and a wide range of professionals in academia, research and policy arena through the IAEA web site. The technical basis of the NFCSS was first published in 2007 as IAEA-TECDOC-1535. Since then, there have been significant improvements in the NFCSS, such as its expansion to include the thorium cycle and other fuel types. The current publication provides comprehensive updates and background information relating to the changes made to the tool since 2007.

The IAEA wishes to thank the experts who took part in the preparation of this publication for their valuable contributions, in particular R. Yoshioka (Japan) for his assistance in the drafting of this publication. The IAEA is also grateful to the Member States that cooperated in this work. The IAEA officers responsible for this publication were H. Tulsidas and K. Sim of the Division of Nuclear Fuel Cycle and Waste Technology.

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1. INTRODUCTION

1.1. BACKGROUND

The Nuclear Fuel Cycle Simulation System (NFCSS) is a scenario based computer simulation tool, implemented in a web based platform, for studying various options of nuclear fuel cycle for nuclear power plants (NPPs). The NFCSS is used to develop illustrative scenarios in support of policy making on nuclear fuel cycles and to assist educational and research activities. It provides answers to questions related to various scenarios of nuclear fuel cycle for periods ranging from a few years to 200 years maximum. The NFCSS is very efficient and reasonably accurate in answering questions such as: the nuclear mineral resources and technical infrastructure needed at each stage of the front end of the nuclear fuel cycle; the amounts of used fuel, actinide nuclides and high level waste generated from a given reactor fleet; and the impact of introducing recycling of used fuel on mineral resource savings and waste minimization.

The development of the NFCSS could be traced to the international symposium on "Nuclear Fuel Cycle and Reactor Strategies: Adjusting to New Realities" at the IAEA in Vienna from June 3 to 6, 1997. In preparation for this symposium, from 1995 an international steering group with representatives from twelve countries and three international organizations (IAEA, Organization for Economic Co-operation and Development (OECD)/Nuclear Energy Agency (NEA) and World Nuclear Association (WNA)) coordinated the work of six working groups. These working groups studied different scenarios of energy consumption and energy mix which involved estimating nuclear electricity production and the associated nuclear fuel cycle requirements.

A new simulation system, named VISTA (the precursor to the NFCSS), was developed in 1996 to fulfil the need for making quick and simple calculations. It was then intensively used to quantify the different scenarios fixed by the working groups of the conference. The NFCSS was initially designed as a standalone spreadsheet tool that could be implemented on computers running Microsoft Office. With the expansion of various web based information services by the IAEA, a web accessible version of the NFCSS was launched in 2003, and from 2005 it was made freely available to Member States and public through the IAEA website. The outcome of these efforts and some case studies were published as IAEA-TECDOC-1535 in 2007 [1].

The NFCSS has also been used internally by the IAEA for estimating spent fuel discharges from civilian reactors worldwide, plutonium and minor actinides (MAs) accumulation in the discharged spent fuel and in the high level waste (HLW). Since NFCSS model requires isotopic composition of spent nuclear fuel as inputs to make estimates of various material accumulations from nuclear reactor operation, a simplified fuel depletion module called Calculation of Actinide Inventory (CAIN) was developed. The CAIN requires a small number of input parameters and gives results in a very short time. Unlike more sophisticated fuel depletion codes like ORIGEN[1] and others, CAIN's computational resource requirement is very minimal and suitable for implementation using various web based platforms. Despite its simplicity and minimalistic approach, the CAIN is very effective and reasonably accurate in estimating isotopic composition of spent fuel discharged from various reactor types.

[1] ORIGEN is a computer code system for calculating the buildup, decay and processing of radioactive materials.

The NFCSS has been used for carrying out fuel cycle assessments for two main commercial nuclear fuels, namely, UO_2 fuel and Pu-doped uranium dioxide (MOX) fuel, and for 7 types of NPPs that compose the global nuclear reactor fleet, i.e. pressurized water reactors (PWRs), boiling water reactors (BWRs), pressurized heavy water reactors (PHWRs), high power channel-type reactors (RBMKs), advanced gas-cooled reactors (AGRs), gas cooled reactors (GCRs) and water-water energetic reactors (WWERs). Recently, the NFCSS has been extended for application to thorium fuel cycles for light water reactors (LWRs). It also has been demonstrated that in principle the NFCSS is capable of modelling fuel cycles of fast reactors (FRs).

The NFCSS can calculate the actinide inventory such as uranium (U), plutonium (Pu), MAs (e.g. Np, Am and Cm) entrained in spent fuels using the CAIN fuel depletion model. For a given nuclear programme size, the NFCSS can provide estimates of material flows and various fuel cycle requirements such as natural uranium resources, enrichment services in separative work unit (SWU), volume of fuel fabrication, volume of spent fuels, accumulation of Pu and MAs, reprocessing volumes and so on. A unique feature of the NFCSS is that it does not need specific reactor core design codes or other proprietary information. This flexibility allows the NFCSS to simulate future uranium needs and other fuel cycle requirements for a reactor park, country, region, or the entire world. The NFCSS is recognized for its speed[2], accuracy and ease of use by a wide range of professionals in academia, research and policy institutions of Member States.

Since 2005 the NFCSS has been widely used by researchers in national labs and academia, by industry analysts, energy planners and policy analysts in Member States working on nuclear fuel cycle options. Based on these experiences, various users requested the IAEA to improve certain aspects of the NFCSS. These include a module for thorium fuel cycle assessments, routines for the initial core loading and the final core discharge, and methods for radiotoxicity and decay heat calculations. Also, a number of trials have been made to investigate fuel cycle options for innovative reactors (e.g. international project on innovative nuclear reactors and fuel cycles (INPRO), and FR) in order to demonstrate its potential applicability.

IAEA has organized consultancy meetings every year from 2009 to 2017 to review NFCSS development by involving consultants, users and fuel cycle experts. It was requested by meeting participants that all changes and improvements made to the NFCSS since it was first publicly accessible more than ten years ago be documented as a timely revision of the publication. This publication also provides the basis for future programming work that will allow increased flexibility and options for NFCSS users.

1.2. OBJECTIVE

Since the publication of IAEA-TECDOC-1535 [1] in 2007, there have been significant improvements in implementation of the NFCSS including a new extension to thorium fuel cycles, methods to calculate decay heat and radiotoxicity, and demonstration applications to the INPRO and fast reactors. This publication provides comprehensive updates and background information relating to the changes made since 2007.

[2] The NFCSS is recommended to use in Internet Explorer.

1.3. SCOPE

This publication provides theoretical background and methods for estimating nuclear fuel cycle requirements for thorium fuel as well as for UO_2 and MOX fuels in various reactor types. More specifically, this publication mainly covers:

- Material flow model for UO_2, MOX and thorium fuel cycles;
- Burnup model for thorium fuel cycles;
- Method for decay heat calculation;
- Method for radiotoxicity calculation;
- Demonstration applications to nuclear fuel cycles for the INPRO and FRs;
- Benchmarking of the NFCSS.

1.4. STRUCTURE

The structure of the publication is organized as follows:

In Section 2, the overall features of the NFCSS are described, including information flow (e.g. key input and output parameters) and various nuclear fuel cycle stages considered in the NFCSS.

In Section 3, nuclear material flow model is described. Resource requirements at each stage of nuclear fuel cycle described in Section 2 are evaluated using this material flow model.

In Section 4, an overview of the burnup model that accounts for nuclear reaction and decay chains of UO_2 and MOX fuel cycles is described. Although details of this simplified fuel depletion model were originally documented in IAEA-TECDOC-1535 [1], their key features are summarized in Annex III of this report for convenience.

In Section 5, Thorium fuel depletion model is described taking into account nuclear reaction and decay chains of thorium.

In Section 6 and Section 7, methods for decay heat and radiotoxicity calculations are described respectively. Templates (e.g. spreadsheets), which are not part of the source programme of the NFCSS, are available for these calculations.

In Section 8, benchmarking exercises based on comparative studies with independent solutions are described.

In Section 9, case studies to demonstrate the application of the NFCSS for advanced fuel cycle initiatives (e.g. INPRO and FRs) are described. A special approach is adopted to FRs, simplifying the complex configuration of the reactor core due to presence of blankets in FRs.

Annex I describes recent modifications of the NFCSS, Annex II describes NFCSS User's Manual. Annex III describes a summary of UO_2 and MOX fuel depletion model. Annex IV contains corrections of errors found in the previous publication (IAEA-TECDOC-1535 [1]).

2. OVERALL FEATURES OF NFCSS

2.1. GENERAL

The NFCSS calculates annual fuel cycle requirements for varying time periods (up to a maximum of 200 years) for various types of commercial power reactors. Calculations can be done for a single reactor or a reactor park or total nuclear fleet of a country or the entire world. Besides calculating requirements of required resources at each stage of the nuclear fuel cycle under various scenarios, volumes and isotopic composition of discharged and/or stored fuels can be estimated according to any recycling strategy specified by the user.

The NFCSS is optimized for accuracy, simplicity and speed, and requires only a few input data and parameters for execution. This convenience allows even non-specialists to develop and model future nuclear energy scenarios. An example of input data can be a future projection of nuclear capacity using historical operational data of NPPs and policy plans made by countries. Data on the historical reactor operations can be obtained from the IAEA database of the Power Reactor Information System (PRIS) [2] and other authoritative publications (e.g. IAEA reference data [3]).

The NFCSS also contains a simplified global reactor database with technical specifications such as reactor physics parameters, neutron flux and cross sections. These are available to the NFCSS users during calculations. Simulations by the NFCSS can also be country specific if relevant data on historical operation and future projections are provided as inputs. Fresh fuel requirements and isotopic compositions in used fuel are then calculated from a set of internal parameters selected by the user. This enables the user to develop an appropriate recycling strategy using stockpiles and profile of spent fuel. Estimation of actinides accumulation, which is critical for assessing future fuel cycle strategies involving the transmutation of minor actinides, is a key feature of the NFCSS simulation.

2.2. INFORMATION FLOW IN NFCSS

The NFCSS is a simulation tool which reads an input deck (a set of input parameters), then calculates and generates a set of output parameters (Fig.1). The input deck includes three groups:

- Strategy parameters: Nuclear capacity variants and reprocessing-recycling strategies, reactor-type mixture and load factors, all on an annual basis;
- Fuel parameters: Fuel discharge burnup, fuel initial enrichment and tails assay - average on annual basis;
- Control parameters: Share of MOX fuel or ThO_2 in the reactor core, lead time and lag time for different processes, loss coefficients, use of depleted or enriched uranium, and the number of reprocessing cycles.

The results are divided into the following two groups:

- Front End: Natural uranium requirements, conversion requirements, enrichment service requirements and fuel fabrication requirements;
- Back End: Spent fuel arisings, total individual nuclides arising including uranium, plutonium and minor actinides, reprocessing requirements.

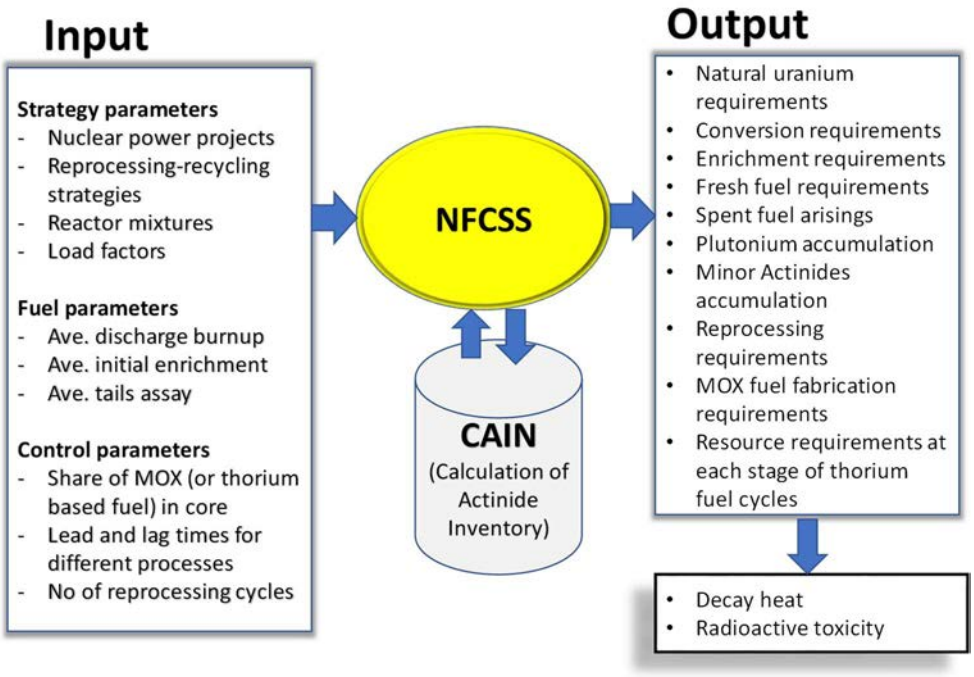


FIG.1. NFCSS information flow.

2.3. NUCLEAR FUEL CYCLE STAGES CONSIDERED IN NFCSS

Nuclear fuel cycle collectively denotes various 'cradle-to-grave' processes involved in making nuclear fuel from raw mineral resources through the final management of discharged fuel from reactors. This starts with the mining of raw mineral resources (i.e. uranium and thorium) and ends with the safe disposal of spent fuel. The elements of commercial fuel cycles are described in the subsequent sections. Figure 2 presents a simplified closed nuclear fuel cycle approach. Basic information on each step can be found from [4].

2.3.1. Mining and milling

Uranium is the most important element for the nuclear industry. Although it is widely distributed in the world, its commercial mining is confined to concentrated ores. Uranium is the only naturally occurring element which can be used to fabricate reactor fuel. The uranium ore is mined and then processed (milled) before it is used. Uranium ore is mined by open pit or underground mining methods. Uranium is extracted from the crushed ore in processing plants or mills using chemical processes. It is also possible to inject chemical solutions to ore beds and dissolve and extract uranium from the ore directly, which is in situ leaching method. This is the first step in the nuclear fuel cycle. The feed for mining and milling process is uranium ore and the product is U_3O_8 concentrate, which is colloquially referred as 'yellowcake' due to its colour and shape.

2.3.2. Conversion

Conversion is the process of purifying uranium concentrate and converting it to the chemical form required for the next stage of the fuel cycle. There are three such forms in common usage: metal, oxide (UO_2 or UO_3) and uranium hexafluoride (UF_6). Each of these is suited for making fuel for a specific reactor type.

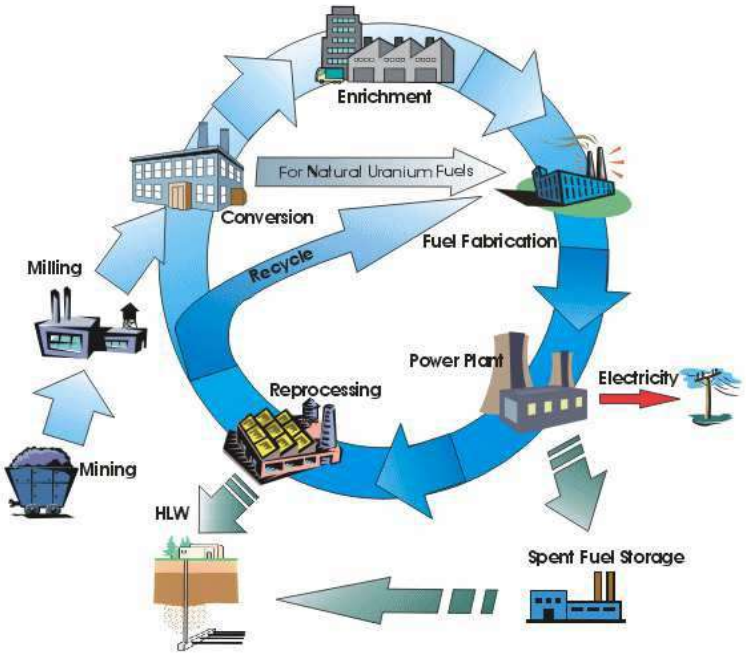


FIG.2. Simplified diagram of a closed nuclear fuel cycle (reproduced from [1]).

Light water reactors (LWRs), the most common reactor type, are fuelled by enriched uranium. Uranium hexafluoride (UF_6) is required for the LWR fuel cycle because it is used as a gas for the enrichment process. For the PHWR fuel cycle, which generally uses natural uranium oxide as the fuel, conversion to UF_6 is not necessary. Uranium is purified and converted to UO_2 or UO_3 in this case. The Magnox fuel cycle uses natural uranium in metallic form.

2.3.3. Enrichment

Natural uranium contains about 0.7% of U-235 and 99.3% of U-238 isotopes. The less abundant isotope (U-235) is the main source of fission energy in all thermal reactors. Although some types of reactors (PHWRs and Magnox) can be directly fuelled with natural uranium, it is impossible to fuel LWRs without enrichment. The special process to enhance the isotopic composition of U-235 from 0.7% to higher enrichment (but below the 5% limit for water cooled power reactor fuels) is called enrichment. There are two commercially available enrichment technologies: gaseous diffusion and centrifuge plants. Both techniques exploit the slight mass difference between U-235 and U-238. The feed for this stage is natural UF_6 and the product is enriched UF_6. The other output of the process is uranium with significantly lower U-235 content (known as enrichment tails or depleted uranium) than natural uranium.

2.3.4. Fuel fabrication

Enriched uranium in UF_6 form is then reconverted to UO_2 powder to make fuel for use in LWRs. This powder is made into pellets, sintered to achieve the desired density and ground to the required dimensions. Fuel pellets are loaded into tubes of Zircaloy or stainless steel and sealed at both ends. These fuel rods are spaced in fixed parallel arrays to form the reactor fuel assemblies. The whole process is referred as fuel fabrication. A similar procedure is adopted for natural uranium oxide fuel PHWRs.

2.3.5. Reactor

The reactor is essentially an irradiator for nuclear fuel. It burns the fuel and produces energy from nuclear fission. A discharged nuclear fuel assembly mostly retains its structural integrity and will be indistinguishable from a fresh fuel assembly—it is their isotopic compositions that will differentiate them. The NFCSS currently focusses on 7 commercial reactor types: PWR, BWR, PHWR, RBMK, GCR, AGR and WWER. As described in Section 9, FR can also be modelled in the NFCSS in a limited way. Since thorium fuel cycles can be modelled (as described in Sections 3 and 5), in principle, the applicability of the NFCSS can be extended to thorium reactors once input parameters are provided as appropriate. The feed for reactor is fresh fuel containing uranium or uranium-plutonium mixed oxide fuel for existing fuel cycle options. The product is used fuel that contains newly generated nuclides such as fission products (Cs, I, etc.), minor actinides (Np, Am, Cm) and plutonium isotopes in addition to the uranium. The biggest part of used fuel is still uranium (accounting for more than 95% by weight for most reactor types).

2.3.6. Reprocessing

A significant amount of fissile material exists in used fuel, which can be reused for nuclear energy production. The discharged fuel assemblies contain a considerable amount of unused U-235 and new fissile nuclides produced during irradiation in the nuclear reactor such as Pu-239. Some fuel cycle options consider extracting the fissile material from used fuel and refabricating it as new fuel assemblies. Uranium-plutonium mixed oxide fuel is the most common fuel that uses reprocessed material. Reprocessing is the process to separate reusable fissile material from the used fuel by means of chemical and physical processes. The feed of reprocessing is used fuel and the products of reprocessing are reusable fissile material and high level waste (HLW).

2.3.7. Used fuel storage

Used fuel which is not reprocessed can be stored temporarily[3] for future use or permanent disposal. Used fuel could be temporarily stored in pools (wet type storage) or in silos (dry type storage).

2.3.8. High level waste storage

The waste from fuel fabrication and reprocessing facilities are classified as HLW and requires careful treating. High level waste is stored in special storage facilities after proper treatment and eventually disposed of.

[3] The duration may range from several years to several decades.

3. NUCLEAR MATERIAL FLOW MODEL

3.1. UO_2 AND MOX FUEL CYCLES

3.1.1. General

The NFCSS is a two-layer computer model to assess the flow of nuclear materials throughout each stage of a nuclear fuel cycle considered, and the quantity and isotopic composition of spent fuel.

As shown in Fig.1, overall nuclear material flow is calculated by the NFCSS main module. Individual nuclide contents are calculated by the CAIN module, which is a simplified fuel depletion code.

The flow of nuclear materials involved in a nuclear fuel cycle can be sketched by tracking the nuclear materials at each step of the nuclear fuel cycle. The NFCSS is capable of simulating multiple fuel cycles with different reactor types. (Figure 3 illustrates the case of once-through UO_2 fuel cycle together with U and Pu recycling in some reactor types.)

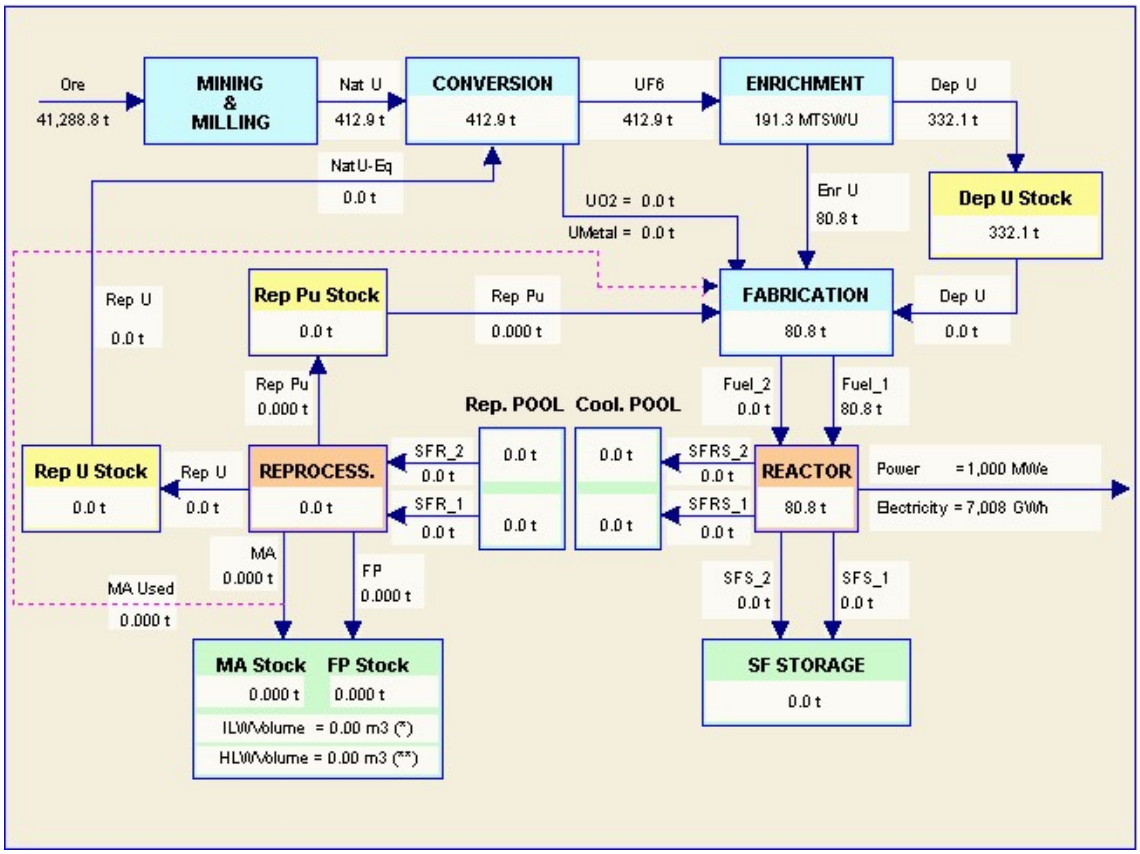


FIG.3. Illustration of material flow simulated by the NFCSS (UOX+MOX fuel case).

Final disposal of spent fuel is not taken into account in the NFCSS.

3.1.1.1. Waiting times and process times

Table 1 represents typical waiting times (lead and lag times) and process times required for each step of a typical thermal reactor fuel cycle. Although there is always waiting or process

times in each step, the NFCSS assumes zero waiting and process times for conversion, enrichment, fuel fabrication and reprocessing in calculating nuclear material flow. Only cooling times in pools are considered in material flow calculations. Cooling time before reprocessing and process time during reprocessing are taken into account for isotopic composition calculation of reprocessed spent fuel.

3.1.1.2. Process losses

Nuclear materials are processed chemically or physically at each stage of the nuclear fuel cycle. Each stage has some losses in processed material. This is accounted for in simulating the actual situation. The NFCSS requires specifying a material loss at each stage as fractional coefficients of the amount of processed material at the stage. If actual data are not known, process loss coefficients are assumed to be zero.

TABLE 1. TYPICAL WAITING AND PROCESS TIME FOR A THERMAL REACTOR CYCLE

Products or services	*Waiting/process time*
Natural uranium procurement	2 years before loading
Conversion to UF_6	1.5 years before loading
Enrichment	1 year before loading
UO_2 fuel fabrication	0.5 year before loading
Spent fuel storage in the reactor pool before transport	2 years after unloading
Spent UO_2 or URE† storage before reprocessing	5 years after unloading
Spent MOX storage before reprocessing	5 years after unloading
Reprocessing (Pu and reprocessed U availability)	1 year
MOX fuel fabrication	1 year
URE† fuel fabrication	0.5 year

† URE: UO_2 fuel using reprocessed uranium.

3.1.2. Input parameters

3.1.2.1. Reactor type

The input parameter ‘reactor type’ provides information on the type of the reactor that is considered in the scenario. A specific number is given to a specific reactor type in a scenario. It is possible to use reactor types which are included in the NFCSS library or to define new reactor types by fuel type and fuel parameters for the reactor.

3.1.2.2. Fuel type

The input parameter ‘fuel type’ provides information on the type of fuel. Three types are considered:

- Uranium (U) fuel;
- Uranium-plutonium (U-Pu) fuel;
- Free content fuel.

3.1.2.3. Nuclear power

The input parameter ‘nuclear power’ provides information on net electric power capacity in MW(e). That is,

[Nuclear power] = [Gross generation of electricity]
– [Usage within the plant such as pump motors]

3.1.2.4. Load factor

The input parameter ‘load factor’ provides information on the ratio of the net electricity produced in the plant to the maximum producible electricity in the plant for the whole year.

3.1.2.5. Thermal efficiency

The input parameter ‘thermal efficiency’ provides information on the ratio of net electric capacity to the total thermal power capacity of the reactor.

3.1.2.6. Discharge burnup

The input parameter ‘discharge burnup’ provides information on the average burnup of the spent fuel at the discharge point.

3.1.2.7. Enrichment

The input parameter ‘enrichment’ provides information on an initial U-235 enrichment in uranium fuel, or an initial total Pu content in MOX fuel[4].

3.1.2.8. Tails assay

The input parameter ‘tails assay’ provides information on the amount of U-235 in depleted uranium from the enrichment process.

3.1.2.9. Fuel residence time

The input parameter ‘fuel residence time’ provides information on the time duration that each of the equilibrium loading fuels must stay in the reactor.

3.1.2.10. Fuel type 2 share

The input parameter ‘fuel type 2 share’ provides information on the average ratio of the amount of second fuel type to the total fuel in the reactor. Fuel type 2 includes MOX fuel and thorium fuels.

[4] The MOX fuel consists of plutonium blended with natural uranium, reprocessed uranium or depleted uranium with a small amount of U-235. Such a small amount of U-235 can be considered for additional fuel content, but it is not counted in for U-235 enrichment.

3.1.2.11. Reprocessing ratio

The input parameter ‘reprocessing ratio’ provides information on the ratio of amount of spent fuel to be reprocessed to the amount of total discharged spent fuel.

3.1.2.12. Uranium source for MOX fuel

The input parameter ‘uranium source’ for MOX fuel provides information on the source of uranium in MOX fuel (depleted uranium or reprocessed uranium).

3.1.2.13. Reprocessed uranium use

When user wants to use reprocessed uranium (fuel type 1), the parameter of reprocessed uranium use should be entered to be yes. If it is selected, the ratio to convert reprocessed uranium to natural uranium is needed. For simplicity, it can be 1.0.

3.1.3. Output parameters

3.1.3.1. Natural uranium requirement

The output parameter ‘natural uranium requirement’ provides information on the amount of natural uranium required to manufacture necessary fresh fuel.

3.1.3.2. Conversion requirement

The output parameter ‘conversion requirement’ provides information on the amount of conversion service requirement.

3.1.3.3. Enrichment service requirement

The output parameter ‘enrichment service requirement’ provides information on the amount of enrichment service requirements (in SWU).

3.1.3.4. Depleted uranium arising

The output parameter ‘deplete uranium arising’ provides information on the amount of depleted uranium arising from enrichment process.

3.1.3.5. Depleted uranium use for MOX fuel

The output parameter ‘depleted uranium use for MOX fuel’ provides information on the amount of depleted uranium used in MOX fuel.

3.1.3.6. Fuel fabrication requirements

The output parameter ‘fuel fabrication requirements’ provides information on the amount of fresh fuel requirement for each fuel type.

3.1.3.7. Electricity production

The output parameter ‘electricity production’ provides information on the amount of net electricity produced in the power plant.

3.1.3.8. Spent fuel discharge

The output parameter ‘spent fuel discharge’ provides information on the amount of each fuel type spent fuel.

3.1.3.9. Spent fuel storage

The output parameter ‘spent fuel storage’ provides information on the amount of spent fuel stored in interim storage facilities for each fuel type.

3.1.3.10. Spent fuel reprocessing

The output parameter ‘spent fuel reprocessing’ provides information on the amount of used fuel reprocessed for each fuel type.

3.1.3.11. Separated Pu amount

The output parameter ‘separated Pu amount’ provides information on the amount of separated Plutonium from reprocessed spent fuel.

3.1.3.12. Amount of used Pu in MOX fuel

The output parameter ‘amount of used Pu in MOX fuel’ provides information on the amount of Plutonium used in MOX fuel.

3.1.3.13. Reprocessed U amount

The output parameter ‘reprocess U amount’ provides information on the amount of separated Uranium from reprocessed spent fuel.

3.1.3.14. MA amount in reprocessing waste

The output parameter ‘MA amount in reprocessing waste’ provides information on the amount of minor actinides (Np, Am, Cm) in HLW from reprocessing process.

3.1.3.15. FP amount in reprocessing waste

The output parameter ‘FP amount in reprocessing waste’ provides information on the amount of fission products (FPs) in HLW from reprocessing process.

3.1.4. Main assumptions

Several assumptions were made for use in simulating the flow of nuclear materials in nuclear fuel cycles. These include:

- All calculations are on an annual base. All reactors are loaded and unloaded, respectively, at the beginning and end of the year. All inputs and results are given and calculated on yearly basis;
- All mass reduction in heavy metals (U, Pu, MA, etc.) is considered as fission product accumulation, regardless there is a small loss of the mass during the operation of the reactor;
- Although every single reactor can be separately accounted for in a scenario, it is convenient to group these reactors based on their neutronic characteristics. In which

case, all inputs should be given yearly so the results of calculation can be obtained as annual averages;

- In addition to NFCSS' built-in module to calculate isotopic composition of spent fuel after discharge, the NFCSS also allows users to provide their own isotopic composition tables. This flexibility allows use of more sophisticated computer codes to calculate the isotopic composition and obtain more precise results. For most users, the inbuilt module fuel depletion code and isotopic composition of used fuel is sufficient to obtain reasonably accurate results;
- There are two modes of operation in the NFCSS. The first mode is called requirement driven mode, in which all fuel cycle facilities work on requirement basis. For example, conversion requirement is determined to deal with fresh fuel requirement without capacity limitation. This means that any amount of material coming into the fuel cycle facility is converted into products immediately. The second mode is capacity driven mode, in which output of each facility is driven by the capacity of the facility and whatever produced in excess of requirement is stockpiled. This mode of operation is currently not available in the web version of the NFCSS;
- Multiple recycling can be simulated putting the fuel composition of spent fuel obtained from the previous recycling step in fuel type 2;
- Material flow is calculated for heavy metals. The unit is tonnes of Heavy Metal expressed as tHM or t-HM unless otherwise noted;
- As regards energy generation by fission, a constant value of 0.97 (MW·d/g-fission) is applied for all fissile nuclides. This value comprises the kinetic energy of FPs and neutrons, decay heat of fission products, etc. (Note that decay heat after shutdown is assessed using NFCSS output, according to the method described in Section 6 of this report.)

3.1.5. NFCSS calculation process

The NFCSS is assumed to be in 'requirement driven mode' of operation and all calculations start from the reactor. First, fresh fuel requirement is calculated for given reactor capacity and other parameters. Then two parallel calculations are performed, one for the front end the other for the back end of the fuel cycle. These calculation processes are shown in Fig.4.

In the front end of the cycle, fresh fuel requirements, enrichment service requirements, depleted uranium amount, conversion requirements and natural uranium requirements are all calculated annually. The only interface between these two calculations is that reprocessed material is introduced from the back end to the front end of the nuclear fuel cycle.

In the back end of the cycle, the amounts of discharged spent fuel, spent fuel reprocessing, spent fuel storage, reprocessed material (U or Pu) and other material arisings such as minor actinides, fission products arisings and HLW arisings are all calculated on annual base.

Material flow calculation algorithm is described below (calculation is performed for each reactor type and each year separately):

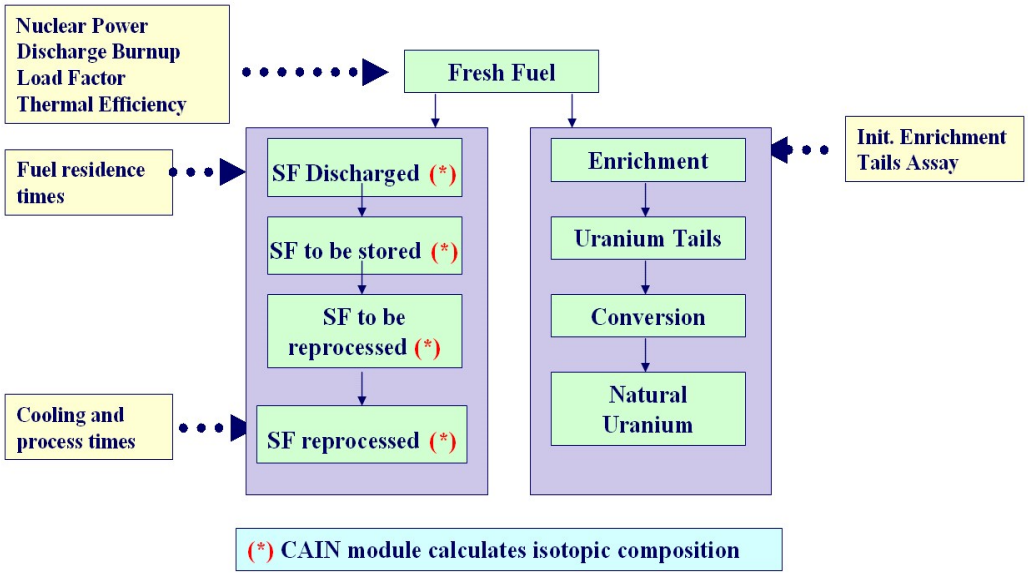
- Fresh fuel requirement is calculated for each fuel type based on the given reactor capacity and other parameters. In the NFCSS, the total reactor capacity for any given year is calculated by:

$$\text{Total Power} = \text{Added Capacity} + \text{Continuous Capacity} - \text{Removed Capacity} + \text{Initial Capacity}. \quad (1)$$

where,

The term ‘Added Capacity’ is the capacity added to the system in given year,
The term ‘Continuous Capacity’ is the capacity coming from previous year,
The term ‘Removed Capacity’ is the capacity removed from the system,
The term ‘Initial Capacity’ is the capacity already existing in the system at the beginning of the scenario period;

- Based on the removed capacity and the fuel residence time in core, discharged spent fuel amount is calculated;
- Using fresh fuel loading and spent fuel discharge, total fuel in core is calculated;
- Amount of spent fuel that will be reprocessed is calculated. This fuel to be reprocessed is routed to spent fuel cooling pool;
- Amount of spent fuel that will be stored in interim storage facility is calculated;
- Spent fuel amount in reprocessing pool is calculated;
- Fuel fabrication requirement is calculated based on the fresh fuel requirement;
- Enrichment requirement is calculated based on fuel fabrication;
- Conversion requirement is calculated based on enrichment and fuel fabrication;
- Natural uranium requirement is calculated based on conversion;
- Individual nuclides are calculated based on overall material flow and the isotopic composition in each step;
- Cumulative stock values are calculated based on the annual accumulation.



Note: SF stands for spent fuel.

FIG.4. NFCSS calculation process.

Mathematical models for calculating the amount of materials required at each stage of nuclear fuel cycle are described in Appendix II of [1].

3.2. THORIUM FUEL CYCLES

3.2.1. General

Section 3.1 describes general information, input parameters, output parameters, main assumptions and calculation process of the NFCSS for application to UO_2 and MOX fuel cycles. Most of these are generic and thus are applicable to thorium fuel cycles. In this Section, the unique features of thorium fuel cycles, which are different from UO_2 and MOX fuel cycles in Section 3.1, are described.

Use of ThO_2 has been of interest to many countries, and a number of publications on thorium utilization have been made by IAEA and OECD/NEA since 2000 [5]–[10]. These reports and others suggest that ThO_2 would be used in various types of reactor such as PWRs, BWRs, PHWRs, high temperature gas reactors (HTGRs), FRs, molten salt reactors (MSRs) [11], accelerator driven system (ADS) [12]. Therefore, it is necessary to include thorium fuel cycle in the NFCSS.

Although thorium is of low order of priority to the nuclear industry currently, some countries have major plans for thorium utilization in future. The biennial publication of IAEA and OECD-NEA on uranium resources (colloquially known as 'Redbook') has estimated the global thorium resources to be around about 6 million tons [13]. This appears to be a significant underestimate because of the lack of industrial demand for thorium and due to the fact that ThO_2 is about four times more abundant than UO_2 in the Earth's crust.

There are several basic features of thorium fuel cycle, such as consideration of different initial fissile materials, selection of fuel cycle options (open vs. closed), and other considerations listed below.

3.2.1.1. Initial fissile materials for thorium cycle

Thorium exists in nature in the form of a single isotope Th-232 and can form the basis of a valuable ^{233}U-$^{232}ThO_2$ fuel cycle. Since natural thorium does not contain fissile materials such as U-235, some fissile material (U-233, U-235, Pu-239) must be added to initiate a thorium fuel cycle. Once the thorium reactor is started, Th-232 absorbs a neutron and generates Pa-233 (which has a half-life of 27 days) and becomes U-233 after another beta decay. Since Th-232 has a larger neutron absorption cross section than U-238 and reproduction factor (η: defined as a number of neutrons produced per neutron absorbed in the fissile nuclide) of U-233 is high, conversion from fertile material (Th-232) to fissile material (U-233) is higher than that in U-238 fuel in thermal reactors.

Table 2 shows a possible matrix of fuel components and reactor types. As explained, materials such as U-233, U-235, low enriched uranium (LEU) and Pu-239 are considered as initial fissile materials. In Table 2, [$^{235}U+ThO_2$] fuel (i.e. 100% enriched U-235 with ThO_2) is not available for commercial LWRs; however, it is listed only for theoretical application of the NFCSS.

In Table 2, only PWR and BWR are shown. The NFCSS may be applicable to other reactors such as PHWR, HTGR, FR and MSR if relevant cross sections of fuel materials for those reactors are provided.

TABLE 2. POSSIBLE FUEL COMPONENTS AND REACTOR TYPES FOR THORIUM FUELS

Fuel component	*PWR*	*BWR*
[^{233}U+ThO_2] fuel	Possible	Possible
([^{235}U+ThO_2] fuel)*	Possible	Possible
[LEU+ThO_2] fuel	Possible	Possible
[Pu+ThO_2] fuel	Possible	Possible

*: [^{235}U+ThO_2] fuel is listed only for theoretical usage of NFCSS.

There is no thorium library in ORIGEN2 for PHWR. The effect of larger neutron absorption cross section of Th-232 becomes larger than in LWR due to the use of natural uranium or slightly enriched fuel in PHWR. At this moment, data for PHWR are not provided.

For FR, thorium may be suitable in the blanket region to achieve higher conversion from Th-232 to U-233; however, data for thorium-fuelled FR are not provided at the moment.

For molten salt reactor (MSR), without considering online reprocessing, refuelling (loading and discharge of nuclear material) process is similar to LWR. The NFCSS can be applied to this MSR case if relevant cross sections are provided. If online reprocessing was assumed for MSR, the situation would be complicated and hence not discussed here.

Although the NFCSS can handle two fuel types (Type-1 and Type-2) in one reactor, Type-1 is designed for LEU fuel (^{235}U + ^{238}U fuel). Accordingly, it is recommended to use Type-2 for thorium fuels. If the reactor contains both LEU and thorium fuels, for example, LEU fuel should be inputted to Type 1 and thorium fuel to Type-2.

Thorium fuel should be declared with 'free content' option which can specify each concentration (weight %) of all actinides for thorium fuel. Table 3 shows a summary of fuels for UO_2 fuel cycle, MOX fuel cycle, and thorium fuel cycle.

TABLE 3. SPECIFICATION OF UO_2, MOX AND THORIUM FUEL CYCLES

Type	*U-cycle*	*MOX-cycle*	*Th-cycle*
Type-1	LEU fuel	(LEU fuel)	(LEU fuel)
Type-2	------	MOX fuel	Th-fuel

3.2.1.2. Open fuel cycle and closed fuel cycle

An open fuel cycle such as current UO_2 fuel cycle or a closed fuel cycle similar to MOX fuel cycle can be adopted for thorium fuel cycle.

Figure 5 shows a once-through fuel cycle for thorium fuel-fuelled thermal reactor (hereafter assuming LWR) without reprocessing. Since reprocessing is not considered for LWR in Fig.5 (upper row), available initial fissile material of thorium-fuelled LWR is limited to LEU (lower row). Instead of LWR in the lower row of Fig.5, PHWR, HTGR and MSR can also be considered for thorium fuel cycle.

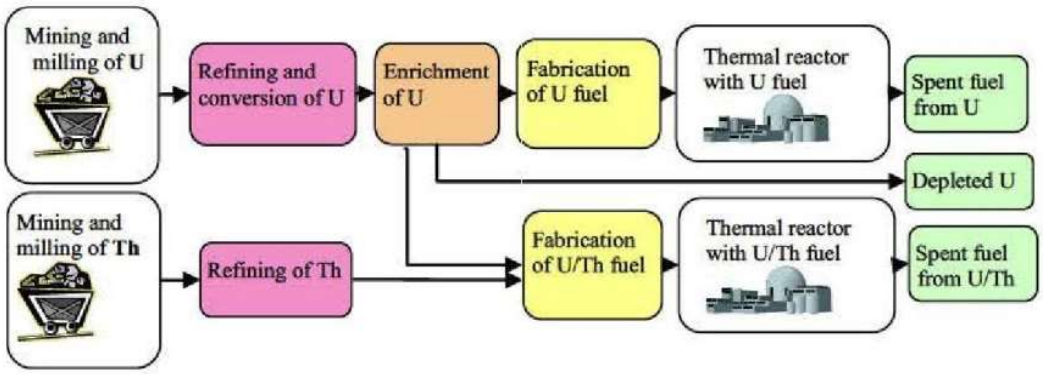


FIG.5. Once-through fuel cycle for Th-fuelled LWR without reprocessing (reproduced from [9]).

Figure 6 shows a closed fuel cycle which comprises LEU-fuelled LWR (top row), Th-fuelled LWR with LEU or U-233 (middle row), and Th-fuelled LWR with recycled Pu or U-233 (bottom row).

It should be noted that the NFCSS calculates data such as required fuel weight, required fuel fabrication weight, discharged fuel weight, and required reprocessing weight, based on the operational assumption of the reactors. That is, the above data may not be consistent with the reprocessed (recycled) amount of Pu or U-233. For example, users need to specify the reprocessing fraction (% of reprocessing fraction for the discharged fuel amount) and reprocessing factory capacity (say 1000 ton/year). If these values are small, then enough fissile (say Pu) is not supplied to the second or third line reactors. Therefore, users need to watch the above for consistency. If FR is included, Fig.6 becomes more complicated, and hence it is not shown here, but it is described in [9].

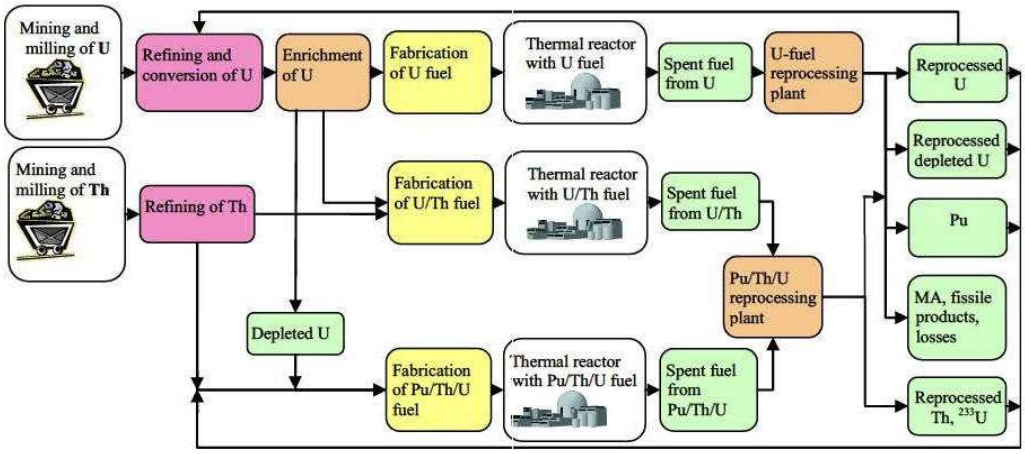


FIG.6. Closed fuel cycle based on LEU-fuelled LWR, Th-fuelled LWR with LEU or U-233, and Th-fuelled LWR with recycled Pu or U-233 (reproduced from [9]).

3.2.2. Input and output parameters

As explained in Table 3, thorium fuel is assigned as Type-2 by specifying each concentration (wt.%) of all actinides as Free Content option. Therefore, several outputs such as enrichment service requirement (in SWU), natural uranium requirement, conversion requirement, and others are not calculated in thorium fuel cycle.

3.2.2.1. Input parameters

Input parameters include: reactor type, fuel type, nuclear power, load factor, thermal efficiency, discharge burnup, fuel residence time, fuel type 2 share, reprocessing share, which are described in Section 3.1.2. Here, the input parameter of fuel type 2 share provides information on the average ratio of the amount of second fuel type to the total fuel in the reactor and implies a thorium fuel.

In addition, a parameter of thorium source for thorium fuel is given as input, which provides information on the source of thorium in thorium fuel (natural thorium or reprocessed thorium).

3.2.2.2. Output parameters

Output parameters include:

- Natural thorium requirement: Provides information on the amount of natural thorium required to fabricate the required fresh fuel assemblies;
- Separated U-233 amount: Provides information on the amount of separated U-233 from reprocessed spent fuel;
- Amount of used U-233 in MOX Fuel: Provides information on the amount of U-233 used in MOX fuel;
- Reprocessed Th amount: Provides information on the amount of separated thorium from reprocessed spent fuel;
- MA amount in reprocessing waste: Provides information on the amount of minor actinides (Np, Am, Cm) in HLW from reprocessing process;
- FP amount in reprocessing waste: Provides information on the amount of fission products in HLW from reprocessing process;
- Fuel fabrication requirement, Electricity production, Spent fuel discharge, Spent fuel storage, Spent fuel reprocessing: See Section 3.1.3.

4. BURNUP MODEL FOR UO_2 AND MOX FUEL CYCLES

4.1.GENERAL

This Section provides a summary of the CAIN module for UO_2 and MOX fuel cycles, incorporated in the NFCSS. The theoretical basis and associated radioactive decay chains of the CAIN module were originally documented in [1] along with the verification and validation results for UO_2 and MOX fuels. In this Section, some physical characteristics and engineering aspects that were not covered in [1] are described. These include: (1) relation between specific power and neutron flux, (2) effect of operation mode, (3) initial core loading and final core discharge, and (4) study of Am-241 cross section.

4.2. CAIN MODEL

The calculation method and associated key input parameters are described in the subsequent sections.

4.2.1. Bateman's equation and its solution

The CAIN module uses the analytical solution of Bateman's equation for a point reactor with one group neutron energy [14]. Its mathematical explanation and solution are described in Annex III of this publication.

4.2.2. Assumptions made in CAIN module for UO_2 and MOX fuel cycles

The CAIN module for UO_2 and MOX fuel cycles makes the following assumptions:

(a) Only U-235 and U-238 are initial nuclides in fresh UO_2 fuel, and the descending nuclides are analytically accounted for by the Bateman's equation. Even though users can provide inputs to other nuclides, e.g. U-236 for UO_2 fuel and Np-237, Am-241, Am-242m, Am-243, Cm-242 and Cm-244 for MOX fuel, these additional nuclide cases have not been verified;
(b) A total of 14 nuclides are accounted for UO_2 and MOX fuel cycles in the CAIN, which include U-235, U-236, U-238, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Np-237, Am-241, Am-242m, Am-243, Cm-242 and Cm-244;
(c) A constant neutron flux and constant cross section for each of nuclides are used throughout the whole burnup period in order to get analytical solutions of Bateman's equation;
(d) For the actinide transmutation chains the following holds:

- Short-lived nuclides (half-life < 8 days) are not taken into account. That is, U-237 (7 days), Np-238 (2 days), Pu-243 (5 hrs), Am-242 (16 hrs), Am-244 (10 hrs) and Am-246 (39 min) are considered to immediately decay to next daughter nuclides.
- Long-lived nuclides (having half-life > 400 year) are considered stable for the whole irradiation period. For example, Am-241 (432 yr) is treated as a stable nuclide, and further transmutation is not taken into account. Meanwhile, decreases of all 14 nuclides by their decay are calculated both in the burnup period and in the cooling period after discharge;

(e) Based on the two assumptions in (d), decays of Pu-238 (87.7 yr), Pu-241 (14.4 yr), Cm-242 (0.447 yr) and Cm-244 (18.1 yr) are accounted for during the period of burnup;
(f) Transmutation is not pursued any more for certain nuclides (shown as mark "x" in Fig.7).

The CAIN module for UO_2 and MOX fuel cycles is based on the above assumptions, and the transmutation chains are simplified as shown in Fig.7.

4.2.3. Inputs for actinides inventory calculations

CAIN requires various inputs to evaluate the actinides inventory in the discharged fuel. They are cross sections and reactor constants such as specific power or neutron flux for the 7 reactor types (PWR, BWR, PHWR, RBMK, AGR, GCR and WWER) handled by the NFCSS.

4.2.3.1. Cross sections for UO_2 fuel and MOX fuel

One group cross section data for the 14 nuclides considered in CAIN module were presented in [1]. Users of the NFCSS can also create their own libraries from other sources. Libraries of UO_2

fuel for the 7 reactor types and MOX fuel for PWR and BWR are incorporated in the NFCSS. With relevant external inputs, the NFCSS can also be applied to FRs.

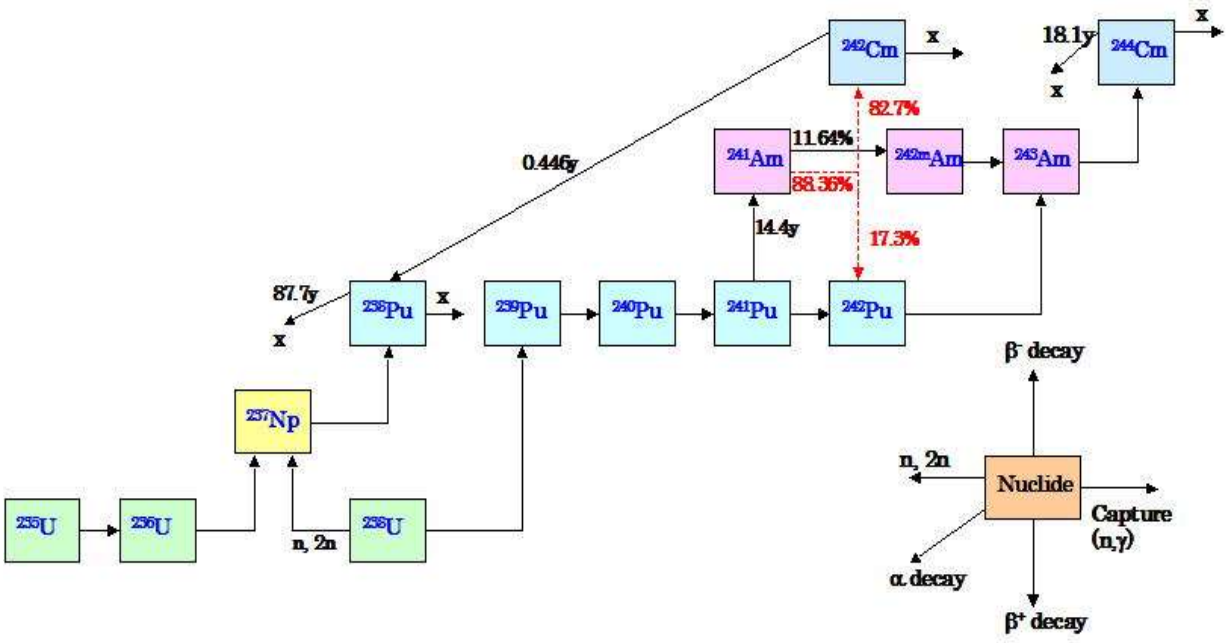


FIG.7. Simplified transmutation model in CAIN for *UO_2 and MOX fuel (reproduced from [1]).*

4.2.3.2. Other constants

Other constants used for actinides inventory calculations by the CAIN include specific power, neutron flux, and others. These are summarized in Annex III of this publication. The neutron flux input is mandatory for initial estimate. However, the final value of neutron flux corresponding to specific power is calculated by the iterative process in the CAIN module.

4.2.3.3. Initial enrichment and discharge burnup

Initial enrichment and discharge burnup are required as input data. Since these are output of reactor core design analysis, these data may not be easily available for NFCSS users. To facilitate providing these input values, relationships between initial enrichment and discharge burnup are provided for UO_2 fuel in 7 reactor types and MOX fuel in PWRs and BWRs (see Annex III, Section III-7). Also, each Pu nuclide fraction (Pu vector) is provided.

4.2.3.4. Relation between specific power and neutron flux

Both specific power (power density) and neutron flux are required as inputs. As described in Section 4.2.3.2, neutron flux can be calculated based on power density, using an iterative process (see Annex Section I-2.1).

4.2.3.5. Effect of operation mode

Load factor is an input for use in evaluating the actual fuel requirement corresponding to actual power generation (electricity and thermal output). The NFCSS assumes 100% full power operation for the CAIN burnup calculation without accounting for the effect of load factor. This assumption will affect the discharged amount of Pu-241 and Am-241 (Pu-241 decays to Am-

241 with half-life of 14.4 year). The impact of this assumption on actinides inventory calculation was investigated and found that after 1-2 decades the errors on Pu-241 and Am-241 are as small as 2-3%. Details are described in Annex Section III-9.

4.2.3.6. Initial core loading and final core discharge

It was not described earlier [1] how to simulate initial core loading and final core discharge. Since this publication, an improved method to resolve this issue has been incorporated in the NFCSS. Details are described in Annex Section III-10.

4.2.3.7. Study on Am-241 cross section

As shown in Fig.7, when Am-241 captures a neutron, there are two reactions which go to the ground-state Am-242 (0.8836) and the meta-stable Am-242m (0.1164). Although these fixed branch fractions are correct for thermal neutron reactors, the above branch fraction to the ground-state Am-242 decreases by 5-10% at fast neutron energy. Since these branch fractions are fixed in the program, there will be small effects for FR on the amount of actinides higher than Am-241. Details are described in Annex Section III-11.

5. BURNUP MODEL FOR THORIUM- FUEL CYCLES

5.1. GENERAL

The detailed burnup chain for thorium fuel cycles is shown in Fig.8. One of the basic assumptions in the CAIN module is to skip nuclides whose half-life is shorter than 8 days [1]. This assumption greatly simplifies the calculation. Therefore, Th-233 (22.3 min.), Pa-234 (1.17m/6.69 h), and U-237 (6.75 day) are skipped in CAIN. As a result, only 7 of the remaining nuclides such as Th-232, Pa-233, U-233, U-234, U-235, U-236 and Np-237 are considered in the CAIN module.

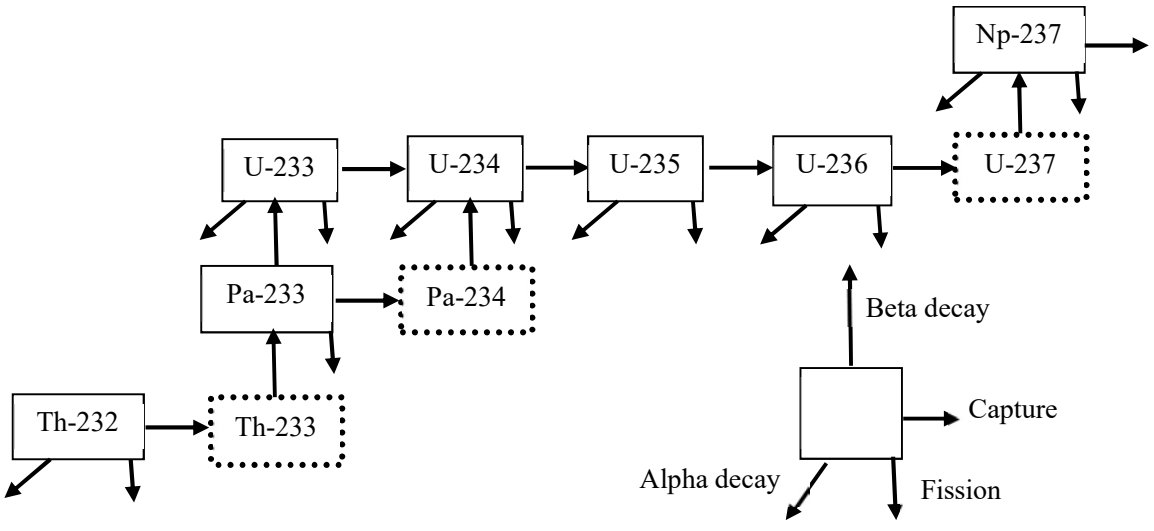


FIG.8. Thorium fuel cycle burnup chain.

Another assumption is to consider nuclides with half-life greater than 400 years as stable [1]. This assumption is introduced because the NFCSS is intended to calculate the actinides inventory for long time periods ranging from several decades to 200 years.

Current NFCSS can handle 7 reactor types namely, PWR, BWR, PHWR, RBMK, GCR, AGR and WWER. The NFCSS can also handle other reactors such as FR with appropriate input data such as cross sections.

Table 4 is the data required for a typical PWR burnup calculation. The third column is the assumption made in the CAIN. The fourth column represents the amount of total and individual nuclides in the annually discharged fuel at a burnup of 45 GW·d/t from a 1000 MW(e) PWR, which is obtained from ORIGEN2 code. The last column is the same data but from a typical MSR.

5.1.1. Study on Th-233 burnup chain

Theoretically, there is another path where Th-233 absorbs a neutron to become Th-234 and decays to Pa-234. This path is benign due to the fact that Th-233 decays very quickly to Pa-233 regardless a high thermal absorption cross section of Th-233 (1500 barns).

TABLE 4. NUCLIDE DATA FOR TYPICAL PWRs AND MSRs

Nuclide	*Half-life*	*Assumption in CAIN code*	*Annual discharge for 45GW·d/t of 1GW(e)-PWR*	*Typical weight in 150MW(e)-MSR-FUJI*
Th-232	1.40E10 year	Stable	25 ton	40 ton
Th-233	22.3 min.	Skipped to Pa-233 (Refer to Section 5.1.1)	----	----
Pa-233	27.0 days	Skipped to U-233 (Refer to Section 5.1.2)	36 kg	20 kg
Pa-234	1.17m/6.69h	Skipped to U-234 (Refer to Section 5.1.2)	----	----
U-232	70.0 year	Ignored (Refer to Section 5.1.3)	1.6 kg	Less than 1 kg
U-233	1.59E5 year	Stable	562 kg	900 kg
U-234	2.46E5 year	Stable	135 kg	70 kg
U-235	7.04E8 year	Stable	21 kg	7 kg
U-236	2.34E7 year	Stable	2.5 kg	0.3kg (Refer to Section 5.1.4)
U-237	6.75 day	Skipped to Np-237	----	----
Np-237	2.14E6 year	Stable	0.1kg (Refer to Section 5.1.4)	0.01kg (Refer to Section 5.1.4)
Pu-238 & other Pu isotopes	----	Ignored (Refer to Section 5.1.5)	0.03 kg	Less than 0.001 kg

5.1.2. Study on Pa-233 burnup chain

There are two paths for Pa-233 to U-234 as shown in Fig.7. Path-1 is beta decay path of Pa-233 to U-233 and neutron capture to U-234. Path-2 is neutron capture of Pa-233 to Pa-234 and beta decay to U-234. That is,

- Path-1: Pa-233(decay)→ U-233(capture) → U-234(capture);
- Path-2: Pa-233(capture)→U-234(capture).

These two paths are taken into account for thorium fuel cycles in the CAIN (refer to Fig.10). The inventory of Pa-233 is calculated with its decay to U-233.

5.1.3. Study on U-232 burnup chain

The nuclide U-232 is generated via several reactions starting from Th-232 as shown in Fig.9. The nuclide U-232 is an important nuclide in thorium fuel cycle from the standpoint of proliferation resistance, because its daughter is a strong gamma emitter. Considering that the weight of U-232 generated is small, U-232 is not accounted for in the CAIN. For future application, however, one prospect is described below.

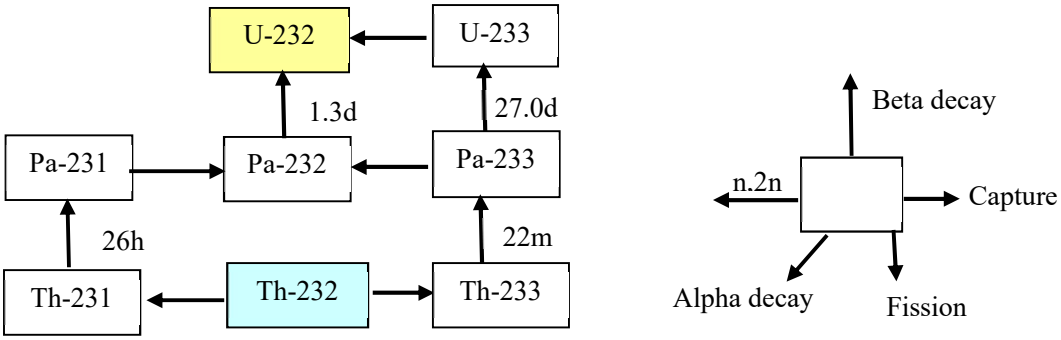


FIG.9. Generation of U-232 in thorium cycle.

There are several paths to reach U-232, but the following 3 paths are most dominant. Although other paths such as Pa-232 (capture) to Pa-233, and Th-230 (natural thorium contains 1 ppm of this isotope) to Th-231 exist, they are not considered as significant ones.

- Th-232 (capture) → Th-233 (beta decay, 22min) →Pa-233 (beta decay, 27days) → U-233 (n,2n) → U-232;
- Th-232 (capture) →Th-233 (beta decay, 22min) → Pa-233 (n,2n) → Pa-232 (beta decay, 1.3days) →U-232;
- Th-232 (n,2n) → Th-231 (beta decay, 26hr) → Pa-231 (capture) → Pa-232 (beta decay, 1.3days) → U-232.

As is explained above, U-232 generation is ignored as represented in Fig.10.

5.1.4. Study on U-236 and Np-237 burnup chains

Since the NFCSS calculates actinide weights in kg, any actinide having its weight less than 1 kg are not shown in the output table. U-236 and Np-237 may not appear in the NFCSS output table for some reactor designs (see Table 4). Nevertheless, U-236 and Np-237 are accounted for in the CAIN module.

Since the half-life of Np-237 is very long and its neutron capture cross section is not large, subsequent chains of Np-237 decay and its neutron capture are not taken into account in the burnup model.

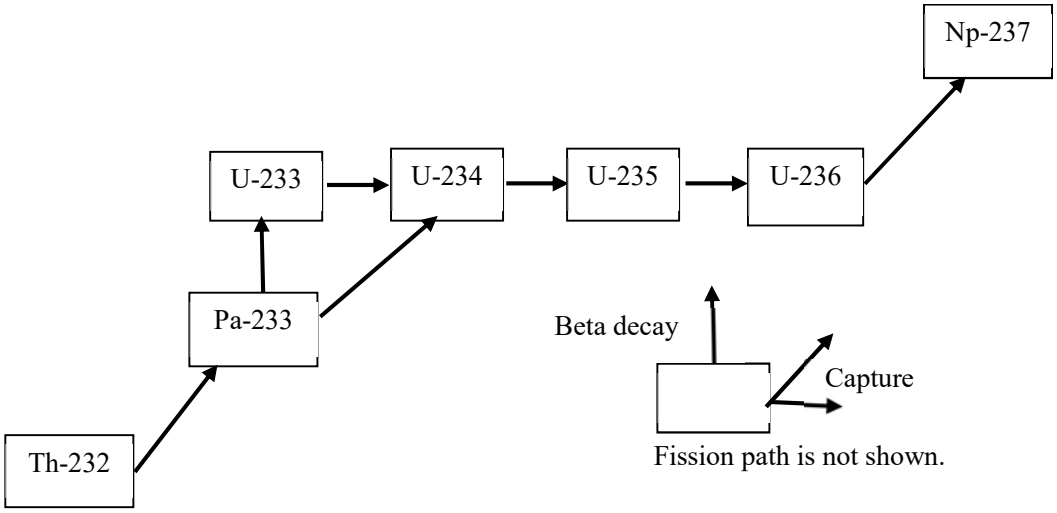


FIG.10. Thorium cycle transmutation model in the NFCSS CAIN module.

5.1.5. Study on Pu-238 burnup chain

Since Pu-238 and other sequential Pu isotopes are transmuted mainly from Np-237, their weights are less than 0.1 kg. Therefore, all Pu generations are ignored in the CAIN module for thorium cycle.

5.1.6. CAIN modules for thorium chains

Based on descriptions in Section 5.1.1 through Section 5.1.5, thorium cycle transmutation chain in the CAIN module can be simplified as shown Fig.10. As stated earlier, further transmutation from Np-237 is not considered in the calculations.

The generic solution for Bateman's equation [14] is given below, if all nuclides are assumed to be stable and hence there are no decay terms in the burnup period.

$$N_n = C_1 \exp(-\sigma_{t1}\,\phi\, t) + C_2 \exp(-\sigma_{t2}\phi\, t) \cdots + C_n \exp(-\sigma_{tn}\phi\, t) \quad (2)$$

where,

$C_1 = N_1^0 \cdot [\sigma_{c1}\sigma_{c2} \cdots \sigma_{cn-1}] / [(\sigma_{t2}-\sigma_{t1}) \cdot (\sigma_{t3}-\sigma_{t1}) \cdots (\sigma_{tn}-\sigma_{t1})]$,
$C_2 = N_1^0 \cdot [\sigma_{c1}\sigma_{c2} \cdots \sigma_{cn-1}] / [(\sigma_{t1}-\sigma_{t2}) \cdot (\sigma_{t3}-\sigma_{t2}) \cdots (\sigma_{tn}-\sigma_{t2})]$,
……
$C_n = N_1^0 \cdot [\sigma_{c1}\sigma_{c2} \cdots \sigma_{cn-1}] / [(\sigma_{t1}-\sigma_{tn}) \cdot (\sigma_{t3}-\sigma_{tn}) \cdots (\sigma_{tn-1}-\sigma_{tn})]$,
σ_{cn} : capture cross section of nuclide n, 10^{-24} cm^2 (=1 barn),
σ_{tn} : total (capture + fission + n2n) cross section of nuclide-n, 10^{-24} cm^2 (=1 barn).

Although further transmutation chains of these 7 nuclides shown Fig.10 are not considered in the CAIN burnup model, decreases of all 18 nuclides by their decay are calculated both in the burnup period and in the cooling period after discharge. Since half-lives of these nuclides are long enough except for Pa-233, this effect would not appear in the actinide inventory.

Figure 10 shows the simplified thorium fuel cycle transmutation model in the CAIN. As described in Section 5.1.2, two burnup chains are proposed for thorium cycle as follows. All nuclides below also decrease by fission reactions too.

- Th-232(capture) → Pa-233(decay) → U-233(capture) → U-234(capture) → U-235(capture) →U-236(capture) →Np-237;
- Th-232(capture) → Pa-233(capture) → U-234(capture) → U-235(capture) → U-236(capture) → Np-237.

5.1.7. Summary of assumptions made in CAIN for thorium fuel cycle

The following assumptions are used in the CAIN for thorium fuel cycle assessments. Refer to Section 5.1.1 through Section 5.1.6 for detailed background and justifications.

(a) Typically, U-233 and Th-232 are considered as the initial nuclides for thorium cycle, and the descending nuclides are analytically calculated using Bateman's equation. But, it is possible to include Pa-233 and/or U-234 as the initial nuclides;
(b) Short lived nuclides (with half-life < 8 days) are skipped. That is, Th-233 (22.3 min.), Pa-234 (1.17m/6.69h), and U-237 (6.75 day) are assumed to decay and go to next nuclide instantly;
(c) The following 7 nuclides are associated with thorium fuel chains: Th-232, Pa-233, U-233, U-234, U-235, U-236 and Np-237. Therefore, the following burnup chains are applied

  - Th-232 (capture)→Pa-233 (decay) →U-233 (capture) → U-234 (capture) → U-235 (capture) →U-236 (capture) → Np-237
  - Th-232 (capture)→Pa-233(capture)→U-234 (capture)→U-235 (capture) → U-236 (capture) → Np-237;

(d) Based on the above assumptions, a total of 18 nuclides are considered in the CAIN model for UO_2, MOX and thorium fuel cycles: Th-232, Pa-233, U-233, U-234, U-235, U-236, U-238, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Np-237, Am-241, Am-242m, Am-243, Cm-242 and Cm-244;
(e) Both cross sections and neutron flux are assumed to be constant throughout the burnup period to simplify the computation;
(f) On the other hand, long lived nuclides (with half-life > 400 year) are assumed to be stable through the irradiation period. That is, 6 nuclides such as Th-232, U-233, U-234, U-235, U-236 and Np-237 are assumed to be stable and their decay chains will not be considered. Meanwhile, decreases of the above 18 nuclides by their decay are calculated both in the burnup period and in the cooling period after discharge from the reactor;
(g) Transmutation is terminated at Np-237 for thorium fuel cycles. This condition is imposed in order to stop the calculation of Bateman's equation at the desired accuracy level set by the CAIN module. This assumption is reasonable because the contribution of further transmutations is very small.

5.2. CROSS SECTION DATA FOR THORIUM FUEL CYCLES IN LWR

5.2.1. General approach

The ORIGEN2 cross section library is applied to the CAIN for thorium fuel cycle simulations. Several nuclear libraries for thorium fuel cycles are incorporated in the ORIGEN2 code [15], and thus an appropriate library needs to be selected based on good understanding of the fundamentals of thorium fuelled core.

Neutron spectrum for thorium fuelled core is represented in Fig.11 and Fig.12.

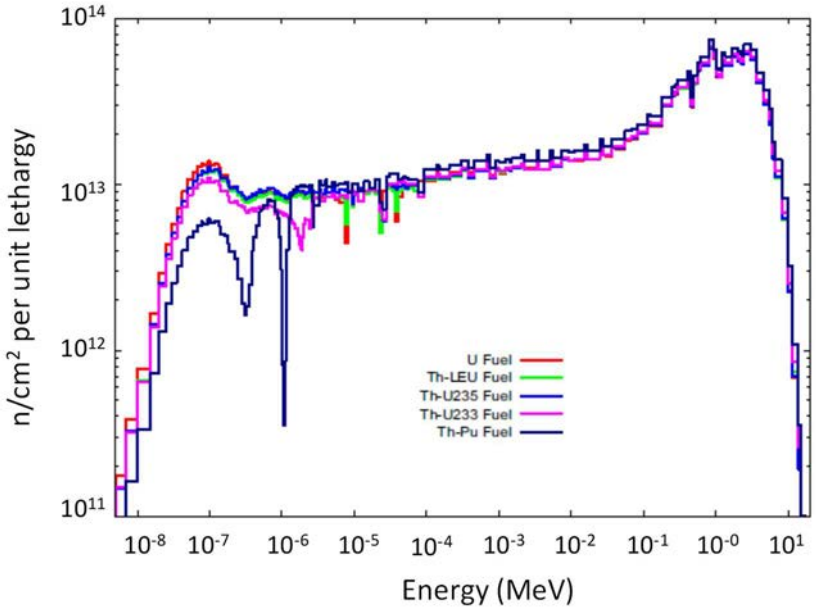


FIG.11. Neutron spectrum in PWR for UO_2, LEU-Th, ^{233}U-Th, ^{235}U-Th and Pu-Th (reproduced from [9]).

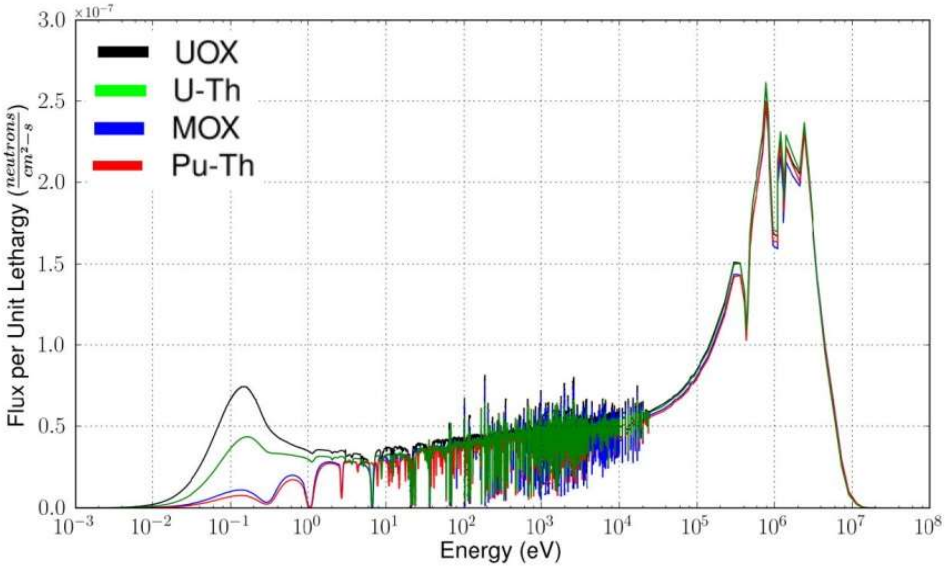


FIG.12. Neutron spectrum in PWR for UO_2, LEU-Th, MOX and Pu-Th at beginning of life (reproduced courtesy of US NRC [16])

The thorium core with U-233, U-235 or LEU is characterized with lower peak of thermal neutrons than the conventional LEU core because the thermal cross section of Th-232 is 3 times higher than that of U-238. Pu-Th core has the lowest peak of thermal neutrons among all of them because most Pu nuclides have larger thermal cross sections than U nuclides. From Fig.12, the neutron spectrum of the Pu-Th core is comparable to that of the MOX core.

Based on the above understanding, cross section for Th core is selected with the following two types. Verification for these selections is discussed in Sections 5.2.4 and 5.2.5.

- Thorium library (ORIGEN2, 214-library) for Th core with U-233, U-235 or LEU;
- MOX library (ORIGEN2, 211-library: PWR-PuPu library) for Th core with Pu.

5.2.2. ORIGEN2 PWR Th-library (214-library)

The Oak Ridge National Laboratory (ORNL) provided PWR thorium-library (214-library) with ORIGEN2 distribution; however, the cross section data of the ORIGEN2 library (214-library) were inconsistent with the ORNL report. As an alternative, the cross sections of 18 nuclides that are modelled in the CAIN and the cross sections of Pa-231, U-232, U-237, Np-238, Pu-236, Pu-243, Am-242 and Cm-243 (totally 26 nuclides) were taken from the original ORNL report (PTD3 case in Table B.1 of [17]). Cross sections of these 18 nuclides are provided in Table 5 for which information was taken from [18] (new214-library).

TABLE 5. ONE-GROUP CROSS SECTIONS FOR PWR/BWR WITH U-233/U-235/LEU-Th FUEL (barn) (reproduced courtesy of ORNL [18])

	$\sigma_c(+\sigma_{ex})$	σ_f	σ_{n2n}	$T_{1/2}(y)$
Th-232	1.1400	0.0250	0.005150	1.40E+10
Pa-233	22.4000	0.1510	0.006953	7.40E-02
U-233	6.3900	53.1000	0.001062	1.59E+05
U-234	14.3000	0.4800	0.002318	2.46E+05
U-235	10.1000	43.9000	0.004828	7.04E+08
U-236	8.0300	0.2070	0.002092	2.34E+07
U-238	**1.5400**	0.1020	0.004828	4.47E+09
Np-237	31.4000	0.5140	0.000485	2.14E+06
Pu-238	34.4000	2.3200	0.000837	8.77E+01
Pu-239	60.0000	106.0000	0.001609	2.41E+04
Pu-240	153.0000	0.5960	0.001127	6.56E+03
Pu-241	37.5000	113.0000	0.002543	1.44E+01
Pu-242	31.9000	0.4330	0.002382	3.75E+05
Am-241	109.6000	1.0900	0.000161	4.33E+02
Am-242m	86.5000	413.0000	0.005955	1.41E+02
Am-243	45.6900	0.4160	0.000000	7.37E+03
Cm-242	5.6000	0.5540	0.000000	4.46E-01
Cm-244	14.2000	0.9020	0.000000	1.81E+01

Cross section values from these two information sources turned out not to be much different except for U-238 capture cross section, where ORIGEN2 library provided 6.69 barns and ORNL report gives 1.54 barns. From the lower capture cross section value of ORNL report, it can be deduced that ORIGEN2 library (214-library) did not account for the self-shielding effect of U-238. ORNL accounted for this shelf shielding effect and published the correct value in their report later. This is the rationale for using the cross section values from the ORNL report in this publication. For most thorium fuel cases, there is no U-238; for LEU-Th fuel case, the self shielding effect exists and affects calculation. Detailed discussions of this effect are described in Section 5.2.4.3.

In summary, the following guidelines were applied during the preparation of cross section values given in Table 5 (also applied to Table 6):

(a) The following 4 nuclides, Th-232, Pa-233, U-233 and U-234 are added for thorium fuel cycles in addition to the 14 nuclides that are considered for UO_2 and MOX fuel in the NFCSS CAIN module. These 14 nuclides include: U-235, U-236, U-238, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Np-237, Am-241, Am-242m, Am-243, Cm-242 and Cm-244;
(b) Cross sections for these 18 nuclides are generated from ORIGEN2 PWR thorium fuel library (214-library for U-Th core, and 211-library for Pu-Th core) with a correction for U-238;
(c) These cross sections are confirmed by verification results from PWR and BWR;
(d) Capture cross sections of Pa-233, Am-241 and Am-243 include excited cross section;
(e) Cross section of [n2n] reaction is used only for U-238 in the CAIN;
(f) If the half-life of any nuclide is greater than 400 year, CAIN assumes them as stable. Although further transmutation chains of these nuclides are not considered in the CAIN burnup model, decreases of all 18 nuclides by their decay are calculated both in the burnup period and in the cooling period after discharge from reactor.

5.2.3. ORIGEN2 PWR Pu-Th library (211-library)

As explained in Section 5.2.1, PWR MOX library (ORIGEN2, 211-library) is applied to PWR Pu-Th fuel with some modification.

ORNL provided PWR MOX Library (211-library) with ORIGEN2 distribution. All cross sections were identical to those in the original ORNL report for MOX fuels (PWR-PuPu case in Table B.1 of [18]). Since Th-232 capture cross section value of 2.93 barns is close to the thermal cross section value, it was inferred that ORIGEN2 library did not account self-shielding effect of Th-232. To account for this self shielding effect, an appropriate small value (0.749 barns), which was found from another original ORNL report for thorium fuels (PTPU case in Table B.1 of [17]), is replaced for use in the CAIN. This modification is validated in Section 5.2.4.4.

Cross sections for all 18 nuclides used in the CAIN to model Pu-Th core in PWRs are presented in Table 6 for which information was taken from [18] except Th-232 (new211-library).

TABLE 6. ONE-GROUP CROSS SECTIONS FOR PWR/BWR WITH Pu-Th FUEL (barn) (reproduced courtesy of ORNL [18])

	$\sigma_e(+\sigma_{ex})$	σ_f	σ_{n2n}	$T_{1/2}(y)$
Th-232	**0.7490**	0.0251	0.005926	1.40E+10
Pa-233	22.6000	0.1647	0.001590	7.40E-02
U-233	5.0790	36.8300	0.003324	1.59E+05
U-234	17.1900	0.4911	0.000485	2.46E+05
U-235	6.3980	22.6900	0.003046	7.04E+08
U-236	8.4870	0.2166	0.003001	2.34E+07
U-238	0.8718	0.1105	0.006263	4.47E+09
Np-237	24.2300	0.5713	0.000529	2.14E+06
Pu-238	15.2600	2.0330	0.000190	8.77E+01
Pu-239	26.0400	46.4500	0.001267	2.41E+04
Pu-240	43.8800	0.6222	0.000509	6.56E+03
Pu-241	16.7200	54.5200	0.008475	1.44E+01
Pu-242	25.5600	0.5354	0.002395	3.75E+05
Am-241	64.3940	0.8959	0.000369	4.33E+02

	$\sigma_c(+\sigma_{ex})$	σ_f	σ_{n2n}	$T_{1/2}(y)$
Am-242m	45.8400	224.4000	0.006493	1.41E+02
Am-243	41.9900	0.4455	0.000233	7.37E+03
Cm-242	5.3410	0.4676	0.000060	4.46E-01
Cm-244	13.8400	0.9332	0.001179	1.81E+01

5.2.4. Verification of ORIGEN2 library for application to thorium fuels in PWR

5.2.4.1. ^{233}U-Th fuel

Nuclide concentrations calculated by ORIGEN2 using Th-library (new214-library) are compared with those by BNL's unit cell based design code for a PWR fuel of 4.3% ^{233}U-Th at a discharge burnup of 61 GW·d/t [19]. As shown in Table 7, ORIGEN2 calculations are reasonably consistent with calculations by the detailed design code for major nuclides.

TABLE 7. ACTINIDES WEIGHT FOR ^{233}U-Th PWR FUEL (grams per initial 1-ton HM) (reproduced courtesy of M. Todosow [19])

Nuclide	*BNL(g)*	*ORIGEN2(g)*	*Error (%)*
Th-232	9.099E+05	9.097E+05	0.0
Pa-231	7.540E+01	6.941E+01	-7.9
Pa-233	1.546E+03	1.422E+03	-8.0
U-232	8.411E+01	9.031E+01	7.4
U-233	1.692E+04	1.869E+04	10.4
U-234	5.599E+03	6.104E+03	9.0
U-235	1.234E+03	1.152E+03	-6.7
U-236	2.708E+02	2.050E+02	-24.3
U-237		5.741E-01	
U-238		2.904E-01	
Np-237	2.048E+01	1.593E+01	-22.2
Np-238	8.497E-02	5.447E-02	-35.9
Np-239	2.061E-04	1.584E-04	-23.1
Pu-236	4.272E-05	1.005E-05	-76.5
Pu-237	3.021E-06	4.213E-06	39.5
Pu-238	5.804E+00	3.888E+00	-33.0
Pu-239	7.695E-01	5.095E-01	-33.8
Pu-240	1.785E-01	1.152E-01	-35.5
Pu-241	1.234E-01	6.297E-02	-49.0
Pu-242	3.408E-02	1.296E-02	-62.0
Pu-243	1.082E-05	4.468E-06	-58.7
Am-241	1.624E-03	8.988E-04	-44.7
Am-242	6.466E-06	3.044E-06	-52.9
Am-243	4.487E-03	1.875E-03	-58.2
Am-242m	3.037E-05	2.185E-05	-28.0
Cm-242	5.430E-04	2.528E-04	-53.4
Cm-243	8.635E-06	5.469E-06	-36.7
Cm-244	9.154E-04	3.923E-04	-57.1
Cm-245	3.936E-05	1.378E-05	-65.0
Cm-246	3.943E-06	1.518E-06	-61.5
Total	9.357E+05	9.357E+05	0.0

Another comparison is made in Table 8 between calculations by ORIGEN2 using Th-library (new214-library) and those reported in an IAEA publication for the PWR fuel of 5.19%^{233}U-Th at a discharge burnup of 45 GW·d/t (Table 3.19 of [9]). ORIGEN2 calculation agrees well with the IAEA publication result for major nuclides.

TABLE 8. ACTINIDES WEIGHT FOR ^{233}U-Th PWR FUEL (grams per initial 1-ton HM)

Nuclide	*BOL(g)*	*IAEA:45G*	*ORIGEN2*	*Error (%)*
Th-232	948 100	921 247	921 900	0.1
Pa-233		1016	1035	1.9
U-233	51 900	24 858	25 510	2.6
U-234		(4,874)*	4,874	
U-235		1,252	648	-48.3
U-236		127	60	-52.7
total	1 000 000	953 374	954 030	0.1

*: The value of U-234 is assumed identical to ORIGEN2.

5.2.4.2. ^{235}U-Th fuel

Nuclide concentrations calculated by ORIGEN2 using Th-library (new214-library) are compared with those reported in an IAEA publication for the PWR fuel of 5.2%^{235}U-Th at a discharge burnup of 45 GW·d/t (Table 3.20 of [8]). ORIGEN2 calculation agrees well with the IAEA publication result for major nuclides as shown in Table 9.

TABLE 9. ACTINIDES WEIGHT FOR ^{235}U-Th PWR FUEL (grams per initial 1-ton HM)

Nuclide	*BOL(g)*	*IAEA:45G*	*ORIGEN2*	*Error (%)*
Th-232	947 962	917 099	918 000	0.1
Pa-233		1129	1140	1.0
U-233		13 121	13 800	5.2
U-234		(1780)*	1780	
U-235	52 038	11 702	12 000	2.5
U-236		6871	6590	-4.1
U-237		12	15	23.3
U-238			9.1	
Np-237		603	687	13.9
Pu-238		182	186	2.3
Pu-239		28	25	-11.0
Pu-240			5.5	
Pu-241			2.8	
total	1 000 000	952 527	954 240	0.2

*: The value of U-234 is assumed identical to ORIGEN2.

5.2.4.3. LEU-Th fuel

Nuclide concentrations calculated by ORIGEN2 using Th-library (new214-library) are compared with those reported in an IAEA publication for the PWR fuel of 26% LEU (5%U-235)-Th at a discharge burnup of 45 GW·d/t (Table 3.17 of [9]). Table 10 shows that ORIGEN2 mostly agrees with detailed design code for major nuclides.

As described in the Section 5.2.2, U-238 capture cross section is modified from 6.69 barns to 1.54 barns in ORIGEN2 library (new214-library). This effect appears only in LEU-Th fuel, because it contains initial U-238. As shown in Table 10, the difference in U-238 concentration is small, and the difference in Pu-239 concentration is improved.

TABLE 10. ACTINIDES WEIGHT FOR LEU-Th PWR FUEL (grams per initial 1-ton HM)

Nuclide	*BOL(g)*	*IAEA:45G*	*ORIGEN2*	*Error (%)*
Th-232	741 835	717 207	719 400	0.3
Pa-233		847	824	-2.7
U-233		11 211	10 600	-5.5
U-234		(1299)*	1299	
U-235	50 348	13 117	12 340	-5.9
U-236		6371	6295	-1.2
U-237		11	13	21.8
U-238	207 817	197 494	199 000	0.8
Np-237		581	646	11.2
Pu-238		179	175	0.0
Pu-239		2465	1856	-24.7
Pu-240		661	687	4.0
Pu-241		658	579	-12.0
Pu-242		233	208	-10.8
Am-241			18	
Am-242m			0.4	
Am-243			41	
Cm-242			6.0	
Cm-244			11	
total	1 000 000	952 334	953 999	0.2

*: The value of U-234 is assumed identical to ORIGEN2.

5.2.4.4. Pu-Th fuel

As explained in Section 5.2.1, neutron spectrum of Pu-Th core is different from U-Th core, but close to MOX core. Therefore, nuclide concentrations calculated by ORIGEN2 using MOX-library (new211-library) are compared with those reported in an IAEA report (Table 3.18 of [9]), for a PWR fuel of 5.5% Pu-Th at a discharge burnup of 45 GW·d/t (see Table 11).

As described in Section 5.2.2, Th-232 capture cross section is modified from 2.93 barn to a smaller value 0.749 barn in ORIGEN2 MOX library (new211-library) for use in Pu-Th fuel analysis. As a result, the difference in Th-232 concentration is small and accordingly the difference in generated U-233 concentration is improved.

Another comparison is made for a higher Pu content PWR fuel (9%) at a discharge burnup of 50 GW·d/t with NRC's NUREG report (Table 6.1 of [16]). Table 12 shows that ORIGEN2 calculations mostly agree with those reported in the NRC report for major nuclides.

TABLE 11. ACTINIDES WEIGHT FOR Pu-Th PWR FUEL (grams per initial 1-ton HM)

Nuclide	*BOL(g)*	*IAEA:45G*	*ORIGEN2*	*Error (%)*
Th-232	945 061	914 852	917 800	0.3
Pa-233		1082	1046	-3.3
U-233		14 158	12 490	-11.8
U-234		2240	1715	-23.4
U-235		535	348	-35.0
U-236		47.8	27.2	-43.1
U-237		0.12	0.09	-26.1
U-238		0.06	0.04	-39.0
Np-237		3.8	2.9	-23.5
Pu-238	549	563	569	0.9
Pu-239	32 416	2113	2240	6.0
Pu-240	12 634	6192	6156	-0.6
Pu-241	6593	4711	5234	11.1
Pu-242	2747	4975	3708	-25.5
Am-241		271	328	21.0
Am-242m		2.8	6.1	114.1
Am-243		1146	1688	47.3
Cm-242		152	139	-8.5
Cm-244		1041	1244	19.5
total	1 000 000	954 085	954 741	0.1

TABLE 12. ACTINIDES WEIGHT FOR Pu-Th PWR FUEL (grams per initial 1-ton HM) (reproduced courtesy of US NRC [16])

Nuclide	*BOL(g)*	*NUREG50G*	*ORIGEN2*	*Error (%)*
Th-232	910 000	886 000	891 000	0.6
Pa-233			658	
U-233		13 400	10 370	-22.6
U-234		1230	1029	
U-235		202	160	-20.6
U-236		17	15	-11.9
U-237		0.04	0.03	-23.3
U-238		0.04	0.05	16.4
Np-237		3.4	3.6	5.6
Pu-238	2214	(1795)*	1795	
Pu-239	49 221	10 500	7269	-30.8
Pu-240	23 544	17 600	14 550	-17.3
Pu-241	8559	10 200	10 390	1.9
Pu-242	6462	7610	6815	-10.4
Am-241		814	806	-1.0
Am-242m			14	
Am-243		1920	2737	42.6
Cm-242			207	
Cm-244			1523	
total	1 000 000	951 291	949 342	-0.2

*: The value of Pu-238 is assumed identical to ORIGEN2.

The difference in Pu-239 concentration was due to different assumptions for fission or transmutations of initial Pu-239, that is, 79% of initial Pu-239 was considered for fission or transmutations in NUREG results, while 85% of initial Pu-239 was considered for fission or transmutations in ORIGEN2 results. As a result, PWR MOX-library (new211-library) can be applied to Pu-Th PWR fuel.

5.2.5. Verification of ORIGEN2 library for application to thorium fuel in BWR

5.2.5.1. ^{233}U-Th fuel

A reference is available for BWR fuel burnup calculation performed by the Chalmers University of Technology for Swedish BWR 10x10 assembly fuel with 3.6% ^{233}U-Th at a discharge burnup of 45 GW·d/t and using its BWR fuel assembly design code [20].

Since there is no BWR thorium library available from ORIGEN2, a PWR Th-library (new214-library) is assumed to be applicable to BWR thorium fuels. Nuclide concentrations calculated by ORIGEN2 are compared with CUT's results. Both are reasonably consistent with each other for major nuclides as shown Table 13.

TABLE 13. ACTINIDES WEIGHT FOR ^{233}U-Th BWR FUEL (grams per initial 1-ton HM) (reproduced courtesy of K.I. Bjork [20])

Nuclide	*BOL(g)*	*CUT:45G*	*ORIGEN2*	*Error (%)*
Th-232	964 000	929 560	926 800	-0.3
Pa-233		(1092)*	1092	
U-233	36 000	17 032	19710	15.7
U-234		4440	4782	7.7
U-235		772	774	0.3
U-236		126	103	-18.2
U-237		0.20	0.22	9.8
U-238		0.09	0.08	-12.4
Np-237		6.66	6.36	-4.6
Pu-238		1.33	1.25	-6.2
Pu-239		0.18	0.14	-19.0
Pu-240		0.040	0.028	-30.9
Pu-241		0.022	0.013	-41.2
Pu-242		0.0056	0.0020	-64.0
Am-241		0.0004	0.0002	-45.1
total	1 000 000	953 030	953 269	0.0

*: The value of Pa-233 is assumed identical to ORIGEN2.

In this case, a specific power of 29.28 kW/kg was used, which was 13% larger than the NFCSS standard value of 25.9 kW/kg. Although this might cause some differences in calculation, the impact is expected to be small. Overall, the application of PWR Th-library (new214-library) to BWR appears acceptable.

5.2.5.2. LEU-Th fuel

Calculation results from ORIGEN2 have been compared with detailed design code (described in Section 5.2.5.1) for the BWR fuel of LEU-Th at a discharge burnup of 45 GW·d/t [20]. Here, LEU fuel was composed of 24% LEU (20% enrichment in LEU; that is 4.9% U-235 in Heavy Metal (HM) and 76% Th in HM. A specific power of 28.92 kW/kg was used, which was 12%

higher than the NFCSS standard value of 25.9 kW/kg. From Table 14, application of PWR Th-library (new214-library) to BWR is reasonably well supported.

TABLE 14. ACTINIDES WEIGHT FOR LEU-Th BWR FUEL GW·d/t (grams per initial 1-ton HM) (reproduced courtesy of K.I. Bjork [20])

Nuclide	*BOL(g)*	*CUT:45G*	*ORIGEN2*	*Error (%)*
Th-232	757 055	733 261	733 300	0.0
Pa-233		(687)*	687	
U-233		10 231	10 940	6.9
U-234		1667	1356	-18.7
U-235	49 080	12 304	11 390	-7.4
U-236		6180	6209	0.5
U-237		6	11	73.1
U-238	193 865	185 168	185 300	0.1
Np-237		455	663	45.6
Pu-238		143	189	31.9
Pu-239		1631	1738	6.6
Pu-240		640	648	1.3
Pu-241		480	551	14.8
Pu-242		226	209	-7.6
Am-241		23	22	-2.0
Am-242m			0.5	
Am-243		50	43	-12.8
Cm-242		6	7	2.8
Cm-244		15	11	-21.0
total	1 000 000	953 171	953 212	0.0

*: The value of Pa-233 is assumed identical to ORIGEN2.

5.2.5.3. Pu-Th fuel

Calculation results by ORIGEN2 and the detailed design code described in Section 5.2.5.1 were compared for Pu-Th BWR fuel (9.57%Pu_t, 6.39%Pu_f) at a discharge burnup of 45 GW·d/t [20]. A specific power of 28.92 kW/kg was used, which was 12% higher than the NFCSS standard value of 25.9 kW/kg.

Considering that neutron spectrum for Pu-Th core is close to MOX core and neutron spectrum between a PWR and a BWR is similar to each other, PWR MOX-library (new211-library) is assumed to be applicable to BWR Pu-Th fuel.

For major nuclides, both results are reasonably consistent with each other (See Table 15). This supports the application of PWR Th-library (new214-library) to BWR.

5.3. OTHER REACTOR CONSTANTS FOR THORIUM FUEL CYCLES IN LWR

Other constants required by the CAIN module are specific power, neutron flux, and reference enrichment.

TABLE 15. ACTINIDES WEIGHT FOR Pu-Th BWR FUEL (grams per initial 1-ton HM) (reproduced courtesy of K.I. Bjork [20])

Nuclide	*BOL(g)*	*CUT:45G*	*ORIGEN2*	*Error (%)*
Th-232	904,300	881,392	889,300	0.9
Pa-233		(474)*	474	
U-233		11,682	9,091	-22.2
U-234		1,172	714	-39.1
U-235		171	94	-45.2
U-236		23	13	-45.3
U-237		0.03	0.02	-36.8
U-238		0.06	0.06	-15.0
Np-237		6.4	5.4	-15.4
Pu-238	2,393	2,029	2,171	7.0
Pu-239	51,869	16,272	11,330	-30.4
Pu-240	22,777	19,369	17,330	-10.5
Pu-241	12,058	8,872	11,410	28.6
Pu-242	6,603	8,460	7,233	-14.5
Am-241		1,289	1,222	-5.2
Am-242m			22	
Am-243		1,626	2,524	55.2
Cm-242		166	221	33.7
Cm-244		714	1,100	54.0
total	1 000 000	953 717	954 253	0.1

*: The value of Pa-233 is assumed identical to ORIGEN2.

5.3.1. Specific power

Specific power (kW/kg) may vary within the same reactor family (e.g. 10-20% difference for different NPPs). Considering that the variation of the specific power on actinides behaviour is benign, typical values of specific power are used for specific reactor types. This constant value of the specific power is used to convert the discharge burnup to the irradiation time (refer to Annex I, Section I-2.1). These specific power values are shown in Table 16.

TABLE 16. SPECIFIC POWER FOR EACH REACTOR TYPES (reproduced from [1])

Reactor Type†	*Specific Power (kW/kg)*
PWR	37.5
BWR	25.9
PHWR	18.8
RBMK	15.75
AGR	10.9
GCR	3.33
WWER	45.8

†: At the moment, thorium fuel cycles in PWRs and BWRs are modelled.

5.3.2. Reference enrichment (or fissile content)

Reference design information on thorium fuel can be taken from NRC's NUREG report [16], which recommends that the following 4 fuels of 4% enriched UO_2 fuel, 5% fissile of LEU-Th fuel, 8% Pu-total (Put) content of MOX fuel, and 9% Put content of Pu-Th fuel are equivalent in reactivity. This is because thermal cross section of Th-232 is three times higher than U-238, and thermal cross sections of most Pu nuclides are significantly higher compared to U-235.

This NRC report does not show any equivalence in reactivity between U-233 and U-235. Based on these it is assumed that ^{233}U-Th fuel and ^{235}U-^{238}U fuel are equivalent in terms of reactivity. The rationales to support this assumption (p.44 of [9]) are: U-233 has higher fission cross section than U-235 which causes higher reactivity; and Th-232 also causes lower reactivity than U-238. These two effects will offset each other.

In summary, the following six fuels are considered as reference designs at 45 GW·d/t discharge burnup. Items (a) and (e) listed below do not include Th fuel, however, they are included for comparative purpose. These reference enrichments (or fissile content) are summarized in Table 17.

(a) 4% enriched UO_2 fuel (4% U-235+96% U-238);
(b) 4%^{233}U-Th fuel (4% U-233+96% Th-232);
(c) 5%^{235}U-Th fuel (5% U-235+95% Th-232);
(d) 5%^{235}U of LEU-Th fuel (5% U-235+20% U-238+75% Th-232);
(e) 8% Pu content of MOX fuel (8% Pu+92% U-238);
(f) 9% Pu content of Pu-Th fuel (9% Pu+91% Th-232).

TABLE 17. REFERENCE FLUX AND ENRICHMENT FOR PWR (reproduced from [1])

Fuel type	*Reference enrichment, or fissile content (weight%)*	*Reference neutron flux (n/cm^2/sec)*	*Reference burnup (GW·d/t)*
^{233}U-Th	4.0% U-233	2.92×10^{14}	45
^{235}U-Th	5.0% U-235	2.74×10^{14}	45
LEU-Th	5% U-235 (25% LEU)	2.55×10^{14}	45
Pu-Th	6% Pu fissile (9.35% Pu)	2.16×10^{14}	45

For implementation of MOX fuel in NFCSS, 7.5% Pu-total content is assumed as equivalent to 4% enriched UO_2 fuel for 45 GW·d/t discharge burnup in terms of reactivity [1]. This 7.5% Pu content is close to the above (e) with 8.0% Pu content.

The enrichment values in (a) to (f) are adopted as reference fissile contents. Pu fuel assumes 64% fissile Pu among all Pu nuclides.

5.3.3. Reference neutron flux

Reference neutron flux, reference enrichment (or fissile content), and reference burnup for PWR are summarized in Table 17, based on the study shown below.

The neutron flux input is mandatory but considered as an initial guesstimate. The neutron flux corresponding to the specific power is calculated in NFCSS through the iterative procedure.

Neutron fluxes for PWR/BWR are derived from ORIGEN2 results. Since single cross section set is applied to different enrichment fuels, actual neutron flux can be modified in the CAIN module using the following Equation (3) for UO_2/MOX fuel [1]. This adjustment using a simple correlation, Equation (3) will increase the speed of calculation.

$$\varphi(a) = \varphi(r) \times (ENR(r)/ENR(a) + 1) / 2 \quad (3)$$

where,

$\varphi(a)$: Actual neutron flux (n/cm^2/sec);

φ(r): Reference neutron flux (n/cm^2/sec);
ENR(a): Actual enrichment or fissile content (wt.%);
ENR(r): Reference enrichment or fissile content (wt.%).

For the thorium cycle, the same formula can be applied, taking into account that the neutron flux becomes higher for lower enrichment fuel at the same power density. Since the neutron flux input is for initial guess, it does not affect the final results.

Figure 13 and Table 18 show the calculated neutron fluxes in terms of initial fissile content by ORIGEN2 for ^{233}U-Th fuel. Here, the discharge burnup was assumed to be proportional to the reference enrichment. Solid line shows Equation (3); it is well consistent with the ORIGEN2 results. The hollow circled point in Fig.13 was taken from Table 3-16 of [9], which has been calculated by the detailed design code at a burnup of 45 GW·d/t burnup.

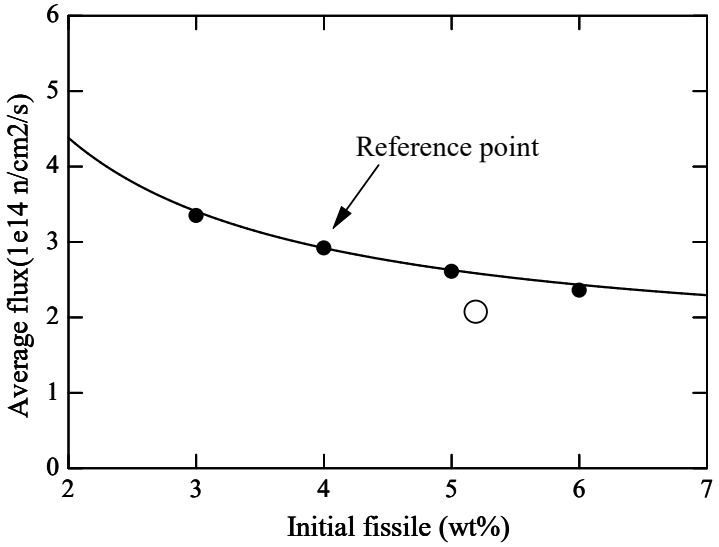


FIG.13. Neutron flux vs. initial fissile content for ^{233}U-Th PWR fuel.

TABLE 18. NEUTRON FLUX VS INITIAL FISSILE CONTENT FOR ^{233}U-Th PWR FUEL

U-233, %	*Flux(E14)*	*Burnup(GW·d/t)*	*Remark*
3	3.35	33.75	
4	2.92	45.00	Reference point
5	2.61	56.25	
6	2.36	67.50	

In Fig.13 to Fig.16, there is a small difference between the solid line (Equation (3)) and the hollow circled point (or cross-marked point). But, the neutron flux is used as an initial guess and does not affect the CAIN burnup results. Therefore, the solid line can be used.

Figure 14 and Table 19 show the calculated neutron fluxes in terms of initial fissile content by ORIGEN2 for ^{235}U-Th fuel. Here, discharged burnup was assumed to be proportional to the reference enrichment. Solid line shows Equation (3) and is consistent with ORIGEN2 results.

The hollow circled point in Fig.14 was taken from Table 3-16 of [9], which has been calculated by the detailed design code at a burnup of 45 GW·d/t.

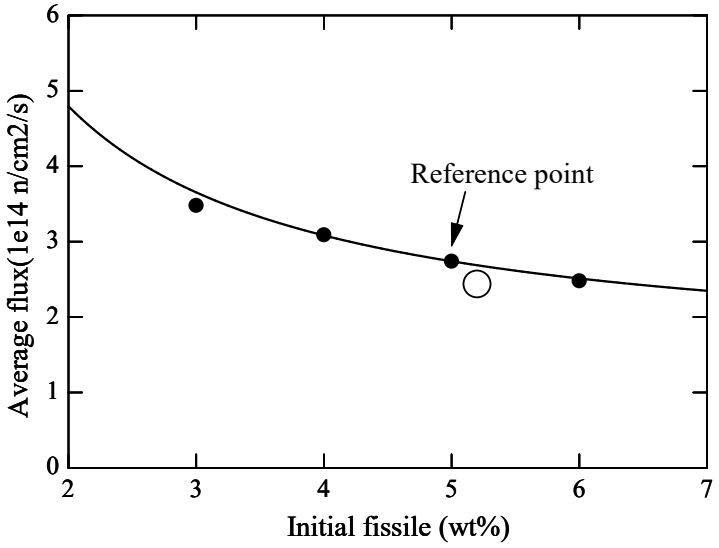


FIG. 14. Neutron flux vs. initial fissile content for ^{235}U-Th PWR fuel.

TABLE 19. NEUTRON FLUX VS INITIAL FISSILE CONTENT FOR ^{235}U-Th PWR FUEL

U-233, %	*Flux(E14)*	*Burnup(GW·d/t)*	*Remark*
3	3.48	27.00	
4	3.09	36.00	
5	2.74	45.00	Reference point
6	2.48	54.00	

Figure 15 and Table 20 show the calculated neutron fluxes in terms of initial fissile content by ORIGEN2 for LEU-Th fuel. Here, discharged burnup was assumed to be proportional to the reference enrichment. Solid line shows Equation (3); it is well consistent with the ORIGEN2 results.

The hollow-circled point in Fig.15 was taken from Table 3-16 of [9], which has been calculated by the detailed design code at a burnup of 45 GW·d/t burnup.

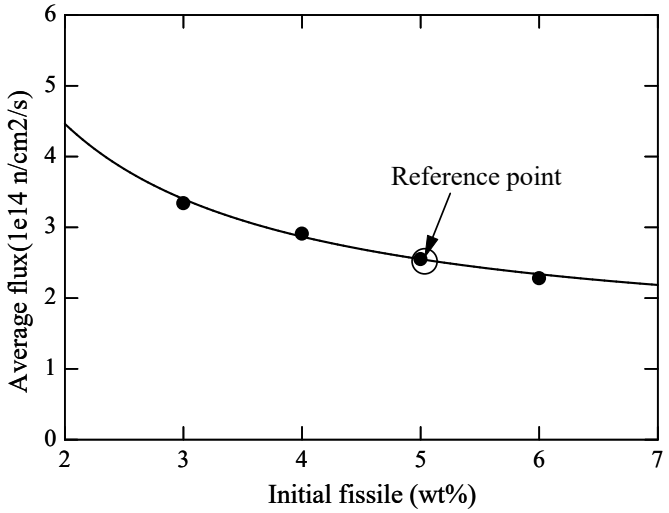


FIG.15. Neutron flux vs. Initial fissile content for LEU-Th PWR fuel.

TABLE 20. NEUTRON FLUX VS INITIAL FISSILE CONTENT FOR LEU-Th PWR FUEL

U-233, %	*Flux(e14)*	*Burnup(GW·d/t)*	*Remark*
3	3.34	27.00	
4	2.91	36.00	
5	2.55	45.00	Reference point
6	2.28	54.00	

Figure 16 and Table 21 show the results calculated by ORIGEN2 for Pu-Th fuel. Here, 64% Pu-fissile content was assumed.

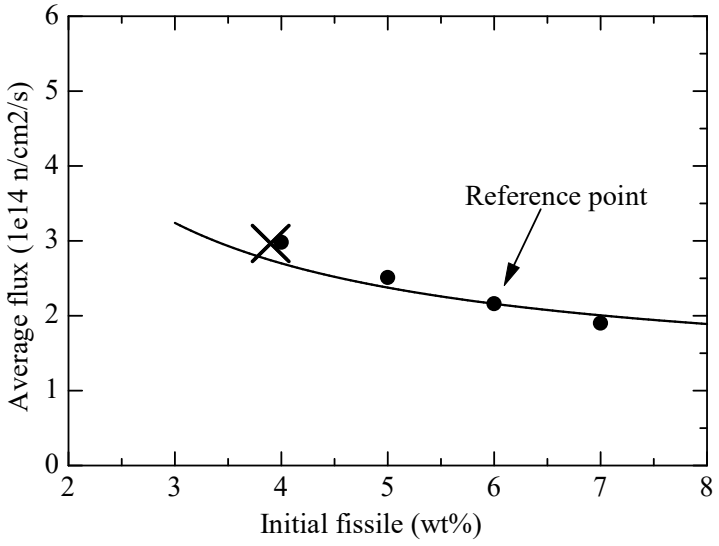


FIG. 16. Neutron flux vs. Initial fissile content for Pu-Th PWR fuel.

TABLE 21. NEUTRON FLUX VS INITIAL FISSILE CONTENT FOR Pu-Th PWR FUEL

Pu fissile, %	*Flux(E14)*	*Burnup(GW·d/t)*	*%Pu$_t$*	*Remark*
4.00	2.980	30.00	6.23	
5.00	2.510	37.50	7.79	
6.00	2.160	45.00	9.35	Reference point
7.00	1.900	52.50	10.90	

Table 22 represents initial concentrations of Pu nuclides (Pu vector) before burnup. These fractional values were estimated based on ORIGEN2 calculation on 4.0% U-235 enriched fuel irradiated to 45 GW·d/t in a PWR; the fuel was cooled for 7 years and reprocessed. To be precise, after Pu is separated in the reprocessing process, Pu-241 decays to Am-241with 14.4 year half-life before actual irradiation in the reactor. Also, Pu may be used with natural U or depleted U. In these cases, Pu vector must be modified.

TABLE 22. ASSUMED PLUTONIUM ISOTOPES FRACTION IN INITIAL Pu-Th FUEL

Pu nuclide	*Wt.%*
Pu-238	2.46
Pu-239	54.69
Pu-240	26.16
Pu-241	9.51
Pu-242	7.18
total	100.00

In Fig.16, discharged burnup is assumed to be proportional to the reference Pu fissile content. Solid line shows Equation (3) and it reproduces the ORIGEN2 results.

Cross mark in Fig.16 shows the result calculated from detailed design code in the IAEA publication (Table 3-16 of [9]) at a burnup of 45 GW·d/t.

5.3.4. Discharged burnup

Table 17 contains the reference burnup for four fuel types. In the NFCSS, the discharge burnup can be estimated using Equation (4) based on the assumption that it is proportional to the reference enrichment.

$$BU(a) = BU(r) \times ENR(a) / ENR(r) \quad (4)$$

where

BU(a): Actual discharged burnup (GW·d/t),
BU(r): Reference burnup (GW·d/t),
ENR(a): Actual enrichment (wt.%),
ENR(r): Reference enrichment. (wt.%).

Figure 17 shows estimated discharge burnups as a function of the reference enrichment, where solid line is for ^{233}U-Th fuel, dotted line for ^{235}U-Th fuel and LEU-Th fuel, and broken line for Pu-Th fuel. Equation (4) is applicable to both PWR and BWR. Since Equation (4) accounts for

the variation in enrichment, the prediction uncertainty due to the linear approach would be small.

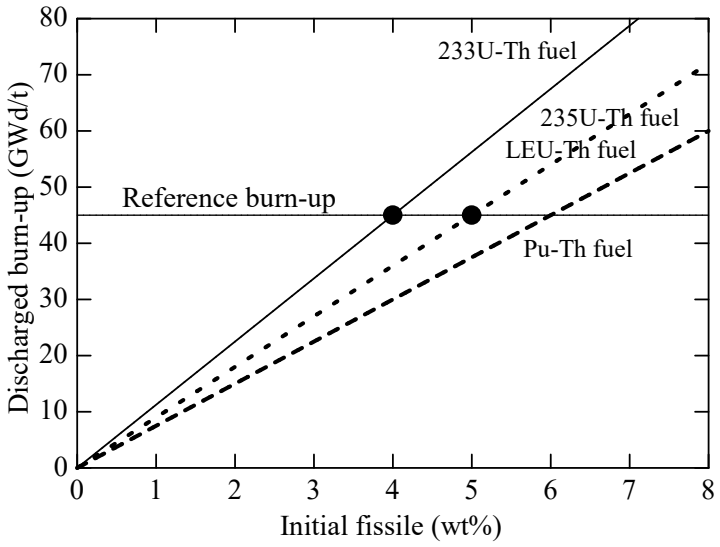


FIG.17. Discharge burnup vs. Initial fissile content for PWR/BWR Th fuel.

5.3.5. Thorium fuel cycles in PWR

Cross sections for 18 nuclides, which are required for the CAIN module, are provided in Table 5 for Th core with U-233 or U-235 or LEU, and in Table 6 for thorium core with Pu. Other input parameters used for the assessment of thorium fuel cycle in PWRs are given in Table 23.

TABLE 23. NFCSS/CAIN INPUTS FOR PWR THORIUM CYCLE (REFERENCE DESIGN)

Fuel type	*^{233}U-Th*	*^{235}U-Th*	*LEU-Th*	*Pu-Th*
Specific Power (kW/kg)	37.5	37.5	37.5	37.5
Cross sections	Table 5	Table 5	Table 5	Table 6
Reference enrichment, or fissile content (wt.%)	4.0	5.0	5.0 (25% LEU)	6.0 (9.35% Pu)
Reference neutron flux (n/cm^2/sec)	2.92x10^{14}	2.74x10^{14}	2.55x10^{14}	2.16x10^{14}
Reference burnup (GW·d/t)	45	45	45	45
Initial fuel composition:				
Th-232 (wt.%)	96.00	95.00	75.00	90.65
U-233 (wt.%)	4.00			
U-235 (wt.%)		5.00	5.00	
U-238 (wt.%)			20.00	
Pu-238 (wt.%)				0.23
Pu-239 (wt.%)				5.11
Pu-240 (wt.%)				2.45
Pu-241 (wt.%)				0.89
Pu-242 (wt.%)				0.67

Input data for neutron flux is mandatory and a guesstimate can be provided as initial value, but the final value of neutron flux corresponding to the specific power is calculated in the NFCSS by the iterative procedure described in Annex I.

For non-reference design of PWR thorium fuel, values in Table 24 are used. Neutron flux and discharge burnup for non-reference design can be estimated using the proposed formula expressed by Equations (3) and (4).

TABLE 24. NFCSS/CAIN INPUTS FOR PWR THORIUM CYCLE (NON-REFERENCE DESIGN)

Fuel type	*^{233}U-Th*	*^{235}U-Th*	*LEU-Th*	*Pu-Th*
Specific Power (kW/kg)	37.5	37.5	37.5	37.5
Cross sections	Table 5	Table 5	Table 5	Table 6
Enrichment, or fissile content (wt. %)	X	X	X ([X+Y]% LEU)	X (Y% Pu)
Neutron flux (n/cm^2/sec)	Fig.13 $=2.92\text{x}10^{14}\times$ (4/X+1) / 2	Fig.14 $=2.74\text{x}10^{14}\times$ (5/X+1) / 2	Fig.15 $=2.55\text{x}10^{14}\times$ (5/X+1) / 2	Fig.16 $=2.16\text{x}10^{14}\times$ (6/X+1) / 2
Discharged burnup (GW·d/t)	Fig.17 =45X / 4	Fig.17 =45X / 5	Fig.17 =45X / 5	Fig.17 =45X / 6
Initial fuel composition				
Th-232 (wt.%)	100-X	100-X	100-X-Y	100-Y
U-233 (wt.%)	X			
U-235 (wt.%)		X	X	
U-238 (wt.%)			Y	
Pu (wt.%)*				Y

*: Each Pu fraction should be determined by Table 22.

Here only once-through fuel cycle is taken into account for thorium fuel cycle because reprocessing of thorium fuel is unlikely to take place on industrial basis in the foreseeable future (p81 of [10]). As described in Section 3.2, however, a closed fuel cycle can be simulated in the NFCSS. If input values of each concentration (in terms of weight %) of all actinides for Th-fuel are provided, the NFCSS/CAIN can handle recycled U-233 or recycled Pu-239.

For uranium fuel cooling time is considered typically to be 6 years, reprocessing time typically 1 year, and the recycled fuel manufacturing time typically 1 year (as described in Section 3.1.9 of [1]). This information for thorium fuels is not known.

5.3.6. Thorium fuel cycles in BWR

Since there is no thorium library available for BWRs in ORIGEN2, the above PWR thorium library is applied to all BWR cases as discussed in Section 5.2.5. That is, PWR thorium library (ORIGEN2, 214-library) is applied to BWR Th core with U-233 or U-235 or LEU, and PWR MOX library (ORIGEN2, 211-library) to BWR Th core with Pu.

Reference design used in the assessment of BWR thorium fuel is given in Table 25. Note that Table 25 is identical to Table 24 for PWR thorium fuel except for neutron flux. The NFCSS assumes that the reference UO_2 design is identical for PWR and BWR, and this assumption would also apply to thorium fuels. The reference neutron flux in Table 25 was calculated by ORIGEN2 as an averaged value up to 45 GW·d/t burnup. Also, the initial input value of neutron flux can be a guesstimate and the final neutron flux corresponding to the specific power is calculated in NFCSS by the iterative procedure.

TABLE 25. NFCSS/CAIN INPUTS FOR BWR THORIUM CYCLE (REFERENCE DESIGN)

Fuel type	*^{233}U-Th*	*^{235}U-Th*	*LEU-Th*	*Pu-Th*
Specific Power (kW/kg)	25.9	25.9	25.9	25.9
Cross sections	Table 5	Table 5	Table 5	Table 6
Reference enrichment, or fissile content (wt.%)	4.0	5.0	5.0 (25%LEU)	6.0 (9.35%Pu)
Reference neutron flux (n/cm^2/sec)	2.06×10^{14}	1.93×10^{14}	1.79×10^{14}	1.51×10^{14}
Reference burnup (GW·d/t)	45	45	45	45
Initial fuel composition:				
Th-232 (wt.%)	96.00	95.00	75.00	90.65
U-233 (wt.%)	4.00			
U-235 (wt.%)		5.00	5.00	
U-238 (wt.%)			20.00	
Pu-238 (wt.%)				0.23
Pu-239 (wt.%)				5.11
Pu-240 (wt.%)				2.45
Pu-241 (wt.%)				0.89
Pu-242 (wt.%)				0.67

For non-reference design of BWR thorium fuel, Table 26 is referred.

Table 26. NFCSS/CAIN INPUTS FOR BWR THORIUM CYCLE (NON-REFERENCE DESIGN)

Fuel type	*^{233}U-Th*	*^{235}U-Th*	*LEU-Th*	*Pu-Th*
Specific Power (kW/kg)	25.9	25.9	25.9	25.9
Cross sections	Table 5	Table 5	Table 5	Table 6
Enrichment, or fissile content (wt.%)	X	X	X ([X+Y]% LEU)	X (Y% Pu)
Neutron flux (n/cm^2/sec)	$=2.06\times10^{14}\times$ (4/X+1) / 2	$=1.93\times10^{14}\times$ (5/X+1) / 2	$=1.79\times10^{14}\times$ (5/X+1) / 2	$=1.51\times10^{14}\times$ (6/X+1) / 2
Discharged burnup (GW·d/t)	FIG.17 =45X / 4	FIG.17 =45X / 5	FIG.17 =45X / 5	FIG.17 =45X / 6
Initial fuel composition				
Th-232 (wt.%)	100-X	100-X	100-X-Y	100-Y
U-233 (wt.%)	X			
U-235 (wt.%)		X	X	
U-238 (wt.%)			Y	
Pu (wt.%)*				Y

*: Each Pu fraction should be determined by Table 22.

5.3.7. Thorium fuel cycles in PHWR

For PHWR, there is no thorium library available in ORIGEN2. Indeed, the effect of thorium in PHWRs will be larger than in LWRs due to low enrichment fuel used in PHWR. At this moment, reliable data for PHWR is not available.

5.4. IMPLEMENTATION IN NFCSS

Current NCFSS has been expanded to model thorium fuel cycles. The following summarizes the incremental features implemented in the NFCSS/CAIN for modelling thorium fuel cycle (for details refer to Sections 5.1 through 5.3).

(a) Reactor types considered for thorium cycle are PWRs or BWRs. Other reactor types such as PHWRs or FRs are not considered for now due to unavailability of reliable information to model them. When appropriate input data (e.g. cross sections) becomes available, impact of thorium fuel cycles in these reactors can also be assessed by the NFCSS;

(b) The following 14 nuclides are taken into account for UO_2 based fuel cycles: U-235, U-236, U-238, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Np-237, Am-241, Am-242m, Am-243, Cm-242, Cm-244. The following four more nuclides are added to model thorium fuel chains: Th-232, Pa-233, U-233 and U-234. Therefore, a total of 18 nuclides are taken into account in the NFCSS;

(c) Two more burnup chains are included in order to model thorium fuel cycle. They are:

- Th-232 (capture)→ Pa-233 (decay) →U-233 (capture) → U-234 (capture) →U-235 (capture) →U-236 (capture) →Np-237
- Th-232 (capture) →Pa-233 (capture)→U-234 (capture)→ U-235 (capture) →U-236 (capture) → Np-237;

(d) Pa-233 is included in the CAIN burnup model although its half-life is as short as 27 days;

(e) U-233 is a typical initial fissile material for thorium cycle, however, Pa-233, U-234, U-235, U-236 or LEU or Pu can be included;

(f) U-232 is not included because its contribution in negligible and generation paths are complicated;

(g) Possible scenarios for combined fuel components and reactor types are shown in Table 2;

(h) Cross sections for thorium cycle can be derived from ORIGEN2 library. The following two libraries are established for application to PWRs and BWRs:

- Thorium library (ORIGEN2, 214-library) for PWR/BWR Th core with U-233, U-235 or LEU
- MOX library (ORIGEN2, 211-library) for PWR/BWR Th core with Pu;

(i) For PHWRs, there is no thorium library available in ORIGEN2. At this moment, reliable data for PHWR is unavailable;

(j) Reprocessing of thorium fuel is not considered here. However, with appropriate inputs of each concentration (in terms of weight %) of all actinides for Th fuel, the NFCSS/CAIN can calculate the used fuel profile for recycled U-233 or recycled Pu-239;

(k) The NFCSS can calculate initial U-235 enrichment of UO_2 fuel corresponding to the discharge burnup provided as an input even if the initial enrichment level of U-235 is not provided by the user. The NFCSS can also calculate actinides inventory with the initial enrichment by solving Bateman's equation. Identical procedure is applied to MOX fuel but using a different formula;

(l) For thorium cycle, however, both reference enrichment and reference burnup need to be provided, and linear relation formula is proposed for non-reference cases.

Validation of the NFCSS with modules to assess thorium fuel cycle should be performed in future.

6. METHOD FOR DECAY HEAT CALCULATION

6.1.GENERAL

Decay heat is one of important parameters for safety assessments in the context of both reactor accident analysis and spent fuel management. Decay heat is generated due to the decay of actinides and fission products (FP), and thus it mainly depends on fuel type, i.e. UO_2 fuel, MOX fuel (plutonium containing fuel) or thorium fuel.

Methods for decay heat calculation are well established for UO_2 and MOX fuels; however, literature on thorium fuel is scant.

There is heat generation by delayed neutrons. After a reactor is shut down, a small number of neutrons are emitted as delayed neutrons and cause fission reactions. These delayed neutrons are emitted by the decay of some FPs. This heating process is accounted for in the kinetic equations used for accident analysis. Since its influence disappears within several minutes after shutdown decay heat due to delayed neutrons is not included in this section.

6.2.CALCULATION METHOD

ORIGEN2 code [15] was used to calculate decay heat for the following two PWR cores with a rated power density of 39.2 MW/t. Since the output of decay heat in ORIGEN2 is given in W/t-HM, decay heat is divided by the rated power density in order to derive fractional heat. Each fuel was burnt up to 45 GW·d/t, and then decay heat was calculated for time periods ranging from 1-sec to 1-million years.

- U-PWR-core: 4% U-235 + 96% U-238;
- Th-PWR-core: 4% U-233 + 96% Th-232.

6.3. DECAY HEAT CHARACTERISTICS IN UO_2 FUEL CORE AND THORIUM FUEL CORE OF PWRS

The identical UO_2-library (PWR-U-205-library) was used for the assessment of the above two cores. This comparison is intended to identify the basic difference between uranium (or U-235) and thorium (or U-233) on fission products and actinides generation. Calculation results of decay heat are shown in Fig.18. In the figure, the Th core shows 10–20% higher decay heat than the U core up to 100 days. For the Th core, a peak of decay heat was present at 0.1 million years.

Decay heat components are shown in Fig.19 for the U core and Fig.20 for the Th core. Both figures show that decay heat by fission products (FPs) is dominant up to 100 years. After 100 years, decay heat by FPs faded out and decay heat by actinides became dominant.

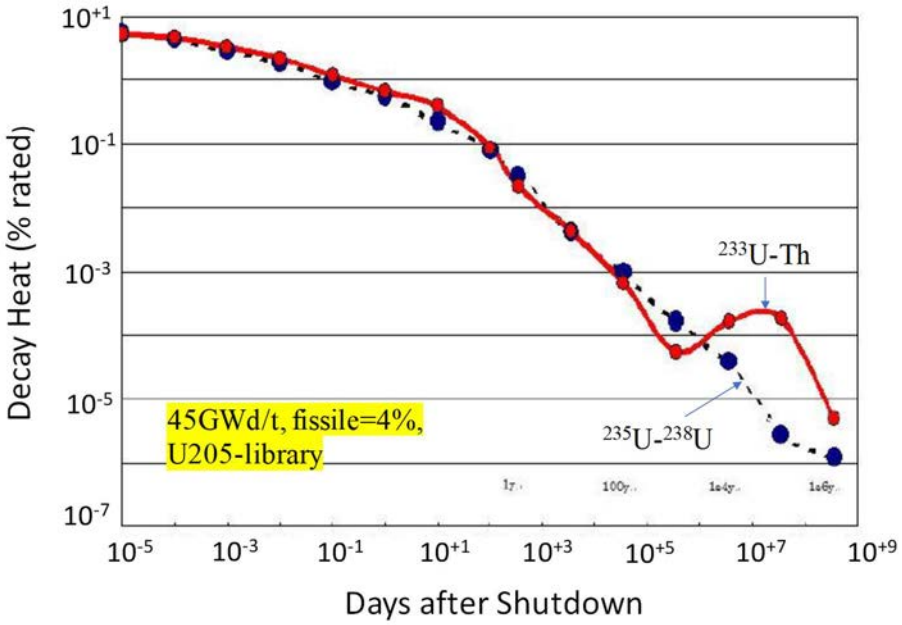


FIG.18. Comparison between the U core and the Th core.

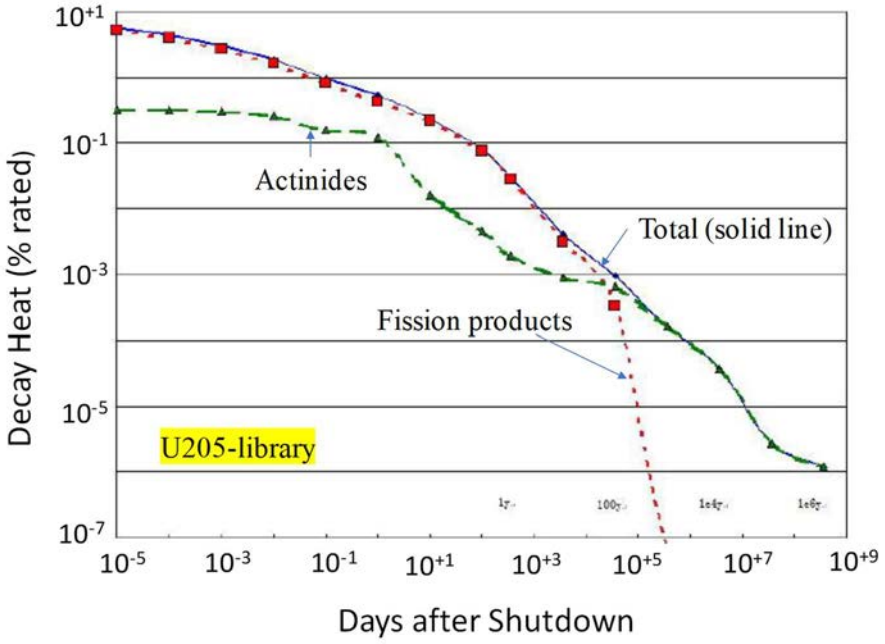


FIG.19. Component of decay heat (U core case).

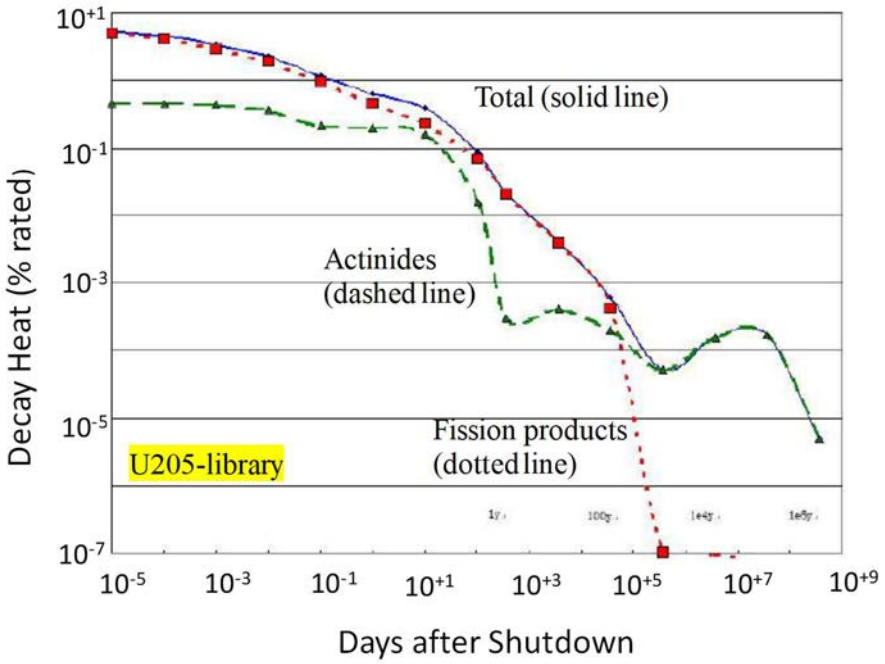


FIG.20. Component of decay heat (Th core case).

As described above, decay heat in the Th core turned out to be 10–20% higher than that of the U core during an early period of cooling after discharge of the fuel. This was attributed to different fission yields between U-233 and U-235. To investigate the primary contributors to the high decay heat in the Th core, decay heat from 10 major FPs has been examined as shown in Fig.21. Specific FPs could not be identified as major contributors.

Top 10 FPs (U core)

1	I-134	2.2
2	Cs-138	2.0
3	Cs-140	1.9
4	Y-96	1.7
5	La-142	1.7
6	Nb-102	1.6
7	Tc-104	1.6
8	La-140	1.5
9	La-144	1.3
10	I-132	1.3

Top 10 FPs (Th core)

1	La-142	2.3
2	Rb-91	2.3
3	Rb-90	2.0
4	Cs-138	2.0
5	Cs-140	1.9
6	Y-96	1.9
7	Rb-89	1.9
8	I-134	1.9
9	La-140	1.9
10	Y-94	1.9

FIG.21. Decay heat of top 10 FPs (% rated).

The cause of the peak decay heat at 0.1 million years in the Th core has been investigated. The contribution of each actinide to decay heat is shown in Fig.22. Here, these nuclides were stemmed from the decay of U-233 (half life: 159 200 years). Daughter nuclides stemmed from the decay of U-233 were: Th-229 (7340 y), Ra-225 (14.9 d), Ac-225 (10.0 d), Fr-221 (14.9 m), At-217 (32.3 ms), Bi-213 (45.59 m), Po-213 (4.2 μs), Pb-209 (3.253 h) and Bi-209 (stable). (Half-life values were taken from [22].) Radioactivity calculations showed peaks of decay heat at around 0.1 million years. This peak is known as transient equilibrium in radiation chemistry [23].

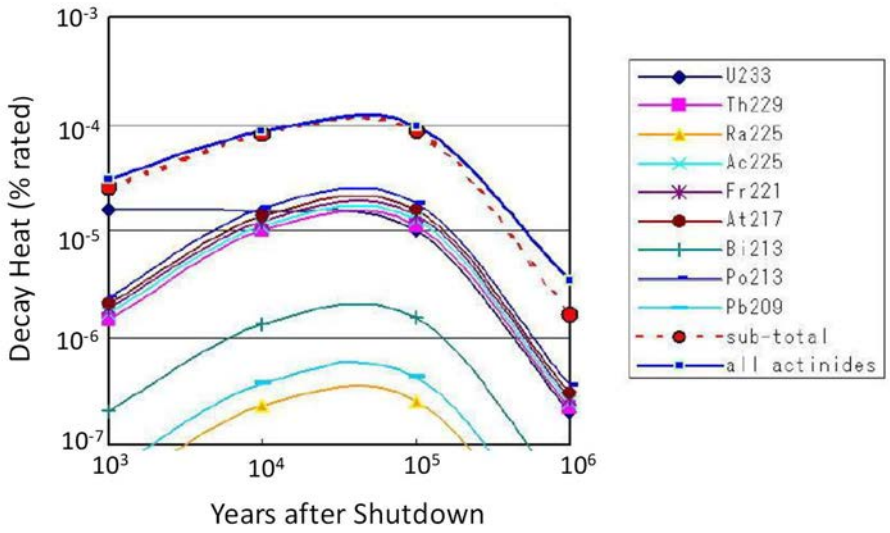


FIG.22. Component of decay heat at its peak (Th core).

6.3.1. Influence of library (Th-library, MOX-library)

ORIGEN2 provides various libraries; one of them is a Th core library (Th214-library) - refer to Sections 5.2.4 and 5.2.5. Two cases were made with the same assumptions except the libraries. As shown in Fig.23, decay heat based on Th-214-library is 10% smaller at 0–10 days than that based on U205-library, and 30% smaller after 1000 years. Although the above difference may be acceptable, Th214-library is applied for decay heat evaluation hereafter.

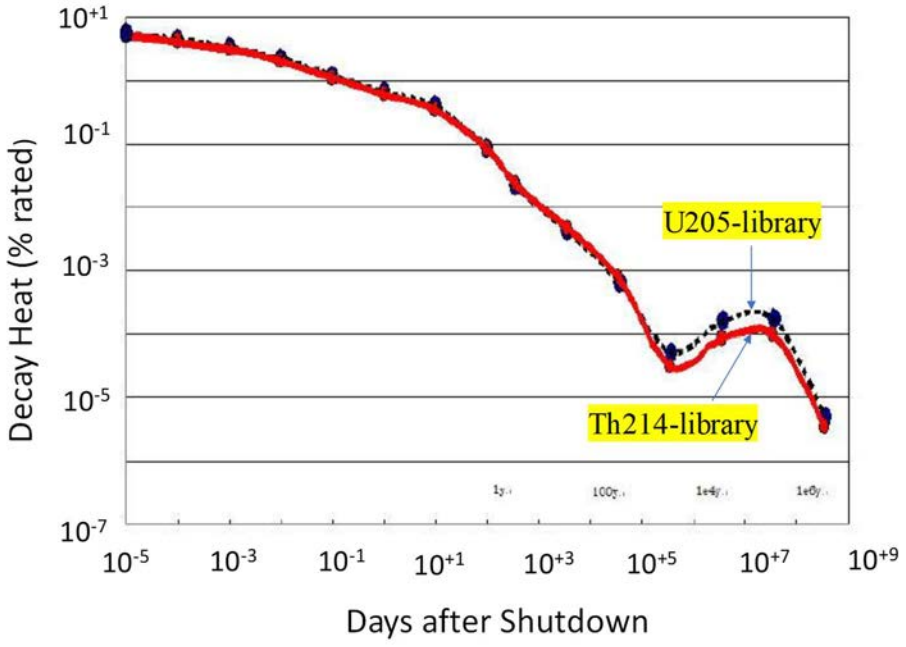


FIG.23. Decay heat for U-library and Th-library.

Another influence of different libraries is studied using MOX211-library. Since MOX-library causes harder neutron spectrum and larger buildup of actinides, it will result in higher decay heat in the long range. Two ThO_2 fuel cases were made with all the same assumptions, except

the application of different libraries. The comparison between U205-library and MOX211-library is shown in Fig.24, and the influence is visibly small.

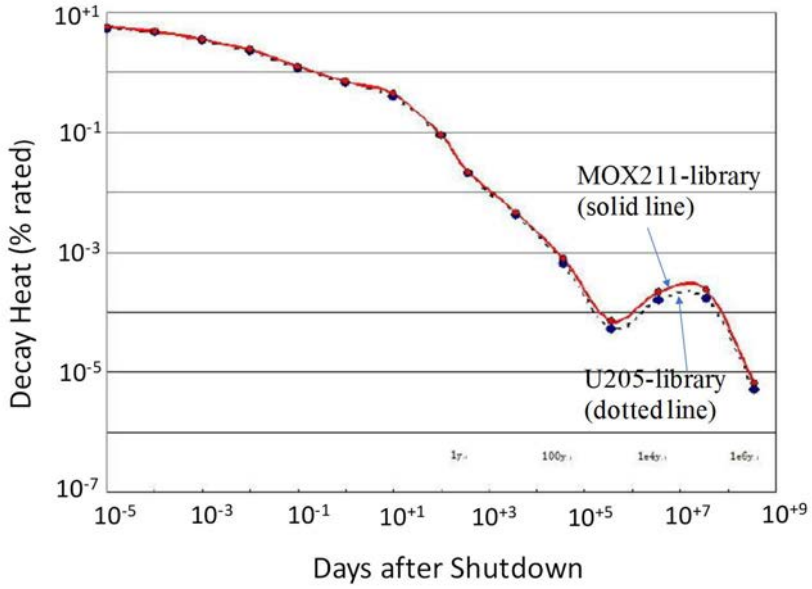


FIG.24. Decay heat for U-library and MOX-library.

6.3.2. Influence of U-233 concentration

In general, higher burnup results from higher fissile content in the initial fuel. The initial U-233 content of 2% case was compared with the referenced 4% case. The result is shown in Fig.25.

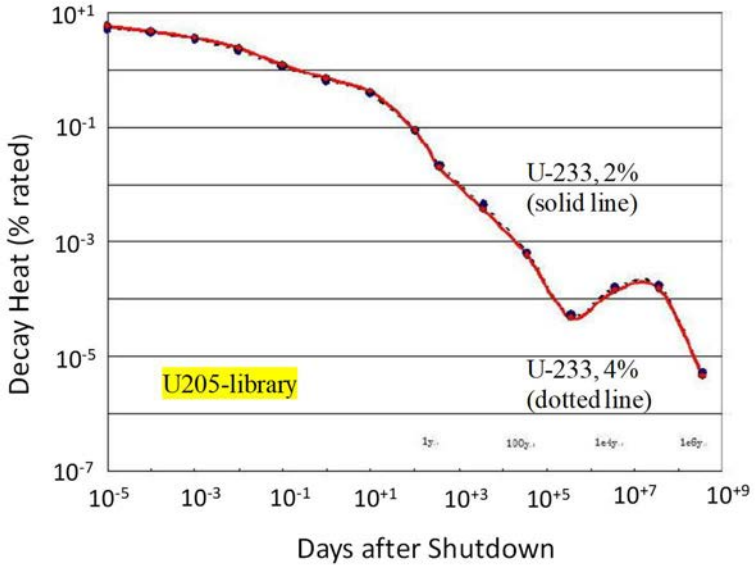


FIG.25. Decay heat for different U-233 contents.

The impact of initial U-233 concentration on decay heat was negligible because both cases assumed an identical burnup (45 GW·d/t). This means that for two cases with different initial concentrations of fissile material, almost identical number of fissions occurred, and almost same amount of FPs and actinides were generated if the discharge burnup was the same.

6.3.3. Influence of burnup

In the NFCSS, the discharge burnup of fuel is specified by the user. In general, higher actinides are present at higher burnup, causing higher decay heat. This effect was studied by using ORIGEN2 code for different PWR fuel types shown in Table 27.

TABLE 27. ENRICHMENT AND DISCHARGE BURNUP CASES

Fuel component	*Case 1*	*Case 2*	*Case 3*
UO_2 (^{235}U-^{238}U)	3 wt.%, 33 GW·d/t	4 wt.%, 45 GW·d/t	5 wt.%, 60 GW·d /t
ThO_2 (^{233}U-^{232}Th)	3 wt.%, 33 GW·d /t	4 wt.%, 45 GW·d /t	5 wt.%, 60 GW·d /t

Figure 26 and Fig.27 show decay heat calculations for UO_2 fuel and ThO_2 fuel, respectively. Decay heat in these figures is plotted in the unit of W/t-HM. Since higher burnup indicates a larger accumulation of actinides and thus results in larger decay heat, there is a positive relationship between burnup and decay heat. Although it is questionable in accuracy, a linear relationship between burnup and decay heat is proposed for simple approach. The method is described below.

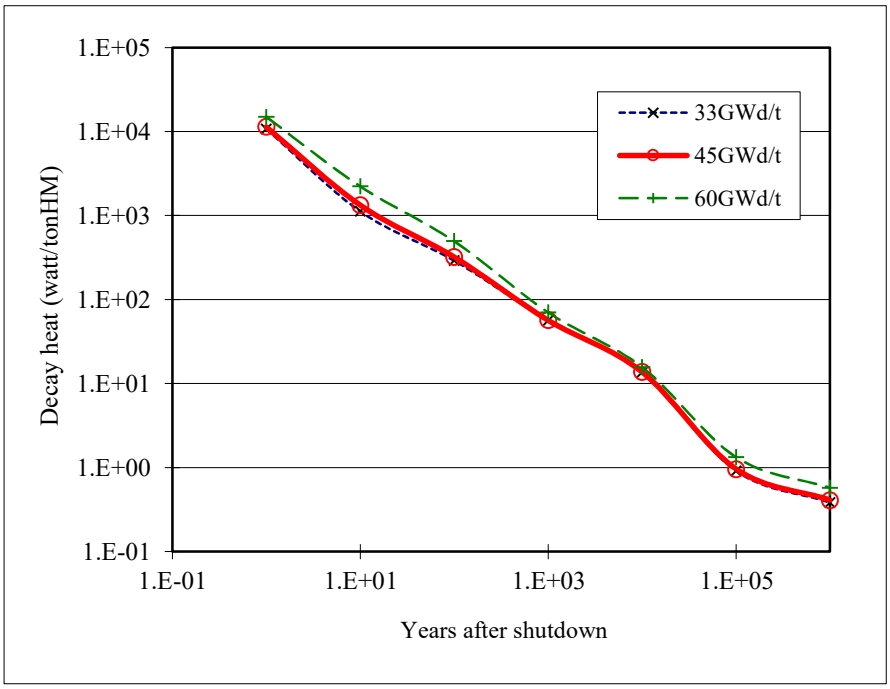


FIG.26. Decay heat for UO_2 fuel.

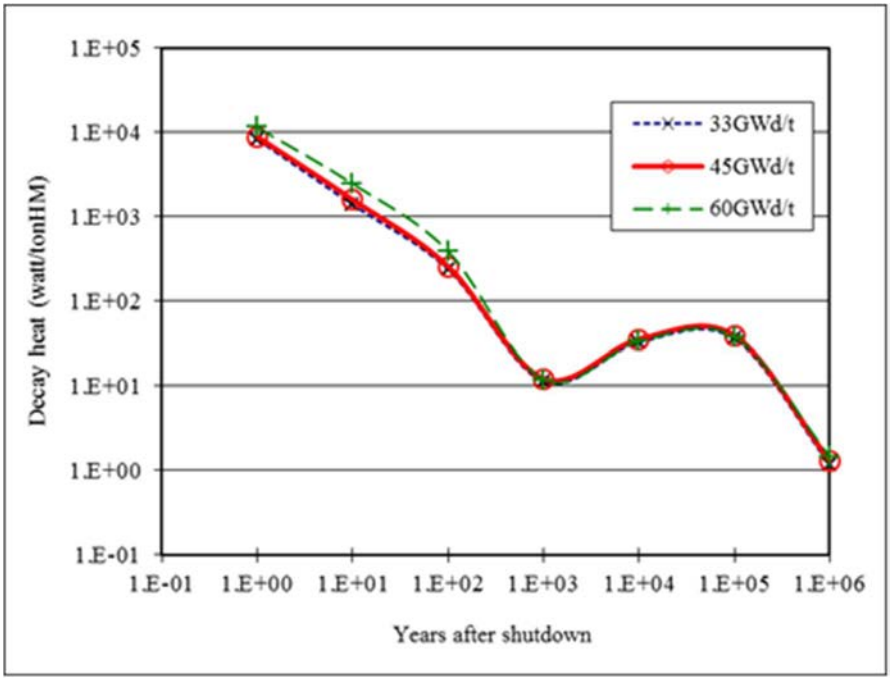


FIG.27. Decay heat for ThO_2 fuel.

Burnup dependence of decay heat is shown in Fig.28 and Fig.29 for UO_2 fuel and ThO_2 fuel respectively, where decay heat (W/t-HM) is normalized to that at the burnup of 45 GW·d/t. In these figures, [BU] shows a linear correlation. Decay heat data at different burnups are not consistent with those calculated by the linear correlation; however, the overall tendency of increased decay heat with burnup is reasonable.

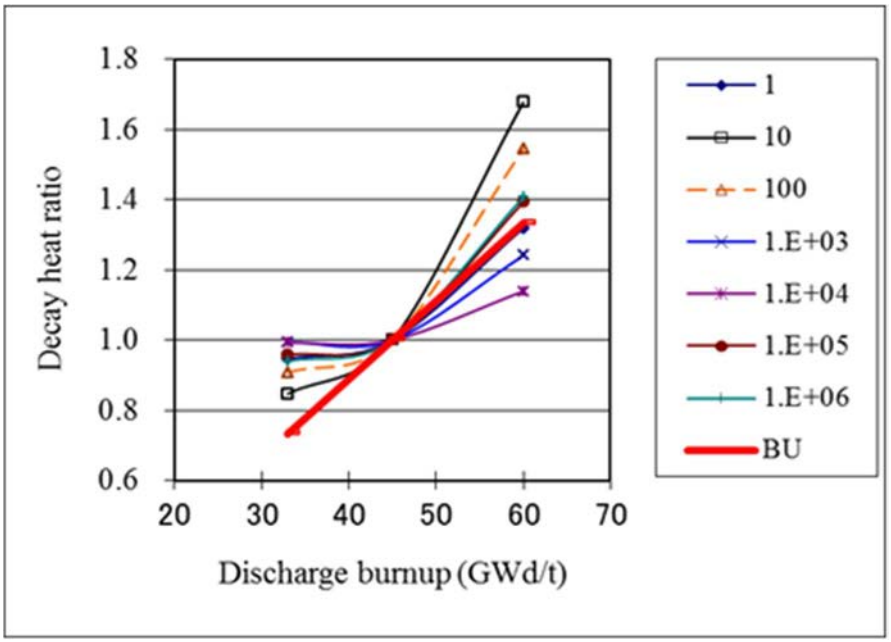


FIG.28. Decay heat ratio for UO_2 fuel, at specified year after discharge.

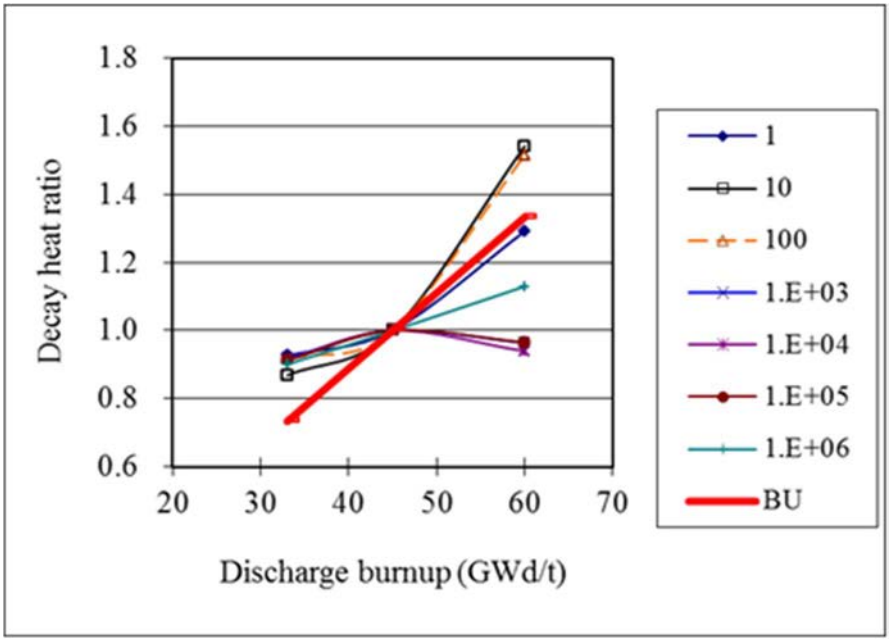


FIG.29. Decay heat ratio for ThO_2 fuel, at specified year after discharge.

Therefore, for a specific purpose of decay heat assessment in the NFCSS, the decay heat at a burnup is adjusted with respect to that calculated at the reference burnup (45 GW·d/t). That is,

$$DH(a) = DH(r) \times BU(a) / BU(r) \quad (5)$$

where,

DH(a): Decay heat for actual discharged burnup (W/t-HM);
DH(r): Reference decay heat for 45 GW·d/t burnup (W/t-HM);
BU(a): Actual burnup (GW·d/t);
BU(r): Reference burnup (45 GW·d/t).

6.3.4. Influence of fast neutron spectrum

It is recognized that decay heat would not be different between thermal neutron spectrum and fast neutron spectrum. As shown in Fig.30 and Fig.31 for U-235 and U-233, fission yields for both spectrums are almost identical, although slight difference between U-235 and U-233 exists [24]. These two figures suggest that decay heat would be similar between thermal neutron spectrum reactor and fast neutron spectrum reactor.

6.4. BENCHMARK

6.4.1. Comparison with measurements

There is only one experimental measurement by Yarnell for U-233 decay heat, which provides the decay heat data up to $1x10^5$ sec (about one day) after 20 000 seconds of irradiation [25]. That is, only FP contribution could be verified in this case.

Figure 32 shows results from ORIGEN2 and measured data for 20 000 sec irradiations of 100% U-235 sample. ORIGEN2 results are consistent with actual measurement and its average of calculated value divided by measurement data is 0.98, where its measurement uncertainty is around 2%. In Fig.32, only one third of the data are plotted in order to simplify its tendency.

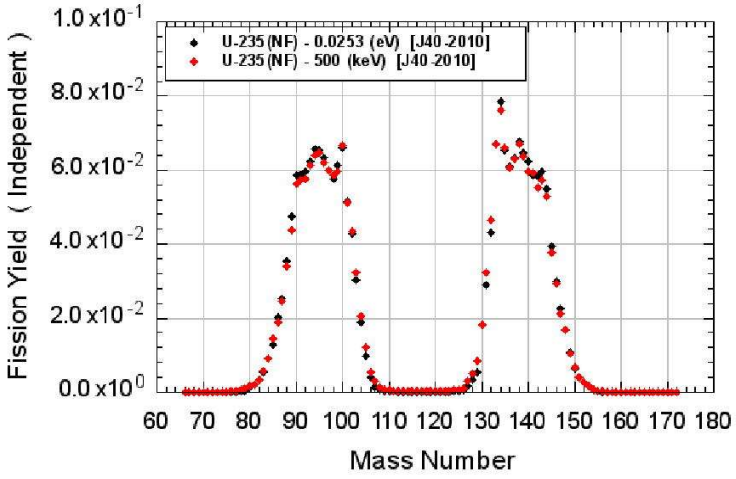


FIG.30. Fission yield for U-235 (reproduced courtesy of Japan Atomic Energy Agency (JAEA)[24]).

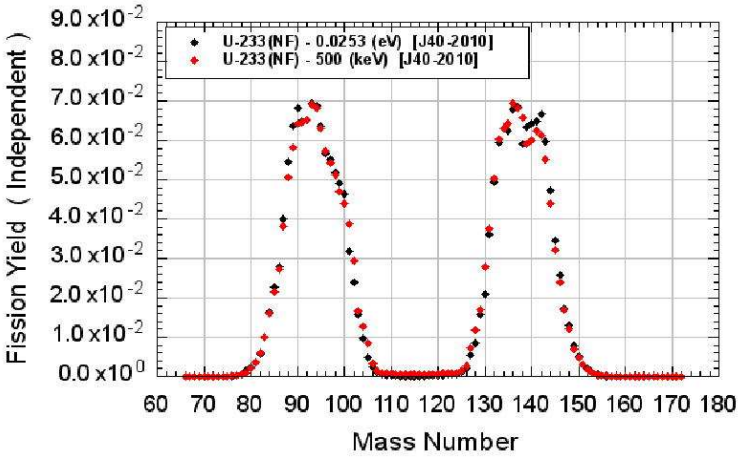
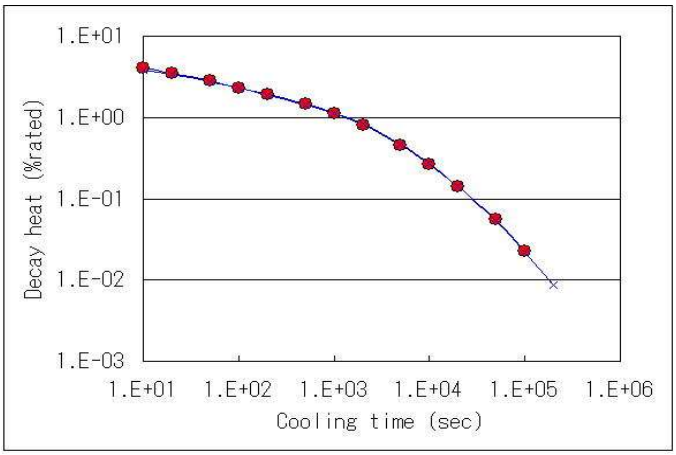


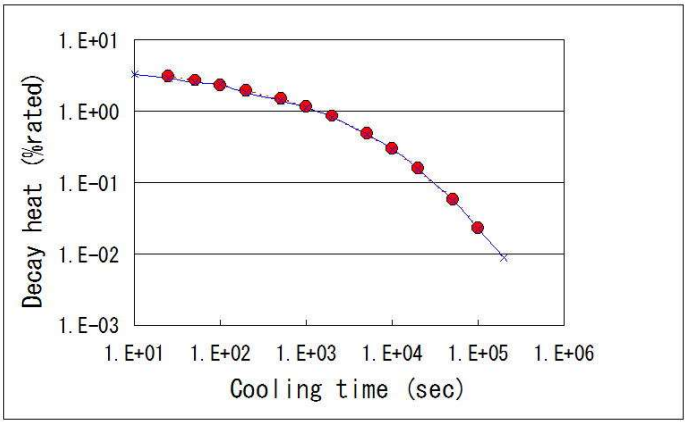
FIG.31. Fission yield for U-233 (reproduced courtesy of JAEA [24]).



(Solid: ORIGEN2 with U205-library, ●: Measurements [25])

FIG.32. Decay heat verification for U-235.

Figure 33 shows results from ORIGEN2 and measured data for 20 000 sec. irradiation of 100% U-233 sample. ORIGEN2 results are consistent with measurement data and its average of calculated value divided by measurement data is 0.95, where its measurement uncertainty is around 5%. In Fig.33 only one third of the data are plotted.



(Solid: ORIGEN2 with U205-library, ●: Measurements [25])

FIG.33. Decay heat verification for U-233.

6.4.2. Comparison with independent calculations

Yarnell's measurement and ORIGEN2 results indicated that decay heat of U-233 would be slightly lower than that of U-235 for short periods of cooling time.

Recent calculations are available from open literature, where updated nuclear cross section libraries were used [26]. The results are shown in Fig.34 for U-235 and Fig.35 for U-233 with Yarnell's measurements, which were reproduced from [26].

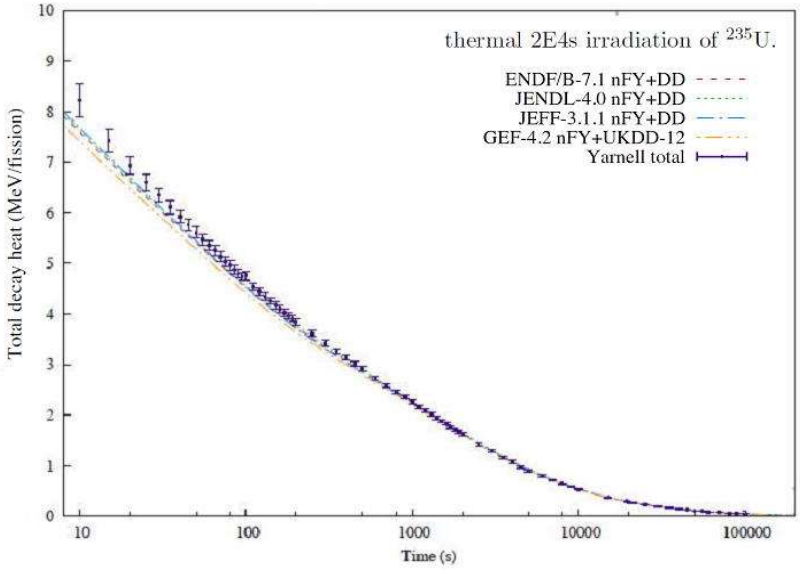


FIG.34. Decay heat comparison for U-235 (reproduced courtesy of Los Alamos Scientific Lab [25]).

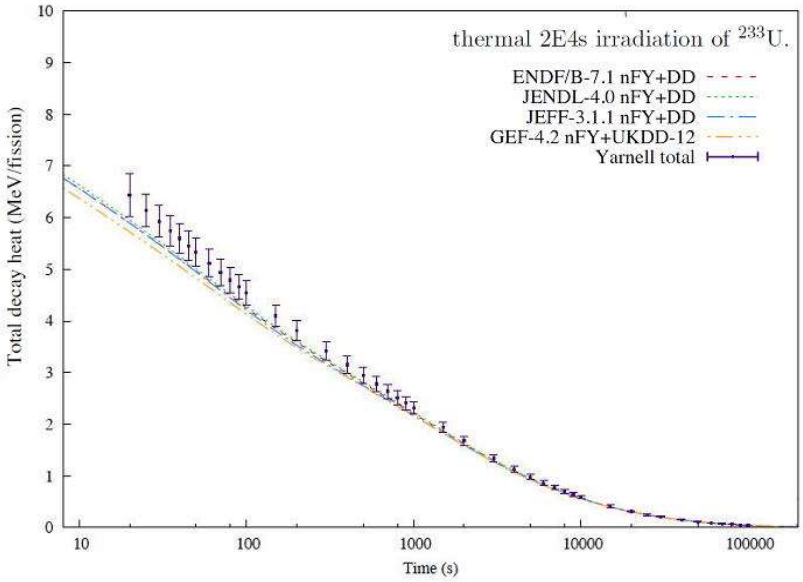


FIG.35. Decay heat comparison for U-233 (reproduced courtesy of Los Alamos Scientific Lab [25]).

Numerical data during a period of cooling time of 20 seconds are shown in Table 28, where decay heat of U-233 is shown to be slightly lower than that of U-235. This confirms that decay heat of U-233 is slightly lower than that of U-235 at short periods of cooling time. ORIGEN2 results are consistent with both measurements and calculations with updated nuclear cross section libraries. Note that this comparison is for 20 000 seconds irradiation case and cannot be generalized for 3–4 years long irradiation case.

TABLE 28. DECAY HEAT COMPARISON BETWEEN U-235 AND U-233 DURING THE PERIOD OF COOLING TIME OF 20 SEC AFTER 20 000 SEC IRRADIATIONS

	U-235 (MeV/fission)	*U-233 (MeV/fission)*
Yarnell's measurement [25]	6.93	6.43 (-7%)
ORIGEN2 (based on 200 MeV/fission)	6.74 (U-220 library)	5.89 (-13%) (Th-214 library)
JENDL-4.0 [24]	6.90	6.00 (-13%)

6.5. DECAY HEAT ASSESSMENTS

6.5.1. Results for the U core and the Th core

Decay heat for the U core was calculated using U220-library for 50 GW·d/t PWR. As for Th core, Th-214 library was used.

As shown in Fig.36, the Th core shows 10% higher decay heat than the U core up to 100 days. Also, there is a peak of decay heat at 0.1 million years for the Th core.

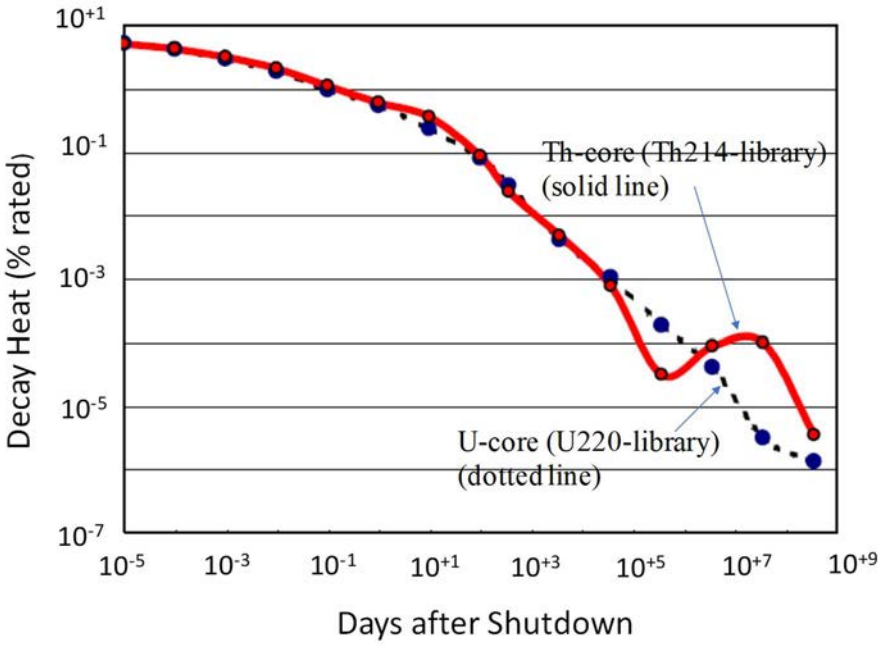


FIG.36. Decay heat for U fuel and Th fuel (long range).

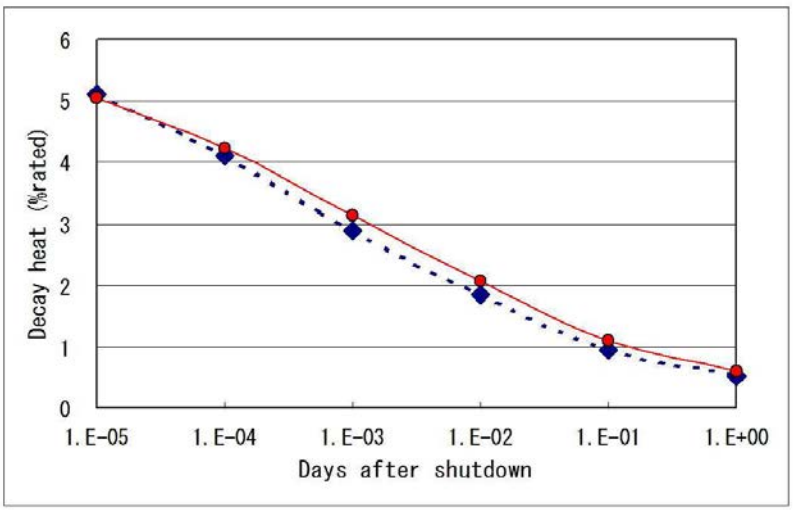
Numerical data of the above assessments are presented in Table 29.

TABLE 29. DECAY HEAT FOR THE U CORE (220-lib) AND THE Th CORE (214-lib) (% RATED)

Time (Sec) *Time (day)*	*0.9* *1E-5*	*9* *1E-4*	*86* *1E-3*	*864* *1E-2*	*1E-1*	*1*	*1E+1*	*1E+2*
U core	5.11 E+00	4.11 E+00	2.89 E+00	1.84 E+00	9.49 E-01	5.32 E-01	2.28 E-01	7.74 E-02
Th core	5.05 E+00	4.23 E+00	3.14 E+00	2.07 E+00	1.10 E+00	5.97 E-01	3.55 E-01	8.44 E-02
Difference (%)	-1.1	2.9	8.8	12.3	15.6	12.2	55.6	9.1

Time(yr) *Time (day)*	*1* *365*	*10* *3650*	*100* *36500*	*1E3* *3.65E05*	*1E4* *3.65E06*	*1E5* *3.65E07*	*1E6* *3.65E08*
U core	2.91 E-02	4.03 E-03	1.03 E-03	1.79 E-04	3.98 E-05	3.02 E-06	1.28 E-06
Th core	2.30 E-02	4.67 E-03	7.46 E-04	3.01 E-05	8.57 E-05	9.54 E-05	3.37 E-06
Difference (%)	-21.0	15.7	-27.2	-83.2	115.2	3058.8	163.2

As for a short-term trend, shown in Fig.37, the Th core shows 10% higher decay heat than the U core up to 1 day, which is important for accident analysis.



Dotted: UO_2 core (U220-library), Solid**:** Th fuel core (Th214-library)

FIG. 37. Decay heat for Th fuel and UO_2 fuel (short range in linear scale).

6.5.1.1. General trend observed in other papers

Figure 38 shows a comparison of the decay heat between the U core and the Th core, taken from [19]. The general trend observed in Fig.38 is consistent with ORIGEN2 result given in Fig.36, although the time span is somewhat different in both figures. In Fig.38, decay heat is presented in units of watt per one PWR fuel assembly. Burnup and decay heat were calculated by a unit-cell code for PWR fuel. UO_2 fuel assembly weight was 467 kg with 4.3% enrichment ^{235}U-^{238}U, and its burnup was 52.5 GW·d/t. ThO_2 fuel assembly weight was 421 kg with 4.3% enrichment ^{233}U-^{232}Th, and its burnup was 60 GW·d/t.

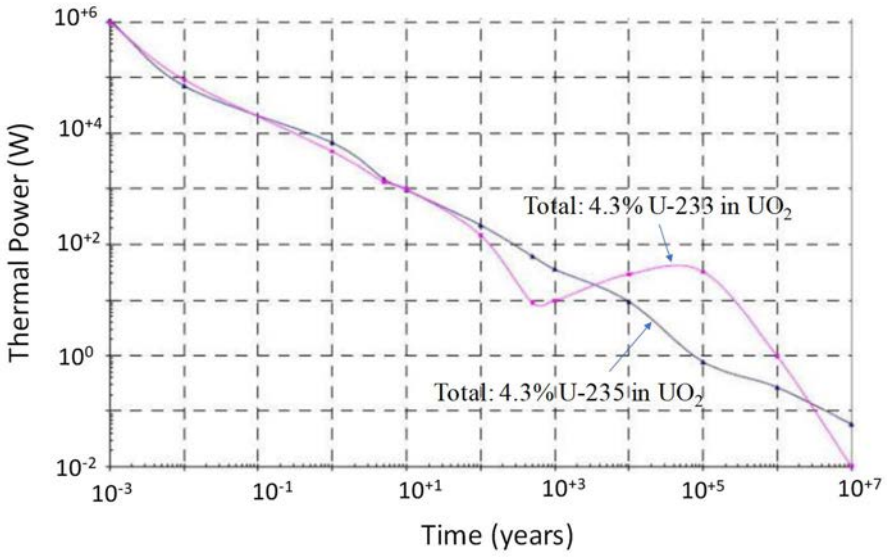


FIG. 38. Decay heat for Th fuel and U fuel (reproduced from [19]).

The Japan Atomic Energy Agency (JAEA) has also published its results on U-233 and U-235 decay heat. Since JAEA's results were calculated using its own code, there might have been

some bias in the results [27] and hence not repeated here. The Argonne National Laboratory has also calculated decay heat for Th core; however, the Th core had a special design with seed and blanket, which is not appropriate for a comparative study [28].

6.5.2. Results for PWR MOX core

Decay heat assessments for PWR MOX core are described in this subsection based on ORIGEN2 calculation. As assumed in Section 4 for MOX fuel, 7.50% Pu-total content fuel is considered as equivalent to 4% enriched UO_2 fuel at the discharge burnup of 45 GW·d/t. For simplicity Pu is considered mixed with 100% U-238.

Table 30 represents Pu vector before burnup based on the ORIGEN2 calculation on the 4.0% enriched UO_2 fuel irradiated to 45 GW·d/t at a PWR; the fuel was cooled for 7 years and reprocessed.

TABLE 30. ASSUMED PLUTONIUM ISOTOPES FRACTION IN INITIAL MOX FUEL

Pu nuclide	*Wt.%*	*% fraction in Put*
U-238	92.50	---
Pu-238	0.19	2.46
Pu-239	4.10	54.69
Pu-240	1.96	26.16
Pu-241	0.71	9.51
Pu-242	0.54	7.18
total	100.00	100.00

The results for both MOX and UO_2 cores are shown in Fig.39 and Table 31 for the discharge burnup of 45 GW·d/t. Here, decay heat data are presented in units of W/t-HM.

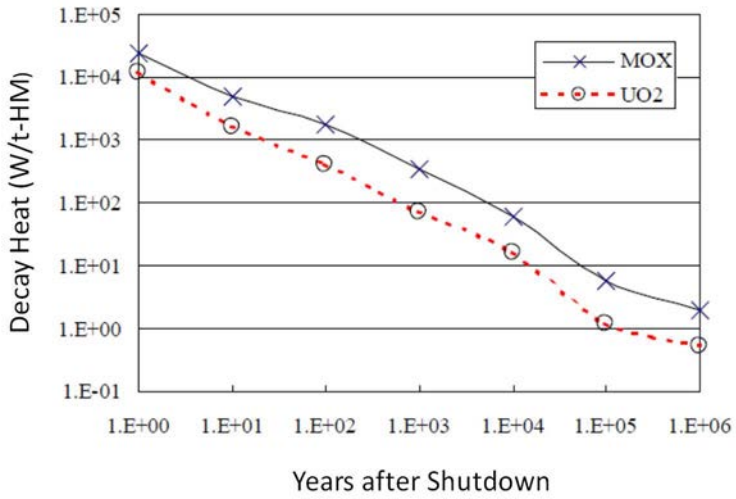


FIG.39. Decay heat for PWR MOX fuel and UO_2 fuel (W/t-HM).

The bottom row of Table 31 shows the ratio of decay heat from the MOX core over from the UO_2 core. the MOX core showed almost 2–4 times higher decay heat than the UO_2 core for time periods ranging from 1 year to 1 million years. This was caused by 4 times larger amount of Pu in the MOX core than the UO_2 fuel at 45 GW·d/t. This also indicates that Pu and its daughter nuclides significantly contribute to decay heat during the long term period of time.

TABLE 31. DECAY HEAT FOR PWR MOX FUEL AND UO_2 FUEL (W/t-HM)

year	*1*	*10*	*100*	*1.00E+03*	*1.00E+04*	*1.00E+05*	*1.00E+06*
MOX	2.424E+04	4.823E+03	1.781E+03	3.359E+02	6.118E+01	5.609E+00	1.896E+00
UO_2	1.141E+04	1.580E+03	4.038E+02	7.017E+01	1.560E+01	1.184E+00	5.018E-01
Ratio	2.12	3.05	4.41	4.79	3.92	4.74	3.78

Figure 40 shows fractional decay heat by actinides for both MOX and UO_2 fuels, which shows that actinide contribution in the MOX fuel is larger than that in the UO_2 fuel from 1 to 1000 years.

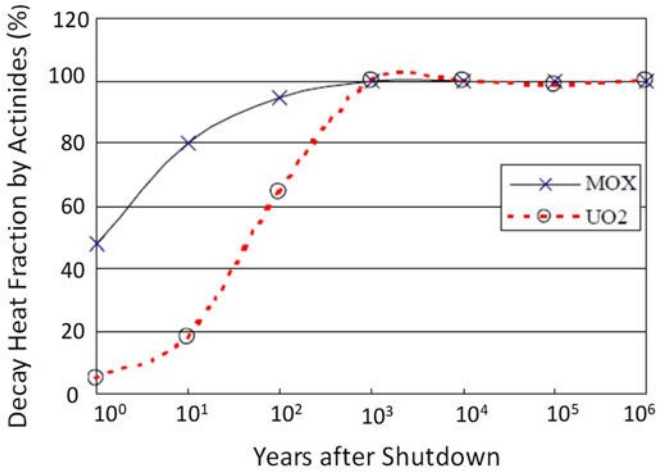


FIG.40. Decay heat fraction by actinides for PWR MOX and UO_2 (%).

Figure 41 shows a comparison of decay heat for the U core and the Th core for a period from 0.01 day to 20 000 days (about 50 years), taken from [29]. Figure 41 is consistent with Fig.39 for the range of first 50 years.

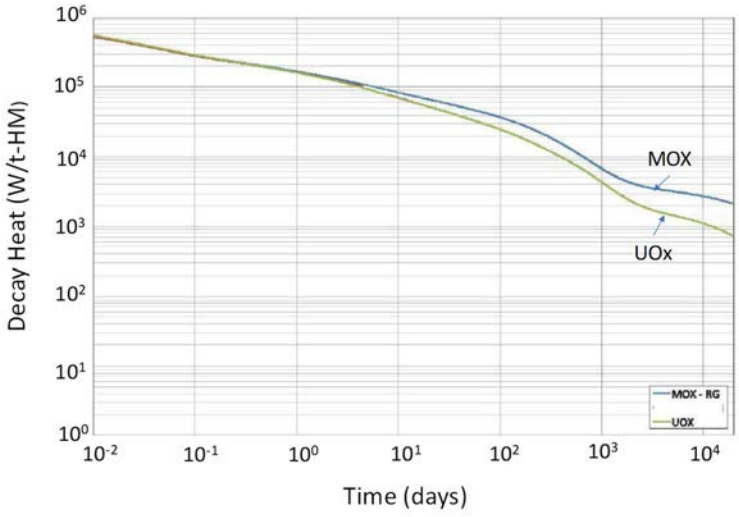


FIG.41. Decay heat for PWR MOX fuel and UO_2 fuel (W/t-HM) (reproduced courtesy of ORNL [29]).

6.5.3. Results for BWR UO_2 core

In general, cross sections between PWRs and BWRs are similar to each other, and thus generate roughly same amount of FPs and actinides. Power density (specific power) could be different between PWRs and BWRs; however, power density does not remarkably affect the accumulation of actinides except for Am-241 at the same burnup condition.

Figure 42 shows decay heat for the BWR UO_2 core, calculated by ORIGEN2 with BWR-U252-library for 4% enrichment UO_2 fuel at a burnup of 45 GW·d/t. Figure 42 shows the previous PWR result too. Here, the decay heat is expressed in units of W/t-HM. Both BWR fuel and PWR fuel are considered to have contained the same U-235 weight in one t-HM and have been discharged at the same burnup.

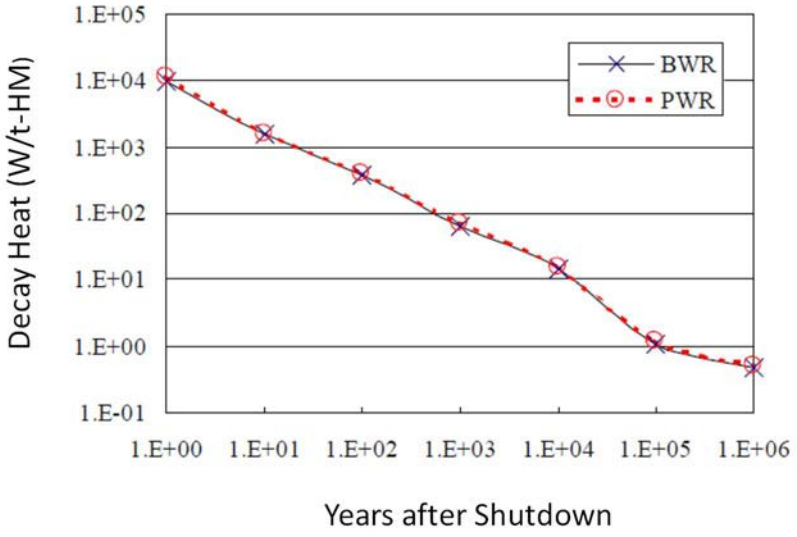


FIG.42. Decay heat for BWR and PWR for UO_2 fuel (W/t-HM).

As a result, almost identical number of fissions and FPs/actinides weight are expected for both fuels. Therefore, decay heat curves for both fuels are also identical as shown in Fig.42. To be precisely, decay heat from the BWR core is 5–10 % smaller than that from PWR for time periods ranging from 10 years to 1 million years due to BWR's softer neutron spectrum and less Pu accumulation.

Figure 43 shows the comparison study of BWR decay heat for U-core and MOX-core by ORNL using its own design code from 0.01 day to 20 000 days (about 50 years) (Fig.15 of [29]). The tendency of these two BWR cores is similar to the previous PWR core case (Fig.41) as shown in Fig.42. These results indicate that BWR decay heat can be calculated by PWR data for UO_2, ThO_2, and MOX fuel.

6.6. IMPLEMENTATION IN NFCSS

From the decay heat assessments using ORIGEN2 for UO_2, ThO_2 and MOX fuel core in PWRs, the overall characteristics of the decay heat were found as follows [21], [30], [31]:

- The Th core has 10% higher decay heat than the U core after shutdown to 1 day;
- After 100 years, the Th core has smaller decay heat than the U core, except the peak that appears between 10 000 to 100 000 years, caused by U-233 and its daughters;

- The MOX core has 2–4 times higher decay heat than the UO_2 core for time periods ranging from 1 year to 1 million years.

Since CAIN calculates weights of only 18 actinides (Th-232, Pa-233, U-233, U-234, U-235, U-236, U-238, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Np-237, Am-241, Am-242m, Am-243, Cm-242 and Cm-244) and does not calculate FPs, direct calculation of decay heat by the CAIN is not possible. Instead, a method of using a lookup table is recommended to calculate decay heat.

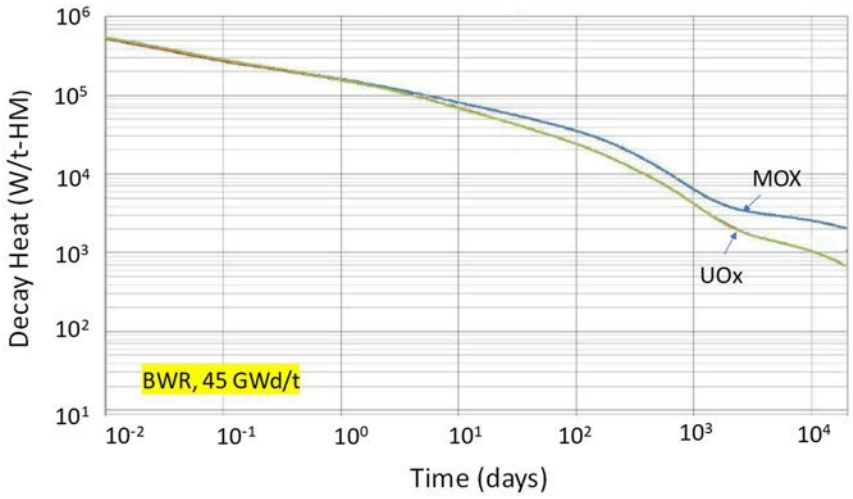


FIG.43. Decay heat for BWR UO_2 and MOX fuel (W/t-HM) (reproduced courtesy of ORNL [29]).

Figure 44 and Table 32 show decay heat results for a burnup of 45 GW·d/t -HM in PWR and BWR. This lookup table data needs to be interpolated in terms of burnup and cooling year.

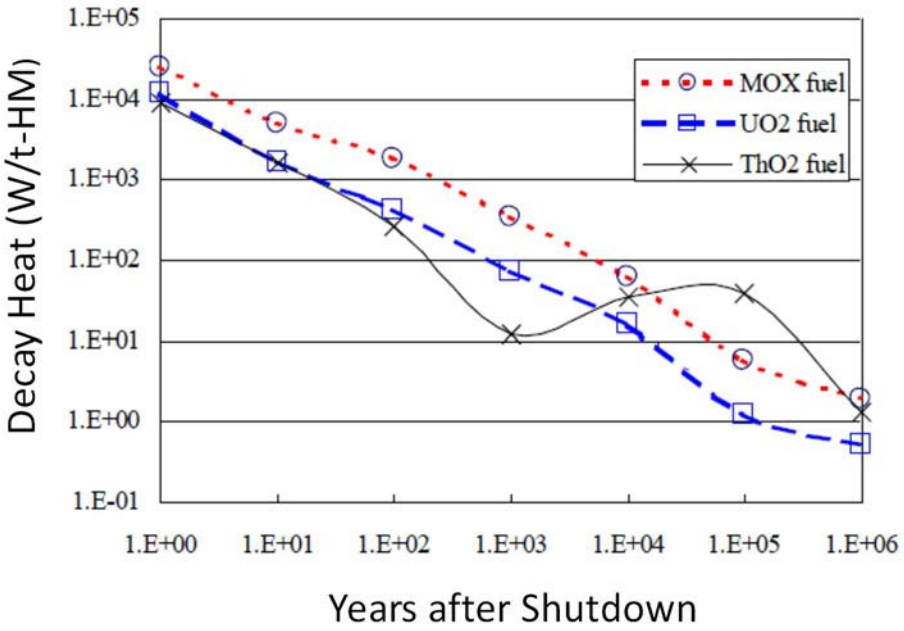


FIG.44. Decay heat for PWR/BWR UO_2/ThO_2/MOX fuel (W/t-HM).

TABLE 32. DECAY HEAT TABLE FOR PWR/BWR UO_2/ThO_2/MOX FUEL (W/t-HM)

year	*1*	*10*	*100*	*1.00E+03*	*1.00E+04*	*1.00E+05*	*1.00E+06*
UO_2	1.141E+04	1.580E+03	4.038E+02	7.017E+01	1.560E+01	1.184E+00	5.018E-01
ThO_2	8.881E+03	1.595E+03	2.574E+02	1.225E+01	3.549E+01	3.920E+01	1.289E+00
MOX	2.424E+04	4.823E+03	1.781E+03	3.359E+02	6.118E+01	5.609E+00	1.896E+00

Interpolation in terms of burnup is done using Equation (6):

$$DH = [DH\text{-reference}] \times BU / 45 \quad (6)$$

where, the reference decay heat (W/t-HM) is shown in TABLE 32 for both PWR and BWR.

If total decay heat is required for the whole fuel batch at the specified year, then the above DH value must be multiplied by the discharged total fuel weight, which is calculated by CAIN.

Interpolation for a specific year is done using:

$$y = y_i + (y_{i+1}-y_i)(x-x_i)/(x_{i+1}-x_i) \quad (7)$$

Here,

$y=\ln(DH)$,
$y_i=\ln(DH_i)$,
$y_{i+1}=\ln(DH_{i+1})$,
$x=\ln(YEAR)$,
$x_i=\ln(YEAR_i)$,
$x_{i+1}=\ln(YEAR_{i+1})$,
$DH=\exp(y)$.

For ThO_2 fuel, 4% U-233 + 96% Th-232 is assumed. For other fuel types such as Pu-ThO_2 fuel, other decay heat tables may be required.

The Excel spreadsheet that calculates decay heat according to the methods described in this section is available from the IAEA web site for the NFCSS:

https://infcis.iaea.org/NFCSS/NFCSSHelp.cshtml.

7. METHOD FOR RADIOTOXICITY CALCULATION

7.1. GENERAL

Radiotoxicity is the required information for managing spent fuel in temporary storage facilities or in geological repositories for permanent disposal. Since radiotoxicity is caused by the decay of actinides and FPs, it mainly depends on the fuel type, i.e. UO_2 fuel, MOX fuel or Th fuel. Methods for radiotoxicity calculation are well established for UO_2 fuel, however, information on radiotoxicity of thorium fuel and MOX fuel are very limited.

In this section, methods for calculating radiotoxicity of UO_2, MOX fuel and thorium fuel are described.

7.2. ASSESSMENT FOR UO_2 FUEL CORE AND THORIUM FUEL CORE IN PWRS

7.2.1. Calculation method

The ORIGEN2 code [15] was used to assess radiotoxicity for the following cores. A constant rated power density of 39.2 MW/t was considered for fuels irradiated to 45 GW·d/t, and radiotoxicity was assessed for time periods up to 1 million years.

(a) U-PWR-core: 4% U-235＋96% U-238, U220-library;
(b) Th-PWR-core: 4% U-233 + 96% Th-232, Th214-library.

Radioactivity calculated by ORIGEN2 was converted to radiotoxicity using Equation (8). Note that ORIGEN2 provides the radioactivity of 1-ton HM (initial Heavy Metal) in units of 'Curie', which needs to be converted to the unit of 'Becquerel'.

$$\text{Radiotoxicity [Sv/t-HM]} = \text{Radioactivity [Bq/t-HM]} \times \text{DCF [Sv/Bq]} \quad (8)$$

where,

Radioactivity [Bq/t-HM] = Radioactivity [Curies/t-HM] × [3.7×10^{10}],
DCF: Dose Conversion Factor (or Dose Coefficient) [Sv/Bq].

Radiotoxicity is an index of toxicity; when a nuclide is taken into a human body, it causes as internal radiation exposure. It depends on type of radiation, energy and impact on human body that is expressed in terms of a dose conversion factor (DCF). Most DCFs can be found from by various references, e.g. [32] and [33]. DCFs of some other nuclides also can be found from [34] and [35], or can be assumed by authors.

These DCF values are applied to adults. In general, DCFs for children are high, and for babies almost 10 times higher than for adults although they ingest only one-tenth of radioactivity due to their lower weights. Since actual influence of radioactivity on the total population is complicated, DCFs for adults are used in this section. DCF is applied to adults who have about 50 years of remaining lifetime, and it considers both physical half-life and biological half-life in the human body within that 50 years.

Two possible paths for internal expose are considered: One is ingestion through mouth by drinking radioactive water etc., and another is inhalation by breathing. Along different paths, DCFs become different each other [32]. For example, the DCF for ingestion of Pu-239 is 2.5×10^{-7} Sv/Bq and the DCF for inhalation of small particles (e.g. 5 micrometre diameter) is 3.2×10^{-5} Sv/Bq which is almost 100 times higher than the former case). Radiotoxicity is generally discussed with ingestion scenario, if it involves spent fuel considering that the primary pathway for radionuclide dispersion is through ingestion. Meanwhile, inhalation scenario is important for reactor accidents.

Radiotoxicity is expressed in units of Sv/t-HM (Sievert/1-ton of initial Heavy Metal). It can also be expressed in Sv/gram-HM, Sv/assembly or Sv/GW(e)/year. In this section, the unit of Sv/t-HM is used.

There is another calculation method using 'ingestion hazard', which is directly computed in ORIGEN2. Ingestion hazard is defined as "the amount of water (m^3) needed to dilute 1 ton of spent fuel in order to reduce potential intake of ingestion below the threshold for the general public set by regulatory authorities". Since there is neither description on supporting data nor

description for this threshold or description of calculation process in the ORIGEN2 manual [15], this method was not adopted. A preliminary study by the authors also indicated that this method would not be appropriate for obtaining accurate results.

7.2.2. Comparison between the U core and the Th core in PWR

Figure 45 shows a comparison of radiotoxicities calculated for the U and Th cores in a PWR. The Th core is 10–90% lower radiotoxicity than the U core up to 1000 years; after 10 000 years, the trend is reversed. There is a radiotoxicity peak at around 0.1 million year. These curves are shown to be similar with decay heat curves. Numerical values of data in Fig. 45 are represented in Table 33.

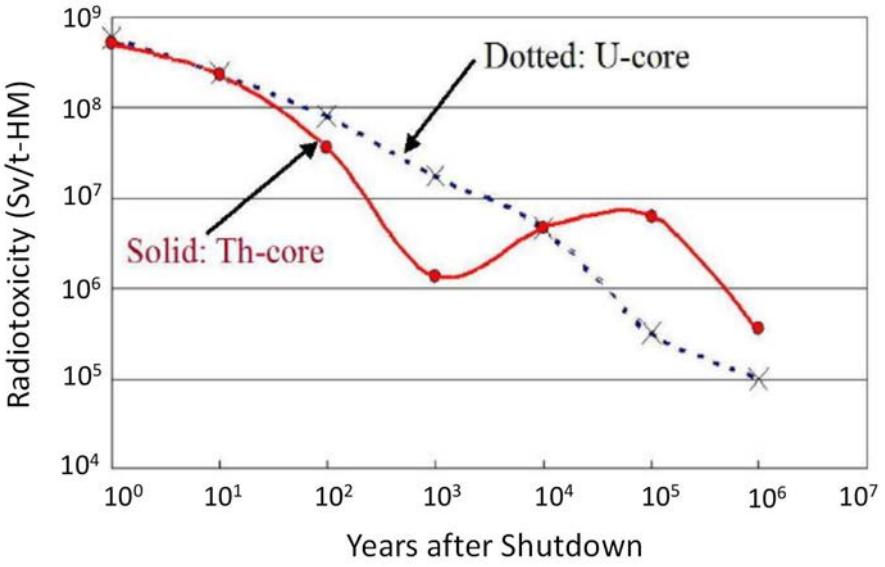


FIG.45. Radiotoxicity for U core and Th core.

TABLE 33. RADIOTOXICITY FOR U CORE AND Th CORE (Sv/t-HM)

year	*1*	*10*	*100*	*1.00E+03*	*1.00E+04*	*1.00E+05*	*1.00E+06*
U core	5.88E+08	2.36E+08	8.18E+07	1.77E+07	4.59E+06	3.30E+05	9.80E+04
Th core	5.18E+08	2.32E+08	3.57E+07	1.32E+06	4.65E+06	6.16E+06	3.51E+05
%	-12.0	-1.9	-56.4	-92.5	1.3	1766.9	258.5

For the U core, the predominant contributor of radiotoxicity during long term storage (e.g. from 10 000 to 100 000 years) is Pu-239, which contributes almost half of the total radiotoxicity.

For the Th core, the main contributor of radiotoxicity during long term storage (e.g. from 10 000 to 100 000 years) is Th-229, whose contribution is close to half the total radiotoxicity. Th-229 is a daughter nuclide of U-233 (half-life: 159 200 year).

Thus, the Th core generates less Pu than the U core and radiotoxicity due to Pu is lower, but a daughter nuclide of U-233 in the Th core causes higher radiotoxicity than the U core during long term storage.

The component of radioactivity is shown in Fig.46 for the U core and Fig.47 for the Th core, respectively. Both figures show that radioactivity from FPs is dominant up to 100 years but decreases rapidly after 100 years. In the long term radioactivity from actinides becomes dominant.

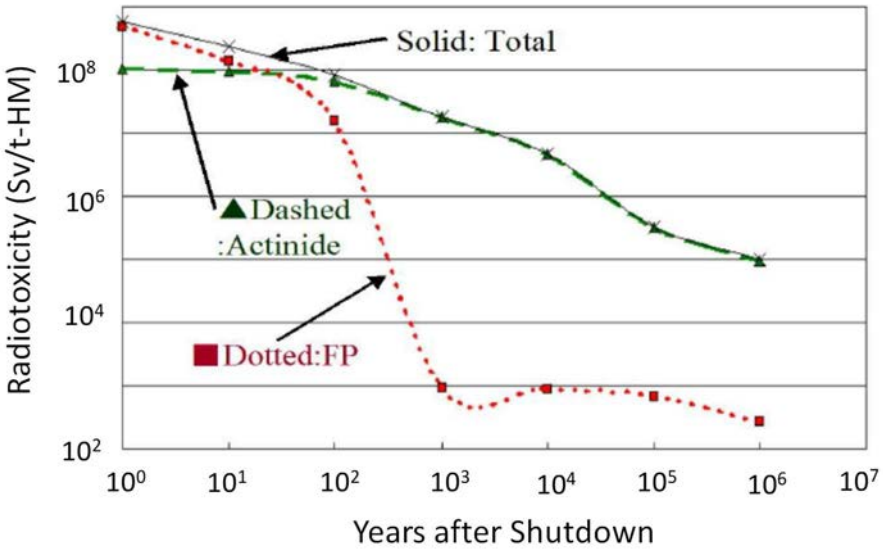


FIG. 46. Component of radiotoxicity for the U core.

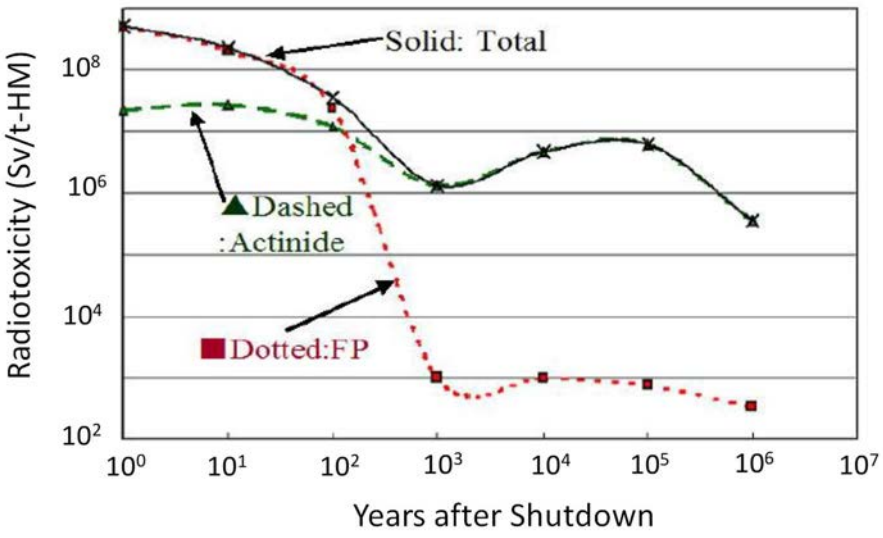


FIG. 47. Component of radiotoxicity for the Th core.

In order to investigate the cause of radiotoxicity peak at 0.1 million year for the Th core, contribution from U-233 and its daughters were evaluated. That is,

- U-233 (Half-life: 159 200 year)→ Th-229 (7340 y) → Ra-225 (14.9 d) → Ac-225 (10.0 d) →Fr-221 (14.9 m) → At-217 (32.3 ms) → Bi-213 (45.59 m) → Po-213 (4.2 μs) → Pb-209 (3.253 h) → Bi-209 (stable).

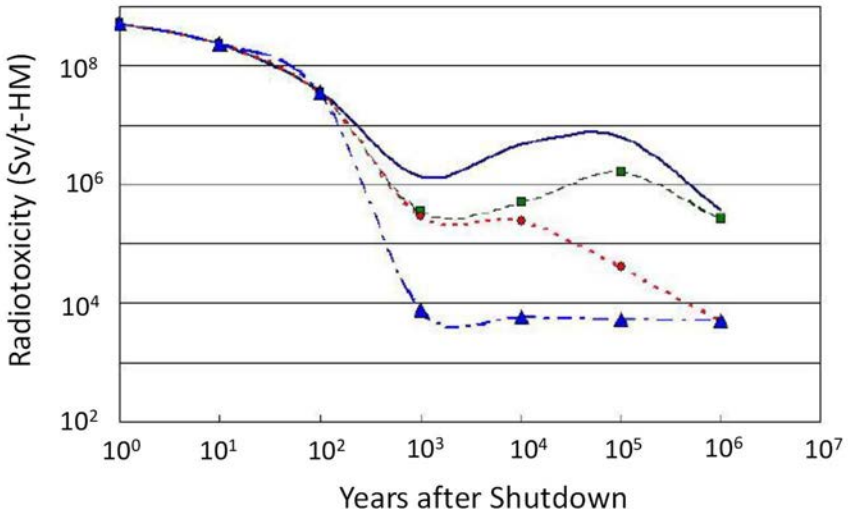
The half-life data here are taken from [22].

In addition to U-233 and its daughters, U-234 and its daughters also contribute to this peak. U-234, generated from U-233 by a neutron absorption, has a very long half-life of 245500 year. The decay chain of U-234 and its daughters is given below:

- U-234 (Half-life: 245 500 year) → Th-230 (75 380 year) → Ra-226 (600 year) →Rn-222 (3.8235 d) → Po-218 (3.10 min) → Pb-214 (26.8 min) →Bi-214 (19.9 min) → Po-214 (164.3 μs) → Pb-210 (22.3 year) → Bi-210 (5.013 d) → Po-210 (138.376 d) → Pb-206 (stable).

This chain also causes the peak and known as transient equilibrium in the theory of radiation chemistry [23].

Figure 48 shows 3 different curves. The top shows the total radiotoxicity. The difference between the top and the second top curves implies the contribution made by U-233 and its daughters. The difference between second top and third top curves implies the contribution made by U-234 and its daughters.



(Solid: Total, ■: Total-^{233}U, ●: Total-^{233}U-^{234}U, ▲: Total-^{233}U-^{234}U-^{231}Pa)

FIG.48. Radiotoxicity for the Th core.

There is still a small peak at around 10 000-year for the third curve. This small peak is caused by the decay of Pa-231, which has a relatively long half-life of 32 760 year. Pa-231 and its daughters cause a small peak or 'transient equilibrium'. In the reactor using thorium fuel, Th-232 absorbs a high energy neutron or gamma, followed by a generation of Th-231 via (n,2n) or (γ,n) reaction. And the following long decay chain is:

- Th-231 (25.52 h) → Pa-231 (32 760 year) → Ac-227 (21.773 year) → Th-227 (18.72 d) → Ra-223 (11.435 d) → Rn-219 (3.96 s) → Po-215 (1.781 ms) → Pb-211 (36.1 min) → Bi-211 (2.14 min) → Tl-207 (4.77 min) → Pb-207 (stable).

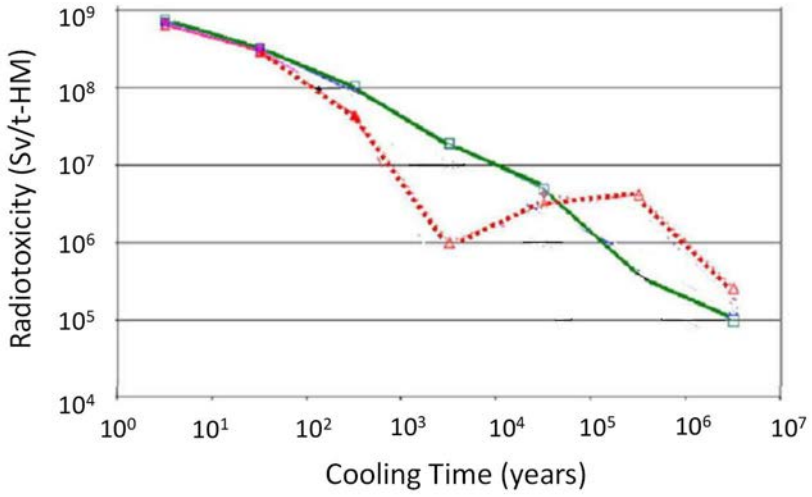
The major contribution to radiotoxicity of actinides up to 100 years is from U-232 and its daughters as shown in Table 39. They are,

- U-232 (Half life: 68.9 year) → Th-228 (1.9116 year) → Ra-224 (3.66 d) → Rn-220 (55.6 s) → Po-216 (0.145 s) → Pb-212 (10.64 h) → Bi-212 (60.55 min) → (Following branch)
  - (Branch ratio: 64 % to) Po-212 (0.299 μs) → Pb-208 (Stable) or
  - (Branch ratio: 36 % to) Tl-208 (3.053 min) → Pb-208 (Stable).

The above results suggest that if the uranium in spent thorium fuel is removed (e.g. by fluorination technology), the radiotoxicity can be reduced significantly.

7.2.3. Comparison with independent calculations

Figure 49 shows radiotoxicity assessment for a Th core performed by British Nuclear Fuels Limited (BNFL) [37]. A fuel assembly design code for PWR fuel was used for burnup and decay; the results displayed in Fig.49 are similar to ORIGEN2 results shown earlier in Fig.45.

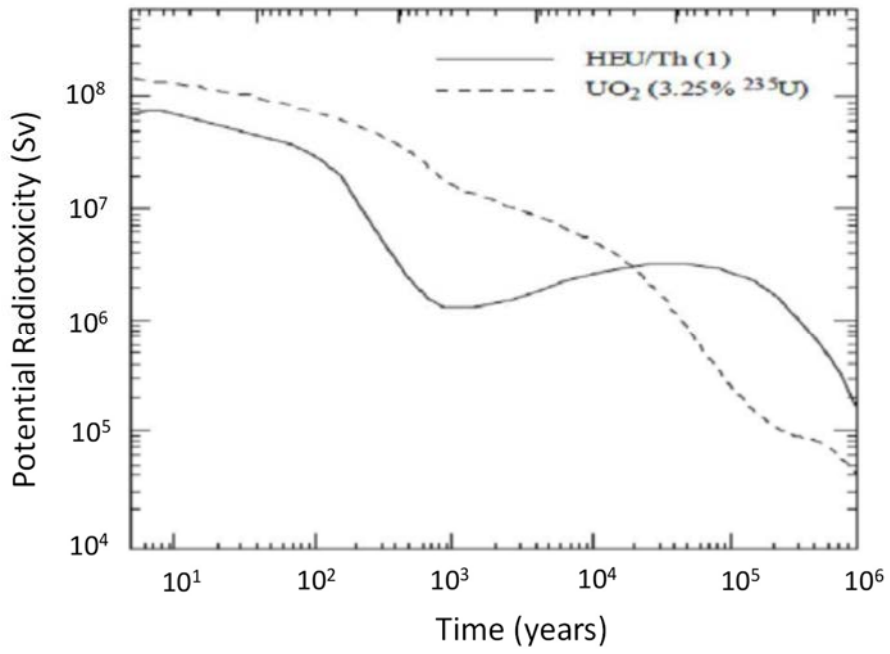


(**Solid**: 4.95% ^{235}U-core, **Dashed**: 4.2% ^{233}U-Th core)

FIG. 49. Radiotoxicity for U core and Th core (reproduced courtesy of BNFL [37]).

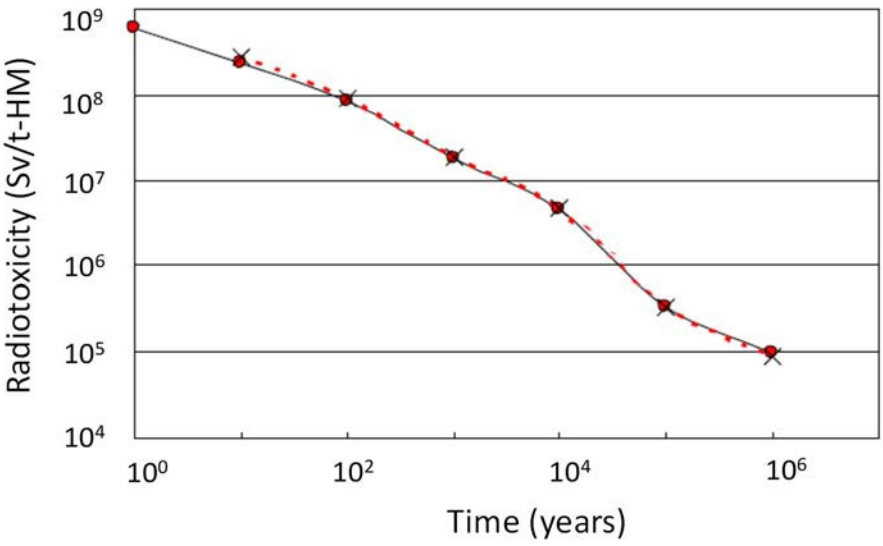
Figure 50 shows radiotoxicity assessment for the U core and the Th core, taken from a paper in IAEA-TECDOC-1319 [6]. These results are different from the results in Fig.45 and Fig.49. Since FP is a main contributor to radiotoxicity up to 100 years, the U core and the Th core should show the same radiotoxicity in this time range. Therefore, this paper is not a suitable benchmark for comparison.

Figure 51 shows radiotoxicity assessment only for a U core, one from [38] and another from ORIGEN2 results. Both calculations agree very well.



(Dashed: 3.25% U-235 core, Solid: Highly enriched ^{235}U-Th core)

FIG. 50. Radiotoxicity for the U core and the Th core (reproduced from [6]).



(●: ORIGEN2, X: IAEA-TRS-435 [38])

FIG.51. Radiotoxicity for the U core.

7.3. ASSESSMENT FOR MOX-CORE IN PWRS

Radiotoxicity for PWR MOX core is described below based on ORIGEN2 calculation. For the assessment, 7.50% Pu-total content (Pu) is assumed to be equivalent to 4.0% enriched UO_2 fuel at 45 GW·d/t discharge burnup. For simplicity, Pu is considered to be mixed with 100% U-238.

Table 34 represents the weight fraction of Pu nuclides (Pu vector) before burnup, which is based on the ORIGEN2 calculation for the 4.0% enriched PWR UO_2 fuel that was irradiated to 45 GW·d/t and reprocessed following cooling for 7 years. This Pu vector is identical to that of MOX fuel considered in the decay heat study.

TABLE 34. ASSUMED PLUTONIUM ISOTOPES FRACTION IN INITIAL MOX FUEL

Pu nuclide	*wt.%*	*% fraction in Pu total content*
U-238	92.50	---
Pu-238	0.19	2.46
Pu-239	4.10	54.69
Pu-240	1.96	26.16
Pu-241	0.71	9.51
Pu-242	0.54	7.18
total	100.00	100.00

Figure 52 shows the radiotoxicity of MOX fuel in comparison with UO_2 fuel. Numerical values are also shown in Table 35 for both MOX fuel and UO_2 fuel, which are discharged at 45 GWd/t. The 4th row of Table 35 is the radiotoxicity ratio of MOX fuel to UO_2 fuel, and radiotoxicity of MOX fuel is 4–5 times higher than that of UO_2 fuel from 10 years to 1 million years.

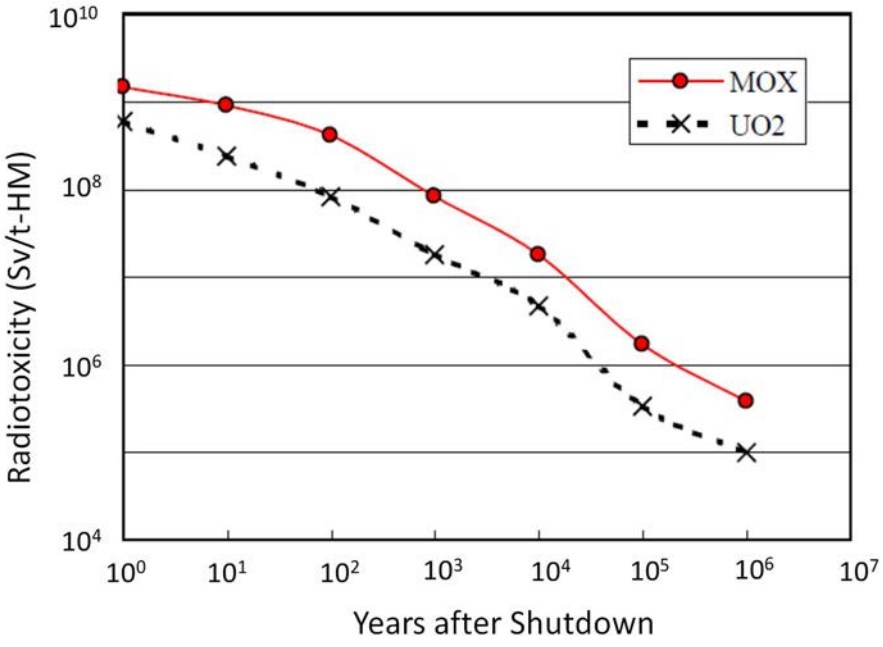


FIG.52. Radiotoxicity for MOX fuel and UO_2 fuel (Sv/t-HM).

TABLE 35. RADIOTOXICITY FOR MOX FUEL AND UO_2 FUEL (Sv/t-HM)

year	*1*	*10*	*100*	*1.00E+03*	*1.00E+04*	*1.00E+05*	*1.00E+06*
MOX	1.457E+09	8.967E+08	4.082E+08	8.205E+07	1.757E+07	1.672E+06	3.728E+05
UO_2	5.878E+08	2.358E+08	8.181E+07	1.770E+07	4.591E+06	3.297E+05	9.797E+04
Ratio	2.5	3.8	5.0	4.6	3.8	5.1	3.8

This is attributed to larger amount of Pu (4 times) in MOX fuel than UO_2 fuel at 45 GW·d/t, and therefore, the contribution of Pu and its daughter nuclides radiotoxicity is high in the MOX fuel during the long term storage. Another factor is contribution from Cm-242 and Cm-244. For example, although the amount of Cm-242 is small, its half-life is very short (162.8 days), and its radiotoxicity is high at early period to 10 years.

Components of radiotoxicity for MOX fuel are shown in Fig.53. Fission products and actinides show similar behaviour with that observed in UO_2 fuel; as described, the contribution of actinide is shown to be large for the period of 1 to 1 million years.

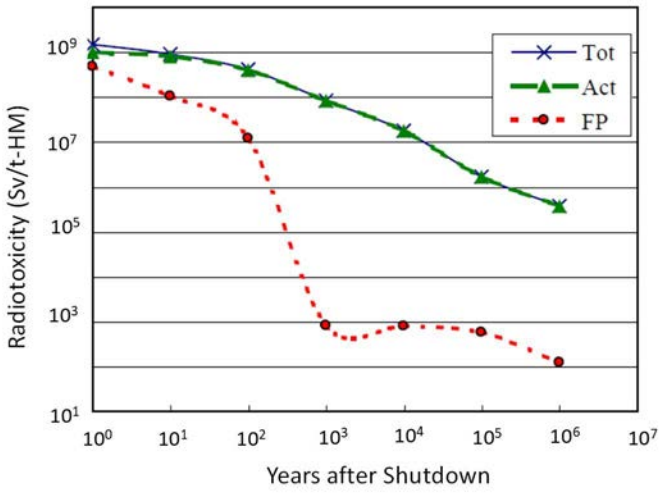


FIG.53. Component of radiotoxicity for MOX fuel (Sv/t-HM).

Figure 54 shows BNFL's results for UO_2 and MOX cores, where burnup and decay are calculated by a fuel assembly design code for PWR fuel [37]. Since this MOX fuel assumes 10.5 wt.% Put content, it is reasonable that radiotoxicity of MOX fuel is slightly higher than results from ORIGEN2 which assumes 7.5 wt.% Pu_t.

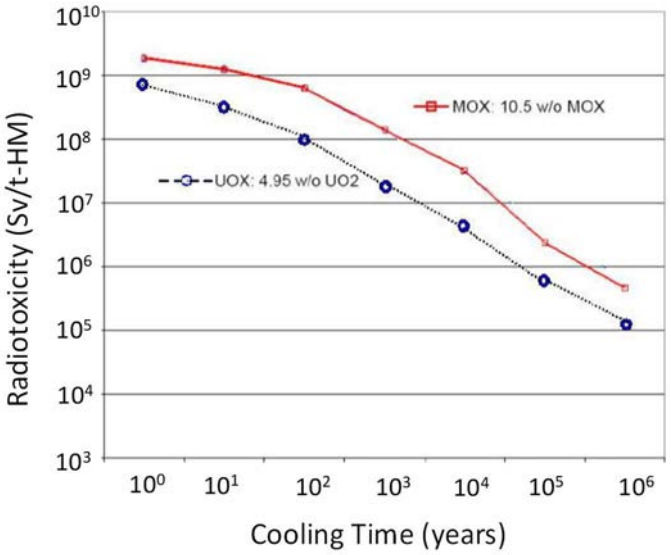


FIG.54. Radiotoxicity for MOX fuel and UO_2 fuel (Sv/t-HM).

7.4. LOOKUP TABLES OF RADIOTOXICITY FOR UO_2, THO_2 AND MOX

Numerical values of radiotoxicity are presented in Table 36 and Table 37 for UO_2 fuel, Table 38 and Table 39 for ThO_2 fuel, and Table 40 and Table 41 for MOX fuel.

In these tables, the first column shows nuclide names in alphabetical order. The second column shows 'DCF' (Dose Conversion Factor, or Dose Coefficient). Most DCF data were taken from [32] and [33]. DCF of some nuclides (*in italic character*) not provided in these two references were supplemented with information from [34] and [35]. Several DCFs were assumed by the author (those with * mark), but these contributions were small. From the third column onwards, radioactivity is shown in units of Sv/t-HM.

In these tables, gaseous nuclides such as Xe, Kr, and Rn are not included because it is impossible to account as "ingestion" for spent fuels.

TABLE 36. RADIOTOXICITY BY FPs OF THE U CORE (Sv/t-HM)

Nuclide	*DCF*	*1 year*	*10 year*	*100 year*	*1.00E+03 year*	*1.00E+04 year*	*1.00E+05 year*	*1.00E+06 year*
Ag-110m	2.80E-09	2.05E+05	2.25E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ba-137m	*1.00E-12*	4.70E+03	3.81E+03	4.77E+02	4.44E-07	0.00E+00	0.00E+00	0.00E+00
Cd-113m	2.30E-08	3.69E+04	2.41E+04	3.35E+02	9.00E-17	0.00E+00	0.00E+00	0.00E+00
Ce-144	5.20E-09	1.04E+08	3.43E+04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cs-134	1.90E-08	1.25E+08	6.07E+06	4.40E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cs-135	2.00E-09	3.94E+01	3.94E+01	3.94E+01	3.94E+01	3.92E+01	3.82E+01	2.91E+01
Cs-137	1.30E-08	6.45E+07	5.24E+07	6.55E+06	6.09E-03	0.00E+00	0.00E+00	0.00E+00
Eu-152	1.40E-09	3.34E+02	2.11E+02	2.15E+00	2.59E-20	0.00E+00	0.00E+00	0.00E+00
Eu-154	2.00E-09	1.01E+06	4.88E+05	3.45E+02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Eu-155	3.20E-10	9.84E+04	2.80E+04	9.63E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ho-166m	2.00E-09	2.73E-01	2.71E-01	2.58E-01	1.53E-01	8.46E-04	0.00E+00	0.00E+00
I-129	1.10E-07	1.66E+02	1.66E+02	1.66E+02	1.66E+02	1.66E+02	1.65E+02	1.59E+02
Nb-94	1.70E-09	1.43E-02	1.42E-02	1.42E-02	1.38E-02	1.01E-02	4.69E-04	2.11E-17
Pd-107	3.70E-11	1.85E-01	1.85E-01	1.85E-01	1.85E-01	1.84E-01	1.83E-01	1.66E-01
Pm-146	9.00E-10	1.36E+02	4.36E+01	5.17E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pm-147	2.60E-10	9.85E+05	9.13E+04	4.30E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pr-144	*5.00E-11*	1.00E+06	3.30E+02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Rb-87	1.50E-09	1.58E-03	1.58E-03	1.58E-03	1.58E-03	1.58E-03	1.58E-03	1.58E-03
Rh-102	2.60E-09	1.46E+02	1.69E+01	7.70E-09	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Rh-106	*1.60E-10*	1.89E+06	3.88E+03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ru-106	7.00E-09	8.28E+07	1.70E+05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sb-125	1.10E-09	4.30E+05	4.52E+04	7.48E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Se-79	2.90E-09	5.70E+01	5.70E+01	5.69E+01	5.64E+01	5.12E+01	1.96E+01	1.32E-03
Sm-146	5.40E-08	6.56E-04	8.17E-04	8.93E-04	8.93E-04	8.93E-04	8.92E-04	8.84E-04
Sm-147	4.90E-08	4.29E-03	8.42E-03	8.84E-03	8.84E-03	8.84E-03	8.84E-03	8.84E-03
Sm-151	9.80E-11	1.43E+03	1.34E+03	6.69E+02	6.53E-01	0.00E+00	0.00E+00	0.00E+00
Sn-126	4.70E-09	1.45E+02	1.45E+02	1.45E+02	1.44E+02	1.35E+02	7.26E+01	1.42E-01
Sr-90	2.80E-08	9.88E+07	7.97E+07	9.36E+06	4.65E-03	0.00E+00	0.00E+00	0.00E+00
Tc-98	2.00E-09	6.97E-04	6.97E-04	6.97E-04	6.97E-04	6.96E-04	6.86E-04	5.91E-04
Tc-99	6.40E-10	3.90E+02	3.90E+02	3.90E+02	3.89E+02	3.77E+02	2.82E+02	1.51E+01
Te-127m	2.30E-09	1.34E+05	1.12E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Zr-93	1.10E-09	9.79E+01	9.79E+01	9.78E+01	9.78E+01	9.74E+01	9.35E+01	6.22E+01
	sum(Sv/t)	4.81E+08	1.39E+08	1.59E+07	8.94E+02	8.67E+02	6.71E+02	2.66E+02

TABLE 37. RADIOTOXICITY BY ACTINIDES OF THE U CORE (Sv/t-HM)

Nuclide	*DCF*	*1 year*	*10 year*	*100 year*	*1.00E+03 year*	*1.00E+04 year*	*1.00E+05 year*	*1.00E+06 year*
Ac-225	2.40E-08	9.24E-05	1.04E-04	1.06E-03	1.61E-01	2.18E+01	5.32E+02	1.17E+03
Ac-227	1.10E-06	3.65E-03	3.33E-02	1.05E+00	1.46E+01	1.44E+02	9.66E+02	1.20E+03
Ac-228	4.30E-10	1.15E-10	1.36E-09	2.73E-08	2.74E-07	3.17E-06	3.89E-05	3.91E-04
Am-241	2.00E-07	3.32E+06	1.75E+07	3.85E+07	9.19E+06	1.60E+03	1.09E+00	0.00E+00
Am-242	3.00E-10	1.16E+02	1.12E+02	7.41E+01	1.22E+00	1.84E-18	0.00E+00	0.00E+00
Am-242m	1.90E-07	7.40E+04	7.11E+04	4.72E+04	7.78E+02	1.17E-15	0.00E+00	0.00E+00
Am-243	2.00E-07	2.47E+05	2.47E+05	2.45E+05	2.25E+05	9.67E+04	2.06E+01	3.04E-03
At-217	1.00E-07*	3.85E-04	4.35E-04	4.41E-03	6.69E-01	9.07E+01	2.22E+03	4.89E+03
Bi-210	1.30E-09	1.30E-07	1.46E-07	1.65E-04	1.17E-01	5.24E+00	4.14E+01	2.11E+01
Bi-211	1.00E-07*	3.33E-04	3.02E-03	9.58E-02	1.32E+00	1.31E+01	8.78E+01	1.09E+02
Bi-212	2.60E-10	5.81E-02	4.32E-01	2.26E-01	4.79E-05	1.03E-05	2.84E-05	2.36E-04
Bi-213	2.00E-10	7.70E-07	8.70E-07	8.83E-06	1.34E-03	1.81E-01	4.44E+00	9.78E+00
Bi-214	1.10E-10	7.13E-10	4.85E-08	2.91E-05	9.90E-03	4.44E-01	3.50E+00	1.78E+00
Cf-249	*3.50E-07*	1.18E-01	1.92E-01	1.61E-01	2.72E-02	5.05E-10	0.00E+00	0.00E+00
Cf-250	*1.60E-07*	6.00E-01	3.73E-01	3.16E-03	1.25E-10	8.73E-11	2.42E-12	6.52E-28
Cf-251	*3.60E-07*	1.24E-02	1.23E-02	1.15E-02	5.74E-03	5.52E-06	0.00E+00	0.00E+00
Cf-252	*9.00E-08*	5.05E-01	4.75E-02	2.55E-12	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cm-242	1.20E-08	6.23E+06	3.70E+03	2.45E+03	4.04E+01	6.10E-17	0.00E+00	0.00E+00
Cm-243	1.50E-07	2.06E+05	1.65E+05	1.85E+04	5.77E-06	0.00E+00	0.00E+00	0.00E+00
Cm-244	1.20E-07	2.16E+07	1.53E+07	4.88E+05	5.34E-10	0.00E+00	0.00E+00	0.00E+00
Cm-245	2.10E-07	3.78E+03	3.78E+03	3.75E+03	3.48E+03	1.67E+03	1.08E+00	0.00E+00
Cm-246	2.10E-07	9.41E+02	9.39E+02	9.27E+02	8.13E+02	2.17E+02	4.08E-04	3.27E-27
Cm-247	1.90E-07	3.02E-03	3.02E-03	3.02E-03	3.02E-03	3.02E-03	3.01E-03	2.89E-03
Cm-248	7.70E-07	3.51E-02	3.51E-02	3.51E-02	3.51E-02	3.44E-02	2.86E-02	4.55E-03
Fr-221	*1.70E-10*	6.55E-07	7.39E-07	7.50E-06	1.14E-03	1.54E-01	3.77E+00	8.31E+00
Fr-223	*2.40E-09*	1.10E-07	1.00E-06	3.17E-05	4.39E-04	4.34E-03	2.91E-02	3.62E-02
Np-235	*5.30E-11*	1.20E-02	3.80E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Np-236	*1.70E-08*	6.44E-03	6.44E-03	6.44E-03	6.40E-03	6.07E-03	3.53E-03	1.55E-05
Np-237	1.10E-07	1.92E+03	1.94E+03	2.51E+03	5.81E+03	6.98E+03	6.78E+03	5.06E+03
Np-238	9.10E-10	1.77E+00	1.70E+00	1.13E+00	1.86E-02	2.80E-20	0.00E+00	0.00E+00
Np-239	8.00E-10	9.89E+02	9.88E+02	9.80E+02	9.01E+02	3.87E+02	8.25E-02	1.22E-05
Pa-231	7.10E-07	3.48E-02	1.19E-01	9.63E-01	9.40E+00	9.30E+01	6.24E+02	7.77E+02
Pa-233	8.70E-10	1.52E+01	1.53E+01	1.98E+01	4.59E+01	5.52E+01	5.36E+01	4.00E+01
Pa-234	5.10E-10	7.66E-03	7.66E-03	7.66E-03	7.66E-03	7.66E-03	7.66E-03	7.66E-03
Pa-234m	*3.10E-12*	3.58E-02	3.58E-02	3.58E-02	3.58E-02	3.58E-02	3.58E-02	3.58E-02
Pb-209	5.70E-11	2.20E-07	2.48E-07	2.52E-06	3.82E-04	5.17E-02	1.26E+00	2.79E+00
Pb-210	6.90E-07	6.88E-05	7.75E-05	8.76E-02	6.21E+01	2.78E+03	2.20E+04	1.12E+04
Pb-211	1.80E-10	5.99E-07	5.44E-06	1.72E-04	2.38E-03	2.36E-02	1.58E-01	1.97E-01
Pb-212	6.00E-09	1.34E+00	9.97E+00	5.21E+00	1.11E-03	2.37E-04	6.54E-04	5.45E-03
Pb-214	1.40E-10	9.07E-10	6.17E-08	3.70E-05	1.26E-02	5.65E-01	4.46E+00	2.27E+00
Po-210	1.20E-06	1.10E-04	1.35E-04	1.52E-01	1.08E+02	4.84E+03	3.82E+04	1.94E+04
Po-211	1.00E-07*	9.31E-07	8.47E-06	2.68E-04	3.71E-03	3.67E-02	2.46E-01	3.06E-01
Po-212	1.00E-07*	1.43E+01	1.07E+02	5.56E+01	1.18E-02	2.53E-03	6.99E-03	5.82E-02
Po-213	1.00E-07*	3.77E-04	4.26E-04	4.32E-03	6.55E-01	8.87E+01	2.17E+03	4.78E+03
Po-214	1.00E-07*	6.50E-07	4.41E-05	2.64E-02	9.00E+00	4.03E+02	3.18E+03	1.62E+03
Po-215	1.00E-07*	3.33E-04	3.02E-03	9.58E-02	1.32E+00	1.31E+01	8.78E+01	1.09E+02
Po-216	1.00E-07*	2.24E+01	1.66E+02	8.68E+01	1.84E-02	3.95E-03	1.09E-02	9.09E-02
Po-218	1.00E-07*	6.48E-07	4.41E-05	2.64E-02	9.00E+00	4.03E+02	3.18E+03	1.62E+03
Pu-236	*8.60E-08*	3.02E+03	3.39E+02	2.93E-03	2.92E-03	2.76E-03	1.61E-03	7.08E-06
Pu-238	2.30E-07	3.76E+07	3.56E+07	1.75E+07	1.51E+04	2.78E-15	0.00E+00	0.00E+00
Pu-239	2.50E-07	3.33E+06	3.33E+06	3.32E+06	3.24E+06	2.54E+06	1.94E+05	3.80E-03
Pu-240	2.50E-07	5.37E+06	5.40E+06	5.44E+06	4.94E+06	1.90E+06	1.37E+02	8.92E-03
Pu-241	4.80E-09	2.94E+07	1.91E+07	2.51E+05	7.97E+01	3.83E+01	2.48E-02	0.00E+00
Pu-242	2.40E-07	2.48E+04	2.48E+04	2.48E+04	2.48E+04	2.44E+04	2.08E+04	4.14E+03
Pu-243	8.50E-11	1.35E-06	1.35E-06	1.35E-06	1.35E-06	1.35E-06	1.35E-06	1.29E-06
Pu-244	2.40E-07	8.61E-03	8.61E-03	8.61E-03	8.61E-03	8.61E-03	8.61E-03	8.57E-03
Ra-223	1.00E-07	3.33E-04	3.02E-03	9.58E-02	1.32E+00	1.31E+01	8.78E+01	1.09E+02

Nuclide	*DCF*	*1 year*	*10 year*	*100 year*	*1.00E+03 year*	*1.00E+04 year*	*1.00E+05 year*	*1.00E+06 year*
Ra-224	6.50E-08	1.45E+01	1.08E+02	5.64E+01	1.20E-02	2.57E-03	7.09E-03	5.91E-02
Ra-225	9.90E-08	3.81E-04	4.30E-04	4.37E-03	6.63E-01	8.98E+01	2.20E+03	4.84E+03
Ra-226	2.80E-07	1.81E-06	1.23E-04	7.40E-02	2.52E+01	1.13E+03	8.92E+03	4.54E+03
Ra-228	6.90E-07	1.84E-07	2.18E-06	4.38E-05	4.40E-04	5.09E-03	6.24E-02	6.27E-01
Th-227	8.80E-09	2.89E-05	2.62E-04	8.31E-03	1.15E-01	1.14E+00	7.62E+00	9.49E+00
Th-228	7.20E-08	1.61E+01	1.20E+02	6.25E+01	1.33E-02	2.84E-03	7.85E-03	6.54E-02
Th-229	4.90E-07	1.89E-03	2.13E-03	2.16E-02	3.28E+00	4.44E+02	1.09E+04	2.39E+04
Th-230	2.10E-07	2.74E-03	5.57E-02	3.61E+00	1.06E+02	1.09E+03	6.68E+03	3.40E+03
Th-231	3.40E-10	2.12E-01	2.12E-01	2.13E-01	2.17E-01	2.51E-01	3.63E-01	3.72E-01
Th-232	2.30E-07	4.18E-07	1.70E-06	1.46E-05	1.47E-04	1.70E-03	2.08E-02	2.09E-01
Th-234	3.40E-09	3.93E+01	3.93E+01	3.93E+01	3.93E+01	3.93E+01	3.93E+01	3.93E+01
Tl-207	*7.10E-12*	2.36E-08	2.14E-07	6.78E-06	9.38E-05	9.27E-04	6.22E-03	7.74E-03
Tl-208	*8.60E-12*	6.91E-04	5.14E-03	2.68E-03	5.70E-07	1.22E-07	3.37E-07	2.81E-06
Tl-209	*6.40E-12*	5.32E-10	6.01E-10	6.10E-09	9.25E-07	1.25E-04	3.07E-03	6.76E-03
U-232	*3.30E-07*	2.45E+02	6.10E+02	2.79E+02	5.93E-02	1.06E-02	6.16E-03	2.72E-05
U-233	5.10E-08	1.23E-02	4.75E-02	4.49E-01	8.72E+00	1.34E+02	1.13E+03	2.49E+03
U-234	4.90E-08	5.12E+01	2.51E+02	1.64E+03	2.97E+03	2.91E+03	2.38E+03	7.08E+02
U-235	4.70E-08	2.94E+01	2.94E+01	2.94E+01	3.00E+01	3.48E+01	5.02E+01	5.14E+01
U-236	4.70E-08	5.92E+02	5.92E+02	5.95E+02	6.21E+02	7.80E+02	8.78E+02	8.55E+02
U-237	7.60E-10	1.14E+02	7.42E+01	9.74E-01	3.09E-04	1.48E-04	9.63E-08	0.00E+00
U-238	4.50E-08	5.20E+02	5.20E+02	5.20E+02	5.20E+02	5.20E+02	5.20E+02	5.20E+02
U-240	1.10E-09	3.94E-05	3.94E-05	3.94E-05	3.94E-05	3.94E-05	3.94E-05	3.92E-05
	sum(Sv/t)	1.07E+08	9.67E+07	6.59E+07	1.77E+07	4.59E+06	3.29E+05	9.77E+04

*: DCF is assumed by the author.

TABLE 38. RADIOTOXICITY BY FPs OF THE Th CORE (Sv/t-HM)

Nuclide	*DCF*	*1 y*	*10 year*	*100 year*	*1.00E+03 year*	*1.00E+04 year*	*1.00E+05 year*	*1.00E+06 year*
Ag-110m	2.80E-09	2.61E+04	2.87E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ba-137m	*1.00E-12*	5.19E+03	4.21E+03	5.27E+02	4.90E-07	0.00E+00	0.00E+00	0.00E+00
Cd-113m	2.30E-08	1.76E+04	1.15E+04	1.59E+02	4.28E-17	0.00E+00	0.00E+00	0.00E+00
Ce-144	5.20E-09	1.12E+08	3.70E+04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cs-134	1.90E-08	1.17E+08	5.66E+06	4.11E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cs-135	2.00E-09	3.96E+01	3.96E+01	3.96E+01	3.96E+01	3.94E+01	3.84E+01	2.93E+01
Cs-137	1.30E-08	7.13E+07	5.79E+07	7.23E+06	6.73E-03	0.00E+00	0.00E+00	0.00E+00
Eu-152	1.40E-09	8.01E+01	5.06E+01	5.16E-01	6.20E-21	0.00E+00	0.00E+00	0.00E+00
Eu-154	2.00E-09	6.30E+05	3.05E+05	2.16E+02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Eu-155	3.20E-10	4.44E+04	1.26E+04	4.35E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ho-166m	2.00E-09	1.81E-02	1.80E-02	1.71E-02	1.02E-02	5.62E-05	0.00E+00	0.00E+00
I-129	1.10E-07	2.97E+02	2.97E+02	2.97E+02	2.97E+02	2.96E+02	2.95E+02	2.84E+02
Nb-93m	*1.20E-10*	1.71E+00	6.08E+00	1.35E+01	1.36E+01	1.35E+01	1.30E+01	8.64E+00
Nb-94	1.70E-09	5.16E-02	5.16E-02	5.14E-02	4.99E-02	3.67E-02	1.70E-03	7.64E-17
Nb-95	*5.80E-10*	1.80E+06	6.06E-10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Nb-95m	*5.60E-10*	5.72E+03	1.95E-12	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pd-107	3.70E-11	2.24E-02	2.24E-02	2.24E-02	2.24E-02	2.24E-02	2.21E-02	2.01E-02
Pm-146	9.00E-10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pm-147	2.60E-10	1.12E+06	1.04E+05	4.88E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pr-144	*5.00E-11*	1.08E+06	3.56E+02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Rb-87	1.50E-09	3.38E-03	3.38E-03	3.38E-03	3.38E-03	3.38E-03	3.38E-03	3.38E-03
Rh-102	2.60E-09	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Rh-106	*1.60E-10*	2.70E+05	5.54E+02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ru-106	7.00E-09	1.18E+07	2.42E+04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sb-125	1.10E-09	7.92E+05	8.33E+04	1.38E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Se-79	2.90E-09	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sm-146	5.40E-08	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sm-147	4.90E-08	4.67E-03	9.35E-03	9.83E-03	9.83E-03	9.83E-03	9.83E-03	9.83E-03
Sm-151	9.80E-11	4.79E+02	4.47E+02	2.24E+02	2.18E-01	0.00E+00	0.00E+00	0.00E+00

Nuclide	*DCF*	*1 y*	*10 year*	*100 year*	*1.00E+03 year*	*1.00E+04 year*	*1.00E+05 year*	*1.00E+06 year*
Sn-123	*7.30E-10*	1.29E+04	2.81E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sn-126	4.70E-09	3.21E+02	3.21E+02	3.21E+02	3.19E+02	3.00E+02	1.61E+02	3.13E-01
Sr-90	2.80E-08	1.59E+08	1.28E+08	1.50E+07	7.47E-03	0.00E+00	0.00E+00	0.00E+00
Tc-98	2.00E-09	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Tc-99	6.40E-10	3.34E+02	3.34E+02	3.34E+02	3.33E+02	3.23E+02	2.41E+02	1.29E+01
Te-125m	8.70E-10	1.53E+05	1.61E+04	2.66E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Te-127	*1.70E-10*	2.03E+04	1.70E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Te-127m	2.30E-09	2.81E+05	2.35E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Y-90	*2.70E-09*	1.53E+07	1.23E+07	1.45E+06	7.20E-04	0.00E+00	0.00E+00	0.00E+00
Y-91	*2.40E-09*	2.37E+06	2.90E-11	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Zr-93	1.10E-09	4.48E-08	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Zr-95	*8.80E-10*	1.21E+06	4.14E-10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
	sum(Sv/t)	4.95E+08	2.04E+08	2.37E+07	1.00E+03	9.73E+02	7.49E+02	3.35E+02

TABLE 39. RADIOTOXICITY ACTINIDES OF THE Th CORE (Sv/t-HM)

Nuclide	*DCF*	*1 year*	*10 year*	*100 year*	*1.00E+03 year*	*1.00E+04 year*	*1.00E+05 year*	*1.00E+06 year*
Ac-225	2.40E-08	7.19E+01	2.32E+02	1.82E+03	1.70E+04	1.12E+05	1.28E+05	2.50E+03
Ac-227	1.10E-06	9.48E+03	4.32E+04	1.39E+05	1.42E+05	1.18E+05	1.75E+04	6.67E+01
Ac-228	4.30E-10	5.52E-01	1.20E+00	1.62E+00	1.62E+00	1.62E+00	1.62E+00	1.62E+00
Am-241	2.00E-07	1.28E+01	8.48E+01	1.92E+02	4.57E+01	3.74E-04	2.39E-07	0.00E+00
Am-242	3.00E-10	1.71E-04	1.65E-04	1.09E-04	1.80E-06	2.71E-24	0.00E+00	0.00E+00
Am-242m	1.90E-07	1.09E-01	1.05E-01	6.95E-02	1.15E-03	1.72E-21	0.00E+00	0.00E+00
Am-243	2.00E-07	1.88E-01	1.87E-01	1.86E-01	1.71E-01	7.33E-02	1.56E-05	2.05E-10
At-217	1.00E-07*	3.00E+02	9.66E+02	7.60E+03	7.08E+04	4.66E+05	5.33E+05	1.04E+04
Bi-210	1.30E-09	2.25E-02	1.75E-02	3.68E-02	2.74E+00	9.91E+01	7.55E+02	1.27E+02
Bi-211	1.00E-07*	8.63E+02	3.93E+03	1.26E+04	1.29E+04	1.07E+04	1.59E+03	6.07E+00
Bi-212	2.60E-10	5.59E+03	1.08E+04	4.63E+03	1.78E+00	9.81E-01	9.81E-01	9.81E-01
Bi-213	2.00E-10	6.00E-01	1.93E+00	1.52E+01	1.42E+02	9.32E+02	1.07E+03	2.08E+01
Bi-214	1.10E-10	5.95E-05	3.01E-04	4.82E-03	2.32E-01	8.38E+00	6.39E+01	1.08E+01
Cf-249	*3.50E-07*	5.75E-09	9.61E-09	8.05E-09	1.36E-09	2.53E-17	0.00E+00	0.00E+00
Cf-250	*1.60E-07*	1.96E-08	1.22E-08	1.03E-10	4.55E-18	3.18E-18	8.85E-20	2.38E-35
Cf-251	*3.60E-07*	4.11E-10	4.08E-10	3.81E-10	1.90E-10	1.83E-13	0.00E+00	0.00E+00
Cf-252	*9.00E-08*	1.11E-08	1.04E-09	5.60E-20	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cm-242	1.20E-08	6.70E+00	5.45E-03	3.61E-03	5.96E-05	8.97E-23	0.00E+00	0.00E+00
Cm-243	1.50E-07	7.23E-02	5.81E-02	6.51E-03	2.03E-12	0.00E+00	0.00E+00	0.00E+00
Cm-244	1.20E-07	6.70E+00	4.75E+00	1.51E-01	1.66E-16	0.00E+00	0.00E+00	0.00E+00
Cm-245	2.10E-07	8.27E-04	8.27E-04	8.21E-04	7.62E-04	3.66E-04	2.38E-07	0.00E+00
Cm-246	2.10E-07	1.11E-04	1.11E-04	1.09E-04	9.59E-05	2.56E-05	4.82E-11	1.20E-34
Cm-247	1.90E-07	2.04E-10	2.04E-10	2.04E-10	2.04E-10	2.04E-10	2.02E-10	1.95E-10
Cm-248	7.70E-07	2.04E-09	2.04E-09	2.04E-09	2.03E-09	1.99E-09	1.66E-09	2.64E-10
Fr-221	*1.70E-10*	5.10E-01	1.64E+00	1.29E+01	1.20E+02	7.93E+02	9.06E+02	1.77E+01
Fr-223	2.40E-09	2.85E-01	1.30E+00	4.18E+00	4.28E+00	3.53E+00	5.28E-01	2.02E-03
Np-235	*5.30E-11*	7.27E-05	2.31E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Np-236	*1.70E-08*	6.52E-05	6.52E-05	6.52E-05	6.48E-05	6.15E-05	3.57E-05	1.57E-07
Np-237	1.10E-07	1.58E+01	1.58E+01	1.58E+01	1.58E+01	1.58E+01	1.53E+01	1.15E+01
Np-238	9.10E-10	2.61E-06	2.51E-06	1.66E-06	2.75E-08	4.14E-26	0.00E+00	0.00E+00
Np-239	8.00E-10	7.50E-04	7.49E-04	7.43E-04	6.83E-04	2.93E-04	6.25E-08	8.20E-13
Pa-231	7.10E-07	9.36E+04	9.36E+04	9.34E+04	9.16E+04	7.57E+04	1.13E+04	4.31E+01
Pa-233	8.70E-10	7.09E+04	1.25E-01	1.25E-01	1.25E-01	1.25E-01	1.21E-01	9.08E-02
Pa-234	5.10E-10	1.54E-03	6.01E-10	6.01E-10	6.01E-10	6.02E-10	6.02E-10	6.10E-10
Pa-234m	*3.10E-12*	7.12E-03	2.81E-09	2.81E-09	2.81E-09	2.81E-09	2.82E-09	2.84E-09
Pb-209	5.70E-11	1.71E-01	5.51E-01	4.33E+00	4.03E+01	2.66E+02	3.04E+02	5.93E+00
Pb-210	6.90E-07	1.19E+01	9.31E+00	1.95E+01	1.46E+03	5.26E+04	4.01E+05	6.77E+04
Pb-211	1.80E-10	1.55E+00	7.08E+00	2.27E+01	2.32E+01	1.92E+01	2.87E+00	1.09E-02
Pb-212	6.00E-09	1.29E+05	2.48E+05	1.07E+05	4.10E+01	2.26E+01	2.26E+01	2.26E+01

Nuclide	*DCF*	*1 year*	*10 year*	*100 year*	*1.00E+03 year*	*1.00E+04 year*	*1.00E+05 year*	*1.00E+06 year*
Pb-214	1.40E-10	7.57E-05	3.84E-04	6.14E-03	2.95E-01	1.07E+01	8.13E+01	1.38E+01
Po-210	1.20E-06	1.94E+01	1.62E+01	3.40E+01	2.53E+03	9.15E+04	6.97E+05	1.18E+05
Po-211	1.00E-07*	2.42E+00	1.10E+01	3.54E+01	3.62E+01	2.99E+01	4.48E+00	1.70E-02
Po-212	1.00E-07*	1.38E+06	2.65E+06	1.14E+06	4.38E+02	2.41E+02	2.41E+02	2.41E+02
Po-213	1.00E-07*	2.93E+02	9.45E+02	7.44E+03	6.93E+04	4.59E+05	5.22E+05	1.02E+04
Po-214	1.00E-07*	5.44E-02	2.74E-01	4.38E+00	2.11E+02	7.62E+03	5.81E+04	9.81E+03
Po-215	1.00E-07*	8.63E+02	3.93E+03	1.26E+04	1.29E+04	1.07E+04	1.59E+03	6.07E+00
Po-216	1.00E-07*	2.15E+06	4.14E+06	1.78E+06	6.83E+02	3.77E+02	3.77E+02	3.77E+02
Po-218	1.00E-07*	5.41E-02	2.74E-01	4.39E+00	2.11E+02	7.62E+03	5.81E+04	9.84E+03
Pu-236	*8.60E-08*	3.78E+00	4.24E-01	2.97E-05	2.95E-05	2.80E-05	1.63E-05	7.16E-08
Pu-238	2.30E-07	1.42E+05	1.32E+05	6.47E+04	5.29E+01	4.09E-21	0.00E+00	0.00E+00
Pu-239	2.50E-07	6.07E+01	6.07E+01	6.05E+01	5.90E+01	4.55E+01	3.41E+00	2.75E-10
Pu-240	2.50E-07	4.15E+01	4.15E+01	4.11E+01	3.74E+01	1.44E+01	1.04E-03	2.44E-09
Pu-241	4.80E-09	1.49E+02	9.66E+01	1.27E+00	1.75E-05	8.38E-06	5.43E-09	0.00E+00
Pu-242	2.40E-07	4.20E-02	4.20E-02	4.20E-02	4.19E-02	4.13E-02	3.52E-02	7.01E-03
Pu-243	8.50E-11	9.11E-14	9.11E-14	9.11E-14	9.11E-14	9.12E-14	9.06E-14	8.71E-14
Pu-244	2.40E-07	2.36E-09	2.36E-09	2.36E-09	2.36E-09	2.36E-09	2.36E-09	2.34E-09
Ra-223	1.00E-07	8.63E+02	3.93E+03	1.26E+04	1.29E+04	1.07E+04	1.59E+03	6.07E+00
Ra-224	6.50E-08	1.40E+06	2.69E+06	1.16E+06	4.44E+02	2.45E+02	2.45E+02	2.45E+02
Ra-225	9.90E-08	2.97E+02	9.57E+02	7.52E+03	7.01E+04	4.62E+05	5.27E+05	1.03E+04
Ra-226	2.80E-07	1.51E-01	7.68E-01	1.23E+01	5.91E+02	2.13E+04	1.63E+05	2.76E+04
Ra-228	6.90E-07	8.85E+02	1.92E+03	2.59E+03	2.59E+03	2.60E+03	2.60E+03	2.60E+03
Th-227	8.80E-09	7.49E+01	3.41E+02	1.10E+03	1.12E+03	9.28E+02	1.38E+02	5.27E-01
Th-228	7.20E-08	1.54E+06	2.98E+06	1.28E+06	4.92E+02	2.72E+02	2.72E+02	2.72E+02
Th-229	4.90E-07	1.47E+03	4.74E+03	3.72E+04	3.47E+05	2.28E+06	2.61E+06	5.09E+04
Th-230	2.10E-07	1.09E+02	1.29E+02	3.23E+02	2.26E+03	2.05E+04	1.22E+05	2.07E+04
Th-231	3.40E-10	2.07E-02	2.07E-02	2.07E-02	2.07E-02	2.08E-02	2.08E-02	2.06E-02
Th-232	2.30E-07	8.65E+02	8.65E+02	8.65E+02	8.65E+02	8.68E+02	8.68E+02	8.68E+02
Th-234	3.40E-09	7.81E+00	3.08E-06	3.08E-06	3.08E-06	3.08E-06	3.09E-06	3.12E-06
Tl-207	*7.10E-12*	6.11E-02	2.78E-01	8.94E-01	9.14E-01	7.57E-01	1.13E-01	4.31E-04
Tl-208	*8.60E-12*	6.64E+01	1.28E+02	5.50E+01	2.11E-02	1.16E-02	1.16E-02	1.16E-02
Tl-209	*6.40E-12*	4.14E-04	1.34E-03	1.05E-02	9.78E-02	6.46E-01	7.34E-01	1.44E-02
U-232	*3.30E-07*	1.48E+07	1.36E+07	5.71E+06	9.86E+02	1.07E-04	6.24E-05	2.75E-07
U-233	5.10E-08	4.00E+05	4.00E+05	4.00E+05	3.99E+05	3.83E+05	2.59E+05	5.06E+03
U-234	4.90E-08	5.60E+04	5.60E+04	5.60E+04	5.59E+04	5.46E+04	4.22E+04	3.30E+03
U-235	4.70E-08	2.86E+00	2.86E+00	2.86E+00	2.86E+00	2.87E+00	2.87E+00	2.85E+00
U-236	4.70E-08	1.04E+01	1.04E+01	1.04E+01	1.04E+01	1.04E+01	1.04E+01	1.01E+01
U-237	7.60E-10	5.79E-04	3.75E-04	4.93E-06	6.77E-11	3.26E-11	2.11E-14	0.00E+00
U-238	4.50E-08	4.08E-05	4.08E-05	4.08E-05	4.08E-05	4.08E-05	4.10E-05	4.13E-05
U-240	1.10E-09	1.08E-11	1.08E-11	1.08E-11	1.08E-11	1.08E-11	1.08E-11	1.07E-11
	sum(Sv/t)	2.22E+07	2.71E+07	1.20E+07	1.32E+06	4.65E+06	6.16E+06	3.51E+05

*: DCF is assumed by the author.

TABLE 40. RADIOTOXICITY BY FPs FOR MOX FUEL (Sv/t-HM)

Nuclide	*DCF*	*1 year*	*10 year*	*100 year*	*1.00E+03 year*	*1.00E+04 year*	*1.00E+05 year*	*1.00E+06 year*
Ag-110	1.00E-09*	2.10E+03	2.30E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ag-110m	2.80E-09	4.41E+05	4.84E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ba-137m	*1.00E-12*	4.90E+03	3.98E+03	4.98E+02	4.63E-07	0.00E+00	0.00E+00	0.00E+00
Cd-113m	*2.30E-08*	6.71E+04	4.37E+04	6.08E+02	1.63E-16	0.00E+00	0.00E+00	0.00E+00
Cd-115m	*1.40E-09*	2.22E+02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ce-141	7.10E-10	1.71E+04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ce-144	5.20E-09	8.66E+07	2.86E+04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cs-134	1.90E-08	1.03E+08	4.99E+06	3.62E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cs-135	2.00E-09	8.15E+01	8.15E+01	8.15E+01	8.14E+01	8.12E+01	7.90E+01	6.03E+01
Cs-137	1.30E-08	6.73E+07	5.47E+07	6.84E+06	6.36E-03	0.00E+00	0.00E+00	0.00E+00
Eu-152	1.40E-09	1.50E+03	9.51E+02	9.68E+00	1.16E-19	0.00E+00	0.00E+00	0.00E+00

Nuclide	*DCF*	*1 year*	*10 year*	*100 year*	*1.00E+03 year*	*1.00E+04 year*	*1.00E+05 year*	*1.00E+06 year*
Eu-154	2.00E-09	1.22E+06	5.91E+05	4.18E+02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Eu-155	3.20E-10	1.45E+05	4.12E+04	1.42E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Gd-153	*2.70E-10*	4.80E+02	3.91E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Nb-95	*5.80E-10*	1.33E+06	4.48E-10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Nb-95m	*5.60E-10*	4.23E+03	1.45E-12	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pm-146	9.00E-10	1.29E+02	4.16E+01	4.94E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pm-147	2.60E-10	1.21E+06	1.13E+05	5.30E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pm-148	*2.70E-09*	6.45E+02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pm-148m	*1.80E-09*	7.63E+03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pr-144	5.00E-11	8.33E+05	2.75E+02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pr-144m	1.00E-09*	2.00E+05	6.60E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Rh-106	1.60E-10	3.51E+06	7.19E+03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ru-106	7.00E-09	1.53E+08	3.15E+05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sb-124	*2.50E-09*	2.03E+03	7.38E-14	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sb-125	1.10E-09	7.29E+05	7.67E+04	1.27E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sb-126m	*3.60E-11*	1.86E+00	1.86E+00	1.86E+00	1.85E+00	1.74E+00	9.33E-01	1.82E-03
Sm-151	9.80E-11	3.10E+03	2.89E+03	1.44E+03	1.41E+00	0.00E+00	0.00E+00	0.00E+00
Sn-119m	5.40E-10*	1.45E+03	1.33E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sn-123	2.10E-09*	3.86E+04	8.42E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sn-126	4.70E-09	2.43E+02	2.43E+02	2.43E+02	2.42E+02	2.27E+02	1.22E+02	2.37E-01
Sr-89	2.60E-09	3.21E+05	8.13E-15	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sr-90	2.80E-08	4.80E+07	3.87E+07	4.54E+06	2.26E-03	0.00E+00	0.00E+00	0.00E+00
Tb-160	*1.60E-09*	4.61E+03	9.50E-11	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Tc-99	6.40E-10	4.14E+02	4.14E+02	4.14E+02	4.13E+02	4.01E+02	2.99E+02	1.60E+01
Te-123m	*1.40E-09*	8.36E+01	4.50E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Te-125m	*8.70E-10*	1.41E+05	1.48E+04	2.45E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Te-127	*1.70E-10*	1.29E+04	1.08E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Te-127m	2.30E-09	1.78E+05	1.49E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Te-129	*6.30E-11*	5.12E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Te-129m	*3.00E-09*	3.74E+03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Y-90	*2.70E-09*	4.63E+06	3.73E+06	4.38E+05	2.18E-04	0.00E+00	0.00E+00	0.00E+00
Y-91	*2.40E-09*	8.62E+05	1.05E-11	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Zr-93	1.10E-09	7.03E+01	7.03E+01	7.03E+01	7.03E+01	7.00E+01	6.72E+01	4.47E+01
Zr-95	*8.80E-10*	8.96E+05	3.06E-10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
	sum(Sv/t)	4.75E+08	1.03E+08	1.18E+07	8.10E+02	7.81E+02	5.68E+02	1.21E+02

*: DCF is assumed by the author.

TABLE 41. RADIOTOXICITY BY ACTINIDES FOR MOX FUEL (Sv/t-HM)

Nuclide	*DCF*	*1 year*	*10 year*	*100 year*	*1.00E+03 year*	*1.00E+04 year*	*1.00E+05 year*	*1.00E+06 year*
Ac-225	2.40E-08	2.91E-05	3.20E-05	5.55E-04	4.24E-01	8.33E+01	2.09E+03	4.62E+03
Ac-227	1.10E-06	2.24E-03	1.23E-02	4.43E-02	5.17E-01	4.11E+01	1.24E+03	1.78E+03
Ac-228	4.30E-10	4.03E-14	1.37E-12	2.70E-10	2.57E-08	1.92E-06	4.70E-05	4.91E-04
Am-241	2.00E-07	3.52E+07	1.05E+08	2.06E+08	4.91E+07	4.02E+04	2.75E+01	0.00E+00
Am-242	3.00E-10	2.98E+03	2.86E+03	1.89E+03	3.13E+01	4.70E-17	0.00E+00	0.00E+00
Am-242m	1.90E-07	1.89E+06	1.82E+06	1.21E+06	1.99E+04	2.99E-14	0.00E+00	0.00E+00
Am-243	2.00E-07	3.65E+06	3.65E+06	3.62E+06	3.32E+06	1.43E+06	3.04E+02	5.09E-02
At-217	1.00E-07*	1.21E-04	1.34E-04	2.31E-03	1.77E+00	3.47E+02	8.72E+03	1.93E+04
Bi-210	1.30E-09	4.65E-08	5.64E-07	1.40E-03	9.72E-01	4.35E+01	3.34E+02	7.04E+01
Bi-211	1.00E-07*	2.04E-04	1.12E-03	4.03E-03	4.70E-02	3.74E+00	1.12E+02	1.61E+02
Bi-212	2.60E-10	1.88E-02	1.16E-01	6.02E-02	1.25E-05	3.14E-06	2.95E-05	2.97E-04
Bi-213	2.00E-10	2.43E-07	2.67E-07	4.62E-06	3.53E-03	6.94E-01	1.74E+01	3.85E+01
Bi-214	1.10E-10	1.26E-08	5.00E-07	2.46E-04	8.23E-02	3.68E+00	2.83E+01	5.96E+00
Cf-249	*3.50E-07*	1.66E+00	2.64E+00	2.21E+00	3.73E-01	6.93E-09	0.00E+00	0.00E+00
Cf-250	*1.60E-07*	4.57E+00	2.84E+00	2.41E-02	5.59E-10	3.91E-10	1.08E-11	2.92E-27
Cf-251	*3.60E-07*	6.20E-02	6.16E-02	5.75E-02	2.87E-02	2.76E-05	0.00E+00	0.00E+00
Cf-252	*9.00E-08*	1.26E+00	1.19E-01	6.37E-12	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Nuclide	*DCF*	*1 year*	*10 year*	*100 year*	*1.00E+03 year*	*1.00E+04 year*	*1.00E+05 year*	*1.00E+06 year*
Cm-242	1.20E-08	8.61E+07	9.46E+04	6.27E+04	1.03E+03	1.56E-15	0.00E+00	0.00E+00
Cm-243	1.50E-07	3.42E+06	2.75E+06	3.08E+05	9.61E-05	0.00E+00	0.00E+00	0.00E+00
Cm-244	1.20E-07	3.72E+08	2.64E+08	8.42E+06	9.23E-09	0.00E+00	0.00E+00	0.00E+00
Cm-245	2.10E-07	9.53E+04	9.53E+04	9.46E+04	8.78E+04	4.22E+04	2.74E+01	0.00E+00
Cm-246	2.10E-07	1.47E+04	1.47E+04	1.45E+04	1.27E+04	3.40E+03	6.37E-03	1.46E-26
Cm-247	1.90E-07	5.05E-02	5.05E-02	5.05E-02	5.05E-02	5.05E-02	5.03E-02	4.83E-02
Cm-248	7.70E-07	4.28E-01	4.28E-01	4.28E-01	4.28E-01	4.20E-01	3.49E-01	5.55E-02
Fr-221	*1.70E-10*	2.06E-07	2.27E-07	3.93E-06	3.00E-03	5.90E-01	1.48E+01	3.27E+01
Fr-223	2.40E-09	6.76E-08	3.69E-07	1.33E-06	1.56E-05	1.24E-03	3.72E-02	5.35E-02
Np-235	*5.30E-11*	2.34E-03	7.42E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Np-236	*1.70E-08*	1.53E-03	1.53E-03	1.52E-03	1.52E-03	1.44E-03	8.35E-04	3.68E-06
Np-237	1.10E-07	2.88E+02	4.05E+02	3.50E+03	2.11E+04	2.74E+04	2.67E+04	2.00E+04
Np-238	9.10E-10	4.54E+01	4.35E+01	2.89E+01	4.77E-01	7.16E-19	0.00E+00	0.00E+00
Np-239	8.00E-10	1.46E+04	1.46E+04	1.45E+04	1.33E+04	5.71E+03	1.22E+00	2.03E-04
Pa-231	7.10E-07	2.74E-02	2.75E-02	3.13E-02	3.34E-01	2.66E+01	7.98E+02	1.15E+03
Pa-233	8.70E-10	2.28E+00	3.20E+00	2.77E+01	1.67E+02	2.17E+02	2.11E+02	1.58E+02
Pa-234	5.10E-10	7.47E-03	7.47E-03	7.47E-03	7.47E-03	7.47E-03	7.48E-03	7.52E-03
Pa-234m	*3.10E-12*	3.49E-02	3.49E-02	3.49E-02	3.49E-02	3.49E-02	3.50E-02	3.52E-02
Pb-209	5.70E-11	2.04E-09	2.47E-08	6.15E-05	4.26E-02	1.98E-01	4.97E+00	1.10E+01
Pb-210	6.90E-07	2.47E-05	2.47E-05	7.45E-01	5.16E+02	2.31E+04	1.77E+05	3.74E+04
Pb-211	1.80E-10	3.68E-07	2.01E-06	7.25E-06	8.46E-05	6.73E-03	2.02E-01	2.91E-01
Pb-212	6.00E-09	4.33E-01	2.69E+00	1.39E+00	2.88E-04	7.25E-05	6.82E-04	6.85E-03
Pb-214	1.40E-10	1.61E-08	6.37E-07	3.13E-04	1.05E-01	4.69E+00	3.60E+01	7.59E+00
Po-210	1.20E-06	3.83E-05	5.21E-04	1.30E+00	8.97E+02	4.02E+04	3.09E+05	6.50E+04
Po-211	1.00E-07*	5.72E-07	3.13E-06	1.13E-05	1.32E-04	1.05E-02	3.15E-01	4.52E-01
Po-212	1.00E-07*	4.62E+00	2.87E+01	1.48E+01	3.08E-03	7.74E-04	7.28E-03	7.31E-02
Po-213	1.00E-07*	1.19E-04	1.31E-04	2.26E-03	1.73E+00	3.40E+02	8.54E+03	1.88E+04
Po-214	1.00E-07*	1.15E-05	4.54E-04	2.24E-01	7.47E+01	3.35E+03	2.57E+04	5.42E+03
Po-215	1.00E-07*	2.04E-04	1.12E-03	4.03E-03	4.70E-02	3.74E+00	1.12E+02	1.61E+02
Po-216	1.00E-07*	7.22E+00	4.48E+01	2.32E+01	4.81E-03	1.21E-03	1.14E-02	1.14E-01
Po-218	1.00E-07*	1.15E-05	4.55E-04	2.24E-01	7.48E+01	3.35E+03	2.57E+04	5.42E+03
Pu-236	*8.60E-08*	7.68E+02	8.62E+01	6.94E-04	6.90E-04	6.54E-04	3.80E-04	1.68E-06
Pu-238	2.30E-07	3.05E+08	2.92E+08	1.44E+08	1.38E+05	7.11E-14	0.00E+00	0.00E+00
Pu-239	2.50E-07	1.02E+07	1.02E+07	1.02E+07	1.00E+07	8.35E+06	6.84E+05	6.36E-02
Pu-240	2.50E-07	1.90E+07	1.96E+07	2.09E+07	1.90E+07	7.33E+06	5.25E+02	1.13E-01
Pu-241	4.80E-09	1.45E+08	9.41E+07	1.24E+06	2.01E+03	9.65E+02	6.26E-01	0.00E+00
Pu-242	2.40E-07	2.37E+05	2.37E+05	2.37E+05	2.37E+05	2.33E+05	1.98E+05	3.95E+04
Pu-243	8.50E-11	2.26E-05	2.26E-05	2.26E-05	2.26E-05	2.26E-05	2.25E-05	2.16E-05
Pu-244	2.40E-07	1.09E-01	1.09E-01	1.09E-01	1.09E-01	1.09E-01	1.09E-01	1.08E-01
Ra-223	1.00E-07	2.04E-04	1.12E-03	4.03E-03	4.70E-02	3.74E+00	1.12E+02	1.61E+02
Ra-224	6.50E-08	4.69E+00	2.91E+01	1.51E+01	3.12E-03	7.85E-04	7.39E-03	7.42E-02
Ra-225	9.90E-08	1.20E-04	1.32E-04	2.29E-03	1.75E+00	3.44E+02	8.64E+03	1.91E+04
Ra-226	2.80E-07	3.22E-05	1.27E-03	6.26E-01	2.09E+02	9.37E+03	7.21E+04	1.52E+04
Ra-228	6.90E-07	6.47E-11	2.20E-09	4.33E-07	4.12E-05	3.09E-03	7.54E-02	7.88E-01
Th-227	8.80E-09	1.77E-05	9.69E-05	3.50E-04	4.08E-03	3.24E-01	9.76E+00	1.40E+01
Th-228	7.20E-08	5.19E+00	3.23E+01	1.67E+01	3.46E-03	8.70E-04	8.18E-03	8.22E-02
Th-229	4.90E-07	5.95E-04	6.54E-04	1.13E-02	8.65E+00	1.70E+03	4.28E+04	9.44E+04
Th-230	2.10E-07	4.10E-02	5.32E-01	3.03E+01	8.84E+02	9.01E+03	5.40E+04	1.14E+04
Th-231	3.40E-10	2.39E-04	3.61E-04	1.59E-03	1.37E-02	1.25E-01	5.18E-01	5.49E-01
Th-232	2.30E-07	1.95E-10	2.23E-09	1.44E-07	1.37E-05	1.03E-03	2.51E-02	2.63E-01
Th-234	3.40E-09	3.83E+01	3.83E+01	3.83E+01	3.83E+01	3.83E+01	3.84E+01	3.86E+01
Tl-207	*7.10E-12*	1.45E-08	7.90E-08	2.85E-07	3.33E-06	2.65E-04	7.96E-03	1.14E-02
Tl-208	*8.60E-12*	2.23E-04	1.39E-03	7.16E-04	1.49E-07	3.73E-08	3.51E-07	3.53E-06
Tl-209	*6.40E-12*	1.68E-10	1.85E-10	3.20E-09	2.44E-06	4.80E-04	1.21E-02	2.66E-02
U-232	*3.30E-07*	7.15E+01	1.63E+02	7.44E+01	1.55E-02	2.51E-03	1.46E-03	6.43E-06
U-233	5.10E-08	4.44E-03	1.06E-02	3.49E-01	2.65E+01	5.17E+02	4.43E+03	9.82E+03
U-234	4.90E-08	5.83E+02	2.23E+03	1.36E+04	2.47E+04	2.41E+04	1.88E+04	1.98E+03
U-235	4.70E-08	3.30E-02	4.99E-02	2.19E-01	1.90E+00	1.72E+01	7.15E+01	7.59E+01

Nuclide	*DCF*	*1 year*	*10 year*	*100 year*	*1.00E+03 year*	*1.00E+04 year*	*1.00E+05 year*	*1.00E+06 year*
U-236	4.70E-08	4.56E-01	1.42E+00	1.17E+01	1.12E+02	7.26E+02	1.11E+03	1.08E+03
U-237	7.60E-10	5.64E+02	3.65E+02	4.81E+00	7.80E-03	3.75E-03	2.43E-06	0.00E+00
U-238	4.50E-08	5.07E+02	5.07E+02	5.07E+02	5.07E+02	5.07E+02	5.08E+02	5.10E+02
U-240	1.10E-09	4.98E-04	4.98E-04	4.98E-04	4.98E-04	4.98E-04	4.98E-04	4.95E-04
	sum(Sv/t)	9.82E+08	7.93E+08	3.96E+08	8.20E+07	1.76E+07	1.67E+06	3.73E+05

*: DCF is assumed by the author.

7.5. IMPLEMENTATION IN NFCSS

In this section, radiotoxicity was assessed for PWR UO_2, ThO_2 and MOX fuel using ORIGEN2 and DCF (Dose Conversion Factor). From these assessments and [30], [36] and [39], the following information is summarized:

- The Th core shows 10–90% lower radiotoxicity than the U core up to 1000 year, and a peak exists at around 0.1 million year. These behaviours are similar to those observed for decay heat.
- The MOX core shows 4–5 times higher radiotoxicity than the U core up to 1 million-year.

Since NFCSS calculates weights of only 18 actinides (i.e. Th-232, Pa-233, U-233, U-234, U-235, U-236, U-238, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Np-237, Am-241, Am-242m, Am-243, Cm-242 and Cm-244) and does not calculate FPs, direct calculation of radiotoxicity by the NFCSS is impossible. Instead, a simple method is suggested for the assessment of radiotoxicity of any burnup fuel in both PWR and BWR based on Fig.55 and Table 42.

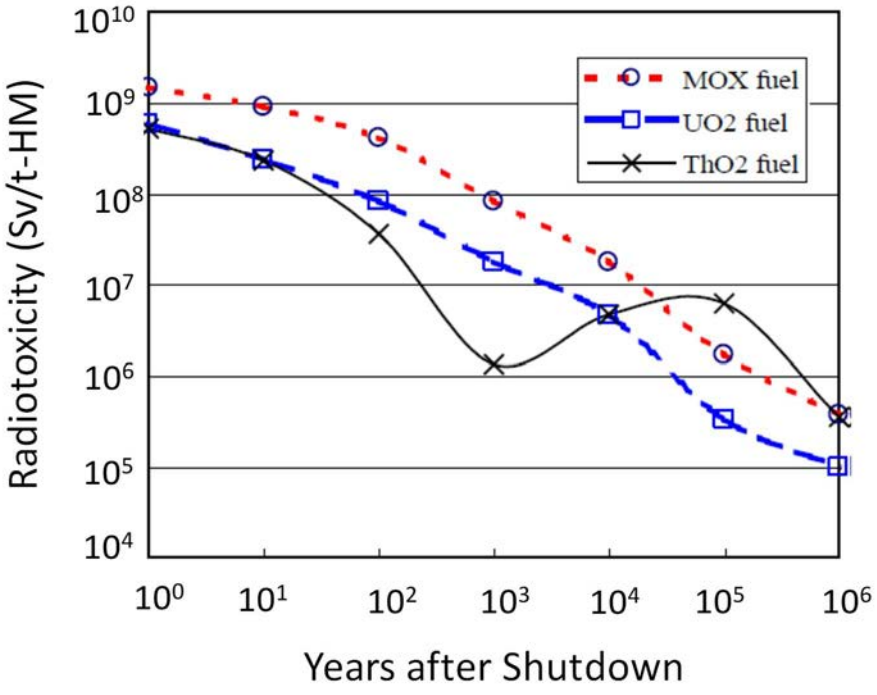


FIG.55. Radiotoxicity for PWR/BWR UO_2/ThO_2/MOX fuel (Sv/t-HM).

TABLE 42. RADIOTOXICITY TABLE FOR PWR/BWR UO2/ThO2/MOX FUEL (Sv/t-HM)

year	*1*	*10*	*100*	*1.00E+03*	*1.00E+04*	*1.00E+05*	*1.00E+06*
UO_2	5.878E+08	2.358E+08	8.181E+07	1.770E+07	4.591E+06	3.297E+05	9.797E+04
ThO_2	5.175E+08	2.316E+08	3.570E+07	1.321E+06	4.651E+06	6.161E+06	3.513E+05
MOX	1.457E+09	8.967E+08	4.082E+08	8.205E+07	1.757E+07	1.672E+06	3.728E+05

Table 42 data need to be interpolated in terms of burnup using the formula

$$\text{Radiotoxicity (SV/tHM)} = [\textbf{Rad-reference}] \times BU / 45 \quad (9)$$

where,

[**Rad-reference**] (reference radiotoxicity in Sv/t-HM) is presented in Table 42.

Although burnup dependence of MOX fuel is not studied here, based on the comparison with decay heat results, it can be reasonably assumed that burnup dependence is similar to UO_2 and ThO_2 fuel.

For ThO_2 fuel, 4% U-233 +96% Th-232 composition is assumed. For other fuel types such as Pu-ThO_2 fuel, other radiotoxicity tables may be required.

If total radiotoxicity is required for the whole batch of the specified year, then the above **Rad** value must be multiplied by the discharged total fuel weight calculated by NFCSS.

Also, if linear interpolation is required for the specified year, which is not shown in Table 42, Equation (10) can be used.

$$y = y_i + (y_{i+1}-y_i)(x-x_i)/(x_{i+1}-x_i) \quad (10)$$

Here,

$y=\ln(Rad)$,
$y_i=\ln(Rad_i)$,
$y_{i+1}=\ln(Rad_{i+1})$,
$x=\ln(YEAR)$,
$x_i=\ln(YEAR_i)$,
$x_{i+1}=\ln(YEAR_{i+1})$,
$Rad=\exp(y)$.

The Excel spreadsheet that calculates radiotoxicity according to the methods described in this Section is available from the IAEA web site for NFCSS:

https://infcis.iaea.org/NFCSS/NFCSSHelp.cshtml.

7.6. OTHER ISSUES

This subsection is related to the recent argument on MSRs. In 1960s, the ORNL proposed an online reprocessing system with MSRs in order to improve the breeding ratio. If this online reprocessing is established, most of the actinides can be transmuted at MSRs itself, and radiotoxicity can be decreased.

The online reprocessing is complicated to be simulated, and thus, comparative assessments have been performed below:

First, radiotoxicity by actinides was compared between the U and Th cores (without reprocessing). The result is shown in Fig.56, which shows actinide radiotoxicity for thorium fuel is lower than UO_2 fuel up to 10 000 years.

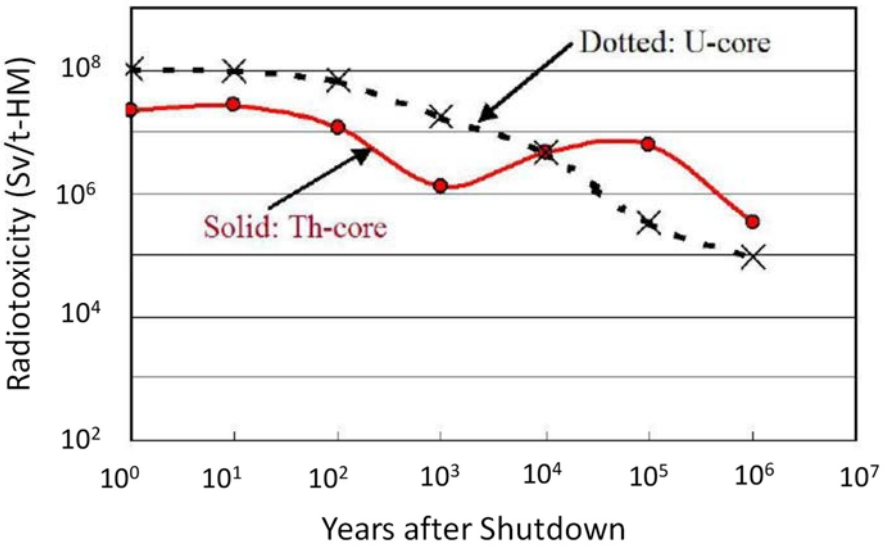


FIG.56. Radiotoxicity by actinides of spent fuel.

If reprocessing is applied to MSRs, most actinides are separated and recycled. Therefore, radiotoxicity during long term storage can be significantly reduced. Further reduction of radiotoxicity can be expected with the separation/recycling of Th and its daughters in addition to U.

An advantage of an MSR with Th fuel is that it has lower radiotoxicity than conventional UO_2 fuel in PWR [40]. Figure 57 shows a comparison of actinide radiotoxicity between U fuel (without reprocessing) and Th fuel (assuming 100% transmutation efficiency based on the above assumptions). In Fig.57 actinide radiotoxicity of a 1 GW(th) plant after 1 year of operation is presented in units of Sv/GW(th)/year and compared with the results from [40].

The conversion procedure is as follows:

The weight of fuel (WT) discharged annually from the reactor of 1000 MW(e) (3000 MW(th)) that operates 365 days at 100% load factor is calculated by Equation (11):

$$\begin{aligned} WT &= [3000\ MW(th)] \times [365\ days] \times 1.0\ (100\ \%\ load\ factor) / [45\ 000\ MW{\cdot}d/t] \\ &= 24.3\ ton/year \end{aligned} \quad (11)$$

If radiotoxicity per 1000 MW(e)·year is required, therefore, the above radiotoxicity should be multiplied by 24.3, that is;

$$Radiotoxicity\ per\ 1000\ MWe\text{-}year = WT \times RD = 24.3 \times RD \quad (12)$$

If radiotoxicity per 1000 MW(th)·year is required, the above radiotoxicity should be multiplied by 24.3/3(GW(th))=8.1. That is;

$$\text{Radiotoxicity per 1000 MW(th)·year} = \text{WT} / 3.0 \times \text{RD} = 8.1 \times \text{RD} \quad (13)$$

is used for conversion.

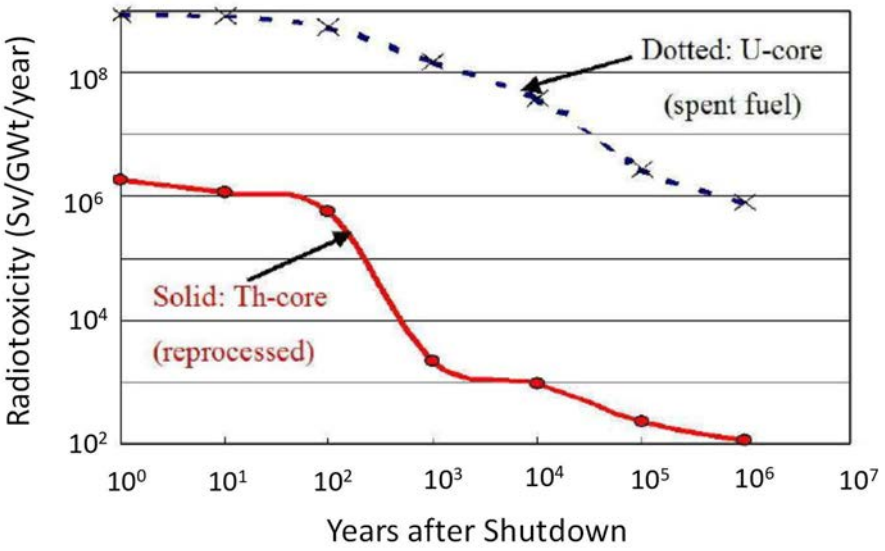


FIG.57. Radiotoxicity only by actinides.

Radiotoxicity due to FPs is dominant up to 100 years, and the above effect appears even after several hundred years. The result is shown in Fig.58, assuming 100% separation and recycling for the Th core. In actual reprocessing, separation efficiency cannot be 100% and new daughter nuclides are generated from recycled U and Th. Hence reduction of radiotoxicity may not be as effective as shown here.

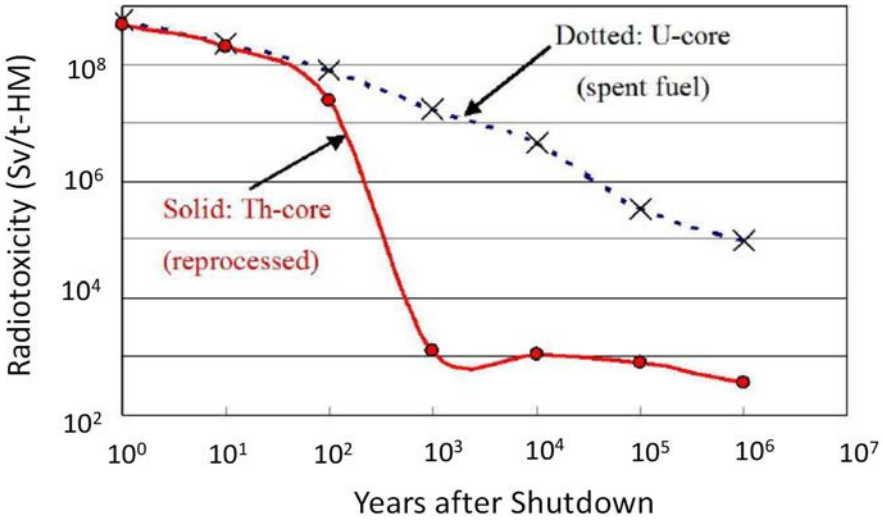


FIG.58. Total radiotoxicity (effect of reprocessing).

8. BENCHMARKING OF NFCSS

8.1. GENERAL

Only partial validation of the NFCSS was performed and documented earlier (See Appendix VI of [1]). The CAIN burnup model results showed reasonable agreement with independent solutions obtained by other codes and with measured data. Specifically, results from the CAIN were consistent with ORIGEN data. The CAIN results for PHWR, RBMK, AGR, and GCR were also reasonably consistent with results from WIMS code except for Pu-241 and Am-241. CAIN values for these two nuclides were 10–30% higher than what was generated by WIMS. When compared with actual measurements for PWR and BWR, the CAIN model provided reasonable accuracy.

In this section, incremental benchmarking exercises of the whole NFCSS are pursued via comparative studies with independent solutions by other codes including HIMMEL, COSAC and MESSAGE.

Benchmarking exercise with HIMMEL code (Section 8.2) is intended to validate the CAIN calculations on nuclide concentrations at the discharge of the fuel. Benchmarking exercises with COSAC and MESSAGE codes aim at validating calculated material flows (e.g. annual fresh fuel requirements, the amount of spent fuel generated) for various operating scenarios of nuclear energy systems.

The results of these benchmarking exercises support the validity of NFCSS applications in qualitative manner. A systematic and comprehensive verification and validation of NFCSS will be needed to quantify the uncertainty of NFCSS applications.

8.2. BENCHMARK WITH HIMMEL CODE

8.2.1. Description of HIMMEL code

For a depletion calculation of a certain reactor fuel, the NFCSS needs input data on specific power and neutron flux at a rated power level. For the common reactor types such as PWR, BWR and PHWR, values of these two input parameters are provided as default values and installed in the NFCSS system library. For other reactor types, users need to provide appropriate values of these input parameters.

Specific power and neutron flux are correlated each other by Equation (14):

$$SP = \phi \times \text{Sum} \left(N_{(i)} \times \sigma_{f(i)} \times E_{f(i)} \right) \quad (14)$$

where,

SP: specific power (W/g),
Φ: flux (n/cm^2-s),
$N_{(i)}$: number density of i-isotope (n/g-HM),
$\sigma_{f(i)}$: fission cross section of i-isotope (barn),
$E_{f(i)}$: energy release per fission of i-isotope (Wsec).

Treating these two input parameters (SP and ϕ) independently may cause some errors because the value of SP at a rated power level is used to determine ‘irradiation-period (day)’ to the discharge burnup BU (MW·d/t) and to determine the initial HM inventory in the NFCSS. At

later stage the NFCSS adjusts the neutron flux value for use in the depletion calculation from the input value (typically a guesstimate) to the value to achieve suitable FP content fit to the burnup BU (MW·d/t) by using a common energy release rate of 0.97 (MW·d/gram-fission).

On the other hand, HIMMEL code [41] determines the neutron flux from the input value of SP using Equation (14). In the depletion calculation, HIMMEL adjusts the flux level at each time step to meet the input SP. While the NFCSS calculates the fuel composition change in one time step for the whole irradiation period, HIMMEL makes four time steps a year and traces the composition change in each time step. HIMMEL does not use the constant of 0.97 (MW·d/g-fission) for the energy generation but adopts different values for different nuclides shown in Table III-3 of Annex III.

8.2.2. Results

The same cross sections installed in the NFCSS were used in HIMMEL calculation. The final flux level in the NFCSS calculation is not known because of lack of printout function at the moment. HIMMEL uses the flux level at each time step at a partial full-power condition that accounts for the load factor. The flux values of HIMMEL shown in the Table 43 to Table 48 are the averaged values for the whole irradiation period. Because NFCSS uses the input value of SP that does not account for the load factor, the irradiation period in the NFCSS calculation is always shorter than in HIMMEL although the same discharge burnup is considered in both calculations. The effect on the load factor and operation mode is described in Annex Section III-9.

Benchmarking was done for six reactor fuel types in the NFCSS library that include PWR UOX 2, WWER UOX1, PWR MOX1, PHWR U1, LMFR Core MOX and LMFR Axial blanket. Six benchmark results are represented in Table 43 to Table 48, respectively. Some findings are:

- Regardless of differences in the number of time steps and in irradiation time for depletion calculation, the discharged fuel compositions were very close to each other. (The biggest difference was 1.5% for Pu-239 in PWR MOX1);

- Systematic differences were found for MAs including Am-241, Am-242m, Cm-242 and Pu-238 with relatively large differences. These differences were caused mainly due to different irradiation time in both codes. NFCSS underestimated the decay effects of isotopes (mainly Pu-241) because of shorter irradiation time than the fuel residence time in reactors. HIMMEL took into account the full decay effect in fuel residence time by using the flux level at a partial full-power operation condition based on the load factor of the reactor.

TABLE 43. BENCHMARK RESULTS ON PWR UOX2

PWR UOX 2 *Enrichment: 4%* *Burnup: 45 GW·d/t* *Load Factor (LF) = 80%*	*NFCSS calculations* *Specific Power (SP) = 38.53 kW/kg* *Irradiation: 1168 days*	*HIMMEL calculations* *SP = 30.82 kW/kg* *Flux = 2.532E+14* *Irradiation: 1460 days*	*Relative error HIMMEL/NFCSS - 1, (%)*
U-235	0.796506	0.796951	0.1
U-236	0.518904	0.518918	0.0
U-238	92.903060	92.919340	0.0
Np-237	0.069401	0.069386	0.0
Pu-238	0.025634	0.025898	1.0
Pu-239	0.540452	0.543697	0.6
Pu-240	0.210179	0.210955	0.4
Pu-241	0.185380	0.185389	0.0

PWR UOX 2 *Enrichment: 4%* *Burnup: 45 GW·d/t* *Load Factor (LF) = 80%*	*NFCSS calculations* *Specific Power (SP) = 38.53 kW/kg* *Irradiation: 1168 days*	*HIMMEL calculations* *SP = 30.82 kW/kg* *Flux = 2.532E+14* *Irradiation: 1460 days*	*Relative error HIMMEL/NFCSS - 1, (%)*
Pu-242	0.078200	0.078123	-0.1
Am-241	0.006268	0.006843	9.2
Am-242m	0.000145	0.000161	11.2
Am-243	0.018332	0.018312	-0.1
Cm-242	0.002194	0.002398	9.3
Cm-244	0.006417	0.006396	-0.3
Total FP	4.638926	4.616708	-0.5

TABLE 44. BENCHMARK RESULTS ON WWER UOX1

WWER UOX 1 *Enrichment: 4%* *Burnup: 45 GW·d/t* *Load Factor (LF) = 80%*	*NFCSS calculations* *Specific Power (SP) = 38.53 kW/kg* *Irradiation: 1168 days*	*HIMMEL calculations* *SP = 30.82 kW/kg* *Flux = 2.652E+14* *Irradiation: 1460 days*	*Relative error HIMMEL/NFCSS - 1, (%)*
U-235	0.939718	0.941301	0.2
U-236	0.505479	0.505387	0.0
U-238	92.634410	92.655550	0.0
Np-237	0.061014	0.060953	-0.1
Pu-238	0.023921	0.024346	1.8
Pu-239	0.6555649	0.658543	0.4
Pu-240	0.204276	0.204826	0.3
Pu-241	0.217476	0.216837	-0.3
Pu-242	0.083149	0.082890	-0.3
Am-241	0.007445	0.008543	14.7
Am-242m	0.000113	0.000131	15.8
Am-243	0.019001	0.018939	-0.3
Cm-242	0.002496	0.002721	9.0
Cm-244	0.006752	0.006703	-0.7
Total FP	4.639097	4.611742	-0.6

TABLE 45. BENCHMARK RESULTS ON PHWR U1

PHWR U 1 *Enrichment: 0.711%* *Burnup: 7 GW·d/t* *Load Factor (LF) = 80%*	*NFCSS calculations* *Specific Power (SP) = 23.97 kW/kg* *Irradiation: 292 days*	*HIMMEL calculations* *SP = 19.18 kW/kg* *Flux = 1.852E+14* *Irradiation: 365 days*	*Relative error HIMMEL/NFCSS - 1, (%)*
U-235	0.237533	0.237535	0.0
U-236	0.071112	0.071113	0.0
U-238	98.582960	98.584560	0.0
Np-237	0.002594	0.002595	0.0
Pu-238	0.000326	0.000286	-12.4
Pu-239	0.265811	0.265858	0.0
Pu-240	0.095692	0.095700	0.0
Pu-241	0.018124	0.018090	-0.2
Pu-242	0.003929	0.003926	-0.1
Am-241	0.000143	0.000181	26.1
Am-242m	0.000001	0.000002	26.2
Am-243	0.000123	0.000123	0.2
Cm-242	0.000049	0.000059	20.1
Cm-244	0.000010	0.000010	0.1
Total FP	0.721588	0.719959	-0.2

TABLE 46. BENCHMARK RESULTS ON PWR MOX1

PWR MOX 1 *Pu enrichment: 7%* *Burnup: 45 GW·d/t* *Load Factor (LF) = 80%*	*Fresh composition*	*NFCSS calculations* *Specific Power (SP) = 23.97 kW/kg* *Irradiation: 292 days*	*HIMMEL calculations* *SP = 19.18 kW/kg* *Flux = 1.852E+14* *Irradiation: 365 days*	*Relative error HIMMEL/NFCSS - 1, (%)*
U-235	0.279000	0.133013	0.134249	0.9
U-236	0.0	0.028528	0.028449	-0.3
U-238	92.72100	90.41615	90.44595	0.0
Np-237	0.0	0.013697	0.013613	-0.6
Pu-238	0.095569	0.093310	0.102992	10.4
Pu-239	4.207340	1.591989	1.615132	1.5
Pu-240	1.514090	1.403817	1.412227	0.6
Pu-241	0.819000	0.871614	0.865784	-0.7
Pu-242	0.364000	0.469313	0.467399	-0.4
Am-241	0	0.065997	0.074993	13.6
Am-242m	0	0.001775	0.002022	13.9
Am-243	0	0.171758	0.170913	-0.5
Cm-242	0	0.013777	0.016382	18.9
Cm-244	0	0.086411	0.085151	-1.5
Total FP		4.638853	4.555631	-1.8

TABLE 47. BENCHMARK RESULTS ON LMFR CORE MOX

LMFR Core *Pu enrichment: 24.03%* *Burnup: 153.977 GW·d/t* *Load Factor (LF) = 85%*	*Fresh composition*	*NFCSS calculations* *Specific Power (SP) = 70.9 kW/kg* *Irradiation: 2172 days*	*HIMMEL calculations* *SP = 60.27 kW/kg* *Flux = 2.247E+15* *Irradiation: 2555 days*	*Relative error HIMMEL/NFCSS - 1, (%)*
U-235	0.22791	0.068691	0.070320	2.4
U-236	0.0	0.029256	0.029275	0.1
U-238	75.74209	64.10078	64.25511	0.2
Np-237	0.0	0.045490	0.045289	-0.4
Pu-238	0.26433	0.152609	0.160056	4.9
Pu-239	13.62501	10.06629	10.13045	0.6
Pu-240	8.07408	7.297717	7.311319	0.2
Pu-241	1.08135	1.074919	1.054857	-1.9
Pu-242	0.98523	0.905084	0.904666	0.0
Am-241	0	0.198227	0.225174	13.6
Am-242m	0	0.005725	0.006697	17.0
Am-243	0	0.141063	0.140241	-0.6
Cm-242	0	0.011582	0.012440	7.4
Cm-244	0	0.030086	0.029456	-2.1
Total FP		15.87248	15.61312	-1.6

TABLE 48. BENCHMARK LMFR AXIAL BLANKET

LMFR Ax blanket *Enrichment: 0.3%* *Burnup: 10.375 GW·d/t* *Load Factor (LF) = 85%*	*NFCSS calculations* *Specific Power (SP) = 23.97 kW/kg* *Irradiation: 292 days*	*HIMMEL calculations* *SP = 19.18 kW/kg* *Flux = 1.852E+14* *Irradiation: 365 days*	*Relative error HIMMEL/NFCSS - 1, (%)*
U-235	0.188083	0.189370	0.7
U-236	0.026752	0.026477	-1.0
U-238	94.35857	94.44395	0.1
Np-237	0.010318	0.010179	-1.3
Pu-238	0.001637	0.001542	-5.8
Pu-239	4.071898	4.026648	-1.1

LMFR Ax blanket *Enrichment: 0.3%* *Burnup: 10.375 GW·d/t* *Load Factor (LF) = 85%*	*NFCSS calculations* *Specific Power (SP) = 23.97 kW/kg* *Irradiation: 292 days*	*HIMMEL calculations* *SP = 19.18 kW/kg* *Flux = 1.852E+14* *Irradiation: 365 days*	*Relative error HIMMEL/NFCSS - 1, (%)*
Pu-240	0.261505	0.254783	-2.6
Pu-241	0.010500	0.009979	-5.0
Pu-242	0.000285	0.000268	-5.7
Am-241	0.000745	0.000835	12.0
Am-242m	0.000006	0.000006	10.6
Am-243	0.000006	0.000005	-6.7
Cm-242	0.000015	0.000015	-1.3
Cm-244	0.00000025	0.00000023	-8.6
Total FP	1.069681	1.035923	-3.2

Table 49 to Table 52 shows benchmark results on thorium fuel cases. In these tables, Pa-233 contents calculated by the NFCSS are about 20 % lower than HIMMEL calculations. This underprediction of Pa-233 content was caused by different methods for neutron flux treatment between NFCSS and HIMMEL. HIMMEL applies burnup-dependent variations of neutron flux, while the NFCSS considered a constant neutron flux. That is, for Pa-233 content calculation, HIMMEL applied higher neutron flux value that corresponds to the specific burnup, 45 GW·d/t. For a short period immediately after discharge of the spent fuel, HIMMEL could provide an estimation close to actual content of Pa-233. For a long period after the discharge, both codes would provide similar results each other, as discussed below.

Since the main objective of the NFCSS is to provide fuel cycle information, the above error for Pa-233 disappears quickly, due to a short half-life of Pa-233 (27 days). After Pa-233 decays to U-233, both NFCSS and HIMMEL results for U-233 show identical content of U-233. The NFCSS calculation of Pa-233 has been verified by comparing with Pa-233 content calculated by ORIGEN2 that also use a constant flux method.

For LEU-ThO_2 fuel (Table 50) and Pu-ThO_2 fuel (Table 51), the NFCSS underpredicted the content of Am-241 compared to HIMMEL. This was also caused by the constant flux method in the NFCSS. The validity of the Am-241 content by the NFCSS was also verified by comparing with ORIGEN2 code calculation.

TABLE 49. BENCHMARK RESULTS ON ^{233}U-ThO_2 FUEL

^{233}U-ThO_2 Core *Specific power = 38.53 MW/t* *Burnup = 45 GW·d/t* *Load factor = 100%*	*Fresh composition*	*NFCSS calculations* *Flux = 3.07E+14*	*HIMMEL Flux = 3.1028E+14*	*Relative error HIMMEL/NFCSS - 1, (%)*
U-235	0	0.07576438	0.077	0.0
U-236	0.0	0.009270391	0.009	0.0
U-238	0.0	0.0	0.0	0.0
Np-237	0.0	0.000547651	0.001	0.0
Pu-238	0.0	0.0	0.0	0.0
Pu-239	0.0	0.0	0.0	0.0
Pu-240	0.0	0.0	0.0	0.0
Pu-241	0.0	0.0	0.0	0.0
Pu-242	0.0	0.0	0.0	0.0
Am-241	0.0	0.0	0.0	0.0
Am-242m	0.0	0.0	0.0	0.0
Am-243	0.0	0.0	0.0	0.0
Cm-242	0.0	0.0	0.0	0.0
Cm-244	0.0	0.0	0.0	0.0

^{233}U-ThO_2 Core *Specific power = 38.53 MW/t* *Burnup = 45 GW·d/t* *Load factor = 100%*	*Fresh composition*	*NFCSS calculations Flux = 3.07E+14*	*HIMMEL Flux = 3.1028E+14*	*Relative error HIMMEL/NFCSS - 1, (%)*
Th-232	96.0	92.57992	92.561	0.0
Pa-233	0.0	0.107026	0.137	-22.0
U-233	4.0	2.100912	2.071	1.5
U-234	0.0	0.4872712	0.492	-1.0
Total FP	0.0	4.639289	4.652	-0.3

TABLE 50. BENCHMARK RESULTS ON LEU-ThO_2 FUEL

LEU-ThO_2 Core *Specific power = 38.53 MW/t* *Burnup = 45 GW·d/t* *Load factor = 100%*	*Fresh composition*	*NFCSS calculations Flux = 2.65E+14*	*HIMMEL Flux = 2.6768E+14*	*Relative error HIMMEL/NFCSS - 1, (%)*
U-235	5.0	1.193555	1.178	1.4
U-236	0.0	0.6288421	0.631	-0.3
U-238	20.0	19.13789	19.132	0.0
Np-237	0.0	0.06695519	0.068	-1.2
Pu-238	0.0	0.01863891	0.019	-1.4
Pu-239	0.0	0.1778549	0.180	-1.4
Pu-240	0.0	0.0659347	0.067	-1.0
Pu-241	0.0	0.05598465	0.057	-1.5
Pu-242	0.0	0.02071291	0.021	-2.1
Am-241	0.0	0.001966255	0.002	14.7
Am-242m	0.0	0.00004475602	0.000	0.0
Am-243	0.0	0.004232795	0.004	-2.9
Cm-242	0.0	0.0005903271	0.001	0.0
Cm-244	0.0	0.001102465	0.001	0.0
Th-232	75.0	72.68827	72.676	0.0
Pa-233	0.0	0.07273804	0.089	-18.7
U-233	4.0	1.090355	1.081	0.9
U-234	0.0	0.1348432	0.138	-2.0
Total FP	0.0	4.639488	4.656	-0.3

TABLE 51. BENCHMARK RESULTS ON Pu-ThO_2 FUEL

Pu-ThO_2 Core *Specific power = 38.53 MW/t* *Burnup = 45 GW·d/t* *Load factor = 100%*	*Fresh composition*	*NFCSS calculations Flux = 2.18E+14*	*HIMMEL Flux = 2.1716E+14*	*Relative error HIMMEL/NFCSS - 1, (%)*
U-235	0.0	0.009150323	0.009	-1.7
U-236	0.0	0.00036674	0.000	0.0
U-238	0.0	0	0.000	0.0
Np-237	0.0	1.42416E-05	0.000	0.0
Pu-238	0.123	0.1166325	0.117	-0.6
Pu-239	5.409	1.096692	1.123	-2.4
Pu-240	1.947	1.603284	1.612	-0.6
Pu-241	1.053	1.053664	1.064	-0.9
Pu-242	0.468	0.580102	0.580	0.1
Am-241	0.0	0.08901003	0.082	9.0
Am-242m	0.0	0.002313472	0.002	5.8
Am-243	0.0	0.1976048	0.197	0.3

Pu-ThO_2 Core *Specific power = 38.53 MW/t* *Burnup = 45 GW·d/t* *Load factor = 100%*	*Fresh composition*	*NFCSS calculations Flux = 2.18E+14*	*HIMMEL Flux = 2.1716E+14*	*Relative error HIMMEL/NFCSS - 1, (%)*
Cm-242	0.0	0.01605335	0.019	-16.5
Cm-244	0.0	0.08662443	0.087	0.0
Th-232	91.0	89.45088	89.469	0.0
Pa-233	0.0	0.04852396	0.066	-26.1
U-233	0.0	0.9390084	0.920	2.0
U-234	0.0	0.07123795	0.074	-3.6
Total FP	0.0	4.638838	4.570	1.5

TABLE 52. BENCHMARK RESULTS ON ^{235}U-ThO_2 FUEL

^{235}U-ThO_2 Core *Specific power = 38.53 MW/t* *Burnup = 45 GW·d/t* *Load factor = 100%*	*Fresh composition*	*NFCSS calculations Flux = 2.86E+14*	*HIMMEL Flux = 2.9050E+14*	*Relative error HIMMEL/NFCSS - 1, (%)*
U-235	5.0	1.072903	1.049	2.2
U-236	0.0	0.6425346	0.645	-0.4
U-238	0.0	0.000	0.000	0.0
Np-237	0.0	0.07155961	0.073	-1.7
Pu-238	0.0	0.02046767	0.021	0.0
Pu-239	0.0	0.000	0.003	-100.0
Pu-240	0.0	0.000	0.001	0.0
Pu-241	0.0	0.000	0.000	0.0
Pu-242	0.0	0.000	0.000	0.0
Am-241	0.0	0.000	0.000	0.0
Am-242m	0.0	0.000	0.000	0.0
Am-243	0.0	0.000	0.000	0.0
Cm-242	0.0	0.000	0.000	0.0
Cm-244	0.0	0.000	0.000	0.0
Th-232	95.0	91.84251	91.810	0.0
Pa-233	0.0	0.09912798	0.127	-22.0
U-233	0.0	1.419846	1.405	1.0
U-234	0.0	0.1917073	0.198	-2.9
Total FP	0.0	4.639336	4.668	-0.6

8.3. BENCHMARK WITH COSAC CODE

8.3.1. Description of COSAC code

COSAC is a simplified computational code developed by ORANO (former AREVA) for nuclear fuel cycle simulation. (COSAC is not publicly available.) This code assesses the spent nuclear fuel inventory for different kinds of nuclear reactors and can calculate their long-term decay heat and radiotoxicity.

COSAC models all the installations where nuclear material stays or is handled in a nuclear fleet such as mines, manufacturing facilities, reactors, cooling pools, intermediate or ultimate storage facilities, reprocessing or partitioning facilities. In COSAC the nuclear material moves from one installation to another according to a time dependent scenario provided by the user through

a Graphical User Interface (GUI). Some initial stockpiles of spent fuel can also be introduced within the simulation to factor already existing stockpile of spent nuclear fuel.

Beside isotopic composition and mass inventory calculations, COSAC allows decay heat and radiotoxicity calculations emitted by the nuclear material from its discharge from a reactor until its reprocessing or final disposal in a geological repository (Fig.59).

COSAC uses simplified methods to compute material isotopic evolutions within each installation as well as material flows between installations. Most of the calculations carried out by COSAC are solutions to matrix equations that enable the code to take into account some complex physics phenomena occurring during the fuel cycle. Burnup of the fuel, radioactive decay of the fuel, decay heat and radiotoxicity release of nuclear material for varying time periods are modelled in COSAC by matrix calculations.

The underlying assumption behind the matrix method for under-flux depletion computation is that fuel depletes linearly according to the initial composition of the fuel as long as fuel discharge occurs at the same reactivity and burnup. For this an equivalency formula is applied to fresh fuel manufactured in COSAC. This equivalency formula adjusts the fissile content to the isotopic composition of fresh fuel. Isotopic compositions are then given as input in the form of vectors and an irradiation matrix is applied to a vector of fuel composition to yield a linear extrapolation of the fuel depletion.

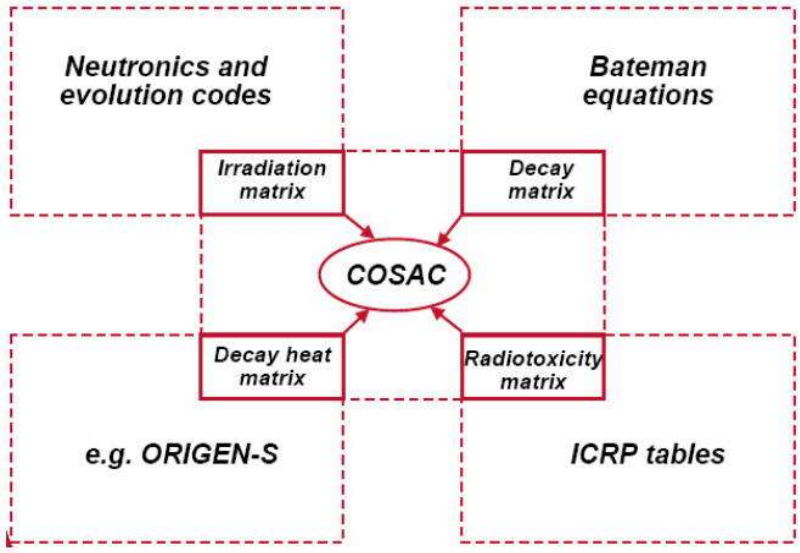


FIG. 59. COSAC and related information.

This approach allows the code to run fast and provides users the flexibility to model most types of reactors, fuels and fuel management options, with theoretically no limit in scaling the time duration for a scenario. PWRs, BWRs, FRs surrounded or not with some fertile blankets and cooled with sodium, lead or whatever material, prismatic high temperature reactors, graphite gas reactors, etc., can be part of the scenario in COSAC as long as the user inputs appropriate irradiation matrices for the reactors considered. Exception is to be mentioned for continuous fuel loading reactors, like pebble bed high temperature reactors or molten salt reactors, which are not presently compliant with the batch loading model used in COSAC for fuelling the reactors.

Output data computed by COSAC can be selected by the user when initializing a scenario. The user can also restrict the number of COSAC calculations to allow only outputs by utility and size. Typically, computational runs last a few minutes or longer depending on the complexity of the scenario. The output file can easily reach a hundred or so megabytes, especially when the scenario is calculated for a century or more. The full list of output data that COSAC can make available is split into several categories:

- Output data related to mass inventories: this type of outputs is related to masses contained in the installations. For instance, one can display with COSAC the mass of Am-241 contained in a storage pool installation, and also its evolution versus time;

- Output data related to mass flows: this type of outputs is related to masses entering or exiting an installation. For instance, one can display with COSAC the plutonium mass exiting a reactor each year;

- Output data related to decay heat: this type of outputs is related to decay heat emitted by the nuclear material contained in an installation. For instance, one can display with COSAC the decay heat emitted by the nuclear material contained in an intermediate storage plant installation;

- Output data related to radiotoxicity: this type of outputs is related to radiotoxicity emitted by the nuclear material contained in an installation. For instance, one can display the radiotoxicity emitted by the nuclear material contained in an ultimate storage installation;

- Other outputs: these output data are related to Separative Work Units (SWU) and produced energy.

The isotopic compositions of the spent fuel inventory and the generated irradiation matrices are entered into COSAC using a GUI that facilitates the planning of the reactor fleet.

From the screen board, the user can create facilities such as:

- Mines;
- Uranium enrichment plants;
- Reactors (different kinds of reactors can be part of the same scenario);
- Spent fuel cooling and intermediate storage facilities;
- Spent fuel reprocessing and partitioning facilities;
- Ultimate disposal facilities (geological repository).

The circulation of the nuclear material flow through various facilities is modelled by connecting the facilities with each other.

Each facility can be customized by the user from the COSAC GUI with specific features. The COSAC GUI can also be used to make post-calculation analysis easier. COSAC output data after computing a scenario can be quite numerous. Post-processing the output data through the COSAC GUI makes understanding of the trends and the optimization of the studied scenario easier. Gateways or plug-ins to Microsoft Office products are also possible by exporting tables and graphs from the COSAC GUI into ‘htm’ or ‘bmp’ format files, and can help the user to complete the COSAC GUI post-processor if necessary.

8.3.2. Results

8.3.2.1. First simple case

The first case is a simple one, where the fleet comprises only PWRs fuelled with UOX fuel with a total capacity of 59.8 GW(e), and the scenario period is considered from 2000 to 2050. Its UO_2 fuel enrichment is 4.2% with a discharge burnup of 50 GW·d/t, thermal efficiency and load factor are assumed to be 34.35% and 80% respectively, and residence time is set at 4 years. Residence time is not necessary to be an integer always, but for this comparison actual residence time is close to 4. Small difference in residence time between two codes does not affect results as shown in Fig.60.

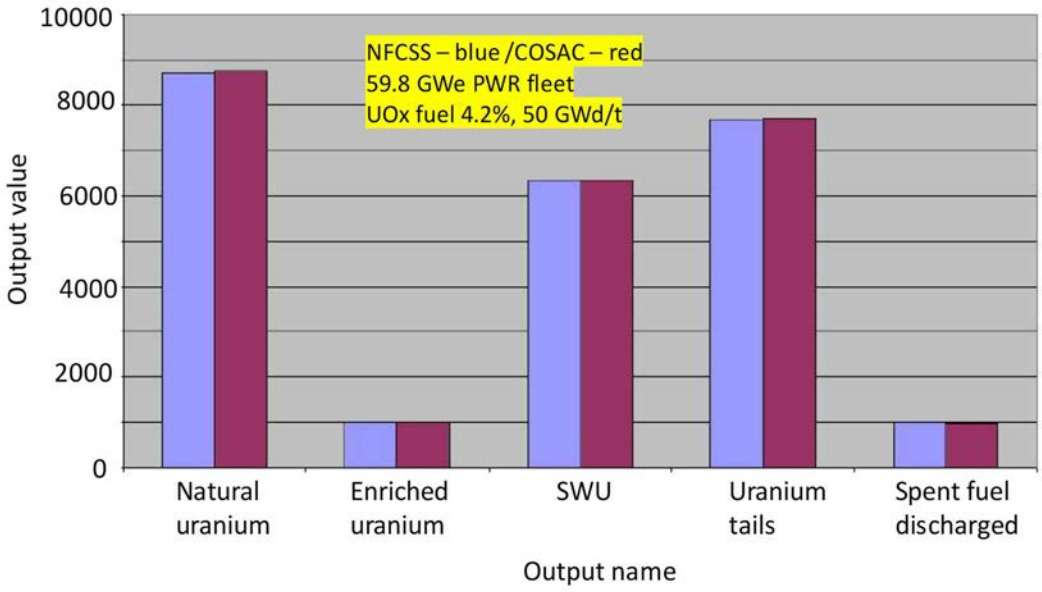


FIG.60. Comparison between NFCSS and COSAC for PWR fleet case.

8.3.2.2. Second complex case

The second case starts with PWR fleet and followed by FBR fleet from year 2000 to 2150 with steady installed power of 60 GW(e). initial fuel enrichment of UO_2 is 4% and UOX-MOX ratio is 30%. Pu content in PWR MOX fuel is 7%, and Pu content in FBR MOX fuel is 25%. For PWR, the following parameters are considered: 33% thermal efficiency, 80% load factor, 4 years residence time, and 45 GW·d/t discharge burnup. For FBR the parameters are: 40% thermal efficiency, 80% load factor, 5 years residence time for core and 8 years residence time for blankets, and 140 GW·d/t discharge burnup for core and 20 GW·d/t discharge burnup for blankets.

In order to compare with theoretical calculations, three periods are chosen below and shown in Fig.61.

- Period 1996–2019 with 42 PWR UOX and 18 PWR 30% MOX;
- Period 2049–2079 with 30 PWR UOX and 30 FBR MOX;
- Period 2094–2150 with 60 FBR MOX.

The results are shown in Fig.62 (Period 1996-2019), Fig.63 (Period 2049-2079) and Fig.64 (Period 2094-2150). In these figures, theoretical calculation uses the following formula;

Annual Fresh Fuel (tons/year) = [Thermal Power (MW(th)) × Number of Reactors × 365.25 (days) × Load Factor] / Discharge Burrup (MW·d/t) (15)

As shown in these figures, NFCSS results, COSAC results, and theoretical calculations are all in agreement with each other.

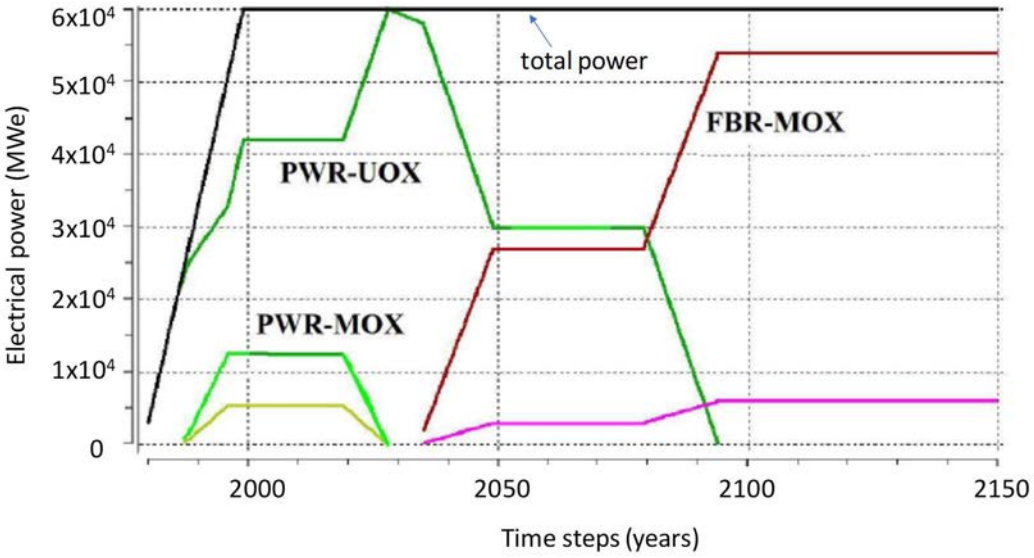


FIG.61. Reactor electric power and its component.

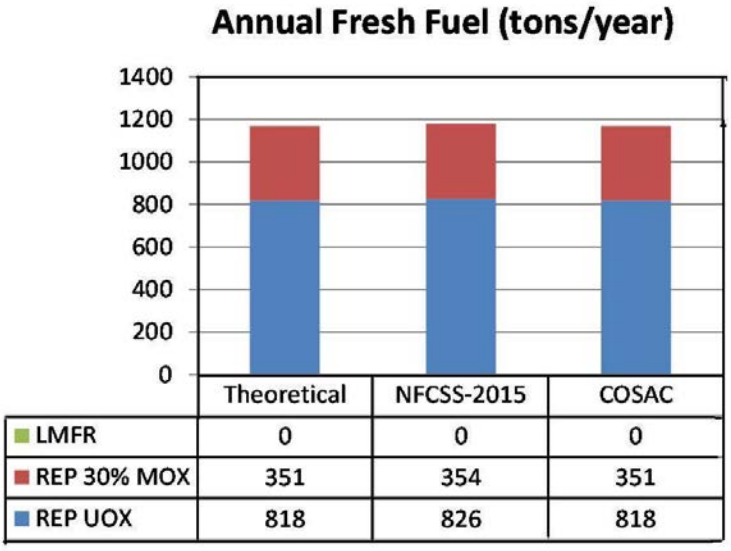


FIG.62. Annual fresh fuel by Theoretical, NFCSS and COSAC (Period 1996-2019).

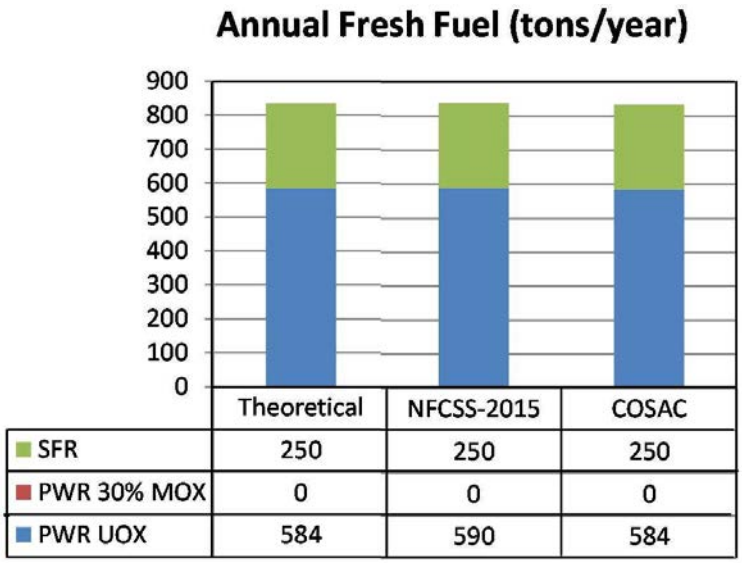


FIG.63. Annual fresh fuel by Theoretical, NFCSS and COSAC (Period 2049-2079).

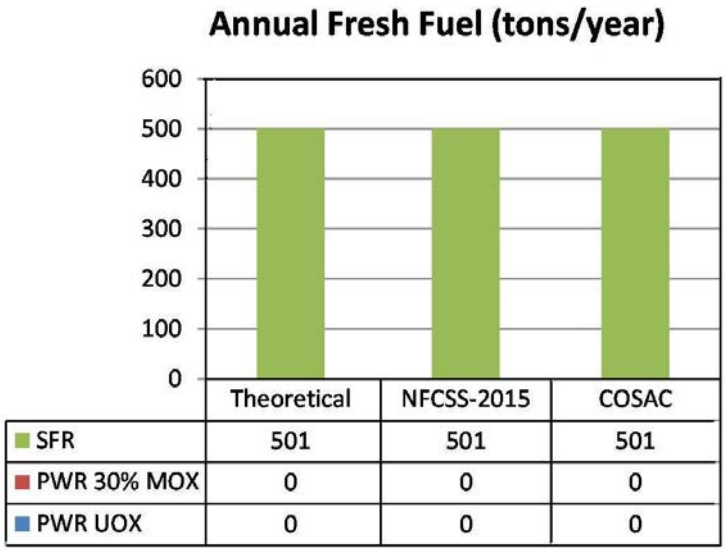


FIG.64. Annual fresh fuel by Theoretical, NFCSS and COSAC (Period 2094-2150).

8.4. BENCHMARK WITH MESSAGE CODE

8.4.1. Description of MESSAGE code

MESSAGE [42] is a tool developed by the IAEA to formulate and evaluate alternative energy supply strategies consistent with user-defined constraints on new investment limits, market penetration rates for new technologies, fuel availability and trade, environmental emissions, etc. The underlying principle of the model is the optimization of an objective function under a set of constraints. The backbone of MESSAGE is the techno-economic description of the modelled energy system. MESSAGE uses projections of energy demand to generate the energy supply system. The most important feature of MESSAGE is its ability to define constraints for all types of energy technologies. The user can limit one technology in relation to other technologies (e.g. the maximum share of wind energy that can be handled in an electricity

network), give exogenous limits on technologies (e.g. a limit on cumulative SO_2 or greenhouse gas emissions) or define additional constraints between production and installed capacity. The model is extremely flexible. It can be used in examining the interaction between energy and electricity markets and climate change policies [43]. In addition to simulating a complete energy system, MESSAGE can also provide a convenient platform for modelling and analysis of nuclear energy systems. This tool can help to produce a description of an entire nuclear energy system with time dependent parameters for long term planning such as: feasibility of a nuclear energy system through correlation and consistency of all nuclear energy system components, constrains and boundary condition imposed on the system; fissile material flows in a close fuel cycle and fuel cycle requirements. MESSAGE also assists users for comparing different reactor fleet options in terms of fuel requirement, volume and toxicity of radioactive waste, etc.

Users can also decide which components to include in the model and each component can be represented with specific details, such as first loading and final unloading of fuel in reactors, cooling time for spent fuel discharged from reactor, lag and lead time for processes, process losses, isotopic composition of spent fuel during the cooling time in storage at the NPP, and reprocessing lag time due to decay of unstable isotopes. However, MESSAGE has some limitations regarding accounting for the decay of plutonium and minor actinides in intermediate stocks.

In order to demonstrate the capabilities of MESSAGE, three nuclear fuel cycle options were simulated, and results were obtained [42]. The major assumptions and boundary conditions for nuclear energy systems as well as data for thermal and fast NPPs (including their respective fuel cycles) are taken from the GAINS (Global Architecture of Innovative Nuclear Energy Systems Based on Thermal and Fast Reactors Including a Closed Fuel Cycle) analytical framework [44].

The first demonstration case describes modelling of a nuclear energy system based on thermal reactors with once-through fuel cycle. The model presents an optimal structure for nuclear power development and allows for assessing the optimal schedule for introduction of various reactor technologies and fuel cycle options, infrastructure facilities, nuclear material flows and wastes, investments and other costs. The reactors and fuels considered are: PHWR using NU fuel; LWR using uranium oxide (UOX) fuel; and advanced light water reactors (ALWR) using UOX fuel. The projection of nuclear demand growth is based on GAINS' high scenario, which assumes a global nuclear energy demand of 5000 GW(e)·year in 2100 and beyond until the end of the modelling period. Historical capacities of NPPs are presented for both LWR and PHWR reactor types. The spent fuel is stored temporarily in these scenarios. After running the MESSAGE tool several times, specific results can be selected and displayed in an interactive mode.

The second case describes modelling a nuclear energy system based on thermal reactors with reprocessing of spent fuel. Plutonium recovered from this process is reused as mixed-oxide (MOX) fuel. This case considers the use of UOX and MOX fuels. UOX fuel is fabricated using natural uranium or reprocessed uranium, while MOX fuel is fabricated from reprocessed plutonium and depleted uranium. It is assumed that a reactor can use MOX for about one-third of its core fuel. Several results can be extracted and analyzed such as nuclear electricity generation, fresh fuel requirements, natural uranium use, reprocessing requirements, and annual investments in NPPs. Front end requirements of the fuel cycle (conversion, enrichment and fuel fabrication) are considered as services in this model. For the back end of the fuel cycle, reprocessing is modelled as a facility with corresponding technical and economic parameters.

The third case provides guidance for building a model nuclear energy system based on thermal and fast reactors in a fully closed fuel cycle. The reactors and fuels considered are PHWRs using natural uranium fuel, LWRs using UOX fuel, ALWRs using UOX fuel, and fast reactors (FR) using MOX fuels for core and depleted uranium for blankets. In this scenario it is assumed that FRs will be introduced in 2020 and achieve 400 GW(e)·year capacity in 2050. After 2050, fast reactors are introduced according to availability of plutonium and economic expediency.

The models representing nuclear energy systems here are not unique. Users can modify the models by adopting a different nuclear fuel cycle modelling approach. Other nuclear energy system issues can also be analyzed with MESSAGE. For example, in the GAINS project, MESSAGE was used to examine the role of research, development and demonstration. The code can also be used to examine the cost components for a nuclear energy system based on a closed nuclear fuel cycle with fast reactors, and to model the world as country groups operating either a thorium fuel cycle based on thermal and fast reactors with spent fuel reprocessing and Pu/U-233 recycling, or MSRs and ADS featuring minor actinide multi-recycling.

Participants in INPRO's GAINS project performed assessments by comparing the results of different codes in order to ensure the credibility of results. Cross-check studies using tools developed by IAEA and organizations from Member States were essential to develop broad consensus and uniformity in support of decision making related to long-term nuclear strategy and energy planning. The cross-check calculations were performed for three scenarios: two cases using once-through fuel cycle with only thermal reactors and one plutonium recycle scenario based on thermal reactors and a break-even fast reactor with a breeding ratio of 1.0. These showed consistent results related to the calculation of indicators in the area of fresh and discharged fuel flows and waste flows. The accuracy of the calculation supports reliable assessment of trends in the consumption of uranium and accumulation of discharged fuel, fissile material and the main components of radioactive waste for the selected scenarios. However, in the case of plutonium multi-recycle scenarios, results could vary significantly depending on how the codes treat approximation of the isotopic vectors of plutonium.

8.4.2. Benchmarking cases

A comparative study between NFCSS and MESSAGE codes was done and is documented here. A scenario, shown in Fig.65, was selected for comparison. This scenario simulates a nuclear fleet comprising LWRs and UOX and MOX moving to FR fleet. The time period considered was 2010–2150 with a constant demand of 60 000 MW(e).

The model simulates LWR units fuelled by UOX and assumed to have 1000 MW(e) of installed capacity with capacity factor of 80%, LWR (MOX/UOX) units which are assumed to have 1000 MW(e) of installed capacity with capacity factor of 80%, and FR (MOX) units which are assumed to have 1000 MW(e) of installed capacity with capacity factor of 85%. LWR (UOX) units use 100% UOX fuel; LWR (MOX/UOX) units use two fuel types: 30% MOX and 70% UOX and FR (MOX) units use MOX fuel for the core and depleted uranium for the blanket. Recycle of plutonium in the form of MOX fuel is also assumed. Figure 66 shows the scenario flow chart for the selected scenario.

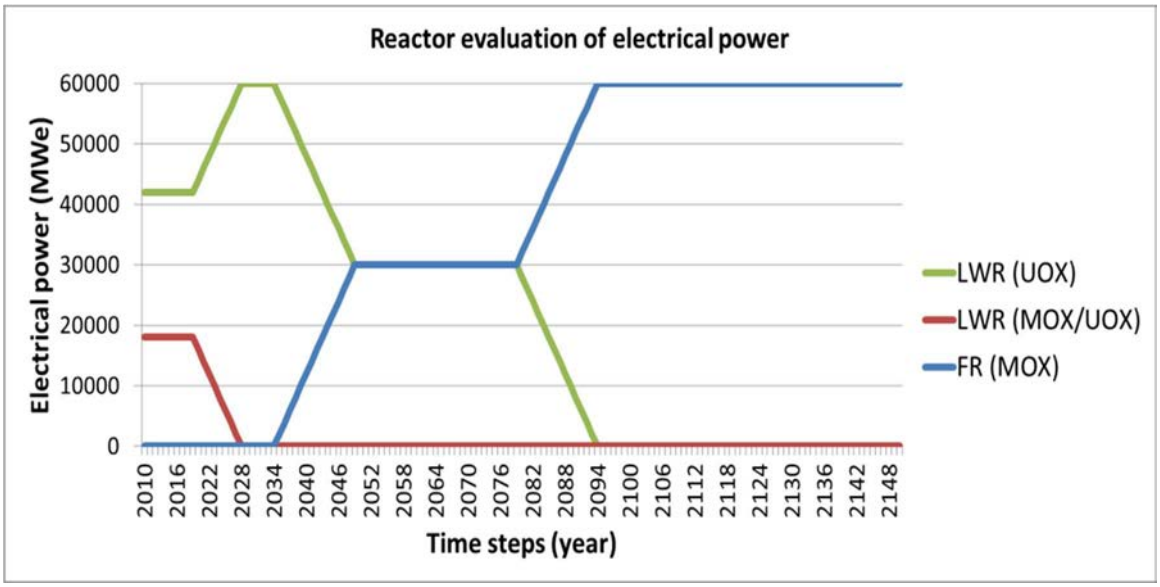


FIG.65. The Reactor evaluation of electrical power.

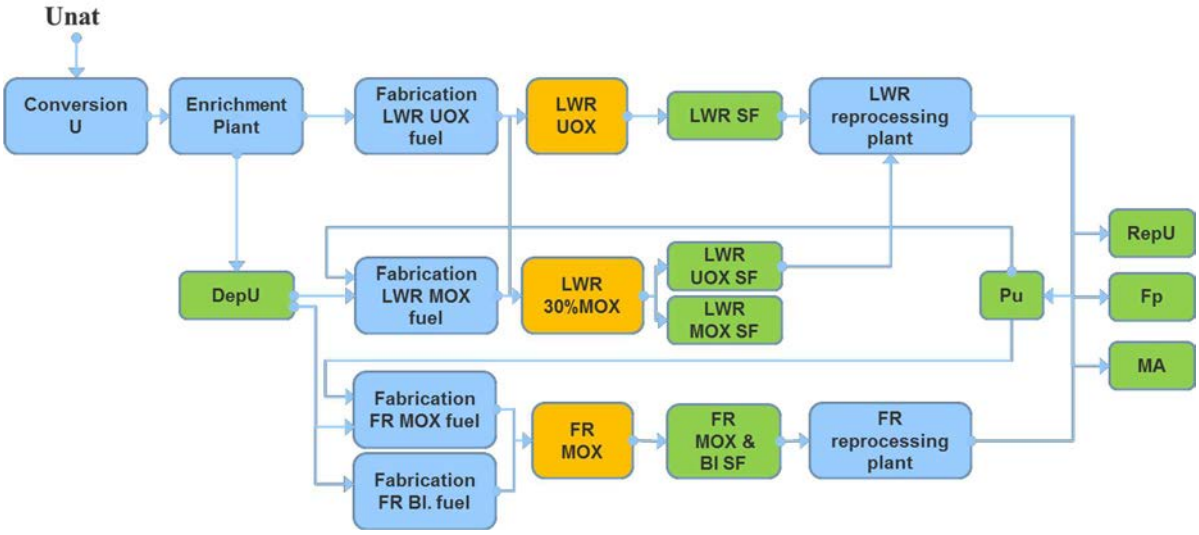


FIG.66. Scenario flow chart.

The technical and economic data of LWR (UOX), LWR (MOX/UOX), FR (MOX) units and their fuel cycle is given in Table 53.

TABLE 53. TECHNCIAL DATA ON REACTORS AND FUEL CYCLE

Item	*Unit*	*UOX 100%*	*MOX 30%*	*MOX 70%*	*CORE MOX*	*BLANKET*
Nuclear capacity	GW(e)	1	1	1	0.9	0.1
Load factor	NA[(1)]	0.8	0.8	0.8	0.8	0.8
Thermal efficiency	NA	0.33	0.33	0.33	0.4	0.4
Discharge burnup	GW·d/t-HM	45	45	45	140	20
Residence time	EFPD	1200[(2)]	1200	1200	1623[(3)]	4000[(4)]

Item	*Unit*	*UOX 100%*	*MOX 30%*	*MOX 70%*	*CORE MOX*	*BLANKET*
Enrichment of fresh fuel	NA	0.04	0.07	0.04	0.25	0.002
Tails assay	NA	0.0025	0.0025	0.0025	0.003	0.003
Cooling time	year	6	7	6	7	7
Power density	kW/kg	37.5	37.5	37.5	86.27	5

Note: (1) NA – Not applicable. (2) 45/37.5*1000=1200, (3) 140/86.27*1000=1623, (4) 20/5*1000=4000

The UOX fuel for LWR has an initial reference enrichment of 4%. The composition to be used in the benchmark is given in Table 54.

TABLE 54. INITIAL COMPOSITION FOR LWR UOX FUEL

Nuclide	*wt. %*
U-235	4
U-238	96

The MOX fuel for LWR has an initial reference enrichment of 7 %. The composition to be used in the benchmark is given in Table 55.

TABLE 55. INITIAL COMPOSITION FOR LWR MOX FUEL

Nuclide	*wt. %*
U-235	0.3
Pu-238	1.36578
Pu-239	60.104860
Pu-240	21.629860
Pu-241	11.700000
Pu-242	5.200000

The MOX fuel for FR has an initial reference enrichment of 22.37 %. The composition to be used in the benchmark is given in Table 56.

TABLE 56. INITIAL COMPOSITION FOR FR MOX FUEL

Nuclide	*wt %*
U-235	0.2
Pu-238	2.272222
Pu-239	59.052080
Pu-240	25.893050
Pu-241	6.806250
Pu-242	5.977083

The fuel for blanket of FR has an initial reference enrichment of 0.2 %. The composition to be used in the benchmark is presented in Table 57.

TABLE 57. INITIAL COMPOSITION FOR FR BLANKET FUEL

Nuclide	*wt %*
U-235	0.2
U-238	99.8

In contrast to NFCSS, the MESSAGE code does not have a depletion module to calculate the evolution of isotopic composition in the fuel. In order to calculate the input data for MESSAGE model with spent fuel reprocessing options, isotopic composition of spent fuel discharged from each type of reactors were taken from NFCSS output data and given in Table 58.

TABLE 58. NUCLIDE GROUP COMPOSITION OF SPENT FUEL AFTER COOLING AND ONE YEAR OF REPROCESSING

Component	*LWR (UOX) spent fuel*	*FR core spent fuel*	*FR blanket spent fuel*
Uranium total	0.9425136	0.6452397	0.9291465
U-235	0.0068005	0.0005172	0.0011301
U-236	0.0052445	0.0002549	0.0001840
Plutonium total	0.0097292	0.2017105	0.0499264
Minor actinides	0.0013493	0.0085250	0.0003044
Fission products	0.046408	0.1445248	0.0206227

8.4.3. Results

In the first part of comparison three equilibrium periods were considered:

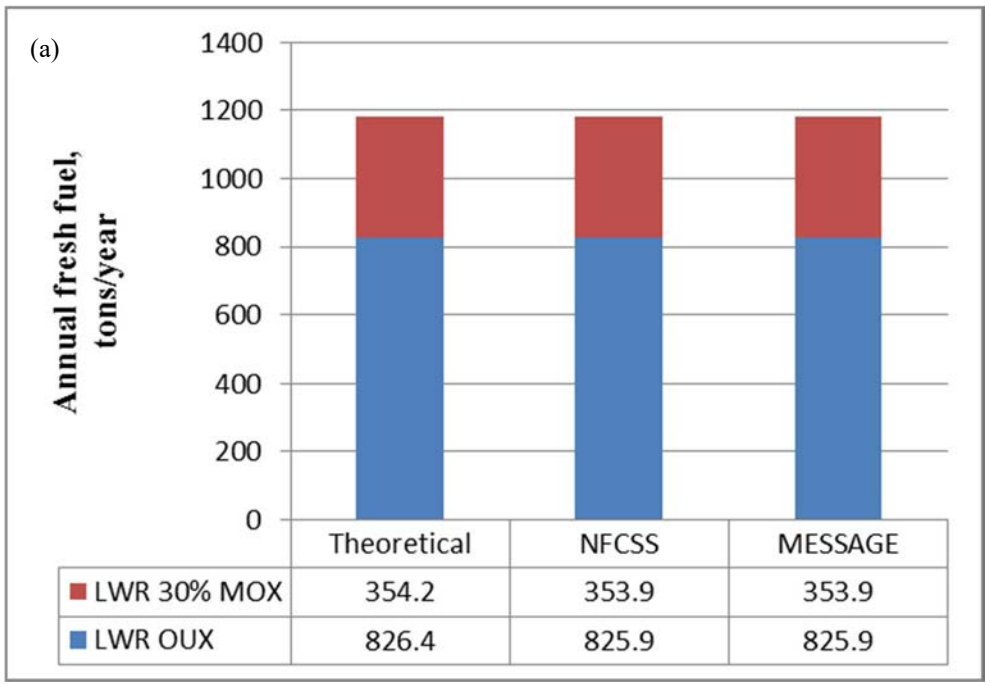
- Period 2010–2019
  - 42 PWR UOX; 42 GW(e); 70% fleet power
  - 18 PWR 30% MOX; 18 GW(e); 30% fleet power
- Period 2049–2079
  - 30 PWR UOX; 30 GW(e); 50% fleet power
  - 30 SFR; 30 GW(e); 50% fleet power
- Period 2094–2150
  - 60 SFR; 60 GW(e); 100% fleet power.

The comparison of the three equilibrium periods is focused on the annual fresh fuel fabrication and spent fuel discharges. The results are presented in Fig.67 to Fig.69. Theoretical values were obtained from the following formulas:

$$Annual\ Fresh\ Fuel = \frac{Pth\ x\ 365.25\ x\ LoadFactor\ x\ NumberOfReactors}{Burnup} \quad (16)$$

$$Spent\ Fuel\ Discharge\ = Annual\ Fresh\ Fuel \quad (17)$$

Results from the NFCSS and MESSAGE are in good agreement for the equilibrium periods as well as with theoretical values.



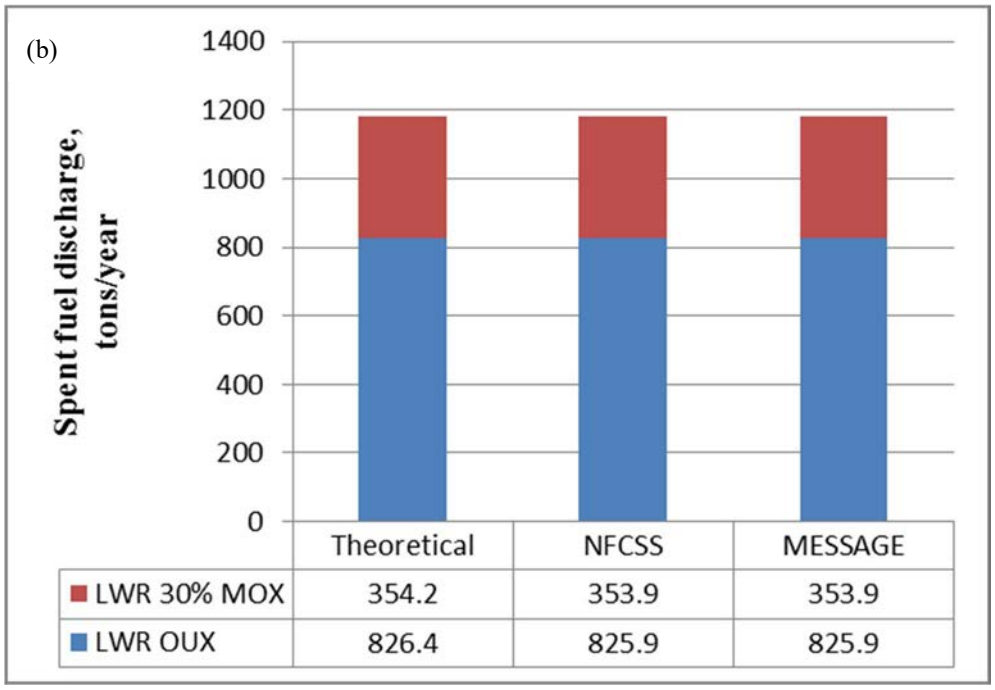


FIG.67. The comparison of (a) annual fresh fuel fabrication and (b) spent fuel discharge in the period 2010–2019.

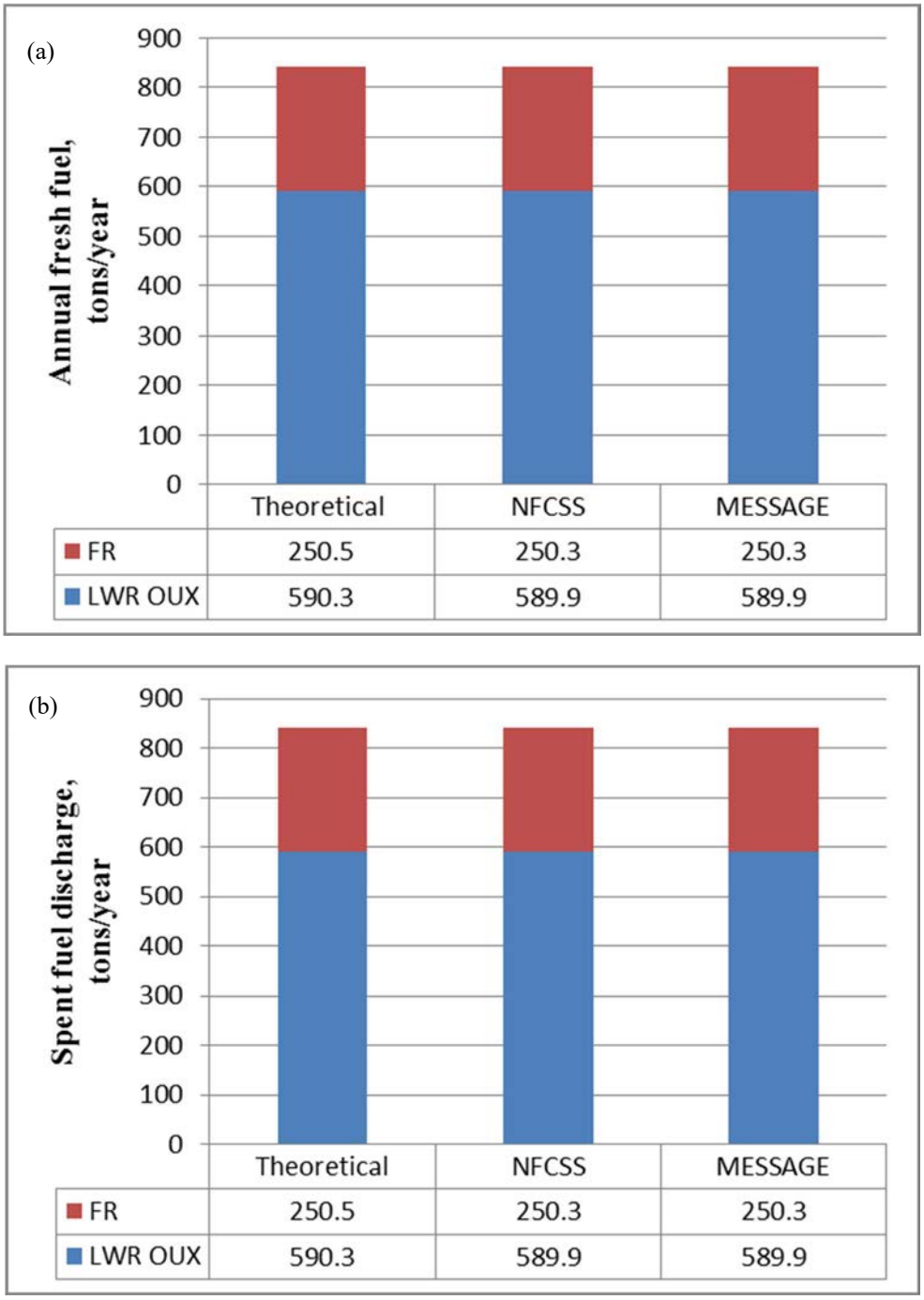
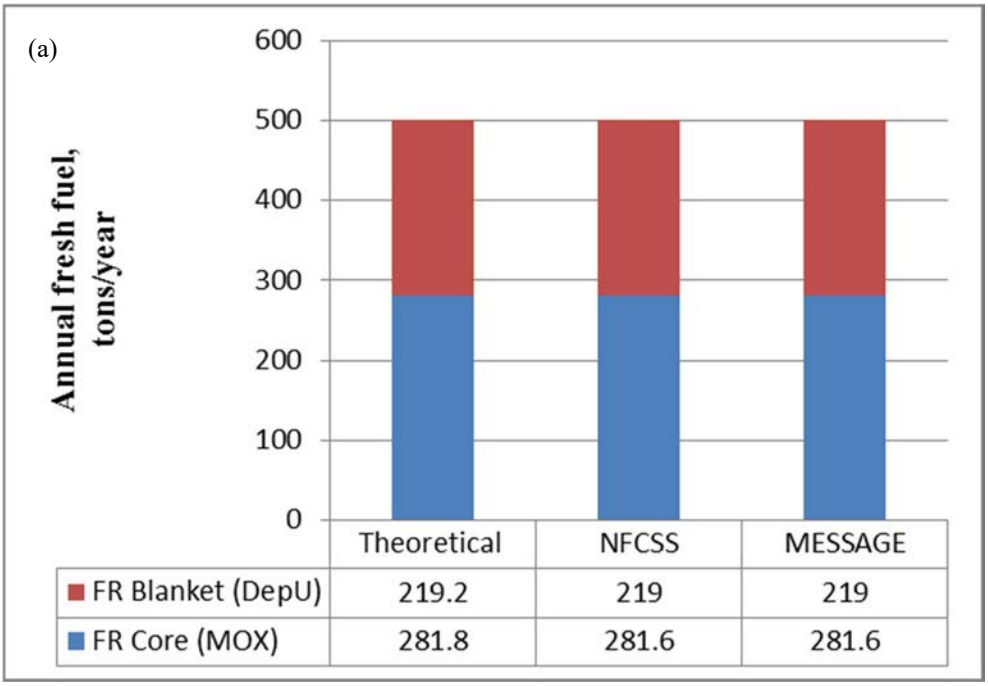


FIG.68. The comparison of annual fresh fuel fabrication (a) and spent fuel discharge (b) in the period 2049–2079.



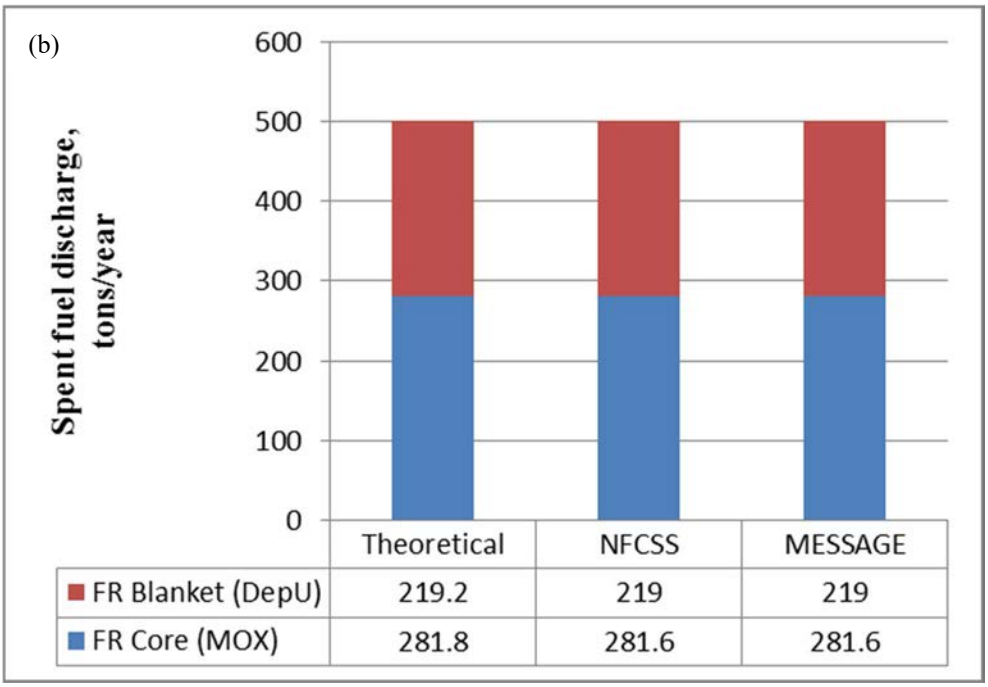
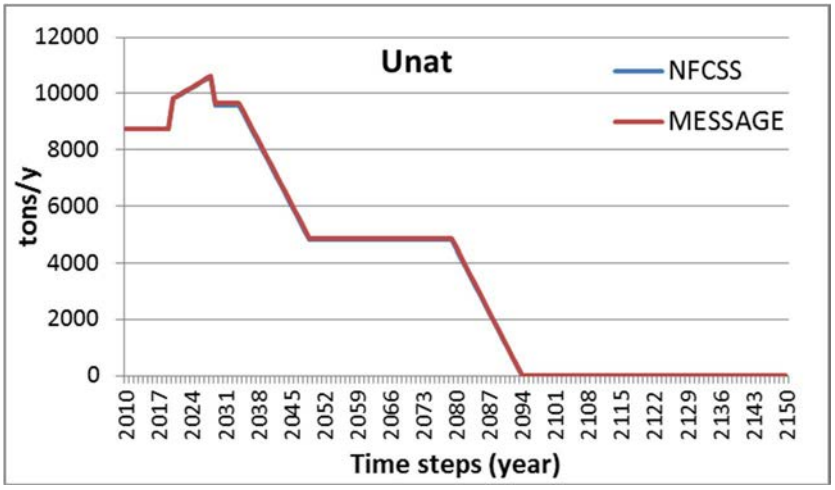


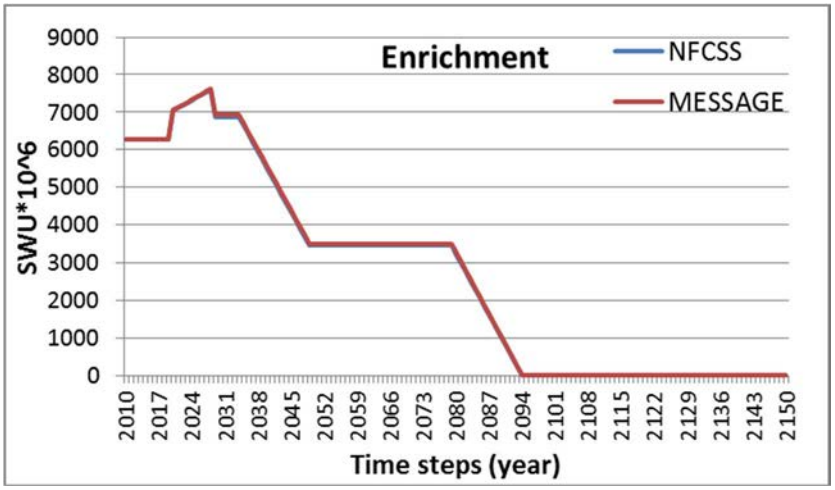
FIG. 69. The comparison of annual fresh fuel fabrication (a) and spent fuel discharge (b) in the period 2094–2150.

In the second part of comparison the entire time period from 2010 to 2150 was considered. The comparison is focused on resources, fuel fabrication, spent fuel discharge, reprocessing spent nuclear fuel, plutonium management and minor actinides, reprocessed uranium and fission products stock area. The results are presented in Fig.70 to Fig.75.

(a)



(b)



(c)

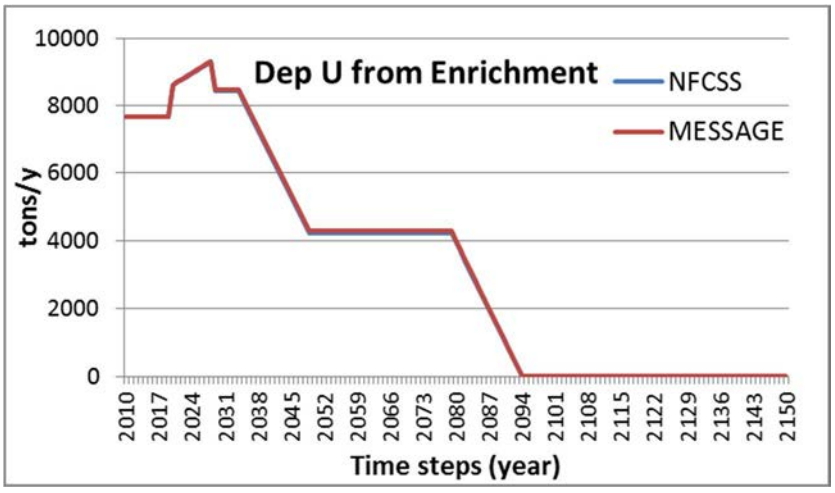
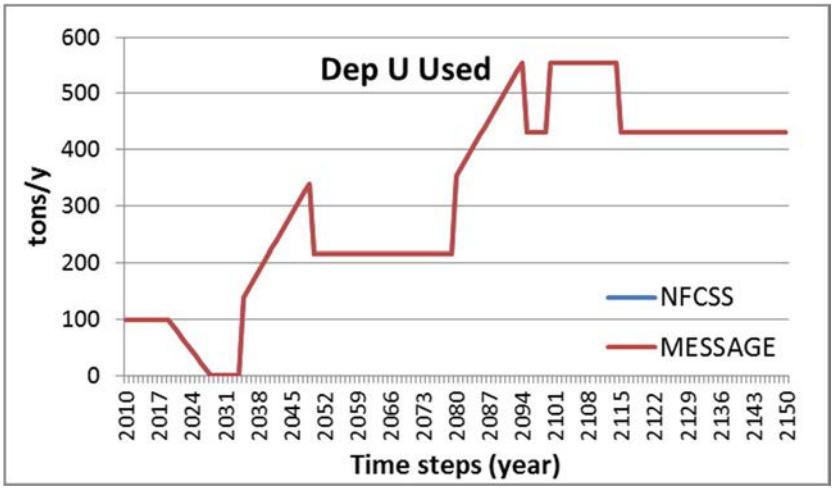


FIG.70. Comparison in the area of resource: (a) Natural uranium, (b) SWU for enrichment, (c) Depleted uranium from enrichment, (d)Used depleted uranium, (e) Depleted uranium stock.

(d)



(e)

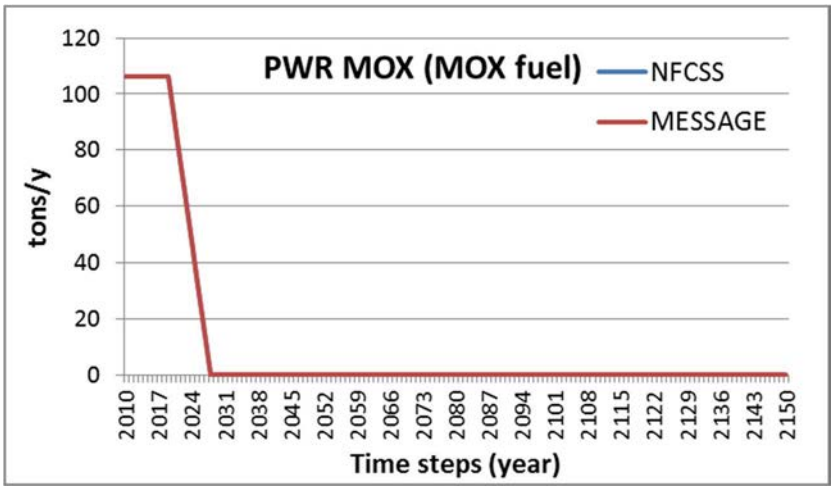
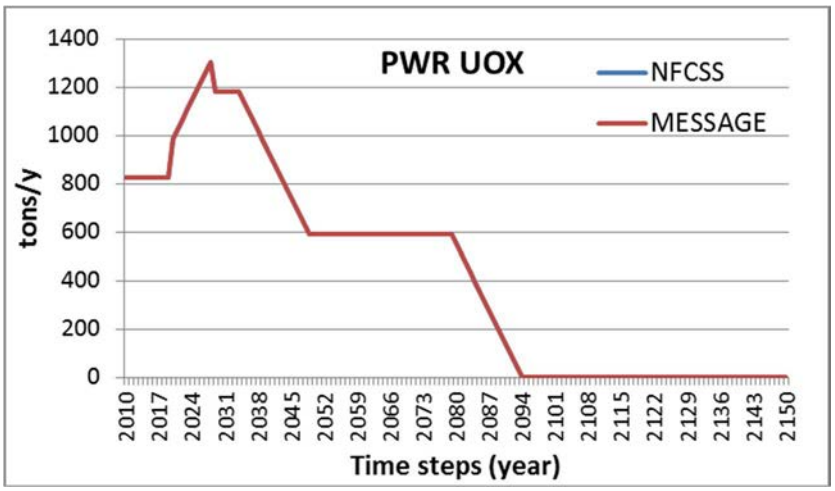


FIG.70. (Continued)

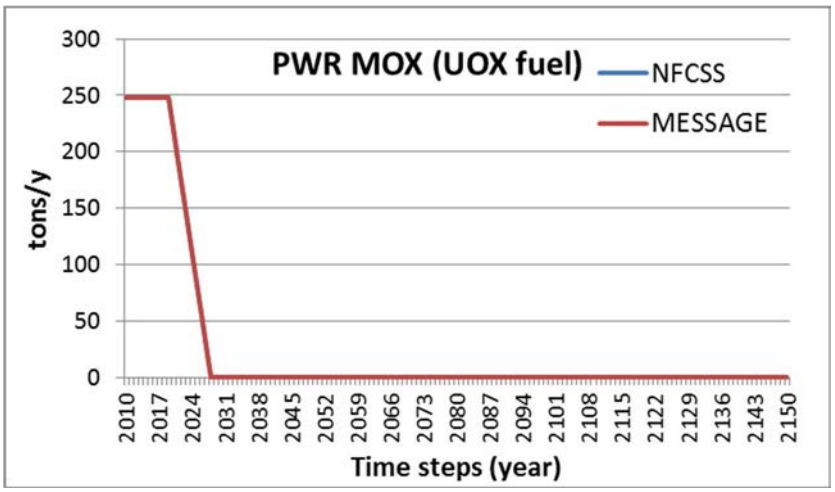
For MESSAGE and NFCSS codes there is a good agreement in estimating resources and this is shown in Fig.70. The maximum deviation for calculations of required amount of natural uranium, SWU for enrichment, depleted uranium from enrichment, used depleted uranium and depleted uranium stock are 1.63% 1.66%, 1.61%, 0.003% and 1.47% respectively.

For fuel fabrication calculations, MESSAGE and NFCSS codes are in good agreement as shown in Fig.71. The maximum deviation for calculations of annual fabrication of UOX fuel for LWR (UOX), UOX fuel for LWR (MOX/UOX), MOX fuel for LWR (MOX/UOX), MOX fuel for FR (core), fuel for FR blanket and Pu used for fabrication MOX fuel for LWR and FR does not exceed 0.011%.

(a)



(b)



(c)

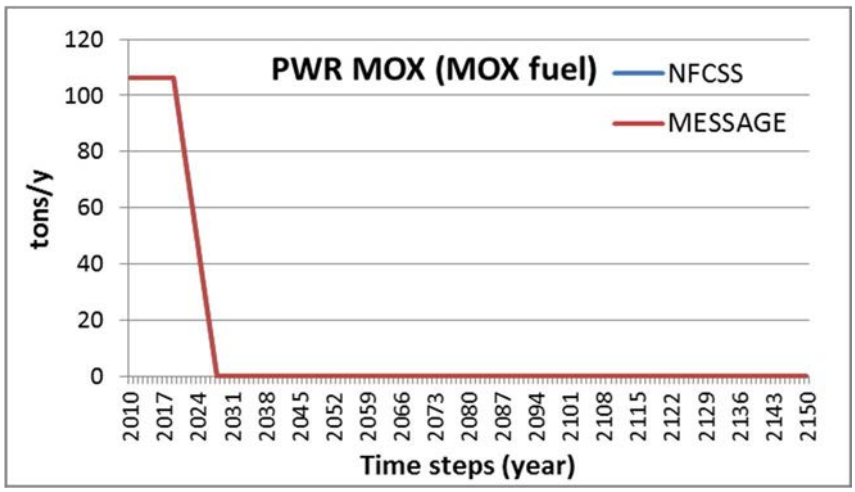
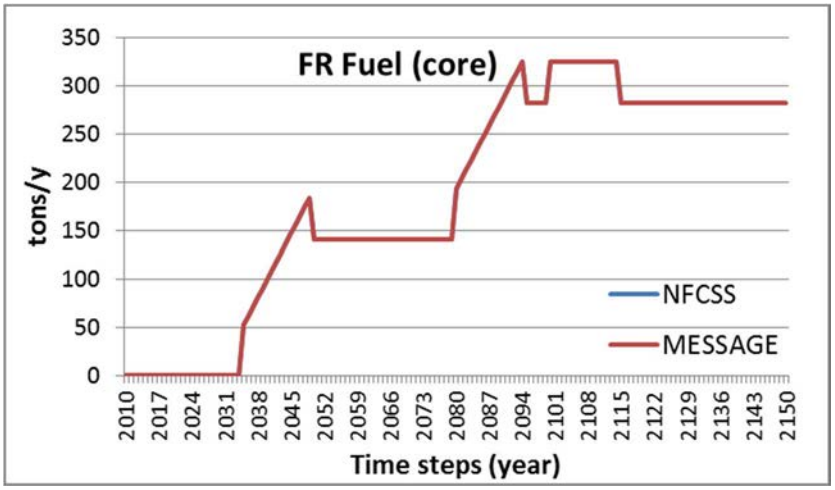
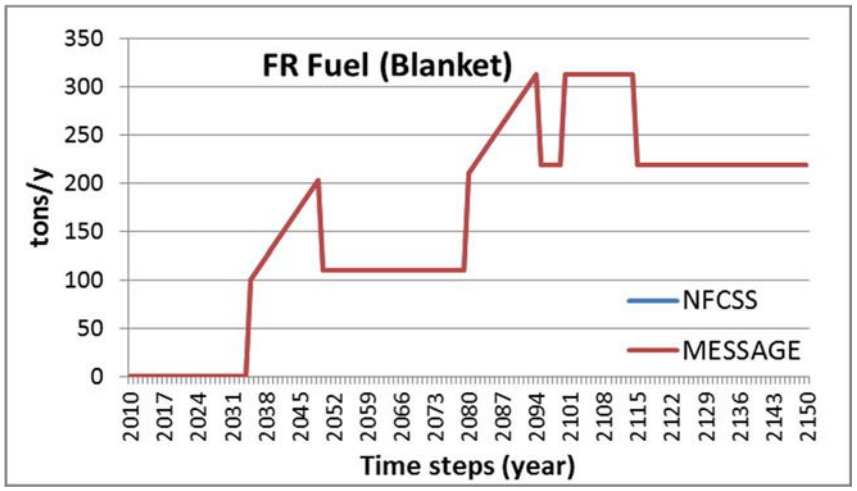


FIG.71. Comparison in the area of fabrication: (a) UOX fuel for LWR (UOX), (b) UOX fuel for LWR (MOX/UOX), (c) MOX fuel for LWR (MOX/UOX), (d) MOX fuel for FR (core), (e) Fuel for FR blanket, (f) Pu used for fabrication of MOX fuel for LWR, (g) Pu used for fabrication of MOX fuel for FR.

(d)



(e)



(f)

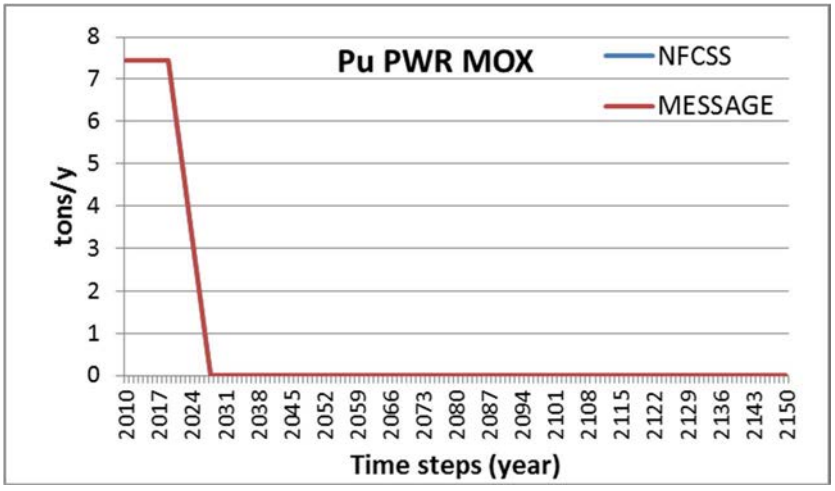


FIG.71. (Continued)

(g)

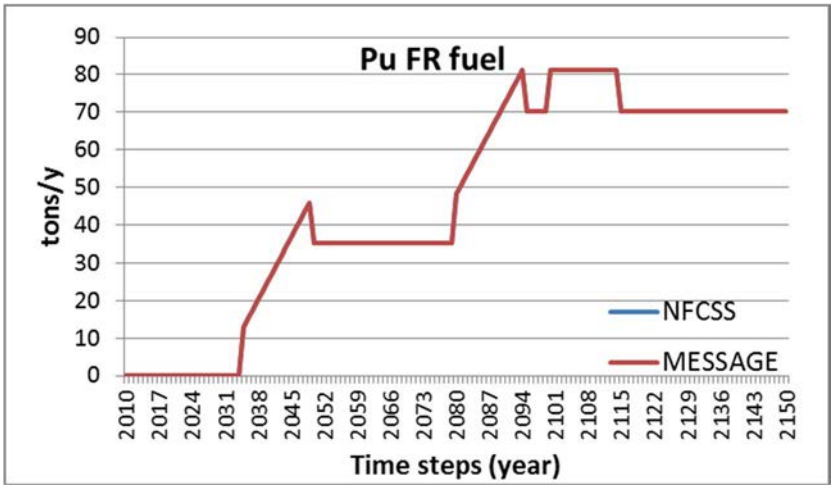
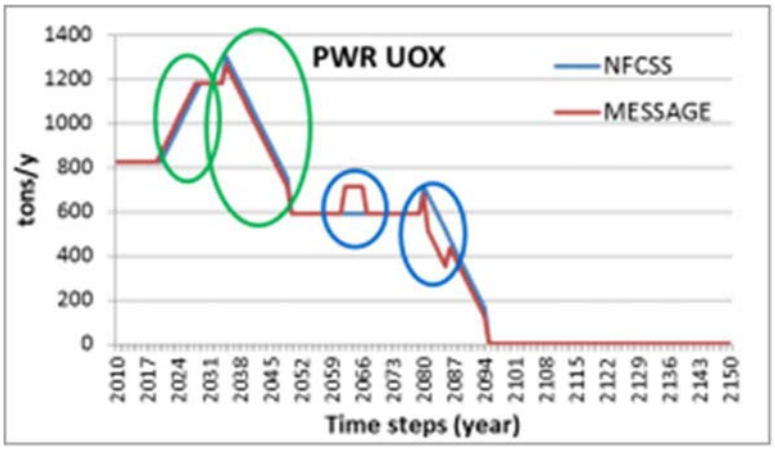


FIG.71. (Continued)

The differences in the results of calculations, shown in circled areas with green line in Fig.72 are caused due to different approaches of the nuclear fuel discharge. In MESSAGE loading and discharge of the nuclear fuel are conducted for one year, while NFCSS simulates this process with one year delay.

(a)



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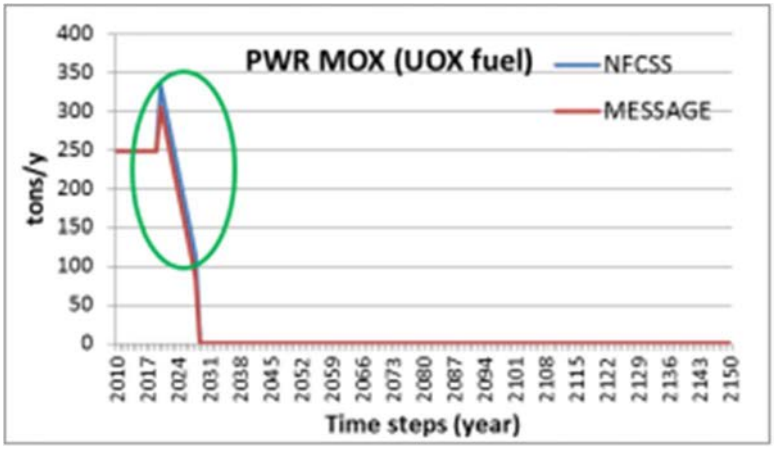
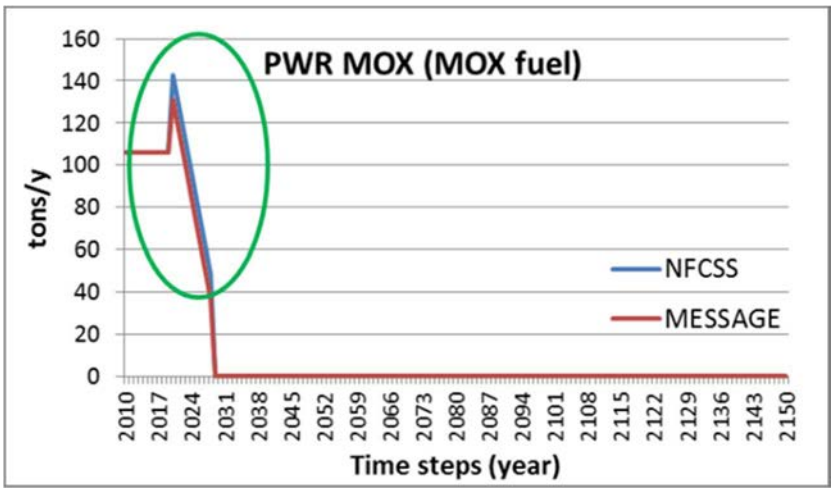
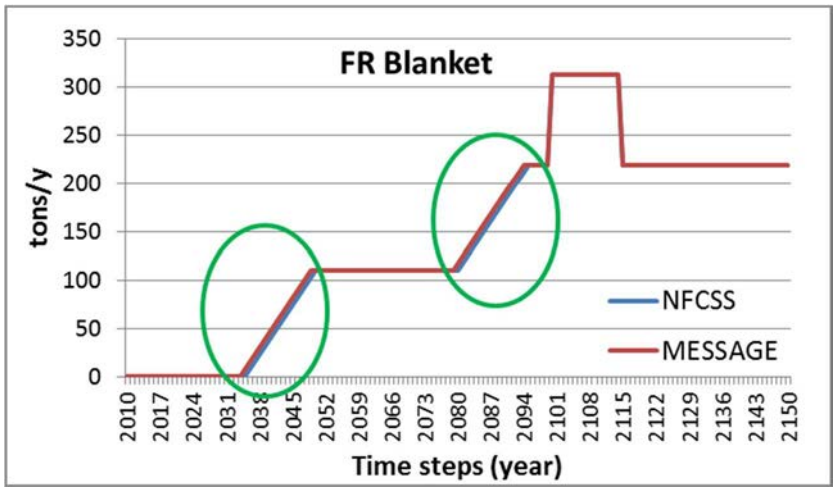


FIG.72. Comparison in the area of spent fuel: (a) UOX SF from LWR (UOX), (b) UOX SF from LWR (MOX/UOX), (c) MOX SF from LWR (MOX/UOX), (d) MOX SF from FR (core), (e) SF from FR blanket.

(c)



(d)



(e)

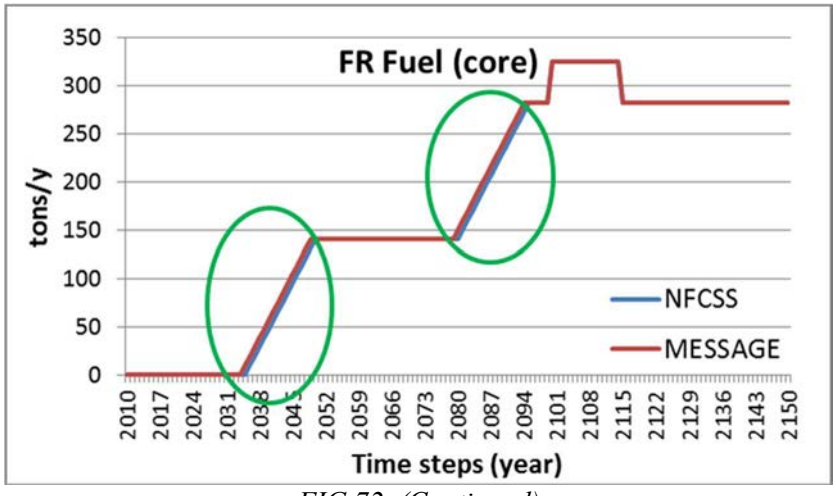


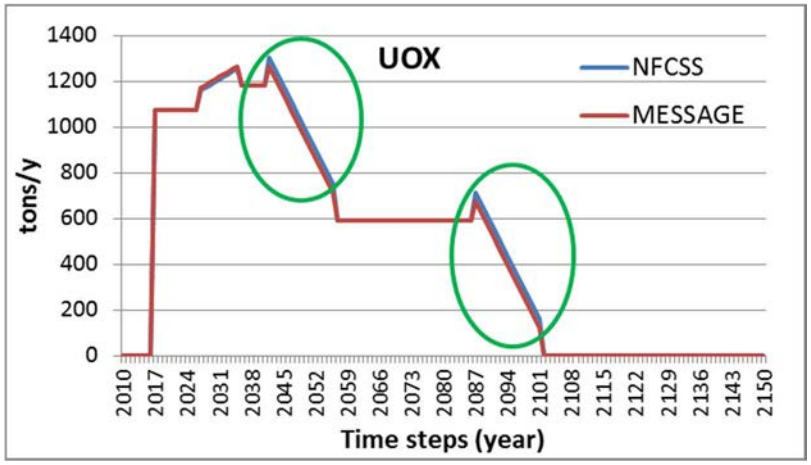
FIG.72. (Continued)

The differences in the results of calculations, shown in circled areas with blue line in Fig.72 (a), are due to different approaches to modelling added and removed capacities. The NFCSS enables to add and remove capacities at any time, while in MESSAGE time for added capacities and technology lifetime are simulated. As a result, increased output data in MESSAGE is associated with decommissioning and discharge of spent nuclear fuel from the

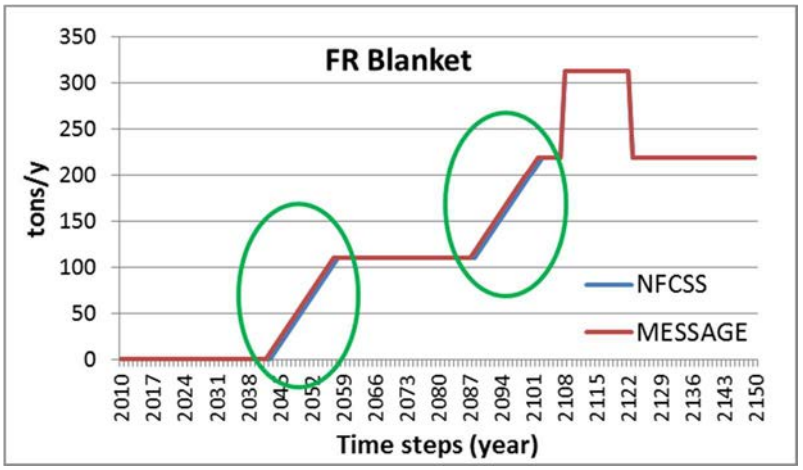
core in the period of 2061–2068, which tends to lowering of the results in the period of 2079–2086.

The differences in the results, shown in circled areas with green line in Fig.73, are due to different amount of the spent nuclear fuel ready for recycling, which occurs as a result of differences in the approaches of nuclear fuel discharge as stated above.

(a)



(b)



(c)

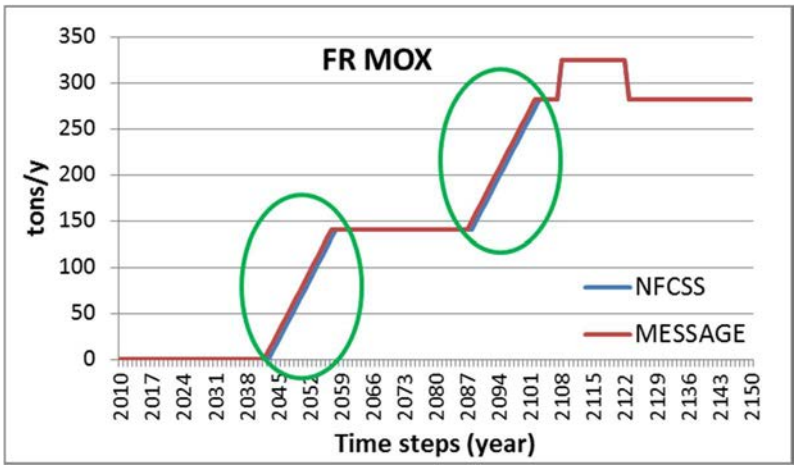
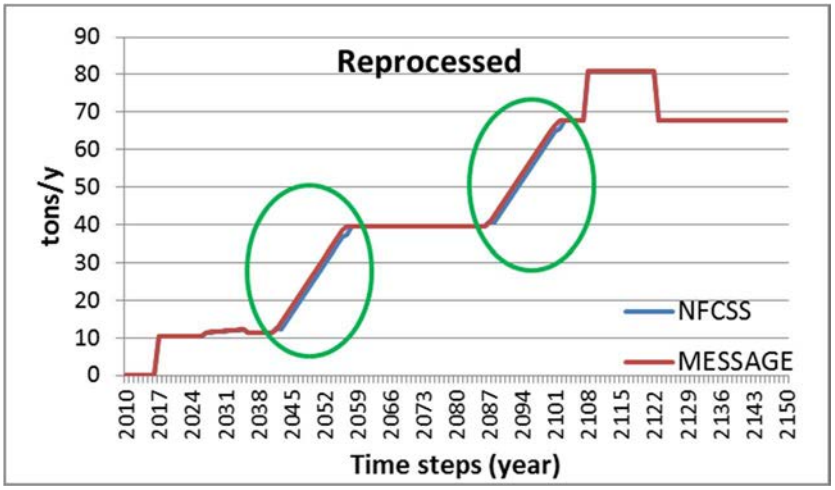


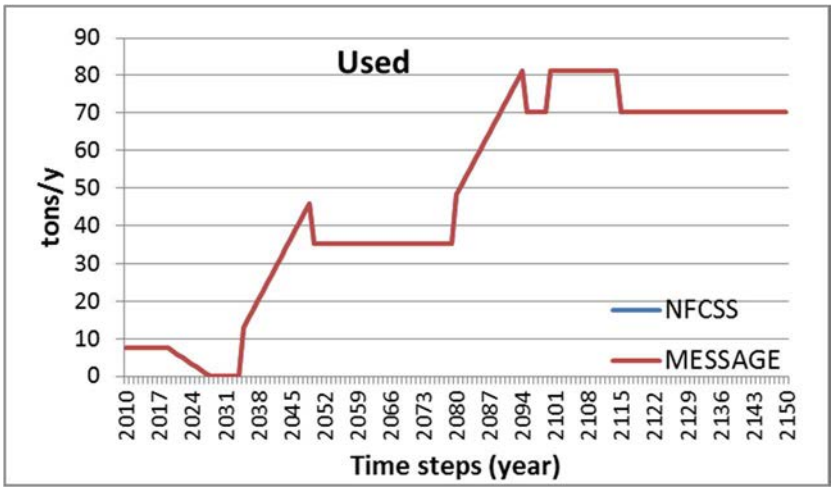
FIG.73. Comparison in the area of reprocessing: (a) Reprocessing UOX SF from LWR), (b) Reprocessing MOX SF from FR core, (c) Reprocessing SF from FR blanket.

Differences in the results, shown in circled areas with green line in Fig.74 (a), are due to different amount of the spent nuclear fuel ready for recycling, which occurs as a result of differences in the approaches of nuclear fuel discharge.

(a)



(b)



(c)

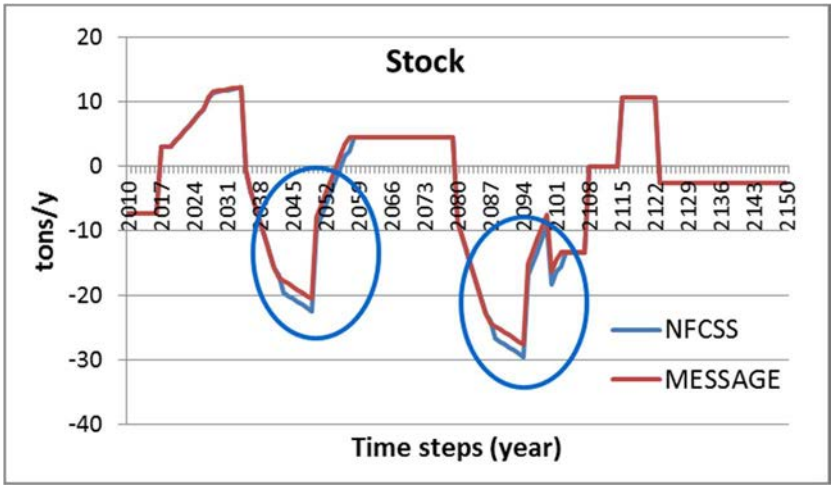
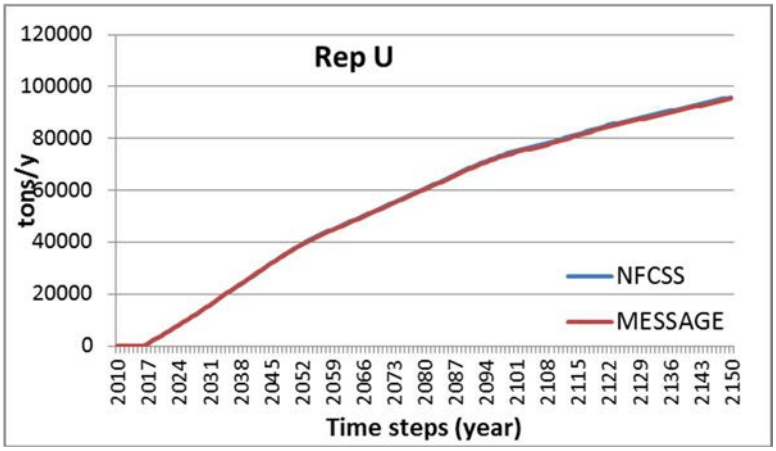


FIG.74. Comparison in the area of plutonium: (a) Reprocessing Pu, (b) Used Pu, and (c) Pu stocks.

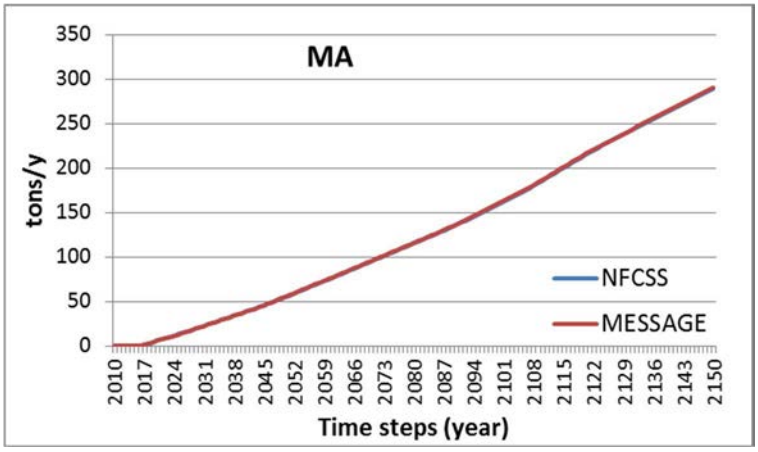
The deviation in the outputs is due to the different amount of reprocessed plutonium which occurs as a result of differences in the approaches of nuclear fuel discharge in NFCSS and MESSAGE.

For MESSAGE and NFCSS codes in stock area there was a good agreement (Fig.75). The maximum deviation for calculations of minor actinides, reprocessed uranium and fission products stocks are 0.82% 0.84%, 0.13% respectively.

(a)



(b)



(c)

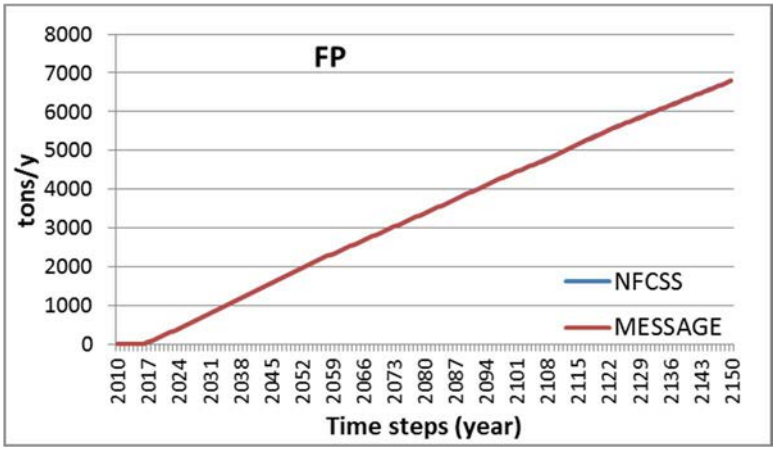


FIG.75. Comparison in the area of stocks: (a) Minor actinides stock, (b) Reprocessed uranium stock, and (c) Fission products stock.

In summary, the following results were obtained from the benchmarking exercises against independent solutions by MESSAGE:

- The NFCSS and MESSAGE show a good agreement of the results for equilibrium periods;
- The discrepancy in the results for spent nuclear fuel was identified during the analysis of the transition periods, which is caused by the differences in the approaches to modelling spent nuclear fuel discharge;
- Different approaches to modelling added and removed capacities lead to the discrepancy in models. This can be avoided by using a more complex modelling of added capacities in MESSAGE;
- For the realization of the suggested scenario the lack of plutonium was detected during nuclear fuel cycle modelling.

9. CASE STUDIES

9.1. GENERAL

NFCSS has been demonstrated to provide reliable results for the nuclear fuel cycle assessments for 7 reactor types. In this section, NFCSS is shown to be applicable beyond the existing reactor types to innovative reactors. Preliminary assessments done for INPRO and FR are described here to support the potential extension of NFCSS' capabilities in future to include advanced reactors and fuel cycle options under development or consideration.

9.2. INPRO MODELLING

9.2.1. Overview

The IAEA's INPRO has performed several assessments on global, regional and national levels to support a sustainable nuclear energy development for the twenty-first century [9],[44]–[47]. In particular, the GAINS project [44] has addressed technical and institutional issues that need to be resolved in developing a global architecture for this purpose and analysing plausible transitions to such architecture. The project has developed a framework, including a common methodological platform, assumptions and boundary conditions, performed sample studies and indicated potential areas for application of the GAINS framework for dynamic assessment of a transition to future sustainable nuclear energy systems. A study of global scenarios and regional trends [45] illustrated the potential contribution of innovative nuclear energy systems employing fast reactors and closed fuel cycles in meeting the global and regional demands for nuclear energy. An INPRO study [44] has investigated the potential role of thorium in supplementing the uranium–plutonium fuel cycle under several scenarios that assumed a significant global expansion of nuclear energy. A Joint Study [46] assessed a national nuclear energy system based on a closed fuel cycle with fast reactors (FRs) regarding its sustainability to determine milestones for the nuclear energy system deployment, and establish frameworks and areas for collaborative R&D work.

Evaluating a transition scenario for a sustainable nuclear energy system in a holistic way needs appropriate modelling tools that provide users with the ability to perform modelling of the scenario under consideration. INPRO modelling activities are based on existing tools such as MESSAGE [47] and NFCSS [1] that have been developed by the IAEA. These tools help produce a description of the entire Nuclear Energy System (NES) with time dependent

parameters for long term planning horizon, confirm the feasibility of a NES through correlation and consistency of all NES components by taking into account all constraints and boundary conditions imposed on the system, balance fissile material in a close fuel cycle, determine fuel cycle requirements and assist the user in the choice of alternatives by comparison of different options regarding need for fuel, volume and toxicity of waste, etc. In addition, the results of material flow analyses can be used as input parameters for assessment by INPRO methodology in some areas. The NFCSS code has been successfully used for modelling of transition scenarios of innovative NESs of the NFCSS application for nuclear energy system modelling within GAINS collaborative project is described in the following subsections.

9.2.2. Input data

Two growth curves have been established for GAINS. In the high growth case, world's nuclear capacity reaches 5000 GW(e)·year, and in the moderate growth case capacity reaches 2500 GW(e)·year and flattens after 2100. The growth curves have 3 periods. Each growth period is modelled linearly to reach a specific level of generation by the end of the specified period:

- 2009–2030: 600 GW(e)·year for the moderate case and 700 GW(e)·year for the high case;
- 2031–2050: 1000 GW(e)·year for the moderate case and 1500 GW(e)·year for the high case;
- 2051–2100: 2500 GW(e)·year for the moderate case and 5000 GW(e)·year for the high case.

The high case based on LWR, HWR, ALWR and FR (with breeding ratio~1.0) is selected as example of NES modelling.

Four reactors types LWR, ALWR, PHWR and breakeven FR (with breeding ratio~1.0) are considered for the GAINS study. ALWRs replace conventional LWR and FRs displace ALWRs after the FRs are introduced. The PHWRs continue at 6% of the total generation independent of the FR introduction. General characteristics of thermal and fast reactors used in scenarios calculation are shown in Table 59, which is summarized from Tables 6.1 – 6.5 of [44].

TABLE 59. GENERAL CHARACTERISTICS OF THERMAL AND FAST REACTORS

Major specifications	*LWR*	*HWR*	*ALWR*	*FR*	
Reactor net electric output, MW	1000	600	1500	870	
Thermal efficiency	0.33	0.3	0.34	0.42	
Average load factor	0.85	0.85	0.85	0.85	
Discharged burnup, MW·d/kg-HM	45	7	60	66 (core)	
Life time, years	40	40	60	60	
Cooling time, years	5	5	5	5	
Uranium enrichment, %	4	0.711	4.9		
				core	blanket
Mass of fuel, HM	78.7	83.4	129.4	12.6	11.7
Fuel residence time, EFPD				420	457
Pu content in fresh fuel, fractional	-	-	-	0.22	-

Corresponding to the reprocessing strategy planned in many countries, in which core fuel and radial blanket subassemblies are dissolved together and reprocessed at the same time, and to make the input for fuel cycle calculation codes more convenient to calculate, the reactor parameters of the fast reactors were homogenized to a one-region core like LWRs or HWRs.

Data on spent fuel for LWRs and PHWRs were calculated with the CAIN module while the details of FR spent fuel was provided by the user independent of the CAIN module.

In GAINS other assumptions were also used regarding reactor and fuel cycle features: uranium enrichment tails assay is equal to 0.2%; fuel reprocessing without losses of heavy metal isotopes; the spent fuel from HWR is stored temporarily; and unlimited uranium supplies.

GAINS framework also imposes constraints on the FR capacity by 2030 and 2050, and on the total Pu inventory in storage. It is intended to have a total capacity of 10 GW(e)·year from FRs in 2030 and 400 GW(e)·year from FRs by 2050 in the high growth case. The Pu inventory in storage is kept close to zero. Many FRs will be introduced after 2050; the FR build rate is only limited by the amount of available Pu and the overall growth rate. GAINS framework also assumes no limitation in the fuel cycle infrastructure such as mining, conversion plant, enrichment plant, fuel fabrication plant, long term storage for spent fuel, interim storage for separated nuclear materials (for instance, Plutonium, MA, FP), reprocessing plant and geological disposal.

The following options with different FR shares are selected to illustrate application of the NFCSS:

- BAU+ is 'business as usual' (BAU) option with evolutionary advancements. The nuclear energy system in the BAU+ option consists of conventional and advanced thermal reactors LWR, PHWR and ALWR using enriched and natural uranium in a once-through fuel cycle;
- BAU+FR is BAU+ option with introduction of a breakeven FR based on a closed uranium-plutonium fuel cycle (including reprocessing of spent fuel from thermal reactors for recycle in FR).

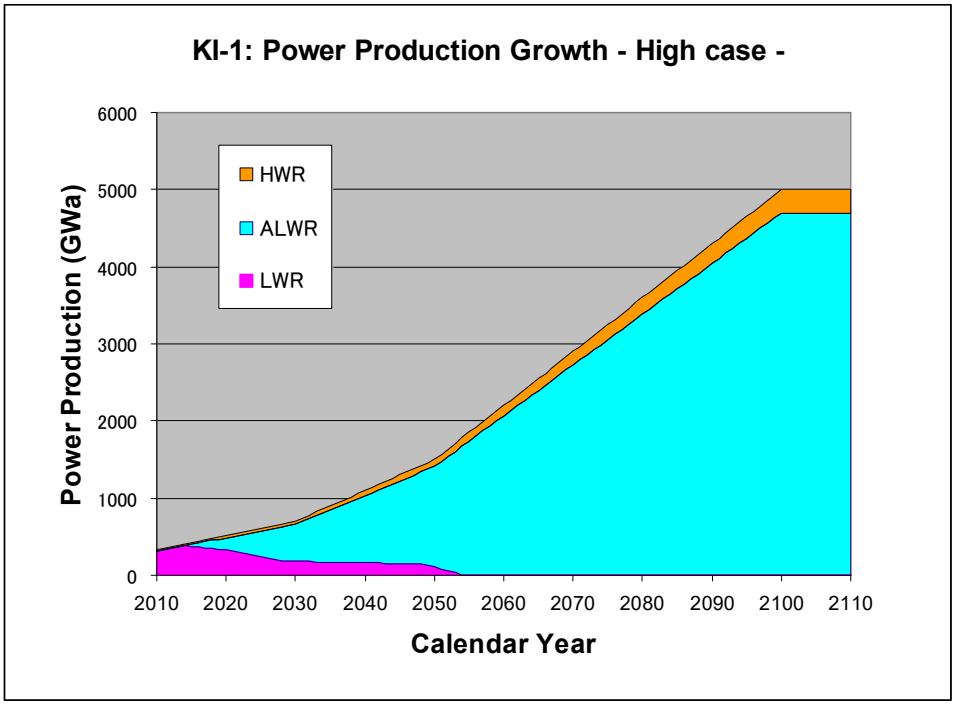
9.2.3. Results of nuclear energy system simulation

Figure 76 shows the trends of power generation for each reactor type in the BAU+ and BAU+FR scenarios. ALWRs are introduced in 2015 and gradually replace LWR, while the share of PHWR is fixed at 6% of total nuclear power capacity. By 2100 the share of fast reactors reaches about 44% of global nuclear energy production. The maximum FR introduction is restrained by zero breeding performance of the breakeven FR.

Cumulative requirements of natural uranium for both nuclear energy system options are shown in Fig.77 (a) and (b). To the end of the century, the total mass of consumed NU would reach 37.8 million tonnes in the BAU+ case. In the BAU+FR case, uranium consumption is 12 million tonnes lower than in the BAU+ case at the end of projection period (i.e., at year 2100). It is clear that currently identified conventional natural uranium resources will be exhausted around 2070 in the BAU+ case and around 2085 in the BAU+FR case.

Thus, transitioning to fast reactors produces a positive effect not only on uranium consumption, but also on the amount of separative work necessary for enriching uranium fuel. Fig.78 (a) and (b) show annual uranium separative work in BAU+ case and BAU+FR case respectively. Because of FR introduction, the values decrease from 750 million SWU to 450 million SWU at 2100.

(a)



(b)

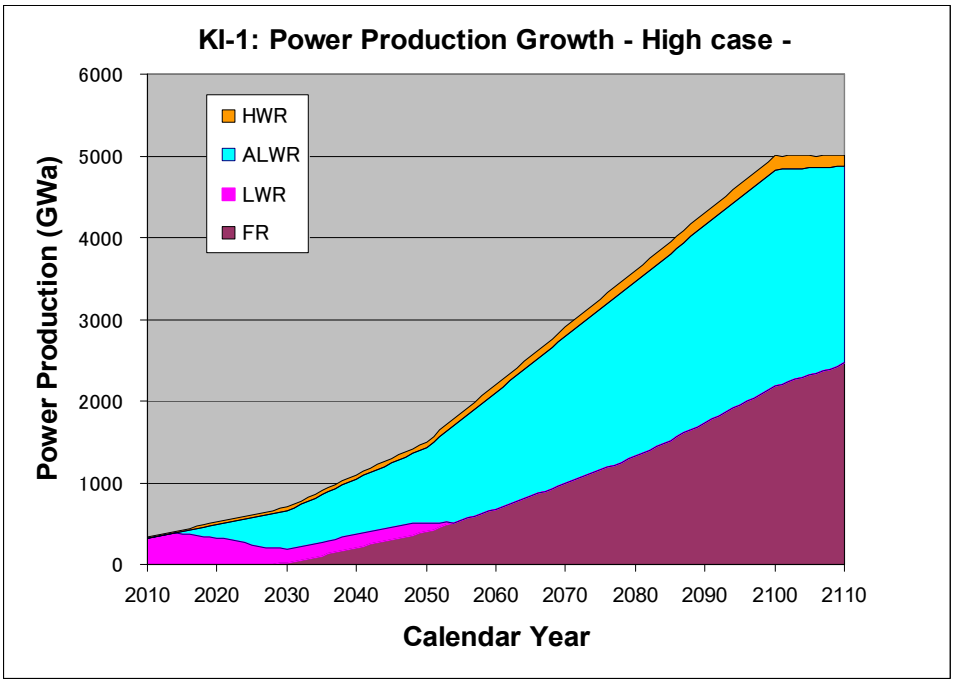
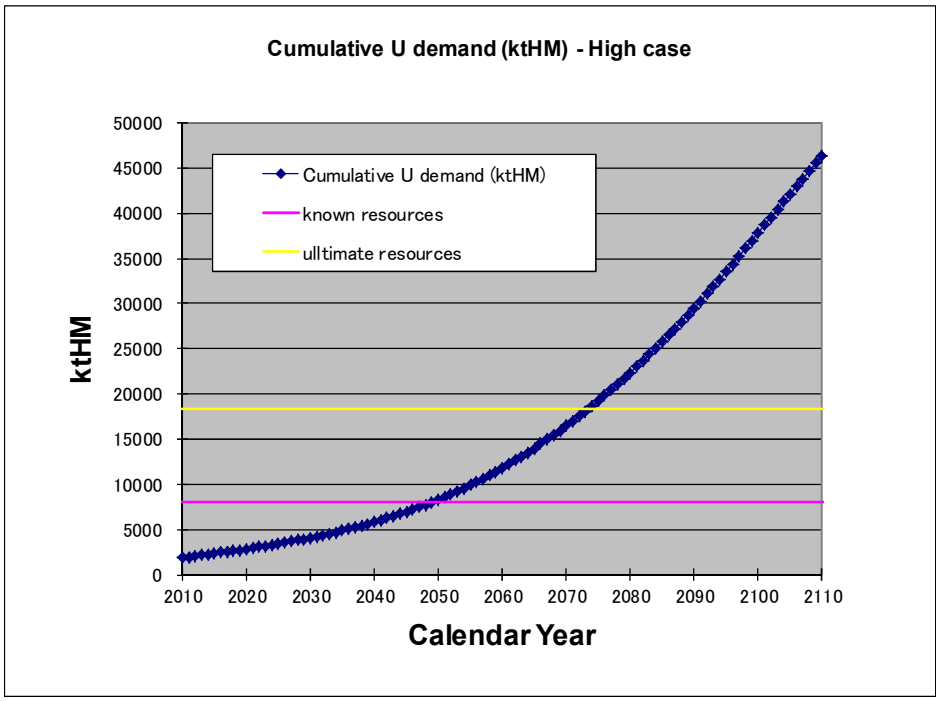


FIG.76. Reactor nuclear power share of (a) BAU+ and (b) BAU+FR.

(a)



(b)

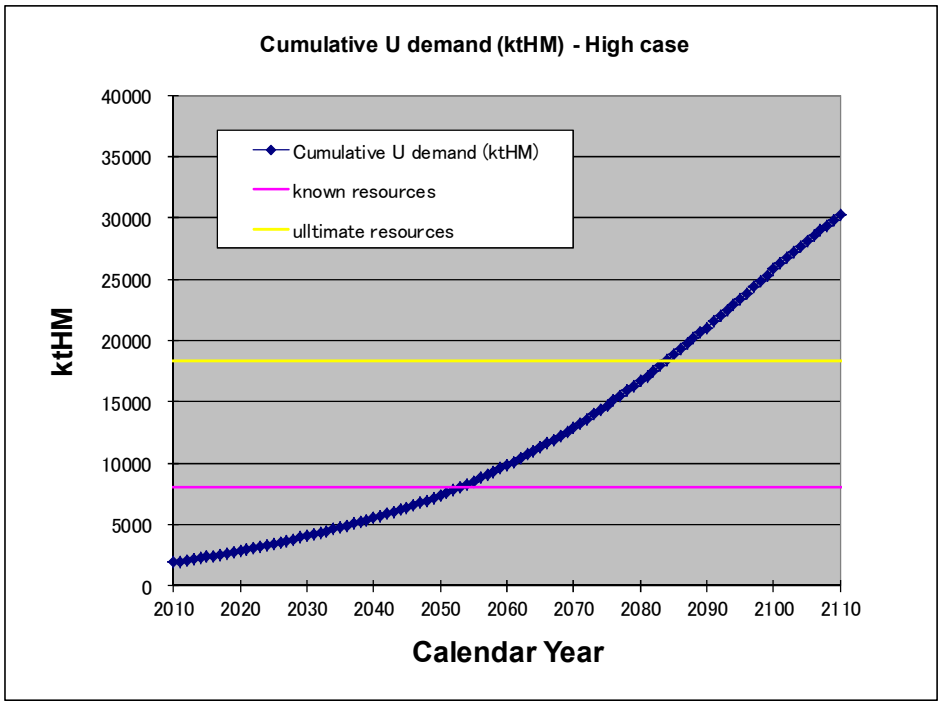
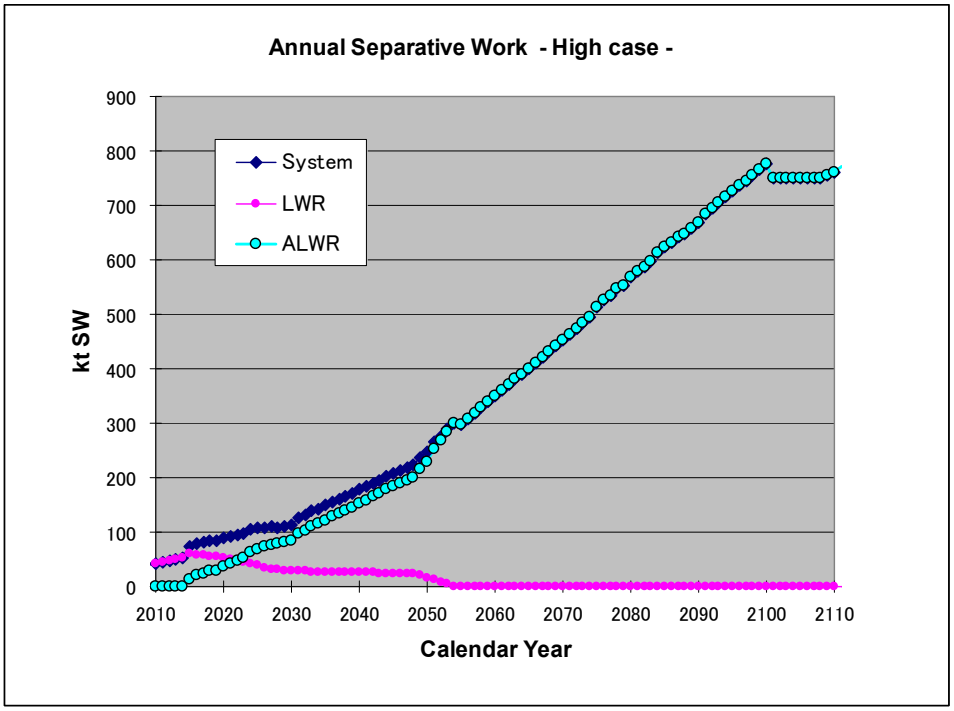


FIG.77. Cumulative natural U demand in (a) BAU+ and (b) BAU+FR.

(a)



(b)

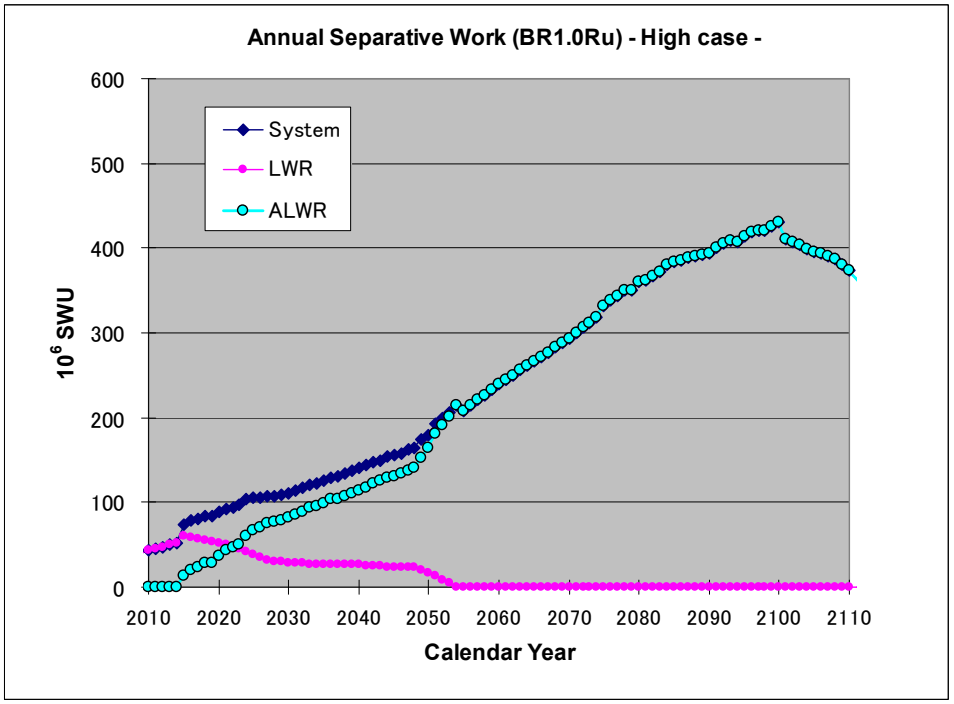
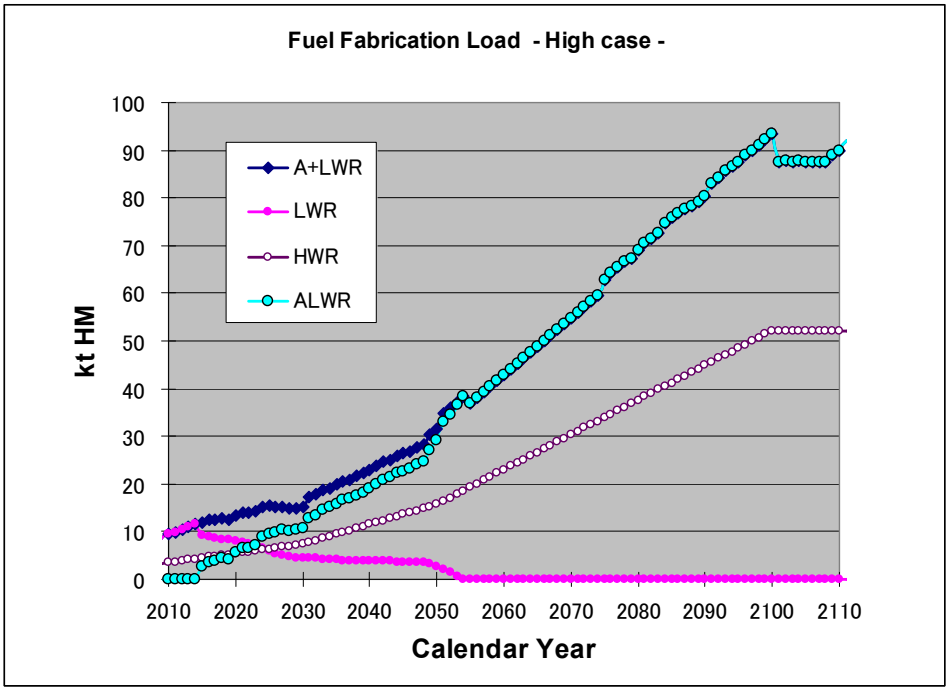


FIG. 78. Annual uranium separative work for a) BAU+ and (b) BAU+FR.

Figure 79 (a) and (b) show annual fuel fabrication load for each reactor type in BAU+ and BAU+FR cases respectively. In BAU+FR case, the fuel fabrication load for ALWR decreases to 50 kt HM at 2100 from 90 kt HM in BAU+. On the other hand, the fuel fabrication load for FR increases to almost the same level as ALWR at 2100. Total fuel fabrication load for all reactors remain same at 130 kt HM as BAU+.

(a)



(b)

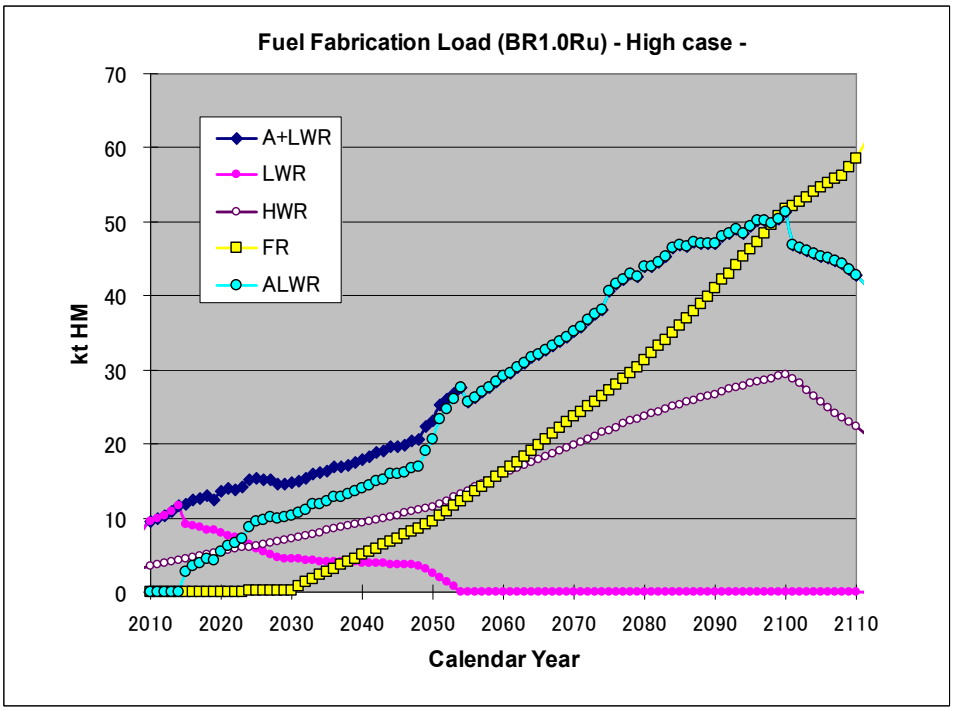


FIG.79. Fuel fabrication load for each reactor in (a) BAU+ and (b) BAU+FR.

Figure 80 shows annual reprocessing load for spent fuels from LWR, ALWR and FR. The requirement for the reprocessing of SF from LWR and ALWR rises stepwise depending on the pace of FR introduction, and the peak value is around 45 kt HM. The requirement for FR SF reprocessing increases monotonically along with the FR capacity increase and reaches almost the same level as the ALWR at the end of the century.

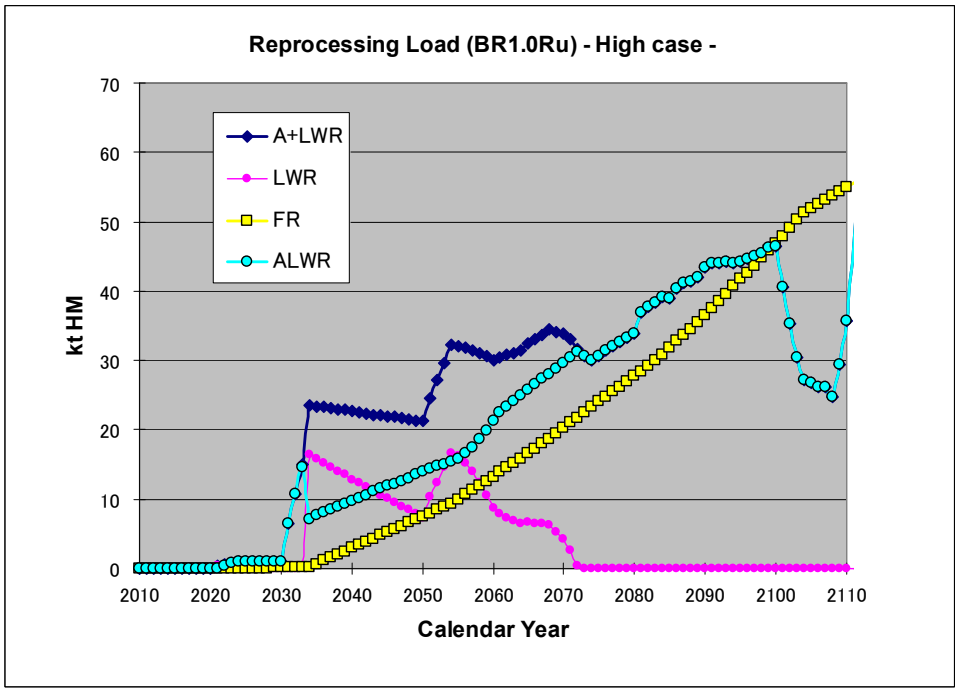


FIG.80. Reprocessing load in BAU+FR.

Figure 81 shows the annual Pu balance between LWR, ALWR and FR. The Pu supply from LWR and ALWR reaches around 600 t in 2100. It should be noted that reprocessing capacities are input data in NFCSS, while they are outputs in GAINS. So, users need to perform considerable additional calculation for reprocessing capacities based on GAINS constraints and incorporate them in the NFCSS calculations.

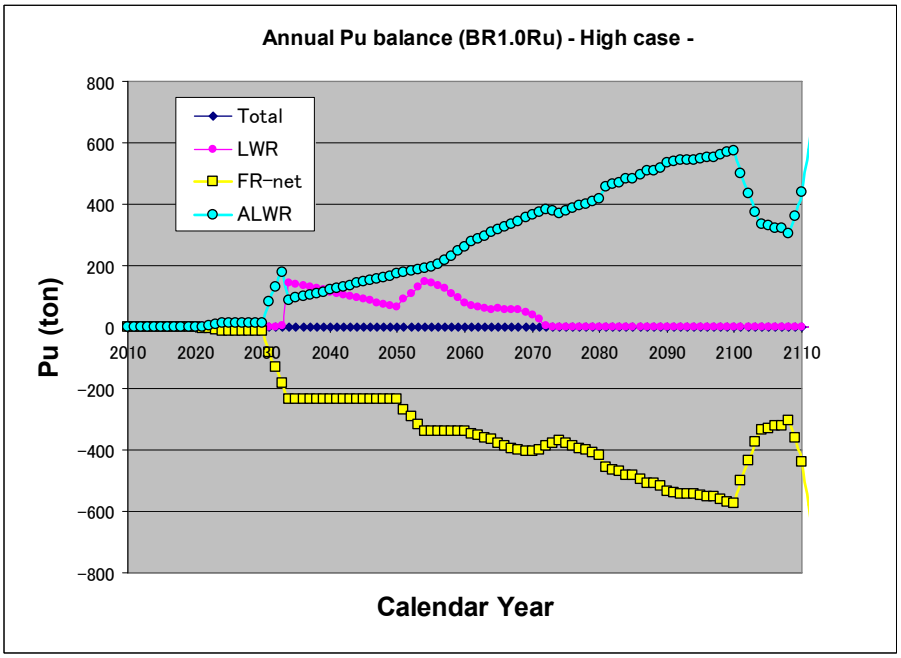
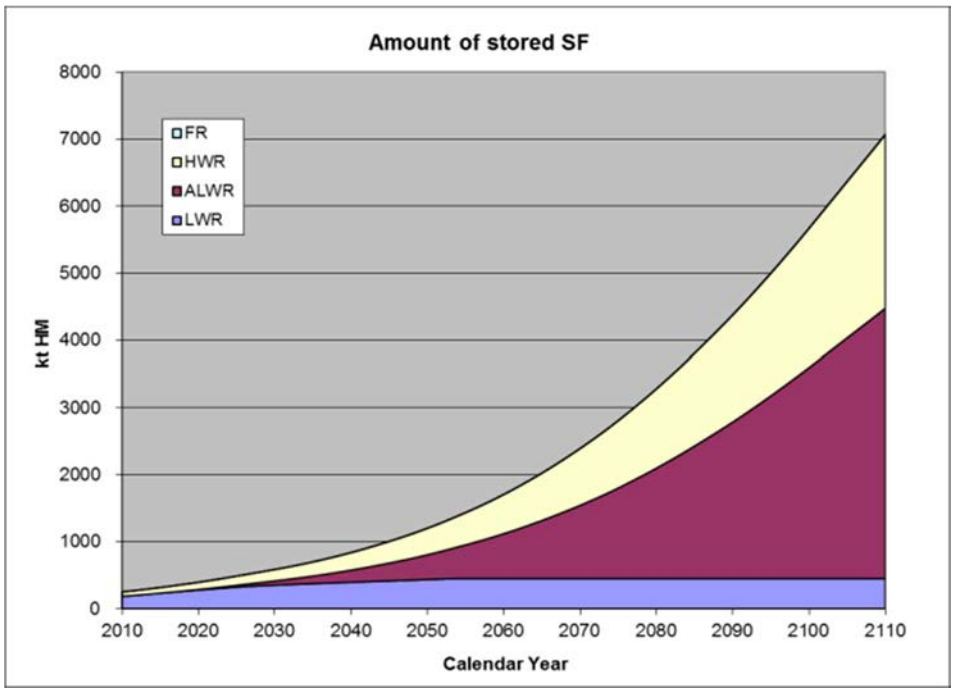


FIG.81. Pu balance among reactors in BAU+FR.

The basic features of the BAU case are sustained growth of thermal reactors with accumulation of spent fuel without recycling. The total amount of spent fuel accumulated by 2100 in the BAU+ scenario reaches 5.5 million tonnes of SF as shown in Fig.82 (a). From Fig.82 (b), LWR spent fuel can be significantly reduced by introduction of fast reactors.

(a)



(b)

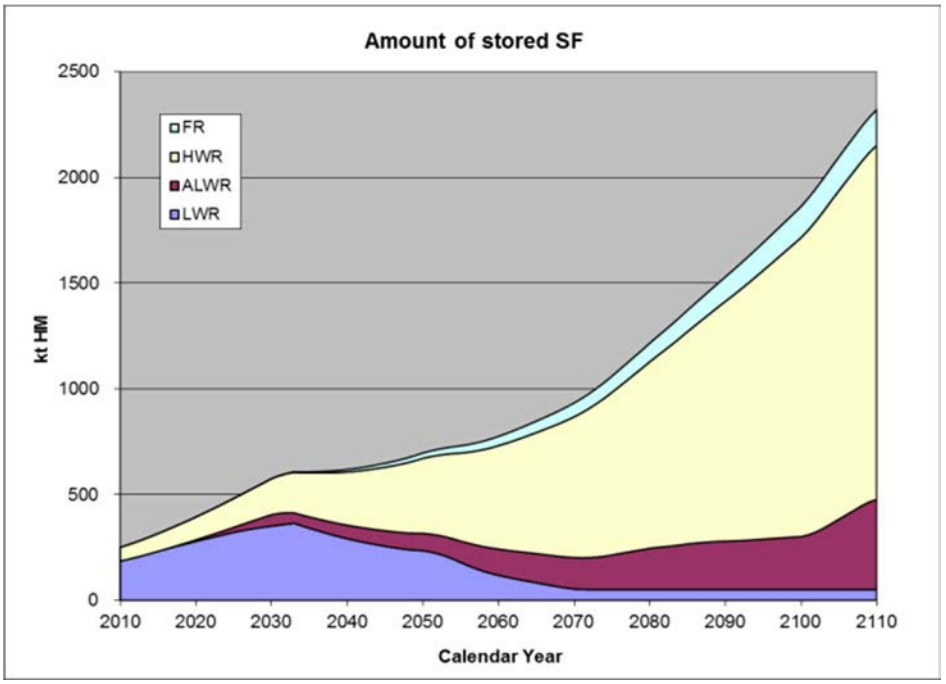


FIG.82. Cumulative amount of SF in (a) BAU+ and (b) BAU+FR.

The NFCSS was successfully used for modelling of the NES selected (listed below) for the INPRO collaborative project GAINS.

- An NES based on thermal reactors with a once-through nuclear fuel cycle without spent fuel reprocessing;

- An NES based on thermal and fast reactors with inclusion of plutonium multi-recycling in fast reactors with mixed oxide fuels.

In summary, NFCSS tool responds well to the main if not all requirements of the nuclear energy system modelling for INPRO collaborative projects. If NFCSS were to perform the INPRO studies, its code and database structure requires further elaboration. However, MESSAGE, NFCSS can be used separately or in modules to perform relevant analysis required for the INPRO assessment.

9.3. FAST REACTOR MODELLING

9.3.1. Overview

When the first publication on the NFCSS was published in 2007 [1], it was not clear whether the NFCSS could handle FRs or not, and the NFCSS application was limited to seven reactor types (PWR, BWR, PHWR, RBMK, AGR, GCR and WWER). In recent NFCSS consultancy meetings held at IAEA, it was proposed to run three imaginary FR reactors, that is, one core, one axial blanket, and one radial blanket, at one reactor site. The NFCSS was developed by presuming one region cores, though it can have two types of fuels such as enriched uranium fuel and MOX fuel. It is not always simple to analyse the mass-flows of FRs using NFCSS, even if we assume the independency between the three regions. This section describes an example of FR modelling based on a reference design data.

9.3.2. Input data

9.3.2.1. Reference design data of the prototype FR

Table 60 represents the specifications of the prototype FR taken from the INPRO/GAINS collaborative project (p.52 of [44]). In GAINS, all nuclear reactors are modelled as one-region core. It means that the designed refuelling data of each region of a FR are totalled to give one region core provided as the design data. That is, the loadings and discharges from the three regions of core, axial blanket and radial blanket at one refuelling are summed and shown in the Table 61 (p.221 of [44]). Table 61 shows the refuelling data of the proto-type FR.

TABLE 60. MAJOR SPECIFICATIONS OF PROTOTYPE FR

Reactor net electric output	MW	500		
Reactor thermal output	MW	1,250		
Thermal efficiency	%	40		
Average load factor	%	85		
Operation cycle length	EFPD	180		
		Core	Axial blanket	Radial blanket
Power share of each region (Note)	%	92	3	5
No of refuelling batches (Note)		3	3	5
Fuel residence time (Note)	EFPD	540	540	900
Specific power density (Note)	MW/t	141.590	7.191	4.467
Average discharged burnup (Note)	MW·d/t	76459	3883	4020
Thermal power of each region (Note)	MW	1150	37.5	62.5

Heavy metal weight share - Initial core and full core discharge - Equilibrium refuelling	% %	29.72 37.37	19.08 24.00	51.20 38.63
Average burnup of whole core	MW·d/t	31,061		
Average residence time of whole core	EFPD	679.06		
Average power density of whole core	MW/t	45.740		
Initial core inventory	t-HM	27.328		
Equilibrium loading	t-HM/year	12.486		

Note: Equilibrium cycle average.

TABLE 61. REFUELLING DATA OF THE PROTOTYPE FR

Isotopes	Initial loading		Reload		Discharge		Full core discharge at retirement	
	kg	%	kg	%	kg	%	kg	%
U-232					8.174E-7	1.129E-8	1.585E-6	5.800E-9
U-233					4.955E-7	6.843E-9	1.385E-6	5.069E-9
U-234	3.635E-5	1.330E-7	9.689E-6	1.338E-7	2.153E-3	2.973E-5	5.177E-3	1.895E-5
U-235	6.267E+1	2.290E-1	1.625E+1	2.243E+1	1.198E+1	1.654E-1	4.861E+1	1.779E-1
U-236	2.497E-5	9.139E-8	5.899E-6	8.143E-8	1.039E00	1.434E-2	3.433E00	1.257E-2
U-238	2.528E+4	9.251E+1	6.566E+3	9.064E+1	6.308E+3	8.711E+1	2.447E+4	8.956E+1
Np-237					7.297E-1	1.008E-2	1.950E00	7.135E-3
Pu-238					2.282E-1	3.151E-3	4.452E-1	1.629E-3
Pu-239	1.363E+3	4.987E00	4.543E+2	6.271E00	4.974E+2	6.869E00	1.678E+3	6.142E00
Pu-240	4.894E+2	1.791E00	1.631E+2	2.252E00	1.786E+2	2.466E00	5.310E+2	1.943E00
Pu-241	1.051E+2	3.845E-1	3.502E+1	4.835E-1	3.112E+1	4.297E-1	9.646E+1	3.530E-1
Pu-242	2.708E+1	9.911E-2	9.028E00	1.246E-1	1.036E+1	1.431E-1	2.992E+1	1.095E-1
Am-241					1.927E00	2.661E-2	4.217E00	1.543E-2
Am-242m					3.587E-2	4.953E-4	6.205E-2	2.271E-4
Am-243					8.079E-1	1.116E-2	1.707E00	6.246E-3
Cm-242					1.153E-1	1.592E-3	2.077E-1	7.602E-4
Cm-244					1.711E-1	2.362E-3	2.845E-1	1.041E-3
Cm-245					8.287E-3	1.144E-4	1.197E-2	4.380E-5
Total FPs					1.987E+2	2.744E00	4.554E+2	1.667E00

Isotopes	Initial loading		Reload		Discharge		Full core discharge at retirement	
	kg	%	kg	%	kg	%	kg	%
Total HM & FPs	27,328.107	100.0	7,243.872	100.000	7,241.501	100.000	27,325.399	100.000
Total U	25,343.780	92.739	6,582.430	90.869	6,321.330	87.293	24,525.374	89.753
Total Pu	1,984.328	7.261	661.443	9.131	717.673	9.911	2,336.169	8.549
Total MAs	0.0	0.0	0.0	0.00	3.795	0.052	8.440	0.031

9.3.2.2. Input depletion conditions for three regions

According to the specifications in Table 59 and Table 60, we can identify the input depletion conditions for NFCSS as follows.

(a) Core
- Reactor net electric power: 460 MW,
- Electric efficiency: 40 %,
- Specific power density (at rated power condition): 141.590 MW/t,
- Average discharge burnup: 76 459 MW·d/t,
- U enrichment: 0.25 %,
- Pu enrichment: 24.431 %,
- Pu vector: Pu-239: Pu-240 : Pu-241 : Pu-242 = 68.69 : 24.66 : 5.29 : 1.36.

(b) Axial blanket
- Reactor net electric power: 15 MW,
- Electric efficiency: 40 %,
- Specific power density (at rated power condition): 7.191 MW/t,
- Average discharge burnup: 3883 MW·d/t,
- U enrichment: 0.25 %.

(c) Radial blanket
- Reactor net electric power: 25 MW,
- Electric efficiency: 40 %,
- Specific power density (at rated power condition): 4.467 MW/t,
- Average discharge burnup: 4,020 MW·d/t,
- U enrichment: 0.25 %.

Normally FR fissile core part has at least two enrichment zones. It's could be simulated as two 'reactors' by the NFCSS.

9.3.2.3. Refuelling scheme of the prototype FR

For the mass flow calculation, LF (load factor) needs to be known to meet the operation cycle of designed FR. Figure 82 schematically shows the operation cycle of the prototype FR. The fuel residence time of core fuel is 540 Effective Full Power Days, that is, 3 periods of 180 day cycle. The fuel residence time of radial blanket fuels is 900 EFPD, that is, 5 periods of 180 day cycle. Therefore, the interval of the operation cycles is determined to be 63 days, and the LF (load factor) to be 74% for use in the mass flow analysis by the NFCSS.

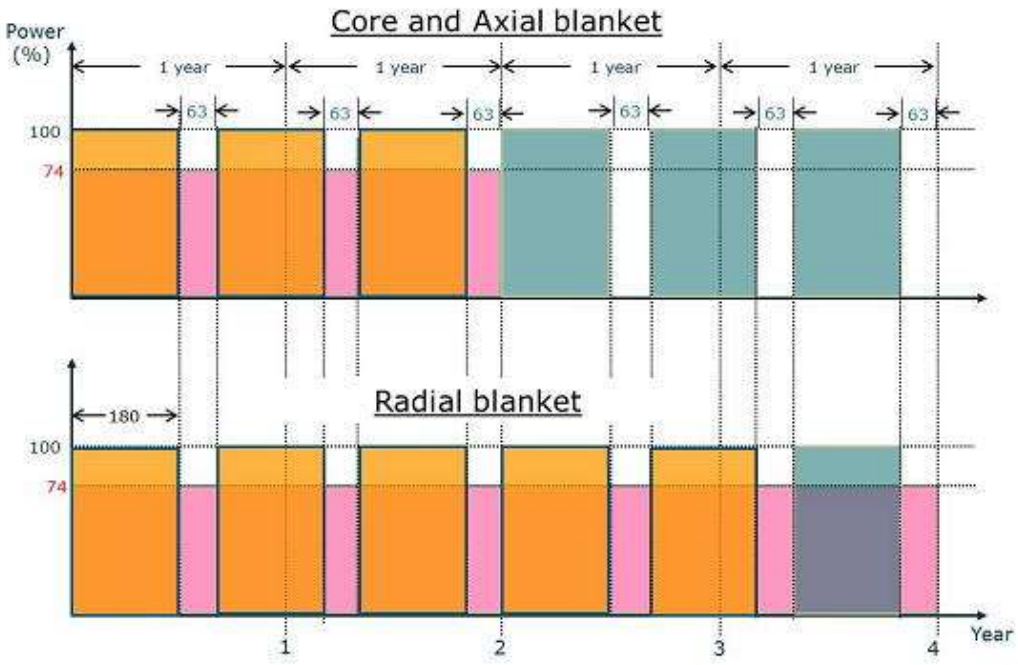


FIG.82. Operation cycle scheme of prototype FR.

9.3.2.4. NFCSS input decks

The mass flow calculation was performed with the cross sections available from NFCSS, and with an assumption of out-of-reactor time of 3 years. The fuel data were copied from the system data of 'LMFR Core MOX (ID: 22)', 'LMFR Axial Blanket (ID: 23)' and 'LMFR Radial Blanket (ID: 54)'. The cross sections of three fuel data are all derived from the ORIGEN2 library.

The inputs for power density, fuel composition and cooling time are revised from the system fuel data of the NFCSS.

Figure 83 shows the fuel data for the core part. The input of the upper figure shows the depletion conditions, the lower figure the cross sections.

Figure 84 shows the inputs of the fuel data for the axial and radial blankets.

9.3.3. Results

9.3.3.1. Isotopic composition results

Table 62 shows heavy metal weights and the compositions in one refuelling for the prototype FR. For the initial loading and reloading, comparison between the design data and the NFCSS has not been made. The design data were taken from [44]. The discharge composition values of core, axial blanket and radial blanket are averaged by weighting the heavy metal weight of each region. As shown in Table 58, the NFCSS results were in good agreement with the design data. Concerning Pu-total and Pu-fissile, the differences are within 1%, uranium within 3%. The difference becomes larger for MA. Overall, the accuracy is within practically acceptable

range for the mass flow analysis of nuclear fuel cycle for medium and long-time horizons. The differences in cross sections can be attributed to information sources.

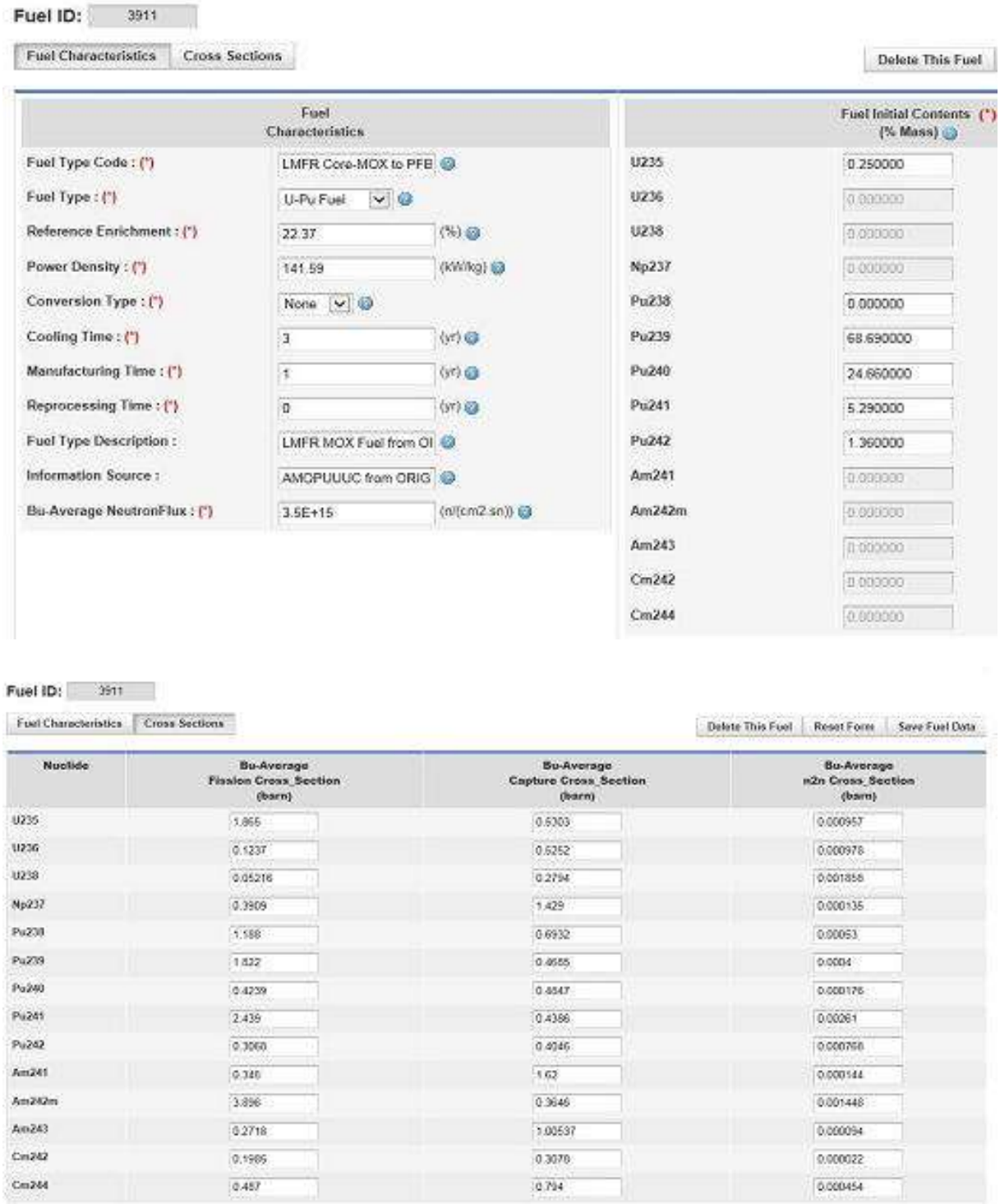


FIG.83. Input of fuel data and the cross section of core part.

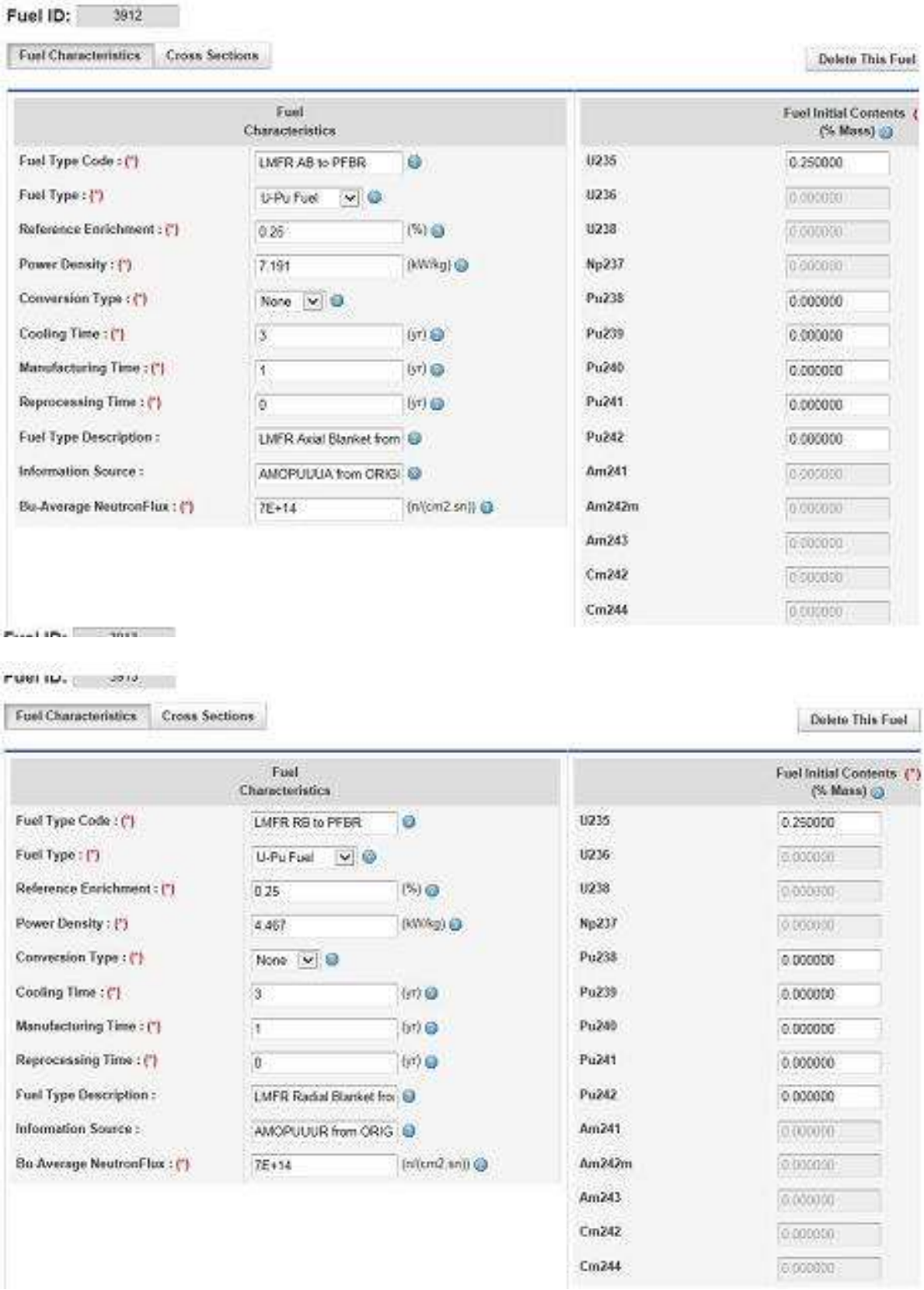


FIG.84. Input of fuel data of axial blanket and radial blanket.

TABLE 62. COMPARISON OF DISCHARGE COMPOSITION BETWEEN DESIGN AND NFCSS

Isotopes	Initial loading – Design data		Reload – Design data		Discharge – Design data		Discharge - NFCSS	
	kg	%	kg	%	kg	%	Composition	NFCSS/Design – 1, %
U-235	62.574	0.229	16.252	0.224	11.981	0.161	0.166	3.4
U-236	0.000	0.000	0.000	0.000	1.039	0.014	0.014	-1.2
U-238	25,281.206	92.510	6,566.178	90.645	6,308.309	84.787	86.985	2.6
Np-237					0.730	0.010	0.013	32.9
Pu-238					0.228	0.003	0.003	1.0
Pu-239	1,362.807	4.987	454.269	6.271	497.401	6.685	6.598	-1.3
Pu-240	489.363	1.791	163.121	2.252	178.560	2.400	2.414	0.6
Pu-241	106.074	0.384	35.025	0.484	31.120	0.418	0.419	0.3
Pu-242	27.064	0.099	9.028	0.125	10.364	0.139	0.419	4.8
Am-241					1.927	0.026	0.146	-0.1
Am-242m					0.036	0.000	0.026	-12.2
Am-243					0.808	0.011	0.000	-5.5
Cm-242					0.115	0.002	0.010	15.3
Cm-244					0.171	0.002	0.002	-56.6
Total Pu	1,984.828	7.261	661.443	9.131	717.673	9.646	0.001	-0.7
Total MAs	0.000	0.000	0.000	0.000	3.067	0.041	9.581	27.5
FisPu	1,467.881	5.371	489.294	6.755	528.521	7.104	0.052	-1.2
Total Am	0.000	0.000	0.000	0.000	2.771	0.037	7.017	-1.8
Total Cm	0.000	0.000	0.000	0.000	0.286	0.004	0.037	-27.7
Total U	25,343.780	92.739	6,582.430	90.869	6,321.330	84.962	0.003	2.6
Total HM	27,328.107	100.000	7,243.872	100.000	7,241.501	97.329	87.165	-0.5
Total FPs	0.000	0.000	0.000	0.000	198.702	2.671	3.202	19.9

9.3.3.2. Pu and MA balance of the prototype FR during the long term operation

Figure 85 shows the Pu and MA stock of each region during the prototype FR operation for 50 years. 'Cooling time', one of important analysis conditions, was set at 3 years for the mass flow analysis by the NFCSS. The Pu stock of whole reactor does not turn to be positive during 50 years of operation, and the deficit Pu is still around 5 tons in 2070. It may be derived from the breeding ratio below 1.2 and the low average discharge burnup of 31 GW·d/t in whole reactor shown in Table 56. Minor actinides and higher order heavy metal isotopes mainly originate in the core part and build up around 0.5 tons at 2070 in this scenario, in which all reprocessed minor actinides are just stored in some storage facility.

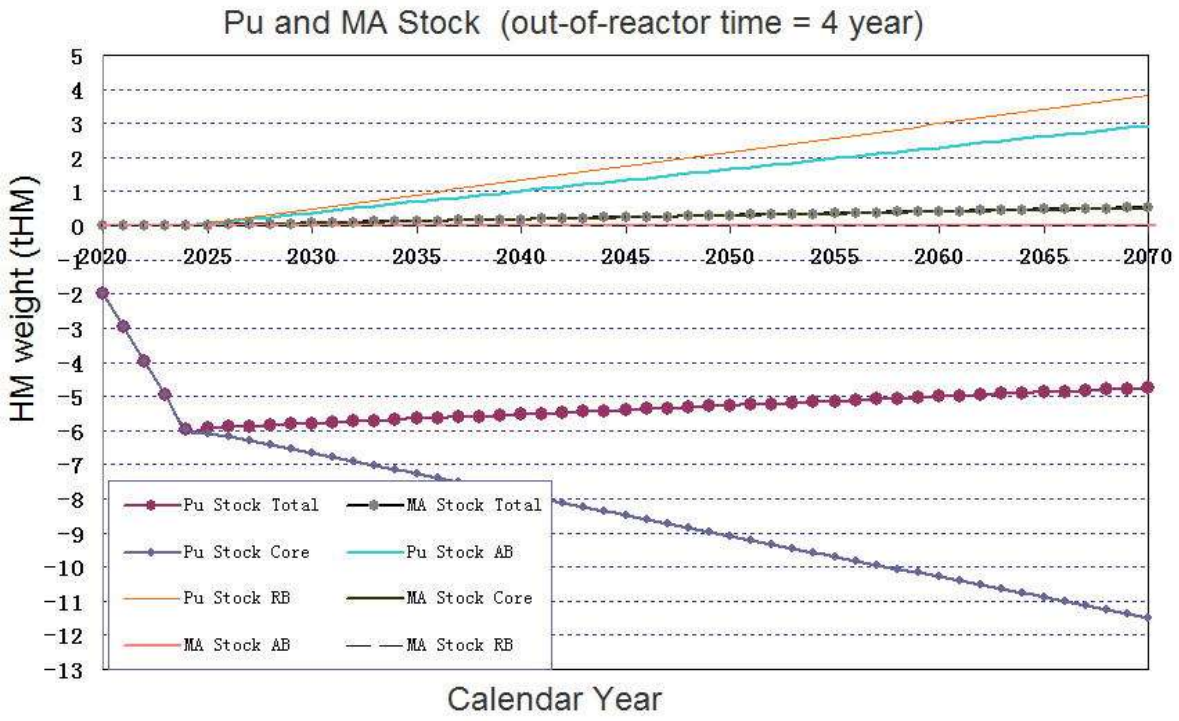


FIG.85. Pu and MA stock during prototype FR operation.

As described so far, the mass flow calculation of FRs can be achieved by the summation of independent reactors, which are one core, one axial blanket and one radial blanket of three one region reactors. As mentioned in the previous section, the discharge isotopic composition estimation by the NFCSS has very good agreement with the design data. Therefore, a long term scenario calculation with FRs can be achieved by using the NFCSS. However, one difficulty in the mass flow analysis using the NFCSS is to keep the power share of three regions in a scenario. With introduction of a new type of reactor, which can add two or three reactors with a constant power shares, mass flow analysis with FRs becomes easier to achieve in the NFCSS.

REFERENCES

[1] INTERNATIONAL ATOMIC ENERGY AGENCY, Nuclear Fuel Cycle Simulation System (VISTA), IAEA-TECDOC-1535, IAEA, Vienna (2007).

[2] INTERNATIONAL ATOMIC ENERGY AGENCY, Power Reactor Information System (PRIS), https://www.iaea.org/pris/

[3] INTERNATIONAL ATOMIC ENERGY AGENCY, Energy, Electricity and Nuclear Power Estimates for the Period up to 2050, IAEA-RDS-1/32, IAEA, Vienna (2012).

[4] World Nuclear Association, http://www.world-nuclear.org/information-library/nuclear-fuel-cycle.aspx.

[5] INTERNATIONAL ATOMIC ENERGY AGENCY, Thorium Fuel Cycle - Potential Benefits and Challenges, IAEA-TECDOC-1155, IAEA, Vienna (2000).

[6] INTERNATIONAL ATOMIC ENERGY AGENCY, Thorium Fuel Utilization: Options and Trends, IAEA-TECDOC-1319, IAEA, Vienna (2002).

[7] INTERNATIONAL ATOMIC ENERGY AGENCY, Potential of Thorium Based Fuel Cycles to Constrain Plutonium and Reduce Long Lived Waste Toxicity, IAEA-TECDOC-1349, IAEA, Vienna (2003).

[8] INTERNATIONAL ATOMIC ENERGY AGENCY, Thorium Fuel Cycle - Potential Benefits and Challenges, IAEA-TECDOC-1450, IAEA, Vienna (2005).

[9] INTERNATIONAL ATOMIC ENERGY AGENCY, Role of Thorium to Supplement Fuel Cycles of Future Nuclear Energy Systems, NF-T-2.4, IAEA, Vienna (2012).

[10] ORGANIZATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT / NUCLEAR ENERGY AGENCY, Introduction of Thorium in the Nuclear Fuel Cycle, Report NEA-7224, OECD/NEA (2015).

[11] DOLAN, T. J. (ed.), Molten Salt Reactors and Thorium Energy, Woodhead Publishing (Elsevier) (2017).

[12] INTERNATIONAL ATOMIC ENERGY AGENCY, Status of Accelerator Driven Systems Research and Technology Development, IAEA-TECDOC-1766, IAEA, Vienna (2015).

[13] ORGANIZATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT / NUCLEAR ENERGY AGENCY, INTERNATIONAL ATOMIC ENERGY AGENCY, Uranium 2016: Resources, Production and Demand, Report NEA-7301, OECD/NEA (2016).

[14] BATEMAN, H., Solution of a System of Differential Equations Occurring in the Theory of Radio-active Transformations, Proc. Cambridge Philosophical Society (1910) 423-427.

[15] CROFF, A.G., A User's Manual for the ORIGEN2 Computer Code, Report ORNL/TM-7175, Oak Ridge National Laboratory (1980).

[16] ADE, B., WORRALL, A., Powers, J., Bowman, S., Flanagan, G., Gehin, J., Safety and Regulatory Issues of the Thorium Fuel Cycle, Report NUREG/CR-7176, Nuclear Regulatory Commission (2014).

[17] CROFF, A.G., BJERKE, M.A., Alternative Fuel Cycle PWR Models for the ORIGEN Computer Code, Report ORNL/TM-7005, Oak Ridge National Laboratory (1980).

[18] CROFF, A.G., BJERKE, M.A., MORRISON, G.W., PETRIE, L.M., Revised Uranium-Plutonium Cycle PWR and BWR Models for the ORIGEN Computer Code, ORNL/TM-6051, Oak Ridge National Laboratory (1978).

[19] TODOSOW, M. et al., “Thorium Based Fuel Cycle Options for PWRs”, paper presented at International Congress on Advances in Nuclear Power Plants (ICAPP '10), San Diego, CA, June 13-17, 2010.
[20] BJORK, K.I. et al., Comparison of Thorium-based Fuels with Different Fissile Components in Existing Boiling Water Reactors, (personal communication, 2015)
[21] YOSHIOKA, R., Decay Heat Study for PWR Thorium Fuel, Study Report, International Thorium Molten-Salt Forum (2013) (in Japanese).
[22] KOREA ATOMIC ENERGY RESEARCH INSTITUTE, Table of Nuclide (2015); http://atom.kaeri.re.kr/,or http://atom.kaeri.re.kr:8080/ton/index.html
[23] http://en.wikipedia.org/wiki/Transient_equilibrium
[24] JAPAN ATOMIC ENERGY AGENCY, Nuclear Data Center, JENDL-4.0 Fission Yield Sub-library [J40-2010], output (2015).
[25] YARNELL, J.L., BENDT, P.J., Calorimetric Fission Product Decay Heat Measurements for ^{239}Pu, ^{233}U and ^{235}U (for thermal neutron irradiation), NUREG/CR-0349, LA-7452-MS, Los Alamos Scientific Lab (1978).
[26] FLEMING, M., SUBLET, J-C., Validation of FISPACT-II Decay Heat and Inventory Predictions for Fission Events, CCFE-R(15)28, UK Atomic Energy Authority (2015).
[27] SON, P.N. et al., An Application Program for Fission Product. Decay Heat Calculations, JAEA-Data/Code 2007-018, JAEA (2007).
[28] YUN, D., KIM, T.K., TAIWO, T.A., Th/U-233 Multi-Recycle in PWRs, ANL-FCRD-309, U.S Department of Energy (2010).
[29] ADE, B.J., GAULD, I.C., Decay Heat Calculations for PWR and BWR Assemblies Fuelled with Uranium and Plutonium Mixed Oxide Fuel Using Scale, ORNL/TM-2011/290, Oak Ridge National Laboratory (2011).
[30] YOSHIOKA, R., KINOSHITA, M., TAKAKI, N., YOSHIDA, T., “Decay Heat Evaluation for Thorium Fuel in PWR”, Transaction of AESJ-2014 Meeting, Tokyo, 2014 (in Japanese).
[31] YOSHIOKA, R., et al., Environment, Waste, and Resources, Woodhead Publishing (Elsevier) (2017) Chapter 9.
[32] INTERNAL COMMISSION ON RADIOLOGICAL PROTECTION (ICRP), Age-dependent Doses to Members of the Public from Intake of Radionuclides, ICRP Publication 72 (1995).
[33] NISHIHARA, K., Data for Estimating Potential Radiotoxicity of Spent Nuclear Fuel, JAEA-Data/Code2010-012, JAEA (2010). (Data are identical to [32]; Report is in Japanese, but an Excel file in English can be downloaded from: http://nsec.jaea.go.jp/ndre/ndre3/trans/DataRadiotoxicity.xls).
[34] CLEMENT, C.H., Compendium of Dose Coefficients based on ICRP Publication 60, ICRP Publication 119 (2012).
[35] KAWAI, K. et al., Dose Coefficients for Radionuclides Produced in High Energy Proton Accelerator Facilities: Coefficients for Radionuclides not Listed in ICRP Publications, JAERI-Data/Code 2002-013, JAEA, (2002).
[36] YOSHIOKA, R., Radiotoxicity Study for PWR Thorium Fuel, Study Report, International Thorium Molten-Salt Forum (2014), in Japanese.
[37] HESKESH, K., “Radiotoxicity of Thorium Fuel Cycles in PWRs”, paper presented at Workshop on Advanced Reactors with Innovative Fuels (ARWIF-2005), Oak Ridge National Laboratory, 16-18 February 2005.

[38] INTERNATIONAL ATOMIC ENERGY AGENCY, Implications of Partitioning and Transmutation in Radioactive Waste Management, Technical Reports Series No.435, IAEA, Vienna (2004) (This publication refers the following article: Magill, J. et al., Impact Limits of Partitioning and Transmutation Scenarios on the Radiotoxicity of Actinides in Radioactive Waste, Nuclear Energy **42** (2003) 263.)
[39] YOSHIOKA, R., KINOSHITA, M., TAKAKI, N., YOSHIDA, T., "Radiotoxicity Evaluation for Spent Thorium Fuel in PWR", Transaction of AESJ-2015 meeting, Hitachi, Japan, 2015 (in Japanese).
[40] DAVID, S., Revisiting the Thorium-Uranium Nuclear Fuel Cycle, Europhysics News **38** (2007) 24.
[41] HAYASHI, H., "Development of Multiple Recycling Analysis Code HIMMEL", Transaction of AESJ-2014 meeting, Tokyo, Japan, 2014 (in Japanese).
[42] INTERNATIONAL ATOMIC ENERGY AGENCY, Modelling Nuclear Energy Systems with MESSAGE: A User's Guide, IAEA Nuclear Energy Series No. NG-T-5.2, IAEA, Vienna (2016).
[43] INTERNATIONAL ATOMIC ENERGY AGENCY, IAEA Tools and Methodologies for Energy System Planning and Nuclear Energy System Assessments, IAEA, Vienna (2009).
[44] INTERNATIONAL ATOMIC ENERGY AGENCY, Framework for Assessing Dynamic Nuclear Energy Systems for Sustainability, Final Report of the INPRO Collaborative Project GAINS, NP-T-1.14, IAEA, Vienna (2013).
[45] INTERNATIONAL ATOMIC ENERGY AGENCY, Nuclear Energy Development in the 21st Century: Global Scenarios and Regional Trends, NP-T-1.8, IAEA (2010).
[46] INTERNATIONAL ATOMIC ENERGY AGENCY, Joint Study: Assessment of Nuclear Energy Systems Based on a Closed Nuclear Fuel Cycle with Fast Reactors (CNFC-FR), IAEA-TECDOC-1639, IAEA (2009).
[47] INTERNATIONAL ATOMIC ENERGY AGENCY, Guidance for the Application of an Assessment Methodology for Innovative Nuclear Energy Systems. INPRO Manual – Overview of the Methodology, IAEA-TECDOC-1575, IAEA (2008).

ANNEX I: SPECFICATION FOR NFCSS PROGRAMME MODIFICATION

I-1. GENERAL

Several modifications have been implemented in the NFCSS. A summary of these modifications is specified in this Annex for future modifications and maintenance of the NFCSS program.

I-2. GENERAL IMPROVEMENTS

There are many small but important improvements that have been incorporated in the NFCSS since the original publication of the NFCSS was published in 2007 [I-1]. These include: output of final neutron flux, initial core loading and final core discharge, and protection against a zero-division in Bateman's equation. A major improvement is expanding the functionality of the NFCSS to cover the thorium fuel cycle.

I-2.1. Output of final neutron flux

In the CAIN burnup module of the NFCSS, both neutron flux and irradiation time are required. Irradiation time can be calculated using discharge burnup and specific power that are given as input:

$$T(\text{sec}) = [Ed \times 1000 \times 24 \times 3600] / SP$$

where,

Ed = Discharge burnup (GW·d/t),
SP = Specific power (kW/kg or MW/t).

In the NFCSS, neutron flux is also given as an input. The input value of neutron flux is only for an initial guess and not used in the CAIN burnup calculation. That is, neutron flux for the CAIN burnup calculation is derived by the following iterative process. However, its final converged value was not printed out. The converged value of neutron flux depends on SP (specific power) and Ed (discharge burnup) and is different across fuel types. For example, when two fuel types are used in one reactor (e.g. UO_2 fuel and MOX fuel), the NFCSS calculates different neutron flux for each fuel type.

The aforementioned iterative process is shown in Fig.I-1.

The iterative process is programmed using ASP (Active Server Pages) language in the CAIN and shown in Fig.I-2.

Figure I-3 illustrates one example of the above iterative process. Neutron flux starts from the initial guess and converges asymptotically to the final values at 8th iteration.

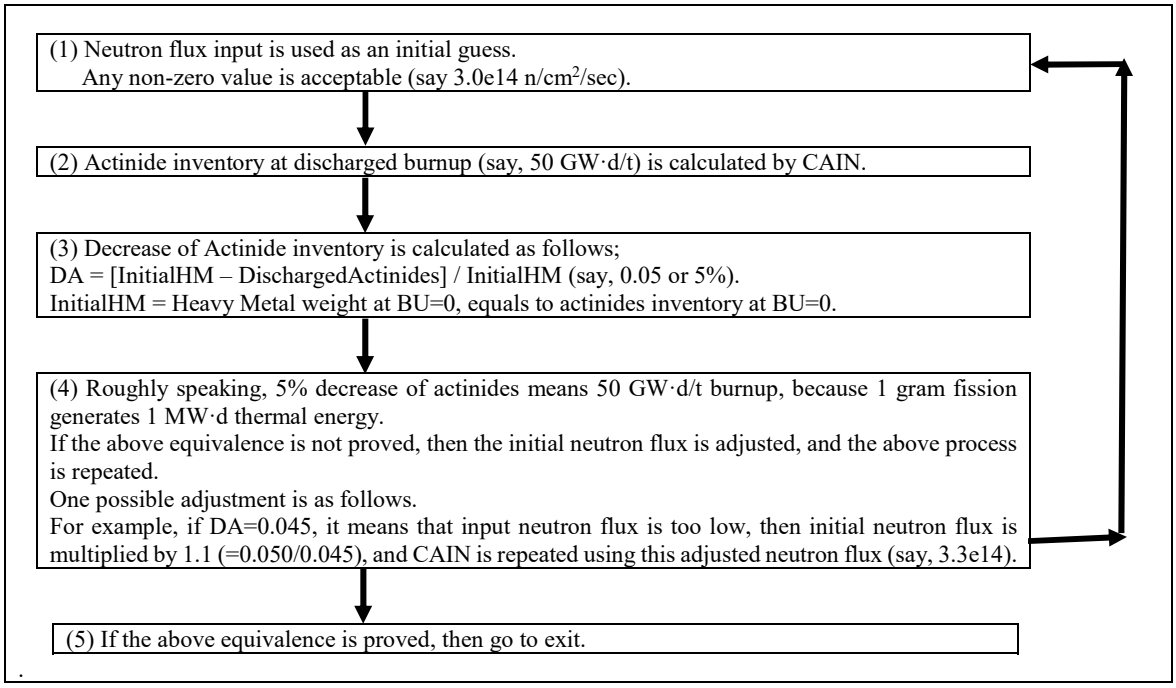


FIG.I-1. Iterative process to find the final value of neutron flux.

```
    ' ------ Start Calculation -----------
    Day = BurnupStep(bustep) * 1000 / KWKG
    Time = Day * 3600 * 24
    Flux_for_Exposure = Burnup_Adjusted_Flux
   'response.Write ("<BR> before i===>CalcActinide bustep:" & bustep )
    Call CalcActinide
   'response.Write ("<BR> i===>CalcActinide" )
    For i = 1 To NNuclide
     Initial_Content(i) = Number_Density(i)
     'Response.Write("<br>xxxInitial_Content(" & i & ")" & Initial_Content(i))
    Next
    Next
    TOTAL = 0
   For i = 1 To NNuclide
      TOTAL = TOTAL + Mass_Density(i)
   Next
   'response.Write ("<BR> Correction of Exposure by " )
   ' ----- Correction of Exposure by " 1 gram fission = 0.97 MWD" ---
    EXPOSURE2 = (100 - TOTAL) * 10 * 0.97
    PHI1 = PHI * Burn / EXPOSURE2
    PHI = PHI1
    NLOOP = NLOOP + 1
   Loop While Abs((EXPOSURE2 - Burn) / Burn) >= 0.0001 ' End of Do Loop
'Loop While 3<2
' ----   end of Exposure iteration
   'response.Write ("<BR> end of Exposure iteration")
```

FIG.I-2. Source code modification for iterative process in FIG.I-1.

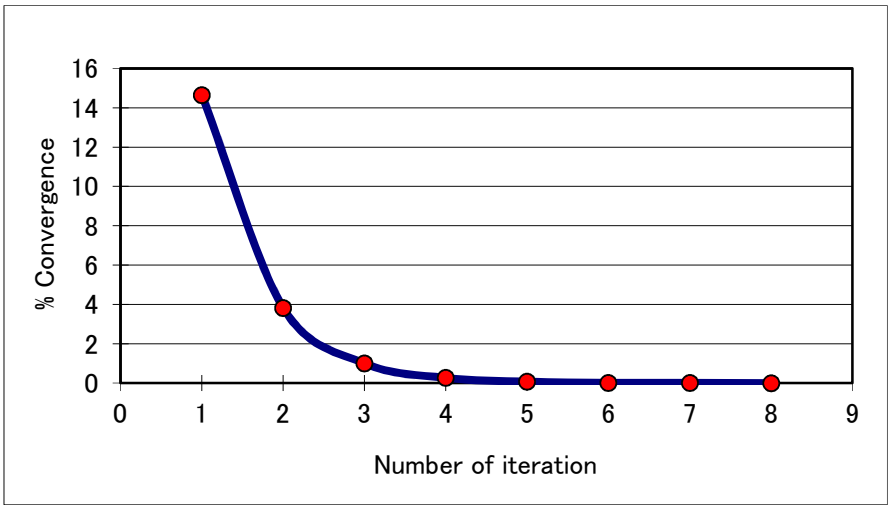


FIG.I-3. Convergence behavior in neutron flux iteration.

Therefore, final converged neutron flux values need to be printed out for each reactor and each fuel type in a separate page as follows (i.e. the following statement is added at the end of the above ASP program).

FinalPHI = PHI

And this 'FinalPHI' is represented in the following page - see Fig.I-4 (right top).

NFCSS Isotopic Composition Result

Reactor Type: UOX + MOX
Fuel: PWR UOX 1

Neutron Flux: 2.58E14(n/(cm2.s))

Beginning of Cycle | End of Cycle | After Cooling

Export All Tables to MS Excel

Import End of Cycle Table

DataYear	Enrichment	Burnup	U235	U236	U238	Np237	Pu238	Pu239	Pu240	Pu241	Pu242	Am241	Am242m	Am243	Cm242	Cm244	TotPu	TotMA
2010	4.00000	45.00000	0.67994	0.52425	93.04687	0.06869	0.02450	0.51137	0.26343	0.15056	0.06494	0.00476	0.00011	0.01461	0.00179	0.00484	1.01480	0.09481
2011	4.00000	45.00000	0.67994	0.52425	93.04687	0.06869	0.02450	0.51137	0.26343	0.15056	0.06494	0.00476	0.00011	0.01461	0.00179	0.00484	1.01480	0.09481
2012	4.00000	45.00000	0.67994	0.52425	93.04687	0.06869	0.02450	0.51137	0.26343	0.15056	0.06494	0.00476	0.00011	0.01461	0.00179	0.00484	1.01480	0.09481
2013	4.00000	45.00000	0.67994	0.52425	93.04687	0.06869	0.02450	0.51137	0.26343	0.15056	0.06494	0.00476	0.00011	0.01461	0.00179	0.00484	1.01480	0.09481
2014	4.00000	45.00000	0.67994	0.52425	93.04687	0.06869	0.02450	0.51137	0.26343	0.15056	0.06494	0.00476	0.00011	0.01461	0.00179	0.00484	1.01480	0.09481
2015	4.00000	45.00000	0.67994	0.52425	93.04687	0.06869	0.02450	0.51137	0.26343	0.15056	0.06494	0.00476	0.00011	0.01461	0.00179	0.00484	1.01480	0.09481

FIG.I-4. Sample screen-shot to show final converged neutron flux.

Since the NFCSS generates an EXCEL file, which is identical to Fig.I-5, the above 'FinalPHI' is also shown somewhere in this file as well.

NFCSS Isotopic Composition Resultss
Beginning of Cycle
Reactor T UOX + MC Neutron F 2.58E14 (n/(cm2.s))
Fuel: PWR UOX 1
If you want to copy data to NFCSS, you should select all columns including headings of the data, copy the data and then goto NFCSS and Import it.

DataYear	Enrichme	Burnup	U235	U236	U238	Np237	Pu238	Pu239	Pu240	Pu241	Pu242	Am241	Am242m	Am243	Cm242	Cm244
2010	4	45	4	0	96	0	0	0	0	0	0	0	0	0	0	0
2011	4	45	4	0	96	0	0	0	0	0	0	0	0	0	0	0
2012	4	45	4	0	96	0	0	0	0	0	0	0	0	0	0	0
2013	4	45	4	0	96	0	0	0	0	0	0	0	0	0	0	0
2014	4	45	4	0	96	0	0	0	0	0	0	0	0	0	0	0
2015	4	45	4	0	96	0	0	0	0	0	0	0	0	0	0	0

FIG.I-5. Sample EXCEL file to show final converged neutron flux.

As described earlier, the input value of neutron flux is used only for an initial guess, although it is a mandatory input parameter. Therefore, the caption and help-guide in the screen-shot of following Fig.I-6 has been modified. That is, a caption is 'Initial guess of neutron flux', and a help guide is 'Initial guess of neutron flux', for example,

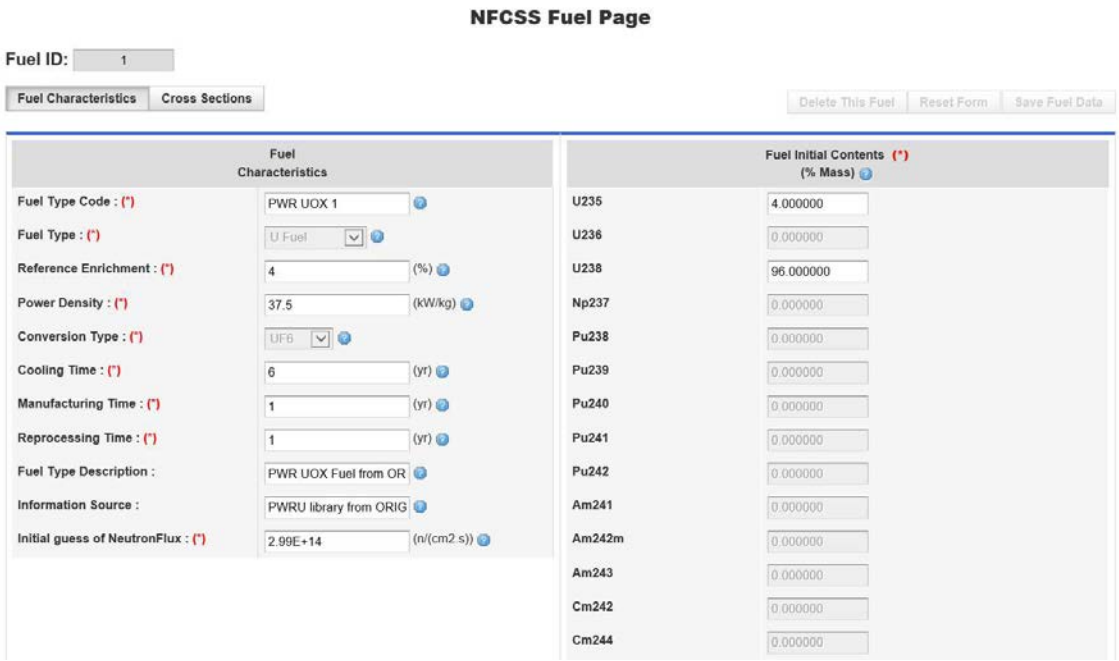


FIG.I-6. "Fuel Characteristics" tab at NFCSS Fuel Page.

I-2.2. Initial core loading and final core discharge

The previous NFCSS publication [I-1] does not describe how to simulate initial core loading and final core discharge. Now, details are shown in Annex II-8 (User's Manual), and there is no necessity to modify the current NFCSS programme.

I-2.3. Protection against a zero division in Bateman's equation

If $[\sigma_{t1}-\sigma_{tn}]$ becomes zero, a zero division occurs in a solution of the Bateman's equation, and this will generate incorrect results. For example, AF_2 (atomic fraction of nuclide-2) is calculated by the Bateman's equation as follow:

$$AF_2 = AF_1(initial)\cdot\left[\left(\frac{\Sigma_{c1}}{\Sigma_{t2}-\Sigma_{t1}}\right)\cdot e^{(-\Sigma_{t1}\cdot\Phi\cdot T\cdot 10^{-24})} + \left(\frac{\Sigma_{c1}}{\Sigma_{t1}-\Sigma_{t2}}\right)\cdot e^{(-\Sigma_{t2}\cdot\Phi\cdot T\cdot 10^{-24})}\right]$$

In order to avoid zero-division when two total cross sections are identical (including the case when both cross sections are zero), a new statement must be added in a subroutine "CALC" of CAIN module as follows:

If $[\sigma_{ti}-\sigma_{tj}]=0$, then New$\sigma_{ti} = \sigma_{ti} + 0.001$

Here, 0.001 is an arbitrary number to avoid a zero division.

A modification in an ASP subprogramme CALC is shown in Fig.I-7.

```
Sub Calc()
   'Response.Write("<br>Start of Calc")
    MAX = LL
    AA = 1
    For l = 1 To MAX - 1
       SCL = SC(l)
       AA = AA * SCL
    Next
     ' -----------
    NII = 0
   'Response.Write("<br>Start of Calc AA " & AA)
    For l = 1 To MAX
      BB = 1
      For k = 1 To MAX
         If k <> l Then
            STk = ST(k)
            STl = ST(l)
   ' Protection against a zero-division
                     If (STk – STl) = 0, then STk = STk + 0.001
            BB = BB * (STk - STl)

         End If
      Next
       CC = AA / BB
       STPT = ST(l) * Flux_for_Exposure * Time * 1E-24
       EEZ = Exp(-STPT)
       NII = NII + CC * EEZ
    Next
     ' ----------
    ni = NII
   'Response.Write("<br>End of Calc   : " )
End Sub 'Calc
```

FIG.I-7. Source code modification to protect against a zero-division.

I-3. INCORPORATION OF IMPROVEMENTS FOR THORIUM FUEL CYCLE

I-3.1. Overview

Bases for modelling thorium fuel cycles in NFCSS are described in detail in Section 5, and a summary of such approach for implementation in NFCSS is provided in Section 5.4.

I-3.2. Cross sections for thorium fuel cycle

Table I-1 and Table I-2 show cross sections for thorium fuel cycle, which are reproduced, respectively, from Table 5 and Table 6 in Section 5. Nuclides designated as No.1 (U-235) through No.14 (Cm-244) are used for UO_2 and MOX fuel, and nuclides designated as No.15 (Th-232) through No.18 (U-234) are those added for thorium fuel cycle. Verification of these cross sections is referred to Section 5.2.4.

The capture cross sections of Pa-233, Am-241 and Am-243 here include excited cross section, and cross section of [n,2n] reaction is used only for U-238 in the CAIN module.

Since Th-232, U-233 and U-234 have a longer half-life than 400 years, CAIN treats them as stable and further transmutation is not considered in burnup chains. Nevertheless, decrease of all these nuclides by their decay is considered in burnup period and cooling period after discharge.

Although Pa-233 has a short half-life (27 days), it is accounted for in the CAIN decay chains for thorium fuel cycle (refer to Section 5.1).

TABLE I-1 ONE-GROUP CORSS SECTIONS (barn) FOR APPLICATION TO U-Th FUEL IN LWRs

No.	*Nuclide*	$\sigma_c(+\sigma_{ex})$	σ_f	σ_{n2n}	$T_{1/2}(y)$
1	U-235	10.1000	43.9000	0.004828	7.04E+08
2	U-236	8.0300	0.2070	0.002092	2.34E+07
3	U-238	**1.5400**	0.1020	0.004828	4.47E+09
4	Np-237	31.4000	0.5140	0.000485	2.14E+06
5	Pu-238	34.4000	2.3200	0.000837	8.77E+01
6	Pu-239	60.0000	106.0000	0.001609	2.41E+04
7	Pu-240	153.0000	0.5960	0.001127	6.56E+03
8	Pu-241	37.5000	113.0000	0.002543	1.44E+01
9	Pu-242	31.9000	0.4330	0.002382	3.75E+05
10	Am-241	109.6000	1.0900	0.000161	4.33E+02
11	Am-242m	86.5000	413.0000	0.005955	1.41E+02
12	Am-243	45.6900	0.4160	0.000000	7.37E+03
13	Cm-242	5.6000	0.5540	0.000000	4.46E-01
14	Cm-244	14.2000	0.9020	0.000000	1.81E+01
15	Th-232	1.1400	0.0250	0.005150	1.40E+10
16	Pa-233	22.4000	0.1510	0.006953	7.40E-02
17	U-233	6.3900	53.1000	0.001062	1.59E+05
18	U-234	14.3000	0.4800	0.002318	2.46E+05

TABLE I-2 ONE-GROUP CORSS SECTIONS (barn) FOR APPLICATION TO Pu-Th FUEL IN LWRs

No.	*Nuclide*	$\sigma_c(+\sigma_{ex})$	σ_f	σ_{n2n}	$T_{1/2}(y)$
1	U-235	6.3980	22.6900	0.003046	7.04E+08
2	U-236	8.4870	0.2166	0.003001	2.34E+07
3	U-238	0.8718	0.1105	0.006263	4.47E+09
4	Np-237	24.2300	0.5713	0.000529	2.14E+06
5	Pu-238	15.2600	2.0330	0.000190	8.77E+01
6	Pu-239	26.0400	46.4500	0.001267	2.41E+04
7	Pu-240	43.8800	0.6222	0.000509	6.56E+03
8	Pu-241	16.7200	54.5200	0.008475	1.44E+01
9	Pu-242	25.5600	0.5354	0.002395	3.75E+05
10	Am-241	64.3940	0.8959	0.000369	4.33E+02
11	Am-242m	45.8400	224.4000	0.006493	1.41E+02
12	Am-243	41.9900	0.4455	0.000233	7.37E+03
13	Cm-242	5.3410	0.4676	0.000060	4.46E-01
14	Cm-244	13.8400	0.9332	0.001179	1.81E+01
15	Th-232	**0.7490**	0.0251	0.005926	1.40E+10
16	Pa-233	22.6000	0.1647	0.001590	7.40E-02
17	U-233	5.0790	36.8300	0.003324	1.59E+05
18	U-234	17.1900	0.4911	0.000485	2.46E+05

I-3.3. Selection of cross sections for thorium fuel cycle (Cross Sections tab at NFCSS Fuel Page)

Thorium fuel cycles are only considered for PWRs and BWRs in the NFCSS for now. The aforementioned two cross section libraries (LWR-Th-U and LWR-Th-Pu) in Table I-1 and Table I-2 are contained in the system library of the NFCSS. These include:

- Fuel ID 5009: LEU-ThO_2 fuel for PWR;
- Fuel ID 5013: (Th,U-233)O_2 fuel for PWR;
- Fuel ID 5014: (Th,Pu)O_2 fuel for PWR;
- Fuel ID 5005: LEU-ThO_2 fuel for BWR;
- Fuel ID 5018: (Th,U-233)O_2 fuel for BWR;
- Fuel ID 5019: (Th,Pu)O_2 fuel for BWR.

Figure I-8 illustrates cross sections of Fuel ID 5009 (LEU-ThO_2 fuel for PWR). It can be seen in Fig.I-8 that the first 14 nuclides are those for uranium fuel cycle and the last four nuclides (Th-232, Pa-233, U-233 and U-234) are for thorium fuel cycle. The first 14 nuclides are numbered as No.1 through No. 14 and the last four nuclides are numbered as No. 15 through No.18 in Table I-1 and Table I-2.

NFCSS Fuel Page

Fuel ID: 5009

Fuel Characteristics | Cross Sections | Delete This Fuel | Reset Form | Save Fuel Data

Nuclide	Bu-Average Fission Cross_Section (barn)	Bu-Average Capture Cross_Section (barn)	Bu-Average n2n Cross_Section (barn)
U235	43.9	10.1	0.004828
U236	0.207	8.03	0.002092
U238	0.102	1.54	0.004828
Np237	0.514	31.4	0.000485
Pu238	2.32	34.4	0.000837
Pu239	106	60	0.001609
Pu240	0.596	153	0.001127
Pu241	113	37.5	0.002543
Pu242	0.433	31.9	0.002382
Am241	1.09	109.6	0.000161
Am242m	413	86.5	0.005955
Am243	0.416	45.69	0
Cm242	0.554	5.6	0
Cm244	0.902	14.2	0
Th232	0.025	1.14	0.00515
Pa233	0.151	22.4	0.006953
U233	53.1	6.39	0.001062
U234	0.48	14.3	0.002318

FIG.I-8. "Cross Sections" tab at "NFCSS Fuel Page" to show additional four nuclides.

Nuclides listed in the same order are also shown in Excel spreadsheet as in Fig.1-9.

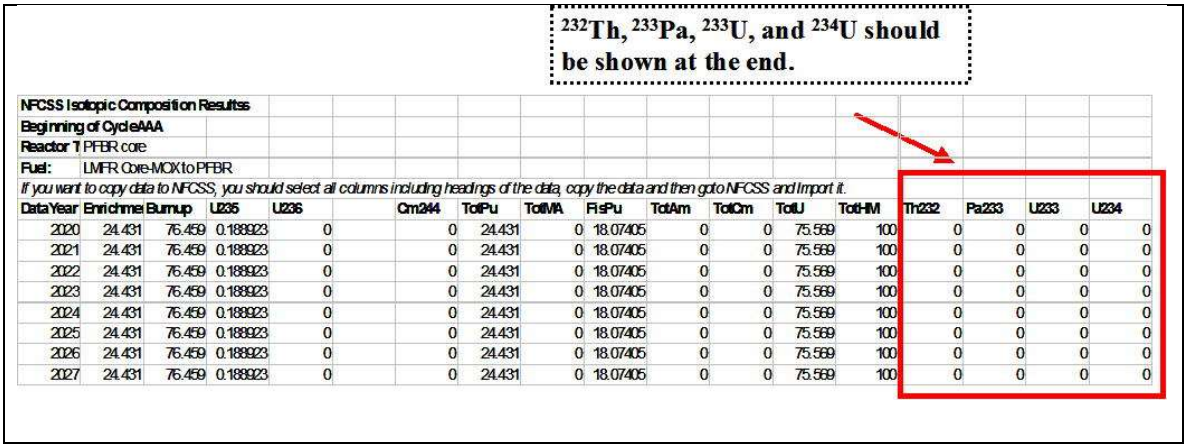


FIG.I-9. Sample EXCEL file to show additional four nuclides

I-3.4. Initial contents of thorium fuel (Fuel Characteristics tab at NFCSS Fuel Page)

Previous version of the NFCSS adopted 14 nuclides from No.1 (U-235) to No.14 (Cm-244), and users could specify the initial contents (weight %) of each nuclide. These nuclides would typically be U-235 for UO_2 fuel, and Pu-238 to Pu-242 for MOX fuel.

Since newly added nuclides are Th-232, Pa-233, U-233 and U-234, the initial contents (in terms of weight %) for these nuclides needs to be included in the input page of the new version of the NFCSS, such as Table I-3. As explained, Th-232, Pa-233, U-233 and U-234 are numbered from No.15 to No.18.

TABLE I-3 LIST OF NUCLIDES IN NFCSS

No.	*Nuclide*	*Initial Content (wt %)*
1	U-235	
2	U-236	
3	U-238	
4	Np-237	
5	Pu-238	
6	Pu-239	
7	Pu-240	
8	Pu-241	
9	Pu-242	
10	Am-241	
11	Am-242m	
12	Am-243	
13	Cm-242	
14	Cm-244	
15	Th-232	
16	Pa-233	
17	U-233	
18	U-234	

Actual specification for initial fuel contents in the input formats is explained according to selected fuel contents in the subsequent sections.

A corresponding Th fuel option can be selected as one of the following fuels by means of a drop-down list as shown in Fig.I-10, besides currently available fuels such as UOX or MOX. One remark here is that the content of each nuclide (wt.%) is fixed in the system library.

If a user wants to generate a completely new fuel, first press the 'Create New Fuel' button at the Fuel List and input all data such as fuel contents and cross sections.

If a user wants to use system cross sections and only to change each nuclide wt.%, generate a 'New fuel' before using this drop-down list. For example, for [5wt.% of 100% enriched U-235 and 95wt.% of Th] fuel scenario, it is possible by generating a 'New fuel' using a copy option from LEU-ThOX fuel, and then specifying 5.0wt.% U-235 and 95wt.% Th-232, then selecting a 'New fuel' here.

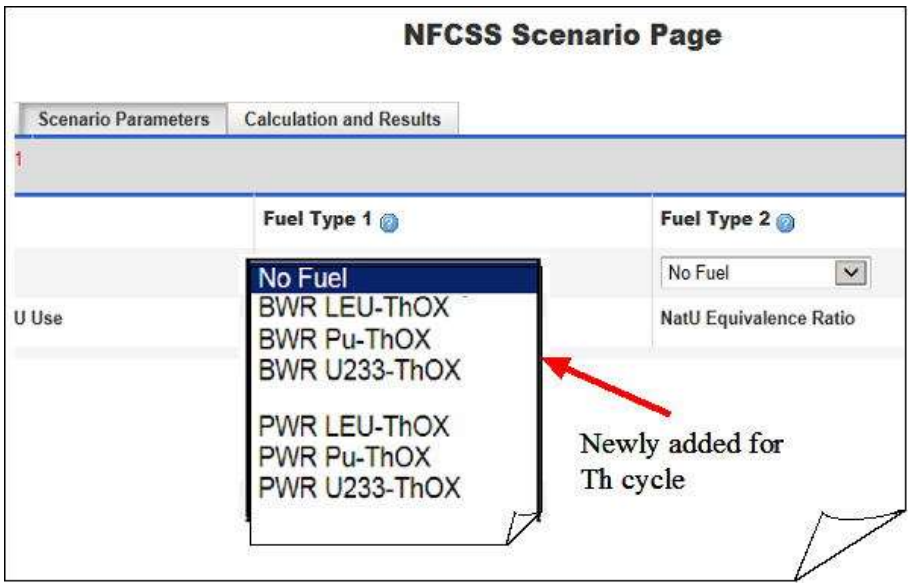


FIG.I-10. Drop-down list in NFCSS Scenario Page (at Scenario Parameter tab).

Current NFCSS gives a help guide (See Fig. I-11) when users move a cursor to the question mark of 'Fuel Content'. As described above, there are 3 fuel contents, which are U-fuel, U-Pu fuel and Free Content fuel. The following help guide is revised based on the above explanation, a sample of which is shown below. Thorium fuel is handled under 'Free Content' fuel. To be distinguished with other fuels that can be handled under Free Content fuel, Conversion Type should be selected as 'Th' from the drop list.

I-3.4.1. (Th,U-233)O_2 fuel

This fuel type would be a simple and typical case, which is composed of only U-233 and Th-232. One simple input style is that a user types a weight % of U-233 (say 4.0) and Th-232 (say 96.0) in the right column of 'NFCSS Fuel Page' (see Fig. I-12).

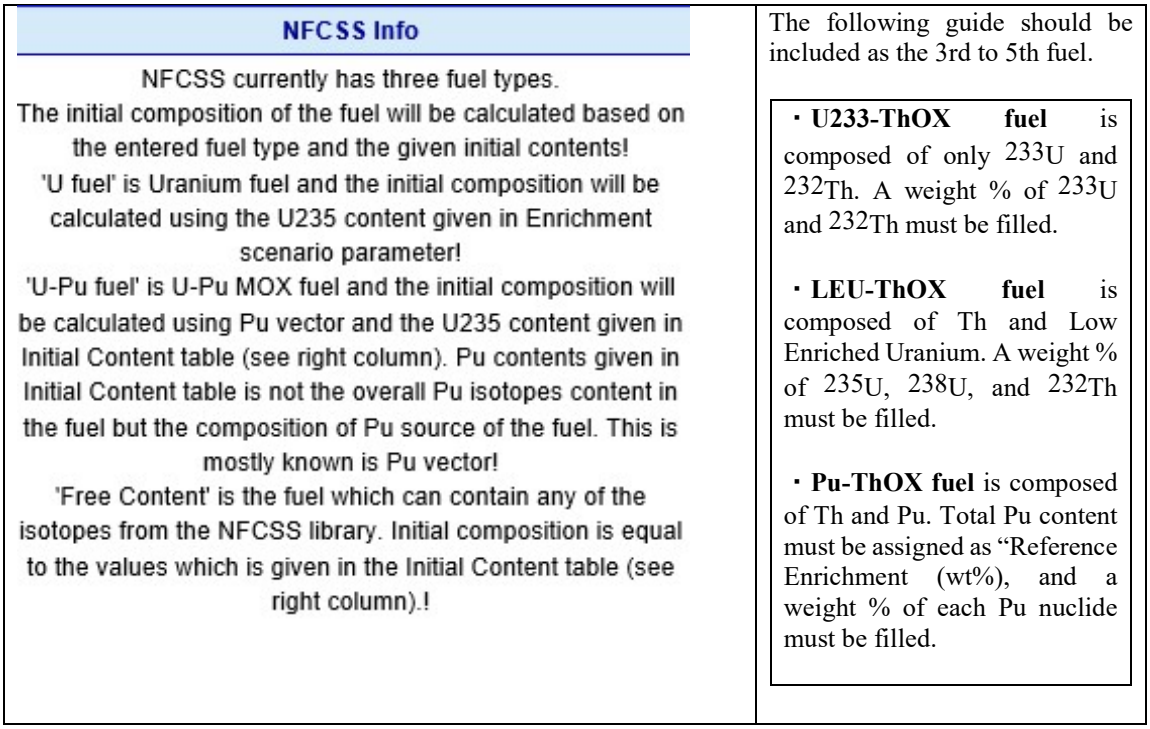


FIG. I-11. Help Guide for Fuel Type in NFCSS Fuel Page.

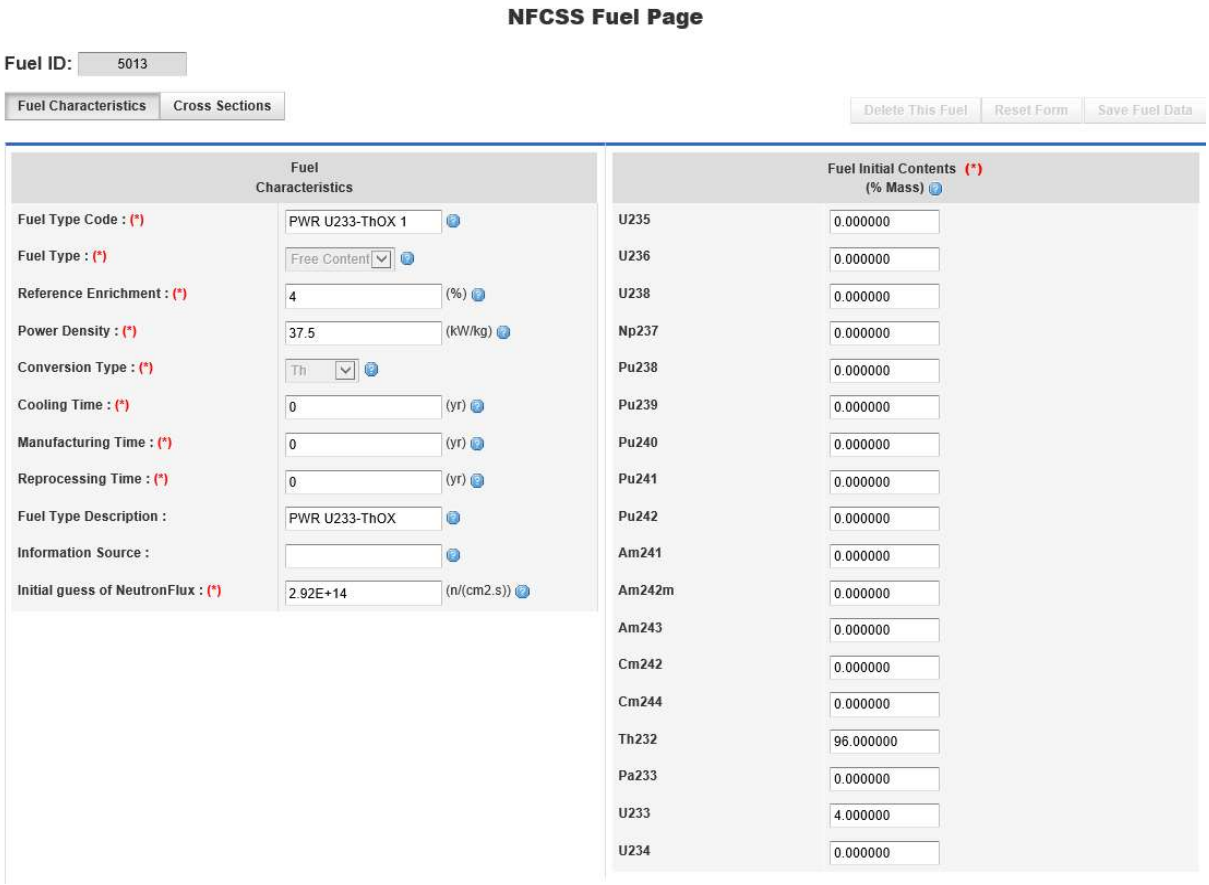


FIG.I-12. Fuel Characteristics tab at NFCSS Fuel Page.

I-3.4.2. (Th,Pu)O2 fuel

This fuel type is composed of thorium and Pu. First of all, total Pu content (say 9.0) is assigned as 'Reference Enrichment' (wt.%). Since Pu is composed of 5 nuclides in NFCSS, users have to type a weight % for each Pu nuclide (Pu-238 to Pu-242), based on the assumed Pu-vector. Then, the content of each of Pu isotopes among 100% is derived, and the rest of total Pu is derived as the content of Th-232 (say 91.0, if Put is 9.0%).

I-3.5. Selection of fuel types for thorium cycle (Scenario Parameters tab at NFCSS Scenario Page)

Figure I-13 is the input page of 'Scenario Parameters' at 'NFCSS Scenario Page'. There are two fuel types. 'Fuel Type 1' is the input for U based fuel, which requires 'Natural Uranium Resources' and 'Separation Work Unit (SWU)'. In general, since Th fuel does not need this information, 'Fuel Type 2' is selected for Th-fuel.

For Th-cycle calculations, (Th,U-235)O_2 fuel and LEU-ThO_2 fuel need special attention. If the initial content of U-235 is non-zero, then some amount of 'Natural Uranium Resources' and 'Separative Work Unit (SWU)' are required. These data are not calculated when users select 'Fuel Type 2'.

It is possible to assign UO_2 fuel as 'Fuel Type 1', and Th fuel as 'Fuel Type 2', in one reactor.

NFCSS requires the following inputs, but it is not required to modify for Th fuel.

(a) Nuclear power: Net electric power capacity in MW;
(b) Load factor;
(c) Thermal efficiency;
(d) Discharge burnup;
(e) Initial U-235 enrichment (or Pu content) for each fuel type.

The following inputs are not required for free content fuel and Th fuel.

(f) Tails assay;
(g) Share of fuel type 2 in the reactor;
(h) Reprocessing ratio for each fuel type;
(i) Use of reprocessed Uranium.

I-3.6. Burnup chains for thorium cycle

Based on the current NFCSS description for U/MOX-cycle (p.53 of [I-1]), there are 28 burnup chains within the irradiation period. The burnup chains for Th-cycle are described as follows.

For the 6 nuclides of Th-cycle (Th-232, U-233, U-234, U-235, U-236 and Np-237) having half-lives longer than 400 years, their further decay is not considered in CAIN burnup chains. Only Pa-233 has a half-life as short as 27 days, and its decay is considered in burnup chains. Decreases of all nuclides by their decay are calculated both in the burnup period and in the cooling period after discharge, regardless of half-life.

Since the NFCSS calculates the actinide weights in unit of 1 kg, any accumulation of actinides weighing less than 1 kg are not shown on the table. Based on the preliminary study, U-236 and Np-237 may not appear in some reactor designs on the NFCSS table. But, for future designs,

U-236 and Np-237 should be included in the CAIN module. Since half-life of Np-237 is very long and its neutron capture cross section is not large, decay of Np-237 and its neutron capture are not considered during the burnup period.

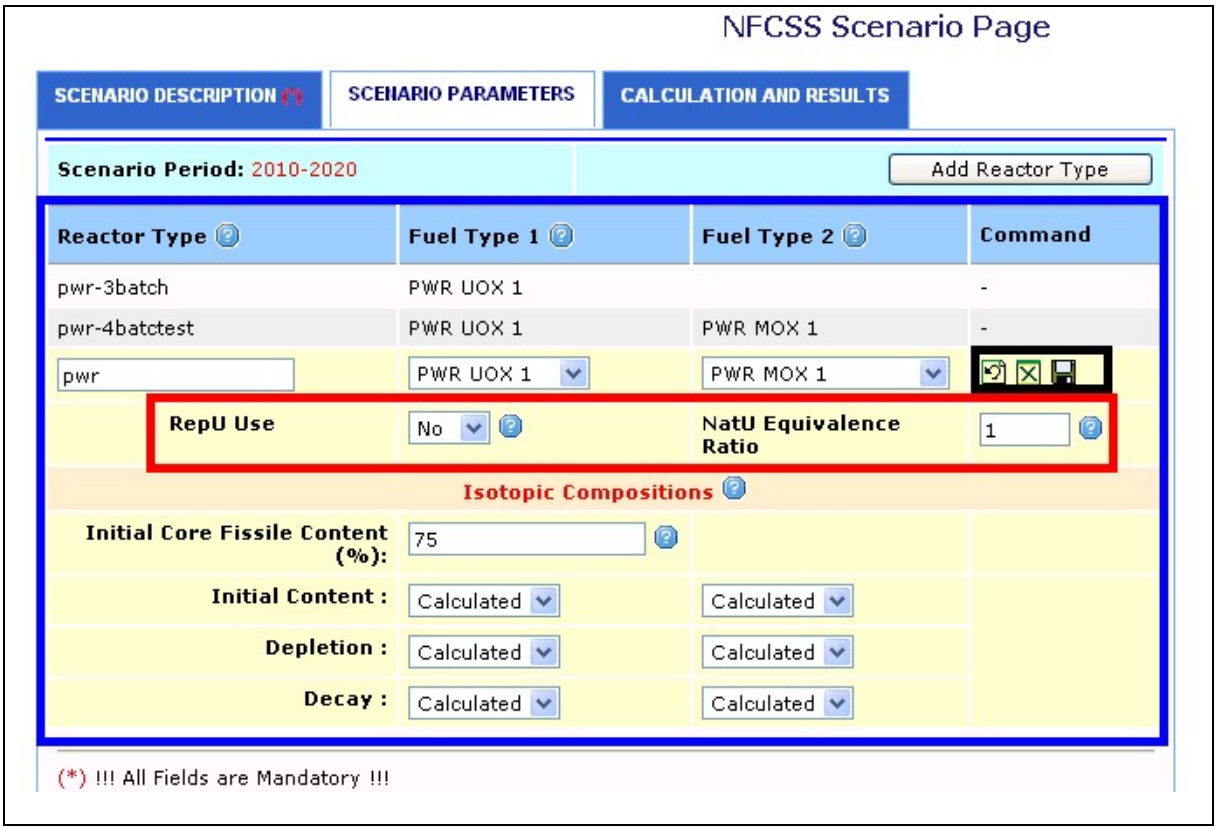


FIG. I-13. Scenario Parameters tab at NFCSS Scenario Page.

So further generation of Pu from Np-237 (Np-237 to Pu-238, and subsequent Pu isotopes) is not assumed for (Th,U-233)O_2 fuel. Since generation of Pu-238 is considered in current U-fuel, this can also be applied to (Th,U-235)O_2 fuel.

One of the most basic assumptions in Bateman's equation is that one equation is required for each initial nuclide. That is, if the fuel is composed of two nuclides such as Th-232 and U-233, two equations are required, even though U-233 appears in burnup chains of Th-232.

Therefore, the following 6 burnup chains are added to the CAIN module. They are 2 paths for Th-232 and 2 paths for Pa-233, and 2 chains starting from U-233 and U-234.

The following 7 nuclides (Th-232, Pa-233, U-233, U-234, U-235, U-236 and Np-237), which appear in the following burnup chains (Table I-4), decrease by fission reaction too.

TABLE I-4 BURNUP CHAINS ADDED TO CAIN FOR THORIUM FUEL CYCLES

No.	New burnup chains for Th cycle
29	Th-232 (capture) > Pa-233 (decay) > U-233 (capture) > U-234 (capture) > U-235 (capture) > U-236 (capture) > Np-237
30	Th-232 (capture) > Pa-233 (capture) > U-234(capture) > U-235 (capture) > U-236 (capture) > Np-237
31	Pa-233 (decay) > U-233 (capture) > U-234 (capture) > U-235 (capture) > U-236 (capture) > Np-237
32	Pa-233 (capture) > U-234 (capture) > U-235 (capture) > U-236 (capture) > Np-237
33	U-233 (capture) > U-234 (capture) > U-235 (capture) > U-236 (capture) > Np-237
34	U-234 (capture) > U-235 (capture) > U-236 (capture) > Np-237

If the initial Th-fuel is composed of other nuclides, such as U-235, U-236, U-238, and/or each Pu nuclide (Pu-238 to Pu-242), and/or each MA nuclide (Np, Am, Cm), then previous burnup chains for U-fuel or MOX fuel should be applied. These 28 burnup chains are shown in Appendix III of the reference [I-1].

Also, the generated nuclides (U-235, U-236, and Np-237) are added to the current burnup chains in CAIN module. For example, if the initial fuel is ^{235}U-Th fuel or LEU-Th fuel, currently existing [Burnup chain-1] is calculated, and its results are added to the above Th burnup chains.

[Burnup chain-1] for initial ^{235}U is as follows (copied from P.53 of the reference [I-1]).

$$^{235}U \xrightarrow{(n,\gamma)} {}^{236}U \xrightarrow{(n,\gamma)} {}^{237}Np \xrightarrow{(n,\gamma)} {}^{238}Pu$$

A modification in ASP programme of the CAIN module to implement Th cycle is shown below in Fig.I-14.

```
' ************************************************************************************
' CHAIN 29 ***************************************************************************
 ' ***********************************************************************************
 ' **** LL=1     LL=2     LL=3     LL=4     LL=5     LL=6     LL7  *********
 ' **** Th232------>Pa233------>U233------>U234------>U235------>U236------>Np237 *********
 ' ***********************************************************************************
If (ChainActive(29) = 1) Then
   Response.Write("<br>Chain 29:")
   'IL(1) = 2: IL(2) = 4: IL(3) = 5:  IL(4) = 6: IL(5) = 7: IL(6) = 8: IL(7) = 9
   IL(1) = 15: IL(2) = 16: IL(3) = 17: IL(4) = 18: IL(5) = 1: IL(6) = 2: IL(7) = 4

   For LL=1 To 7
      Response.Write("<br>Chain 29")
      Response.Write("<br>SIGC("&i&")" & SIGC(i))
      Response.Write("<br>SIGT("&i&")" & SIGT(i))
      i=IL(LL)
      SC(LL) = SIGC(i)
      ST(LL) = SIGT(i)

          ' ---------- LL=2 ------  I=16 : Pa233 (decay to U233) -----
       If LL = 2 Then SC(2) = SDECAY(16)

      Call Calc
      If Err.Number <> 0 Then
         Response.Write("Error chain 29: " & Err.Description)
         response.end
      end if
      Response.Write("<br>Initial_Content(IL(1))" & Initial_Content(IL(1)))
      NDI = NI * Initial_Content(IL(1))

      If i=1 then NDI=NDI+Number_Density(1)  '+++Add U235+++
            If i=2 then NDI=NDI+Number_Density(2)  '+++Add U236+++
      If i=4 then NDI=NDI+Number_Density(4)  '+++Add Np237+++
      Number_Density(i) = NDI

     Number_Density(i) = NDI + Number_Density(i)
     Response.Write("<br>Number_Density("&i&")" & Number_Density(i))
   Next

End if
```

FIG.I-14. Modification of source code of CAIN to incorporate the burnup chain of thorium fuel cycles.

```
 ' ********************************************************************************
 ' CHAIN 30 ********************************************************************************
 ' ********************************************************************************
 ' *****  LL=1    LL=2    LL=3    LL=4    LL=5    LL=6  *********
 ' *****  Th232------>Pa233------>U234------>U235------>U236------>Np237 *********
 ' ********************************************************************************
If (ChainActive(30) = 1) Then
   Response.Write("<br>Chain 30:")
   'IL(1) = 2: IL(2) = 4: IL(3) = 5:  IL(4) = 6: IL(5) = 7: IL(6) = 8
   IL(1) = 15: IL(2) = 16: IL(3) = 18: IL(4) = 1: IL(5) = 2: IL(6) = 4

   For LL=1 To 6
      i=IL(LL)
      SC(LL) = SIGC(i)
      ST(LL) = SIGT(i)

      Call Calc
   If Err.Number <> 0 Then
      Response.Write("Error chain 30: " & Err.Description)
      response.end
   end if
      NDI = NI * Initial_Content(IL(1))
      'Changed as discussed in the meeting – 20101006
   if i<>15 then  Number_Density(i) = NDI + Number_Density(i)

      ' Do not add Th232 (i=15) because of redundancy. Others must be added as follows.
      If i=18 then NDI=NDI+Number_Density(18)  '+++Add U234+++
            If i=1 then NDI=NDI+Number_Density(1)    '+++Add U235+++
            If i=2 then NDI=NDI+Number_Density(2)    '+++Add U236+++
            If i=4 then NDI=NDI+Number_Density(4)    '+++Add Np237+++
            Number_Density(i) = NDI

      end if
   Next

End if

 ' ********************************************************************************
   ' AS suggested by Ki Seob - 2017-09-08
 ' CHAIN 31 ********************************************************************************
 ' ********************************************************************************
 ' *****  LL=1    LL=2   LL=3    LL=4    LL=5    LL=6  *********
 ' *****  Pa233------>U233------>U234------>U235------>U236------>Np237 *********
 ' ********************************************************************************
If (ChainActive(31) = 1) Then
   Response.Write("<br>Chain 31:")
   IL(1) = 16: IL(2) =17: IL(3) = 18:  IL(4) = 1: IL(5) = 2: IL(6) = 4

   For LL=1 To 6
      i=IL(LL)
      SC(LL) = SIGC(i)
      ST(LL) = SIGT(i)
```

FIG.I-14. (Continued)

```
      ' ---------- LL=1 ------  i=16 : Pa233 (decay to U233) -----
      If LL = 1 Then SC(1) = SDECAY(16)

      Call Calc
      NDI = NI * Initial_Content(IL(1))

      ' Do not add Pa233 (i=16) because of redundancy.
     If i<>16 then Number_Density(i) = NDI + Number_Density(i)
     end if
)
   Next

End if

 ' ***************************************************************************
   ' AS suggested by Ki Seob - 2017-09-08
 ' CHAIN 32 ****************************************************************
 ' ***************************************************************************
 ' *****  LL=1     LL=2    LL=3    LL=4    LL=5   ********
 ' *****  Pa233------>U234------>U235------>U236------>Np237 *********
 ' ***************************************************************************
If (ChainActive(32) = 1) Then
   Response.Write("<br>Chain 32:")
   IL(1) = 16: IL(2) =18: IL(3) = 1:  IL(4) = 2: IL(5) = 4

   For LL=1 To 5
      i=IL(LL)
      SC(LL) = SIGC(i)
      ST(LL) = SIGT(i)

      Call Calc
      NDI = NI * Initial_Content(IL(1))
      Number_Density(i) = NDI + Number_Density(i)
   Next

End if

' ***************************************************************************
   ' AS suggested by Ki Seob - 2017-09-08
 ' CHAIN 33 ****************************************************************
 ' ***************************************************************************
 ' *****  LL=1    LL=2    LL=3     LL=4   LL=5   ********
 ' *****  U233------>U234------>U235------>U236------>Np237 *********
 ' ***************************************************************************
If (ChainActive(33) = 1) Then
   Response.Write("<br>Chain 33:")
   IL(1) = 17: IL(2) =18: IL(3) = 1:  IL(4) = 2: IL(5) = 4

   For LL=1 To 5
      i=IL(LL)
      SC(LL) = SIGC(i)
      ST(LL) = SIGT(i)

      Call Calc
      NDI = NI * Initial_Content(IL(1))
      Number_Density(i) = NDI + Number_Density(i)
   Next

End if
```

FIG.I-14. (Continued)

```
' ************************************************************************************
   ' AS suggested by Ki Seob - 2017-09-08
 ' CHAIN 34 ************************************************************************
 ' ************************************************************************************
 ' *****  LL=1    LL=2    LL=3    LL=4   *******
 ' *****  U234------>U235------>U236------>Np237 *********
 ' ************************************************************************************
If (ChainActive(34) = 1) Then
   Response.Write("<br>Chain 34:")
   IL(1) = 18: IL(2) =1: IL(3) = 2:  IL(4) = 4

   For LL=1 To 4
      i=IL(LL)
      SC(LL) = SIGC(i)
      ST(LL) = SIGT(i)

      Call Calc
      NDI = NI * Initial_Content(IL(1))
      Number_Density(i) = NDI + Number_Density(i)
   Next

End if

   'Response.write ("<br>End of CalcActinide Total_Mass : " & Total_Mass )
   'Response.write("<br>NNuclide="& NNuclide)

For i = 1 To NNuclide
    Response.write("<br>i=" & i)
    Mass_Density(i) = Number_Density(i) * MASS(i) / Total_Mass * 100
   Response.write("<br><b>Mass_Density("& i & ")-> " & Mass_Density(i) & "</b>")
Next

End Sub 'CalcActinide
```

FIG.I-14. (Continued)

I-3.7. Decay chains for thorium cycle

In [I-1] there are 14 decay chains after fuel discharge. The following 4 decay chains after fuel discharge are added to CAIN module for Th fuel cycle (Table I-5). Here, “x” means to stop further decays. It is noted that only generated U-233 from Pa-233 decay is added to the inventory of discharged U-233. Other nuclides (Th-232, U-233, U-234) have very long half-life, and these decays would appear only if users calculate very long span after fuel discharge.

TABLE I-5 ADDITIONAL DECAY CHAIN FOR THORIUM FUEL CYCLES

No.	Decay chains
15	Pa-233 (decay) > U-233 > “x”
16	Th-232 (decay) > “x”
17	U-233 (decay) > “x”
18	U-234 (decay) > “x”

As for other nuclides such as U-238 or Pu-239 and other minor actinides, existing chains (Decay chain-1 to 14) are calculated, and its results are added to the above Th burnup chains.

A modification in the ASP programme of NFCSS for thorium fuel is shown in Fig.I-15.

```
 ' ************************************************************
 ' CHAIN 15 *******  Decay of Pa233  ************************
 ' ************************************************************
 ' *****  LL=1       LL=2                 *****
 ' *****  Pa233 ------>U233                 *****
 ' ************************************************************
 IL4(1) = 16: IL4(2) = 17
   For LL = 1 To 2
      i = IL4(LL)
      ST(LL) = SDECAY(i)
      SC(LL) = SDECAY(i)
         Call Decay(DecayTime)
      NDI = ni
      NDI = NDI * ND1(IL4(1))
     If i = 17 Then NDI = NDI + Number_Density(17) ' +++++ Add U233 +++++
      Number_Density(i) = NDI
   Next

' ************************************************
 ' CHAIN 16 *******  Decay of Th232   ***************************
 ' ************************************************************
 ' *****  LL=1                                 *****
 ' *****  Th232                                *****
 ' ************************************************************
 IL4(1) = 15
For LL = 1 To 1
i = IL4(LL)
ST(LL) = SDECAY(i)
 SC(LL) = SDECAY(i)
Call Decay(DecayTime)
NDI = ni
Number_Density(i) = NDI * ND1(IL4(1))
next

' ************************************************
 ' CHAIN 17 *******  Decay of U233   ***************************
 ' ************************************************************
 ' *****  LL=1                                 *****
 ' *****  U233                                *****
 ' ************************************************************
 IL4(1) = 17
For LL = 1 To 1
i = IL4(LL)
ST(LL) = SDECAY(i)
 SC(LL) = SDECAY(i)
Call Decay(DecayTime)
NDI = ni
Number_Density(i) = NDI * ND1(IL4(1)) + Number_Density(17)  ' +++ Add U233 in chain 15 ++++
next

' ************************************************
 ' CHAIN 18 *******  Decay of U234   ***************************
 ' ************************************************************
 ' *****  LL=1                                 *****
 ' *****  U234                                *****
 ' ************************************************************
 IL4(1) = 18
For LL = 1 To 1
i = IL4(LL)
ST(LL) = SDECAY(i)
 SC(LL) = SDECAY(i)
Call Decay(DecayTime)
NDI = ni
Number_Density(i) = NDI * ND1(IL4(1))
next
```

FIG.I-15. Modification of source code of CAIN to incorporate the decay chain of thorium fuel cycles.

I-4. OTHER IMPROVEMENTS THAT ARE NOT DIRECTLY INCORPORATED IN NFCSS

I-4.1. Decay heat calculation

Decay heat is one of the important parameters to perform safety assessments for reactor accident analysis and radioactive waste management. However, current NFCSS does not provide information on decay heat in output. Since decay heat depends on fuel weight and fuel type, it can be calculated only using the NFCSS output table data. Therefore, it will be practical to provide a supplementary programme (for example, an independent EXCEL programme) which can calculate decay heat. Another reason for this proposal is that NFCSS projections are limited to a maximum period of 200 years, whereas decay heat issue is a very long-term issue and can be relevant for even million years.

Table 32 and Fig.44 in Section 6 provide decay heat from UO_2, ^{233}U-ThO_2, and MOX fuel applicable to any discharge burnup in both PWR and BWR. An interpolation formula is also described in Section 6.6.

Figure I-16 shows a schematic diagram to calculate decay heat at a certain year. Since the NFCSS provides discharged fuel weight and fuel type at Year-1 2 3 etc., decay heat at a certain year (year-X) can be calculated year wise. Then, the summation of these decay heat gives total decay heat at year-X. This calculation can be performed for one reactor or multiple reactors in one country.

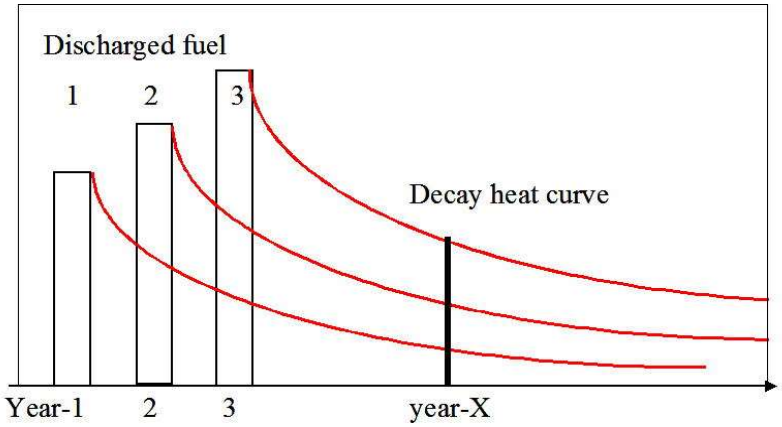


FIG.I-16. Schematic diagram to calculate decay heat.

I-4.2. Radiotoxicity calculation

Radiotoxicity is also an important parameter in fuel cycle calculations, especially for analysis concerning spent fuel storage and geological radioactive waste disposal.

The NFCSS does not provide radiotoxicity information. Since radiotoxicity depends on fuel weight and fuel types; it is only calculated using the NFCSS output table data. It will be practical to provide a supplementary programme (for example, an independent EXCEL programme) which can calculate radiotoxicity. Since radiotoxicity, like decay heat, lasts for a very long period (up to million years) and the NFCSS projections are limited to a maximum of 200 years, adding a module for radiotoxicity calculation will be a valuable enhancement of the NFCSS features. Table 42 and Fig.55 in Section 7 provide the radiotoxicity of UO_2, ^{233}U-ThO_2 and

MOX fuel for any burnup fuel in PWR or BWR. An interpolation formula is also described in Section 7.5.

Figure I-17 shows a schematic diagram to calculate radiotoxicity at certain year. Since the NFCSS provides discharged fuel weight and fuel type at Year-1 2 3 etc., radiotoxicity at a certain year (year-X) can be calculated year-wise. Then, the summation of these radiotoxicities gives the total radiotoxicity at year-X. This calculation can be performed for one reactor or multiple reactors in one country.

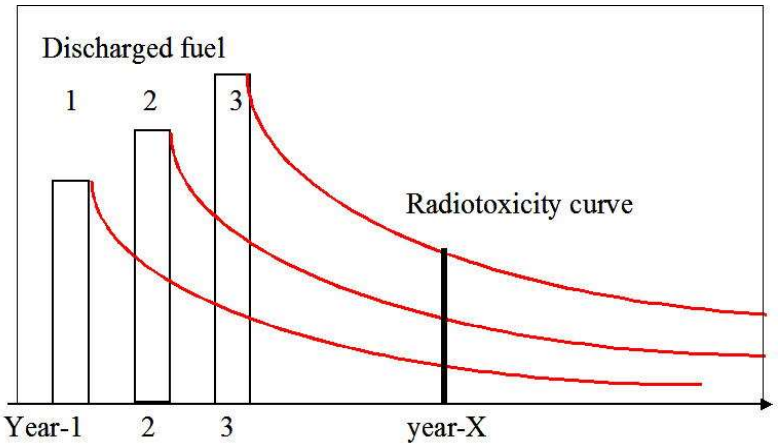


FIG. I-17. Schematic diagram to calculate radiotoxicity.

I-4.3. Influence of operation mode on Pu-241 decay

The NFCSS has an input of Load Factor (LF), but the NFCSS assumes 100% power operation in the CAIN burnup calculation. Since the CAIN does not include load factor effect, the influence of this assumption is investigated in Annex III-9 for nuclides such as Pu-241, Am-241 and Am-242m.

For long term evaluation of more than a decade, difference due to this assumption becomes benign as small as 2–3%.

When the NFCSS is applied to a single reactor simulation for a short-time period (e.g., several years' operation), however, the difference may no longer become negligible on the inventory of Am-241 and Am-242m (e.g. as large as 20–30%).

Therefore, the load factor effect should be incorporated in the CAIN burnup calculation in the next software update of the NFCSS. Because of its small effect for most of the fuel cycle evaluations, this modification is yet to be incorporated in the NFCSS.

I-4.4. Residence time input

As explained in Section 4.2.3, RT (Residence Time) is a mandatory input provided in integers such as 1, 2, 3 etc., or according to the following formula:

RT (year) = integer value of [BU/SP/365/LF]

where,

BU: Discharge burnup (MW·d/t),
SP: Specific Power (MW/t),

LF: Load Factor (fraction).

In the actual burnup calculation in the NFCSS, however, RT is calculated using the following formula, which does not include LF:

RT = BU / SP / 365

RT is a mandatory input but never used. Users should note this procedure because this was not described in the earlier NFCSS publication [I-1].

I-4.5. Study on Am-241 cross section

When Am-241 captures a neutron, there are two reactions: (a) go to Ground-state Am-242 (about 10%) and go to (b) Meta-stable Am-242m (about 90%), as described in Section 4.2.3. Since this branch fraction (BF) is almost constant at thermal neutron energy, BF is fixed in the NFCSS programme.

Also, BF decreases at high neutron energy and thus for application to FBR the above fixed BF would cause small error in the inventories of the above nuclides. At this moment, this is not corrected because the inventories of the above nuclides are small in most FBR designs.

REFERENCES TO ANNEX I

[I-1] International Atomic Energy Agency, Nuclear Fuel Cycle Simulation System (VISTA), IAEA-TECDOC-1535, IAEA, Vienna (2007).

ANNEX II: NFCSS USER'S MANUAL

II-1. GENERAL

The NFCSS is a web based simulation tool for performing various nuclear fuel cycle calculations over time and allows users to create various growth scenarios. According to an input specification on 'reactor type', a new scenario is generated, and new fuel types and data sets for a reactor (or a group of reactors) are defined for use in the defined scenario.

The entire NFCSS system is stored in the servers of IAEA in Vienna. The web executable and scenario data and results obtained by registered users are also stored in the database servers of IAEA. This approach has the following advantages:

(a) There is no need to install any type of software in client computers;
(b) Users can access the NFCSS and their scenario data and results virtually using any computer in the world which has internet connection;
(c) NFCSS software updates can be applied virtually any time. Applying patches and fixes is very easy because there is only one executable running for all users;
(d) The users can use reactor and fuel types existing in the NFCSS library or create their own reactor and fuel types.

Some technical features are given below:

(a) The programme has been fully tested and operational on Microsoft Internet Explorer;
(b) The NFCSS application is an ASP (Active Server Page) application running on IAEA's web server, and the codes were originally written in Visual Basic;
(c) The scenario data and results are stored centrally in IAEA's database servers in Vienna;
(d) Exporting data to and importing from Microsoft Excel is available for some of the functions in NFCSS.

This manual describes a UO_2 fuel or MOX fuel case. Some remarks on Th fuel are described in Section 5 and Annex I.

II-2. PROGRAMME OPERATION

Since NFCSS is a scenario based simulation tool, the user has to define the scenario to run the system. The list of ordered steps to successfully run the NFCSS simulation tool is given below.

(a) Access iNFCS–NFCSS as an IAEA Nucleus (http://nucleus.iaea.org) registered user. A free Nucleus user account is required to create and save users own scenarios;
(b) Scenario preparation
    1) User should Create New Scenario or Select Scenario to work.
    2) User should edit scenario description (the scenario period is important).
    3) User should select the reactor and fuel types for the selected scenario.
    4) User should enter scenario data for each of the reactor and fuel types in the selected scenario;
(c) Calculations and results

1) User should perform isotopic composition calculations for each fuel type in each reactor type in the selected scenario or provide isotopic composition table.
2) User should perform material flow calculation for each reactor type in the selected scenario.
3) User should perform overall material flow calculation for all reactor types in the selected scenario.

The following subsections explain each of the above steps in details and provide explanation for every input parameter.

II-3. ACCESS TO THE SCENARIOS PAGE

Authorized Nucleus users can access the NFCSS Scenarios after login. The NFCSS web site has 7 tab-pages and one of the tab pages is Scenarios. The user should select Scenarios tab (See Fig.II-1).

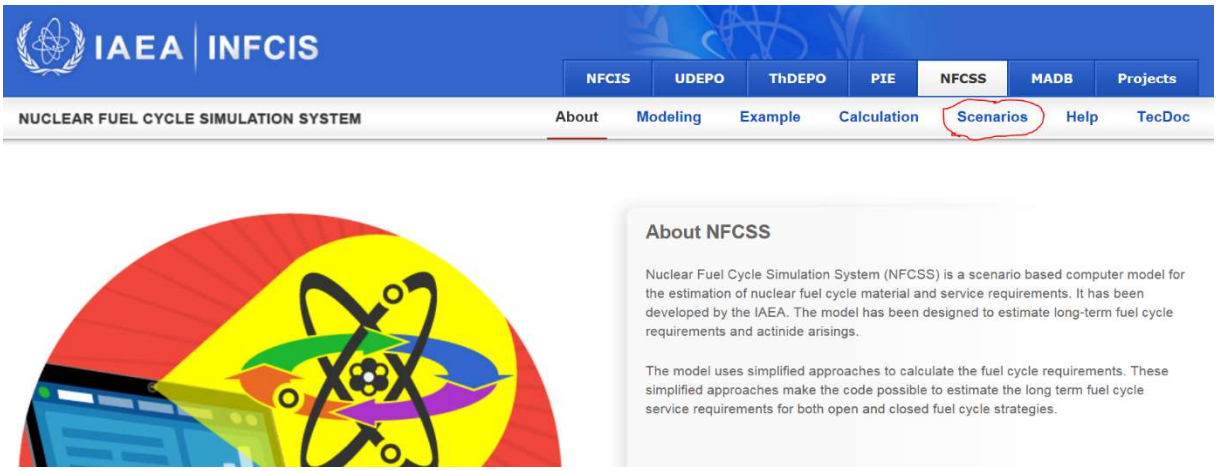


FIG.II-1. The Scenario tab of NFCSS

Authorized Nucleus users will be able to see three demo Scenarios (Fig.II-2). They will be able to build and save their own scenarios.

The NFCSS is accessed from the Scenarios tab (Fig.II-2). There is a breadcrumb (a kind of navigation system) in this page to quickly access to the different parts of the system. First shortcut in the breadcrumb is the link to the scenario list. The user can create a new scenario, delete an existing scenario or select one of the existing scenarios to work with in this Scenario List Page. The second shortcut in breadcrumb is the link to the Fuel List page. The third link is to the Reactor List page. The last shortcut in the breadcrumb is the link to the Selected Scenario Page in which the users can edit scenario data and run the scenario. The breadcrumb is always available in the NFCSS in all pages.

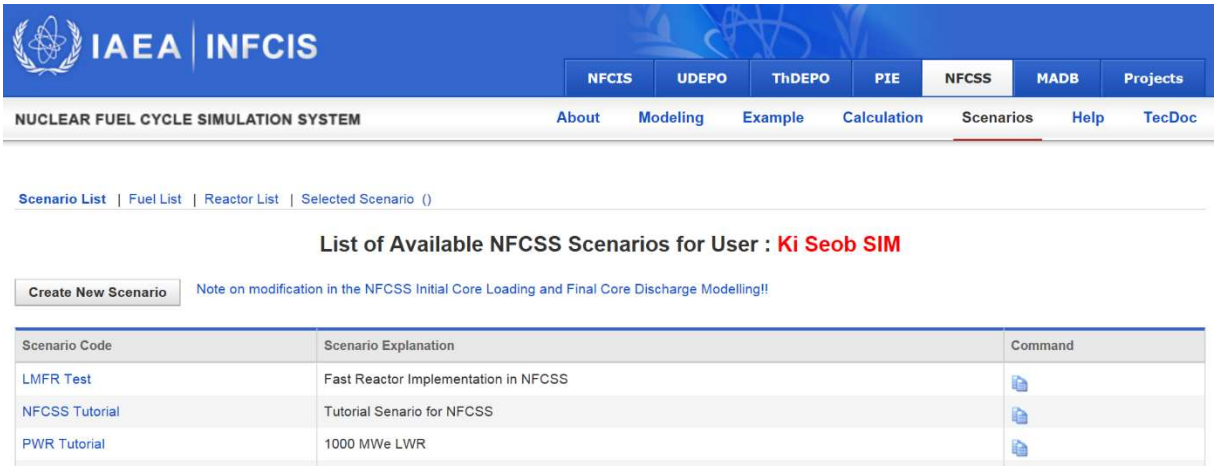


FIG.II-2. NFCSS Scenarios page.

Another feature of the NFCSS application is that there is always confirmation dialogs when the user wants to add or delete something. For example, when the user wants to create a new scenario, a dialog like Fig.II-3 is displayed.

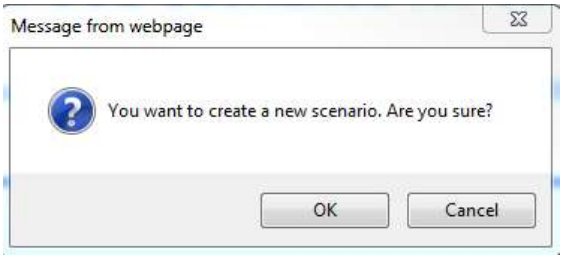


FIG.II-3. Confirmation dialog for creating a new scenario.

II-4. SCENARIO PREPARATION

II-4.1. Creating a new scenario

The user can use the **Create New Scenario** button (in Fig.II-2) to create a new scenario. After confirmation (Fig.II-3), the NFCSS will create a new scenario and displays the Scenario Page for the newly created scenario. The default code for the new scenario will be 'New Code'.

II-4.2. Copying an existing scenario

The user can copy one of his/her existing scenario in order to start a new study with similar data. The copying scenario is done by clicking button in the Scenario List page. After a confirmation dialog, the NFCSS copies the selected scenario with all the data. The isotopic composition and material flow results are not copied. Calculations must be done for the newly created scenario after changing the data if necessary.

II-4.3. Deleting an existing scenario

The user can use the button to delete an existing scenario. After confirmation, the NFCSS will delete the selected scenario and all related data and result records from the database.

II-4.4. Selecting an existing scenario to work with

The user can select one of the existing scenarios to work with from the Scenario List page. There are links to the Scenario Page for each scenario in the list. The user needs to click on the Scenario Code for the scenario to work with.

II-4.5. Editing scenario description (Scenario Page)

Following the selection of working scenario, NFCSS displays the Scenario Page. Scenario Page is the centre of defining, running and post-processing a scenario. Figure II-4 shows the NFCSS Scenario Page (headings for the web site is not displayed). There are three tab-pages in the NFCSS Scenario Page. The lower part of the scenario page is the main part of the page and displays different options depending on the selected tab page.

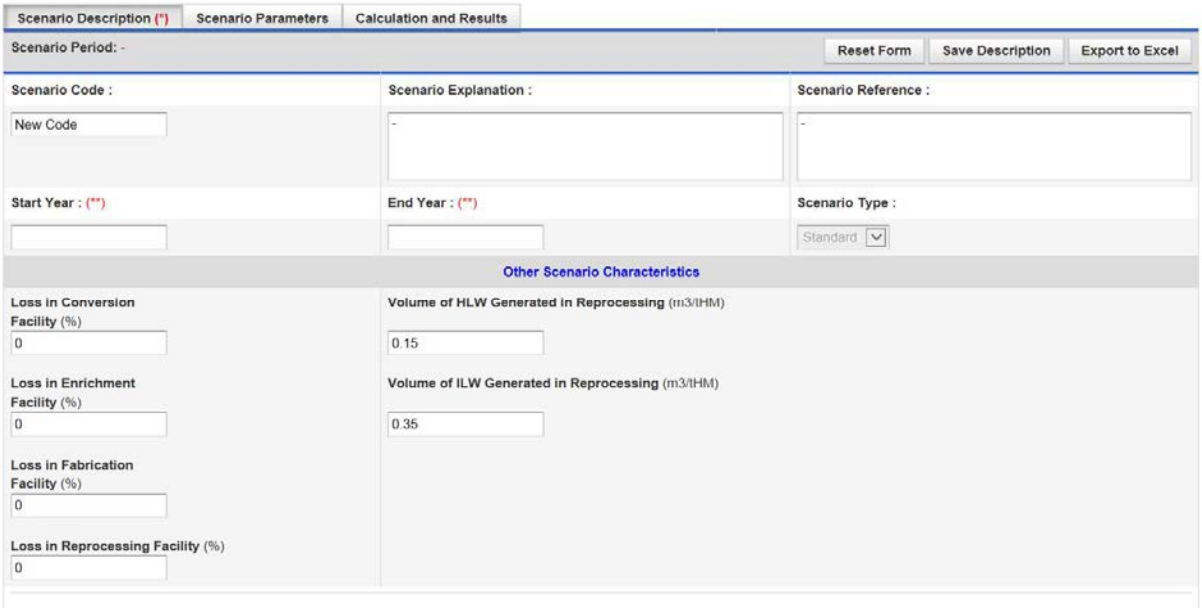


FIG.II-4. Scenario Description page in NFCSS.

After creating a new scenario, the first thing to do is to enter the general scenario description data. The **Scenario Description** tab page in scenario page provides tools to do this (Fig.II-4).

The explanation of each input parameter and the possible options are:

- **Scenario Code**: The identification code of the scenario. The text can be entered freely in this field up to 50 characters.
- **Scenario Explanation**: The explanatory information about the scenario. This field is a free text field of any length.
- **Scenario Reference**: The source(s) of information which is used to define the scenario, if any. For example, the user can use IAEA Nuclear Power Estimates to analyse the worldwide situation in the future. This is a free text field with any length.
- **Start Year**: Beginning of the scenario period. The data should be entered in integer format.
- **End Year**: End of scenario period. The data must be entered in integer format. Note that the start and end year difference defined in the scenario must be not greater than 200 years.

- **Loss in Conversion Facility (%), Loss in Enrichment Facility (%), Loss in Fabrication Facility (%), Loss in Reprocessing Facility (%)**: Loss coefficients at steps in the nuclear fuel cycle. The loss is given in percent. The material loss is calculated at the beginning of the step and remains unchanged for the rest of the calculation.
- **Volume of HLW Generated in Reprocessing**: The volume of the high level waste generated during the reprocessing of spent fuel per tonne Heavy Metal of reprocessed spent fuel.
- **Volume of LLW Generated in Reprocessing**: The volume of the low and intermediate level waste generated during the reprocessing of spent fuel per tonne Heavy Metal of reprocessed spent fuel.

Following the entry of each data, user must save the page before continuing the work. In order to save the scenario description, the user should click on the **Save Description** button at the upper right location of Scenario Page.

The user can export whole scenario data to Microsoft Excel to locally store the scenario data and results, or work on it in Microsoft Excel. In order to export scenario description including all the data to Microsoft Excel, **Export to Excel** button is used.

II-4.6. Selecting reactor types and associated fuel types (Scenario Page)

After scenario description, **Scenario Parameters** tab page in scenario page (Fig.II-4) is used to specify reactor and fuel types and data for the scenario parameters for each of the reactor and fuel type. Scenario Parameters page (Fig.II-5) includes the list of reactor types which is included in the selected scenario. If no reactor type is selected, the list will be empty. There are four parts in this page: 'Reactor Type', 'Fuel Type 1', 'Fuel Type 2' and 'Command'.

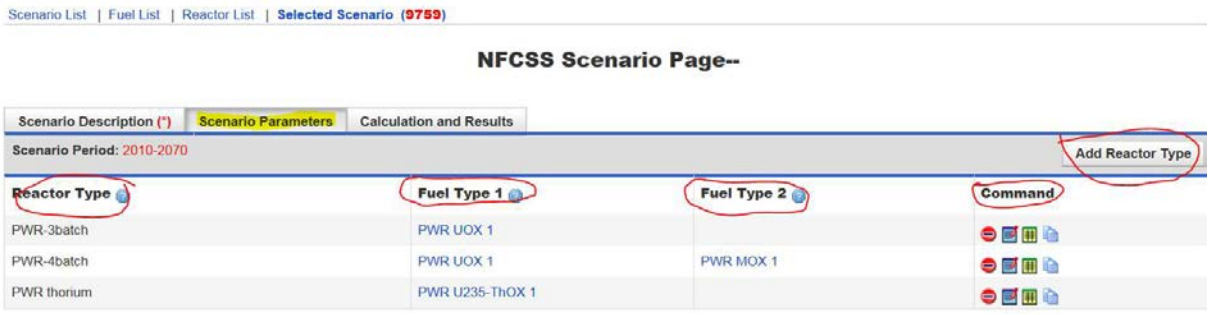


FIG.II-5. Scenario Parameters page in the NFCSS.

A button **Add Reactor Type** is used to add new reactor type to the scenario. Scenario period is also displayed in this page to remind the user.

Commands are used, respectively, to delete the selected reactor type and its related data, to edit reactor and fuel type characteristics, to add new reactor type using the characteristics of existing one, and to edit scenario parameters (e.g. nuclear capacity, enrichment level, etc.) for the selected reactor type.

Figure II-6 illustrates editing of "Scenario Parameters" page using the command in Fig.II-5. In Fig. II-6,

- **Reactor Type**: Free text information for the reactor type up to 50 characters.
- **RepU Use**: If user wants to use reprocessed uranium in the fuel type 1, it should be 'Yes'. If it is selected, the ratio to convert reprocessed Uranium to natural uranium is needed. For simplicity set this ratio to 1.
- **Fuel Type 1**: The type of fuel for Fuel Type 1 (fuel from natural material, usually uranium fuel). The fuel type should be selected from a predefined fuel list. The list includes the fuel types from the NFCSS built-in fuel library and the fuel types which have been added by the user. The data for those built-in fuel types cannot be changed by the users. However, the users can create their own fuel types to be used in their scenario. After addition of a fuel to the system by the user, only the user who owns the fuel type can use that specific fuel type in his/her scenario. The Fuel Types are explained in Annex II-6.
- **Fuel Type 2**: The type of the fuel for the Fuel Type 2 (fuel from reprocessed material or depleted uranium, usually MOX fuel). The fuel type should be selected from a predefined fuel list. which includes the fuel types from the NFCSS built-in fuel library and the fuel types which have been added by the user. If the reactor type does not use second fuel type, No Fuel option must be selected from the list.
- **Initial Core Fissile Content**: Initial core fissile content is defined as a percentage of the fissile content of equilibrium cycle fuel loading. The initial loading enrichment for fresh core is not the same as the equilibrium cycle loading enrichment since not entire initial core has to stay in the reactor for the whole residence time. The initial core loading enrichment is less than the equilibrium cycle loading enrichment. There is a box to enter the core fissile content ratio to determine initial core requirements in the NFCSS. The calculation procedure is also different for final core discharge and the methodology used in the NFCSS is discussed in Annex II-8.

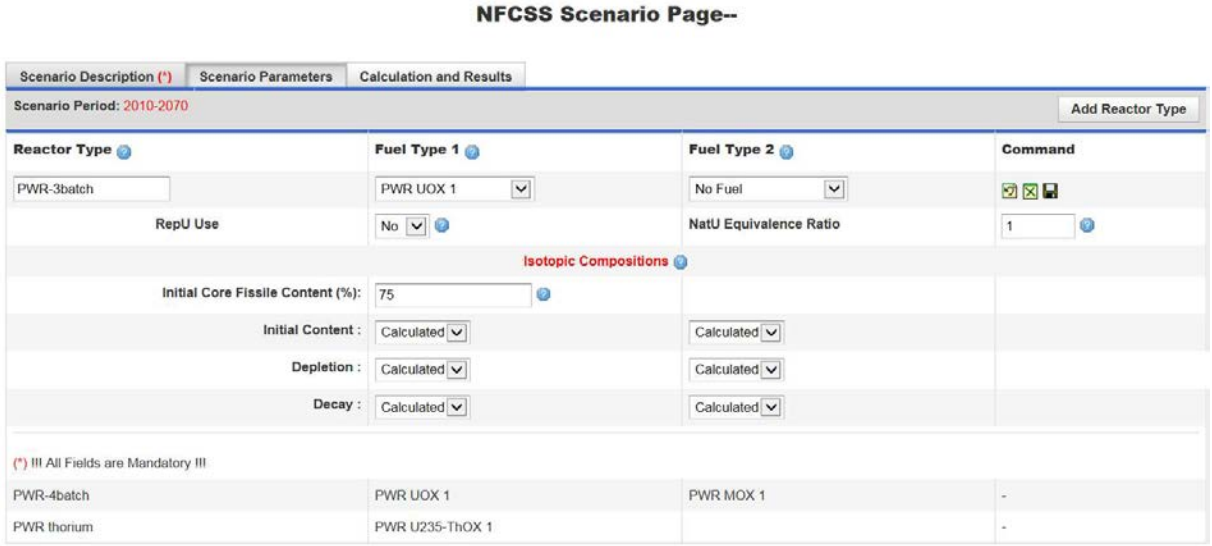


FIG.II.6. Editing of reactor type and associated fuel types.

- **Initial Content**: The flag to indicate how initial content of fuel will be entered. The NFCSS can calculate initial fuel content from the given enrichment or fissile content or the user can provide the table for initial content for each year. In later case, the initial content table should be provided in 'Isotopic Composition' page.
- **Depletion**: The flag to indicate how isotopic composition of spent fuel during discharge will be entered. The NFCSS can calculate it if it has cross section library for

the fuel or the user can provide the table for isotopic composition for each year. For the latter case, the initial content table should be provided in 'Isotopic Composition' page.

- **Decay**: The flag to indicate how isotopic composition of spent fuel after cooling will be entered. NFCSS can calculate it if it has half-lives for the fuel or the user can provide the table for isotopic composition for each year. For the latter case, the initial content table should be provided in 'Isotopic Composition' page.

The commands  in Fig.II-6 are used, respectively, to cancel all last edits and reset the form, to cancel editing and close reactor type edit mode, and to save the last edits.

II-4.7. Editing scenario parameters data (Scenario Data Page)

The command  in Fig.II-5 is used to edit the scenario parameters data for each the reactor types and associated fuel types. Figure II-7 is displayed when the user selects editing scenario parameters data.

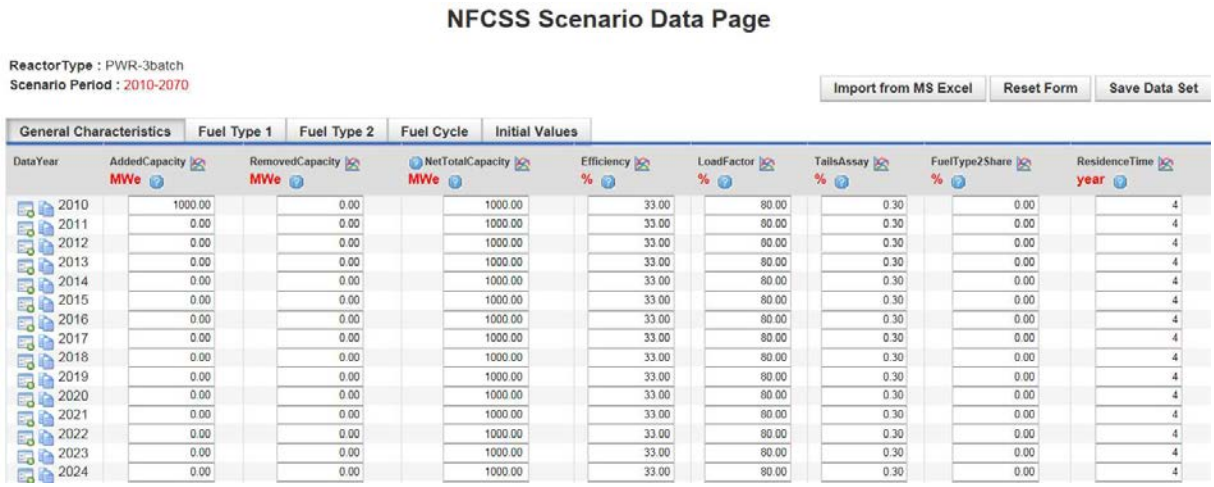


FIG.II-7. Scenario Data page.

The scenario data page consists of several parts: There are five different tab pages for 'General Characteristics', 'Fuel Type 1', 'Fuel Type 2', 'Fuel Cycle' and 'Initial Values' (Fig.II-7).

When a new reactor type is added to the scenario, records for scenario parameter data are also created with "0.0" values in each of the scenario parameter. The user can later edit the data records to complete the scenario. The easiest data entry is done through Microsoft Excel since Microsoft Excel is known to many computer users already and it provides easy editing features in tabular form. In this case, the data can be prepared in Microsoft Excel and then imported into NFCSS using **Import from MS Excel** button.

For this the data has to be prepared in the same column structure in Microsoft Excel. The option to exporting data was explained earlier. The exported data can be used to prepare new data set or to modify existing ones and can be imported back to the NFCSS. The other way to enter data is to use the NFCSS for the entire exercise and there is a practical way in the NFCSS to enter data. In most cases, the data for several parameters is constant for the scenario period. The NFCSS can utilize this option by providing easy data preparation tool.

For any year (each row in the table represents a year in the NFCSS scenario since the NFCSS makes calculations annually) the data can be entered by selecting a predefined reactor type from the reactor list. In order to do this, button from Data Year column (leftmost column in the table) can be used. After confirmation, Reactor Type Selection Page will be displayed (Fig.II-8). The left part of the page shows the list of reactor types available to the user and the right part of the page shows the details of the active reactor type. The active reactor type can be changed by clicking on the reactor type name (2nd column in the Fig.II-8).

The active page will always be displayed in different background colour in the list. If the active reactor type is selected as base data, button in the Command column of the list should be used. After clicking on the button, the data from selected reactor type will be copied to the given year.

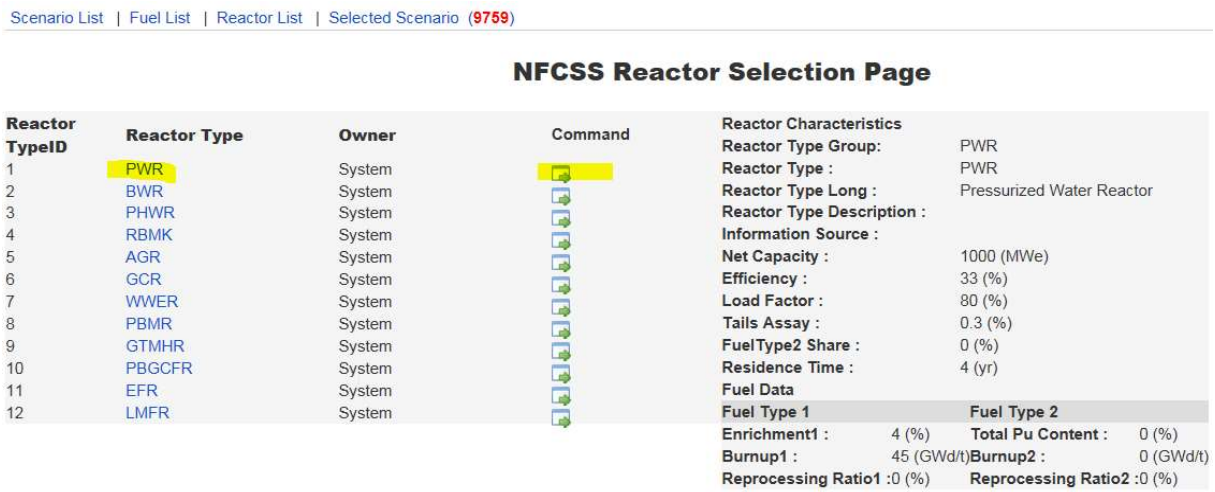


FIG.II-8. Reactor type selection page.

If the user wants to enter the data manually for any year, it can be done in the table directly. After entering the data manually, it should be saved using **Save Data Set** button each time before executing any other command. There is another easy tool for the users to enter data to the NFCSS. If the scenario data is not changed for the whole scenario period or part of it, there is a command to copy the data from any year to the rest of the scenario period. For this, the user should click button in the leftmost column of the data page (Fig.II-7). This button automatically generates data for every year of the scenario period after the selected year.

There is only one thing to do later. Since the 'Added Capacity' and 'Removed Capacity' are used to calculate 'Net Total Capacity', the data for 'Added Capacity' and 'Removed Capacity' should be entered individually for each year of the scenario period later.

Saving data will re-calculate 'Net Total Capacity' each time.

Explanations of each field in this page (All parameters should be entered for the selected reactor type and the data should be calculated in annual average for a given year):

- **Added Capacity (MW(e)):** Net electric capacity added to the system.
- **Removed Capacity (MW(e)):** Net electric capacity removed from the system.

- **Net Total Capacity (MW(e)):** Total net electric capacity. This column is automatically calculated by the system using the data given for initial power, added and removed capacity.
- **Thermal Efficiency (%):** The ratio of net electric capacity to the total thermal energy produced in the reactor.
- **Load Factor (%):** The ratio of the net electricity produced in the plant to the maximum producible net electricity in the plant for the whole year.
- **Enrichment Tails Assay (%):** The amount of U-235 in depleted uranium from the enrichment process.
- **Fuel Type 2 Share (%):** The average ratio of the amount of second fuel type to the total fuel for the reactor type. Fuel type 2 is MOX fuel for the most of the existing reactor types, if any.
- **Residence Time (year):** The time duration that each of the equilibrium loading fuels must stay in the reactor. In reality, multi-batch fuel management schemes are used in reactors and a fraction of core refuelled. If n is the number of fuel batches, the fraction of core refuelled is 1/n. If the operating cycle length is T_c then the residence time to be used in the NFCSS is equal to (nT_c) (closest integer must be given to the NFCSS). The NFCSS calculates annual average loading or discharge instead of actual loading of every operating cycle.
- **Discharge Burnup (GW·d/t-HM):** The average discharge burnup of the spent fuel at the discharge point for each of the fuel type.
- **Enrichment (%):** Initial fissile U-235 in Uranium fuel or Initial Total Pu content in MOX fuel for each of the fuel type.
- **Reprocessing Ratio (%):** The ratio of amount of spent fuel to be reprocessed to the amount of total discharged spent fuel. Some portion of the spent fuel is delivered to cooling pool for reprocessing and the rest is delivered to interim storage facilities. The reprocessing ratio defines the amount of spent fuel which is sent to the cooling pool for reprocessing for given year and not the amount of reprocessed spent fuel for the given year.
- **Capacities of fuel cycle facilities (t-HM or SWU):** The alternative running mode of the NFCSS is 'Capacity Driven Mode' which will be implemented in the future requires the capacities of each fuel cycle facility. Only reprocessing facility capacities have been implemented so far.
- **Reprocessing Capacity (t-HM):** The maximum amount of reprocessing which can be performed in given year.
- **Initial Reactor Power (MW(e)):** Total net electric capacity of selected reactor type at the beginning of the scenario period. The reactor is assumed to be running in equilibrium mode at the beginning of the scenario period. This data should be supplied in the initial data section and it is not part of data import from Microsoft Excel.
- **Initial Reprocessed Pu Stock (t-HM):** The total amount of Reprocessed Pu which is available for recycling at the beginning of scenario period.
- **Initial SF Stock (t-HM):** The total amount of spent fuel (for each fuel type) which is ready for reprocessing at the beginning of the scenario period.

II-4.8. Considerations for Scenario Parameters Data

While specifying parameters for different reactor types, consistent data set should be entered. For this, the following considerations should be in order:

(a) Enrichment and Burnup relations can be derived depending on reactor types.
For PWR, the discharge burnup and enrichment relation is

Bd = 12.9xε −10.0 for 3-batch core

Bd = 13.7xε -10.02 for 4-batch core

Here ε is defined as enrichment and Bd is defined as discharge burnup.

For PHWR

Bd = 22.26xε - 6.830

where ε is enrichment level of fuel in percent, Bd is the discharge burnup (GW·d/t-HM);

(b) Enrichment of Fuel Type 2 to Enrichment of Fuel Type 1 relation can be derived by keeping equal fissile content in each fuel type. For example, if the enrichment of fuel type is 4 %, it is equivalent to 4% fissile. The fissile content of the second fuel type will be the same if same discharge burnup level is used. So, if the fissile content in Pu in MOX fuel is about 60%, then the total Pu content in the MOX fuel should be at least 6.66 %;

(c) Specific power of fuel and discharge burnup relation: Specific power is entered in the fuel type information. The specific power is defined as the power produced in unit amount of fuel. Specific power is only used to calculate the irradiation period of the fuel and that is used to calculate isotopic composition of the spent fuel after irradiation. However, consistent discharge burnup, residence time and specific power need to be entered in order to keep the accuracy higher. The relation between those three is defined as $SP = B_d / RT$;

(d) Fuel type should be consistent with the burnup;

(e) First Core Loading Requirements:
To define initial fuel loading requirements, initial core enrichment ratio needs to be specified depending on fuel cycle scenarios and target burnup for initial core. In real practice, different reactors apply different enrichment levels for initial core loading. For instance,

- TURKEY POINT-PWR-2200 MW(th) 3.1, 2.55, 1.85 w/o enriched fuels,
- INDIAN POINT #2-PWR-2758 MW(th) 3.2, 2.7, 2.2 w/o enriched fuels,
- GINNA PWR 1300-MW(th) 3.48, 2.78, 2.44 w/o enriched fuels,
- AP-1000 (PWR) 3415 MW(th) 2.35–4.45 w/o eq. 4.8 w/o.

To define initial core enrichment ratio, the following procedure is suggested:

- Assume number of batches is n (in the NFCSS this is residence time since each batch is assumed one year), enrichment of reload fuel at equilibrium core is ε_{eq}, enrichment of discharged fuel at the end of cycle is ε_d;
- Since enrichment (fissile material weight percent) decreases linearly as a function of burnup, the following model might help define equilibrium composition of fuel batches at the end of each cycle and use the equilibrium cycle results to define initial core requirements. That is, the core average enrichment in initial core is

$$\varepsilon_{initial-core-ave} = \frac{\left((n+1)\varepsilon_{eq} + (n-1)\varepsilon_{d}\right)}{2n}$$

For PWRs, let us assume that n = 3, ε_d= 1.5 w/o and ε_{eq} = 3.2 w/o. Then,

$\varepsilon_{initial\text{-}core\text{-}ave}$ = 2.5 w/o.

II-5. CALCULATIONS AND RESULTS

The last tab page in Scenario Page is the Calculations and Results page (Fig.II-4). This tab page is used to make all calculations in the NFCSS and then see the results (Fig.II-9).

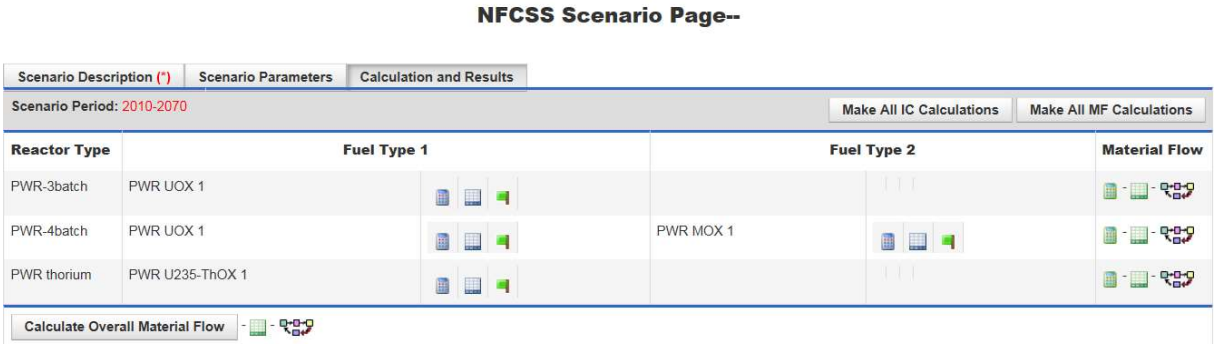


FIG.II-9. Calculation and Results tab page in Scenario page.

Calculations and Results tab page displays the list of each reactor type and associated fuel types (Fig.II.9). The calculations should be performed in the correct order in order to get the appropriate results. The correct order of the calculations is:

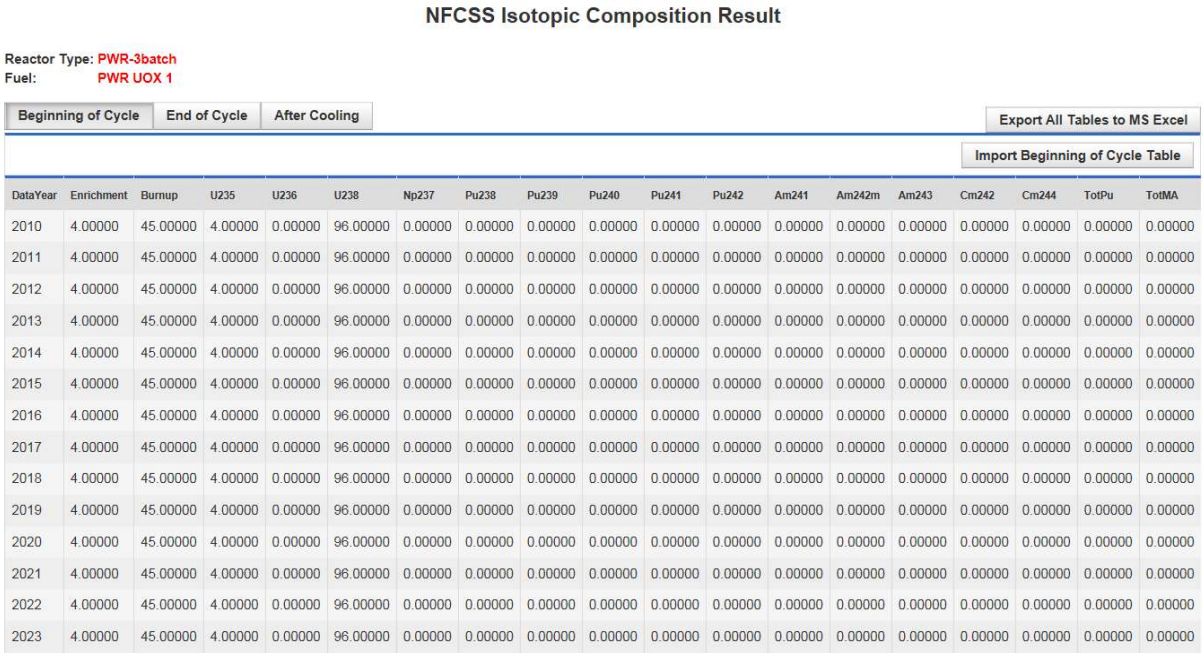
(a) Isotopic composition calculations for each fuel type in each reactor type;
(b) Material flow calculations for each reactor type;
(c) Overall material flow calculations.

II-5.1. Isotopic composition calculation (Scenario Page)

In order to start the NFCSS calculations, the user first needs to make sure that isotopic compositions of initial fresh fuel, spent fuel at discharge time and spent fuel after a cooling period. The compositions could be provided as tables or could be calculated by the NFCSS depending on the selected options in definition of fuel types.

In order to perform isotopic composition calculations, initial composition of fresh fuel and other fuel parameters have to be provided. If all data is correctly entered for a fuel type, button is used to perform isotopic composition of spent fuel. The calculation may take several seconds depending on the length or scenario period. The button is available for each of the fuel types for each of the reactor types. The button is used to see the result of isotopic composition calculation for each fuel type.

If the isotopic composition is to be provided by the user, button is again used. When the user clicks on button, isotopic composition page is displayed (Fig.II-10).



DataYear	Enrichment	Burnup	U235	U236	U238	Np237	Pu238	Pu239	Pu240	Pu241	Pu242	Am241	Am242m	Am243	Cm242	Cm244	TotPu	TotMA
2010	4.00000	45.00000	4.00000	0.00000	96.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2011	4.00000	45.00000	4.00000	0.00000	96.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2012	4.00000	45.00000	4.00000	0.00000	96.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2013	4.00000	45.00000	4.00000	0.00000	96.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2014	4.00000	45.00000	4.00000	0.00000	96.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2015	4.00000	45.00000	4.00000	0.00000	96.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2016	4.00000	45.00000	4.00000	0.00000	96.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2017	4.00000	45.00000	4.00000	0.00000	96.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2018	4.00000	45.00000	4.00000	0.00000	96.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2019	4.00000	45.00000	4.00000	0.00000	96.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2020	4.00000	45.00000	4.00000	0.00000	96.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2021	4.00000	45.00000	4.00000	0.00000	96.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2022	4.00000	45.00000	4.00000	0.00000	96.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2023	4.00000	45.00000	4.00000	0.00000	96.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

FIG.II-10. Isotopic Composition page.

This page has three tab-pages for each of the cycle positions: 'Beginning of Cycle', 'End of Cycle' and 'After Cooling'. The page has also **Import Beginning of Cycle Table** and similar buttons to import isotopic composition from MS Excel. **Export All Tables to MS Excel** button is to export isotopic compositions to MS Excel.

In order to import the table from MS Excel, the same column structure (order of the columns and number of columns are important) has to be prepared in MS Excel. Then the data should be selected together with the header row and copied into clipboard (Ctrl-C makes it in MS Excel). After having the data in Clipboard, button is used to import data from MS Excel to the NFCSS. Similarly, button can be used to export data from NFCSS to MS Excel.

The lower part of the isotopic composition page displays the data for each year and each isotope (and some isotope groups).

II-5.2. Material flow calculations for each reactor type (Scenario Page)

After completing isotopic composition calculations or providing the isotopic compositions, the user can make material flow calculations for each of the reactor types. Figure II-11 shows the command bar for the material flow calculations, where the 1st button is used to perform material flow calculations for the selected reactor type, the second button is used to see the material flow result in table form and the last button is used to see the material flow result in diagram form. If the isotopic compositions are not ready for any reactor type, the command bar will display a warning message.

When the user clicks on button the NFCSS starts material flow calculations. The calculation is completed usually in less than a minute depending on the length of scenario period. During the calculations the NFCSS displays a wait message on the screen. After completing the calculations, the NFCSS returns to the Calculations and Results tab page.

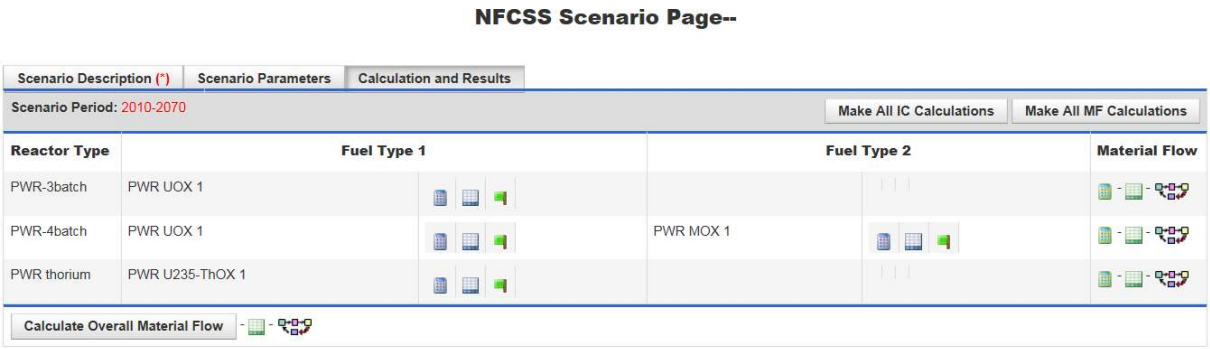


FIG.II-11. Calculation and Result tab page showing material flow buttons.

Following the calculation, the user can see the results. The results can be displayed in two different formats: tabular and diagrammatic. When the user clicks button, material flow result page is displayed for the selected reactor type (Fig.II-12). This page consists of four tab-pages: 'General', 'Front End', 'Back End' and 'Nuclide Group' tab pages provide the different results from the material flow calculation. The table displays the pre-selected result columns from the NFCSS full result table. The selection of columns by the users will be implemented in future.

NFCSS Nuclear Material Flow Result

Reactor Type :PWR-3batch

General | Front End | Back End | Nuclide Groups

Year	TypeCapacity (MWe)	Electricity (GWh)	F2Share (%)	Enri_1 (%)	Bu_1 (GWd/t)	Rep_1 (%)	Enri_2 (%)	Bu_2 (GWd/t)	Rep_2 (%)
2010	1000	7008	0.000	4.000	45.00	0.000	0.000	0.00	0.000
2011	1000	7008	0.000	4.000	45.00	0.000	0.000	0.00	0.000
2012	1000	7008	0.000	4.000	45.00	0.000	0.000	0.00	0.000
2013	1000	7008	0.000	4.000	45.00	0.000	0.000	0.00	0.000
2014	1000	7008	0.000	4.000	45.00	0.000	0.000	0.00	0.000
2015	1000	7008	0.000	4.000	45.00	0.000	0.000	0.00	0.000
2016	1000	7008	0.000	4.000	45.00	0.000	0.000	0.00	0.000
2017	1000	7008	0.000	4.000	45.00	0.000	0.000	0.00	0.000
2018	1000	7008	0.000	4.000	45.00	0.000	0.000	0.00	0.000
2019	1000	7008	0.000	4.000	45.00	0.000	0.000	0.00	0.000
2020	1000	7008	0.000	4.000	45.00	0.000	0.000	0.00	0.000
2021	1000	7008	0.000	4.000	45.00	0.000	0.000	0.00	0.000
2022	1000	7008	0.000	4.000	45.00	0.000	0.000	0.00	0.000
2023	1000	7008	0.000	4.000	45.00	0.000	0.000	0.00	0.000

FIG.II-12. Material Flow Result page in table form.

The user can see the graph for each of the result column by clicking on button in each column heading of Fig.II-12. The chart form is shown in Fig.II-13.

The user can see calculation results of material flow in diagram by clicking on button in Fig.II-11. The result is shown in Fig.II-14. The user can get the chart for results of each of the fuel cycle steps by clicking on the box of steps. The mouse cursor will automatically change when the mouse comes over a chartable parameter in the diagram.

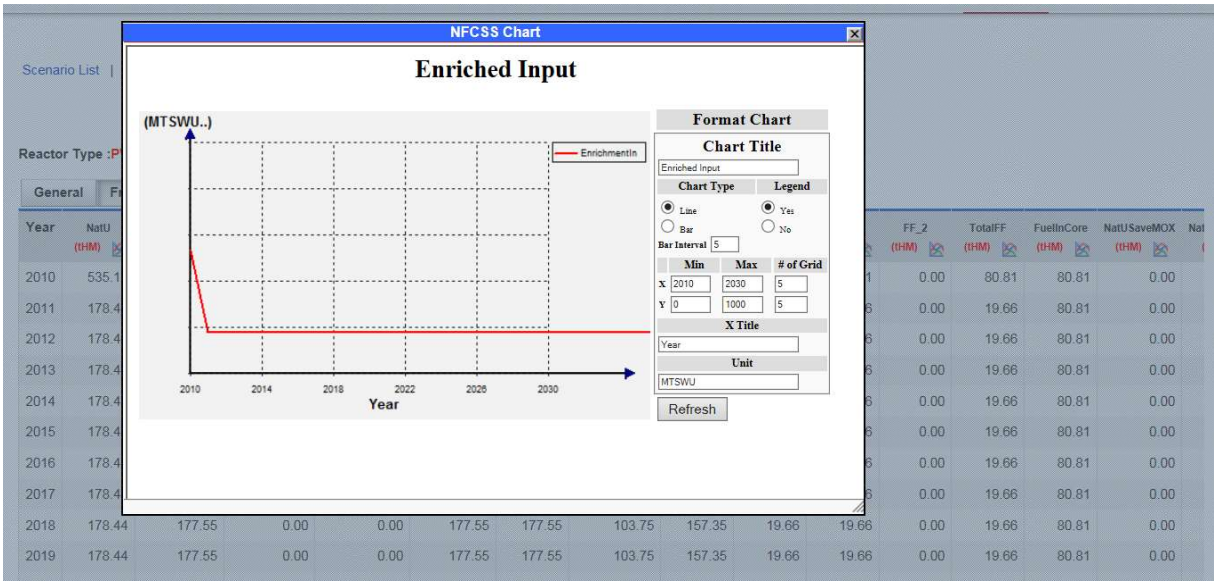


FIG.II-13. Example result in chart.

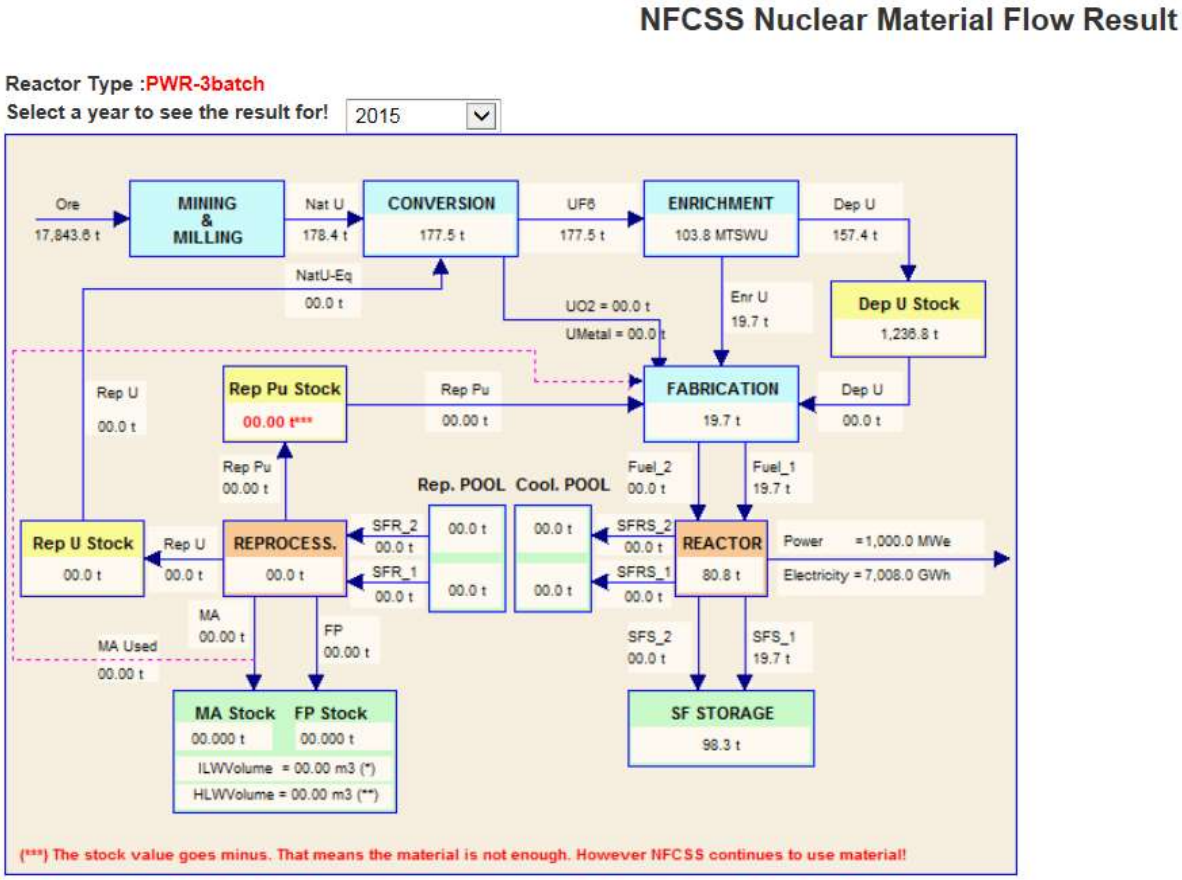


FIG.II-14. Material Flow Result in flow diagram form for a specific year.

The NFCSS calculates and displays below outputs (and more) in addition to the summary of some input parameters for selected reactor type for each year:

- **Nuclear Capacity:** The total net electric capacity;
- **Electricity:** The total electricity amount generated in the power plant;
- **Natural Uranium Requirement:** The amount of natural uranium required to manufacture necessary fresh fuel;
- **Conversion Requirement:** The amount of conversion service requirement. Conversion service requirement is calculated for the end product from the conversion facilities. For example, for conversion to UF_6 the only requirement for conversion to UF_6 is calculated and not conversion to UF_4 if it is done in a different facility;
- **Enrichment Service Requirement:** The amount of enrichment service requirements (SWU);
- **Depleted Uranium Arising:** The amount of depleted uranium arising from enrichment process;
- **Fuel Fabrication Requirements (for two fuel types):** The amount of fresh fuel requirement;
- **Total Fuel in Reactor Core:** The total amount of fuel loaded in the reactor core;
- **Natural Uranium Saving due to Use of MOX:** Saved amount of natural uranium resulting from MOX fuel use;
- **Natural Uranium Saving due to Use of reprocessed Uranium:** Saved amount of natural uranium resulting from reprocessed uranium use;
- **Spent Fuel Discharge (for two fuel types):** The amount of spent fuel discharged out of the reactor;
- **Spent Fuel Storage (for two fuel types):** The amount of spent fuel stored in interim spent fuel storage facilities;
- **Spent Fuel reprocessing (for two fuel types):** The amount of spent fuel reprocessed;
- **Separated Pu amount:** The amount of Plutonium separated from reprocessed spent fuel;
- **Used Pu in MOX fuel:** The amount of separated Plutonium used in MOX fuel;
- **Depleted Uranium Used in MOX fuel:** The amount of depleted uranium used in MOX fuel;
- **Separated U amount:** The amount of separated Uranium from reprocessed spent fuel;
- **MA amount in Reprocessing Waste:** The amount of Minor Actinides (Np, Am, Cm) in HLW from reprocessing process;
- **FP amount in Reprocessing Waste:** The amount of Fission Products in HLW from reprocessing process.

II-5.3. Overall material flow calculations

The material flow results of each reactor type can be combined using overall material flow calculations. **Calculate Overall Material Flow** button (Fig.II-11) is used to make overall material flow calculations. The result of the combination is displayed as table or diagram similar to the result for each reactor type.

All calculations can be done only by clicking. However, depending on the performance of the server at the time of user request, the programme operation may or may not be completed, in which case all calculations have to be individually performed.

II-6. WORKING WITH FUEL TYPES

One of the important features of the NFCSS simulation system is the CAIN module to calculate isotopic composition of spent fuel at discharge or after cooling. The description of the CAIN module is given in Annex III and Section 5. In order to make the isotopic composition calculations, the CAIN requires some parameters of the fuel as inputs. These are mainly initial content of the fuel, the specific power of the fuel, burnup average one group-neutron cross sections and an initial guess of burnup average neutron flux. All these parameters form the fuel type information. The NFCSS has a built-in fuel type library which includes a number of typical fuel types for the existing and planned reactor types.

II-6.1. Fuel Type List

The users can access the available fuel type list by selecting Fuel List link from the NFCSS breadcrumb (Fig.II-15).

FIG.II-15. Fuel List in NFCSS breadcrumb.

This gives the list of fuel types which are available to the user. The list will show the fuel types from the NFCSS built-in library and the user's own fuel types. Fuel types entered by other users will not be displayed in this list.

The fuel list page is shown in Fig.II-16. The list shows the names of each fuel type and the owner. Clicking on the fuel type name displays the fuel data page for the selected fuel type.

List of available fuels for User : Ki Seob SIM

Create New Fuel

Fuel ID	Fuel Type	Owner	Command
1	PWR UOX 1	System	
2	PWR MOX 1	System	
3	PWR UOX 2	System	
4	PWR UOX 3	System	
5	BWR UOX 1	System	
6	BWR MOX 1	System	
7	BWR UOX 2	System	
8	PHWR U 1	System	
9	PHWR U 2	System	
10	RBMK U 1	System	
11	AGR U 1	System	
12	GCR U 1	System	

FIG.II-16. The Fuel List page.

II-6.2. Adding a new fuel type

In addition to the selection of the fuel type from the built-in library of the NFCSS, the users can add their own fuel types to the fuel list. Fuel types added by the users will only be available to the creator of the specific fuel type.

Create New Fuel button is used to create a new fuel type and to add it to the library. The newly created fuel type will be displayed at the end of the list. The user then goes to the fuel data page to define the details of the new fuel type by clicking on the name of the new fuel type.

II-6.3. Copying existing fuel type

The users can copy one of the existing fuel types from the list to create a new fuel type. They can later revise the data for the newly created fuel type and use in their scenario. In order to copy the fuel type, button from the command column of the fuel list table should be used. After that a new fuel type will be added to the end of the list with "New Fuel" name and with the same data as copied fuel type.

II-6.4. Editing fuel type

Clicking on the name of the fuel type opens the fuel data page for the selected fuel type. The fuel data page is shown in Fig.II-17. The page has two parts: command part and data part. The data part consists of two tab-pages: 'Fuel Characteristics' and 'Cross Sections'. In the fuel characteristics tab page, fuel parameters such as specific power, reference enrichment etc. are entered. In the cross section tab page, fission, capture and (n,2n) cross sections are entered. After entering the data, the data needs to be saved by clicking on the **Save Fuel Data** button.

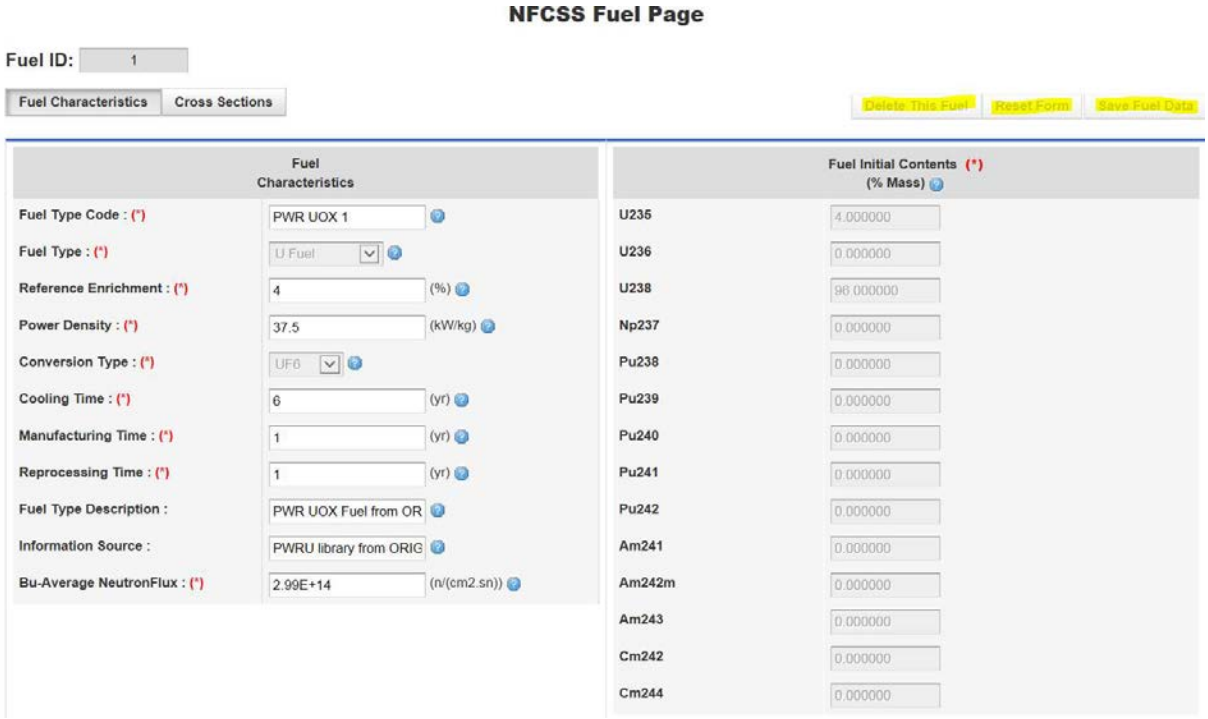


FIG.II-17. Fuel Data page.

If the user wants to delete one of their own fuel types, **Delete This Fuel** button should be used. The user can cancel the last edit any time and reset the data to the status on last save by clicking **Reset Form** button.

The description of the fuel parameters and possible options are described below:

- **Reference Enrichment (%):** Enrichment level of reference fuel from which the cross sections are calculated. This parameter has no effect on the NFCSS calculations;

- **Power Density (kW/kg):** Power density (or specific power) of the fuel. Power density is used to determine the irradiation period which is used in the CAIN module to calculate isotopic composition of spent fuel during the discharge time. It is also used to calculate the initial core loading requirements. This parameter must be consistent with Residence Time and Discharge Burnup data in the scenario data part;
- **Fuel Type Code:** A short code to represent the fuel type;
- **Fuel Type:** The type of the fuel. NFCSS has currently three types of fuel in its library;
- **U Fuel**, **U-Pu Fuel** and **Free Content:** The calculation of initial content is different for each fuel type. The details are given in Initial Content parameter below;
- **Conversion Type:** Type of conversion which is necessary to manufacture the fuel. There are three types of conversion. **UF6** is used for enriched fuel. **UO2** is typically used for PHWR fuels and **UMetal** is used for GCR fuels. For enriched uranium fuels, reconversion to UO_2 after enrichment is not considered as a conversion step. It is considered as internal part of fuel manufacturing;
- **Cooling Time (year):** Minimum time required for cooling before reprocessing the fuel;
- **Manufacturing Time (year):** Minimum time required for manufacturing the fuel;
- **Reprocessing Time(year):** Minimum time required for reprocessing the fuel;
- **Fuel Type Description:** Free text for description of the fuel type;
- **Information Source:** The reference where the fuel type information is received from;
- **Burnup Average Neutron Flux (n/cm^2/s):** Burnup average one group neutron flux.

NFCSS Fuel Page

Fuel ID: 1

Fuel Characteristics | Cross Sections

Delete This Fuel | Reset Form | Save Fuel

Nuclide	Bu-Average Fission Cross_Section (barn)	Bu-Average Capture Cross_Section (barn)	Bu-Average n2n Cross_Section (barn)
U235	46.71	10.46	0
U236	0.1975	7.541	0
U238	0.1004	0.9021	0.00553
Np237	0.5244	32.12	0
Pu238	2.465	34.67	0
Pu239	106.2	58.61	0
Pu240	0.584	104	0
Pu241	118.1	38.68	0
Pu242	0.4146	31.72	0
Am241	1.123	118.8	0
Am242m	466	98	0.00567
Am243	0.3959	49.487	0
Cm242	0.5591	5.801	0
Cm244	0.8746	13.82	0

FIG.II-18. Cross Sections part of Fuel Data page.

- **Fuel Initial Contents:** The table used to calculate the initial compositions of the fresh fuels.
  - If the fuel is **U Fuel** type, initial content has no meaning since the content will be calculated from the given enrichment level.
  - If the fuel is **U-Pu Fuel** the initial content must give the Pu vector which gives the contents of Pu isotopes in total Pu amount and the enrichment of uranium part of

the fuel. In this case the initial content will be calculated from given total Pu content.
    - If the fuel is **Free Content** the initial content must be entered as complete since the initial content of the fuel is not pre-defined.
- **Cross Sections (barn):** Burnup average one group fission, capture and [n2n] cross sections for each isotope in the fuel (Fig.I-18).

II-7. WORKING WITH REACTOR TYPES

The NFCSS has a built-in reactor library which includes a number of typical reactor types under operation, construction, and planning in different countries.

II-7.1. Reactor type list

Users can access the available reactor type list by selecting Reactor List link from the NFCSS breadcrumb (Fig.II-19).

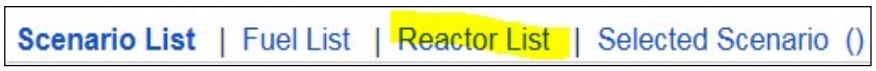


FIG.II-19. Reactor List in NFCSS breadcrumb.

This gives the list of reactor types available to the user. The list will show the reactor types from the the NFCSS built-in library and the user's own reactor types. Reactor types of other users will not be displayed in this list.

The fuel list page is shown in Fig.II-20. The list shows the names of each reactor type and the owner. Clicking on the reactor type name displays the reactor data page for the selected reactor type.

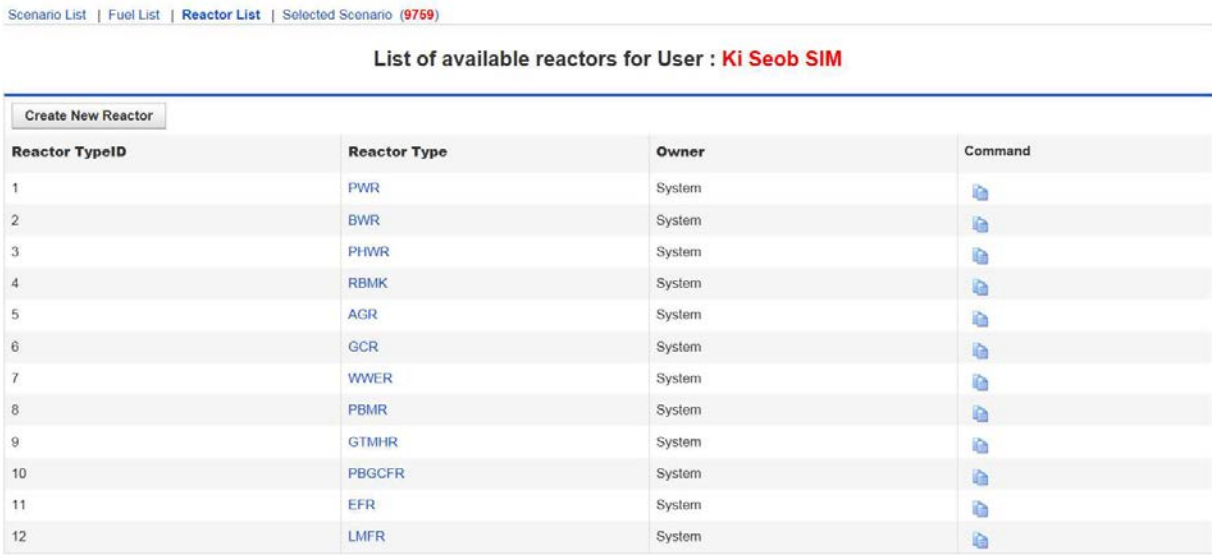


FIG.II-20. The Reactor List page.

II-7.2. Adding a new reactor type

In addition to the selection of the reactor type from the built-in library of the NFCSS, users can also add their own reactor types to the reactor list. Reactor types added by users will only be available to the creator of the specific reactor types.

Create New Reactor button is used to create a new reactor type and to add it to the library. The newly created reactor type will be displayed at the end of the list. The user then goes to the reactor data page to define the details of the new reactor type by clicking on the name of the new reactor type.

II-7.3. Copying existing reactor type

Users can copy one of the existing reactor types from the list to create a new reactor type. They can later revise the data for the newly created reactor type and use in their scenario. In order to copy the reactor type, button from the command column of the reactor list table should be used. After that a new reactor type will be added at the end of the list with 'New Reactor' name and with the same data as copied reactor type.

II-7.4. Editing reactor type

Clicking on the name of the reactor type opens the reactor data page for the selected reactor type. The reactor data page is shown in Fig.II-21. The page has two parts: command part and data part. After entering the data, the data should be saved by clicking on the **Save Reactor Data** button.

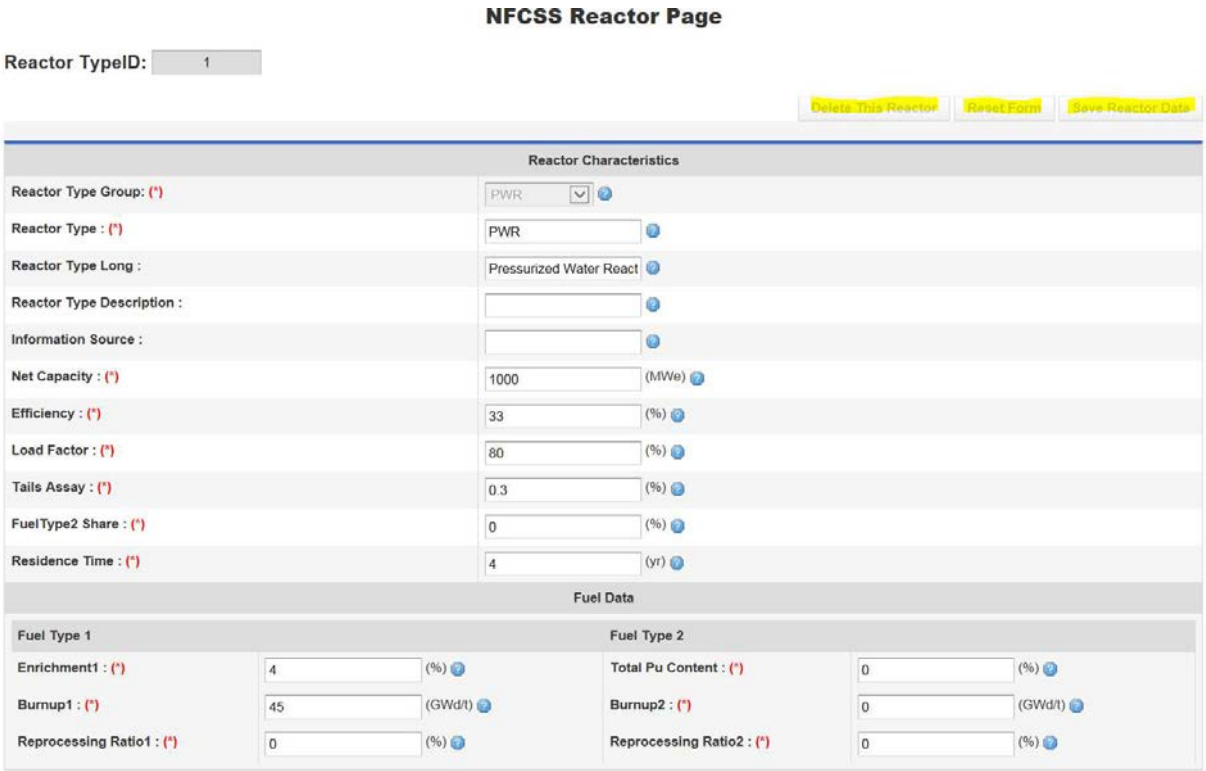


FIG.II-21. Reactor Data page.

If the user wants to delete one of owned reactor types, **Delete This Reactor** button should be used. The user can cancel the last edit any time and reset the data to the status on last save by clicking **Reset Form**.

The description of the fuel parameters is given in the input parameters description in Section 3.1.2.

II-8. INITIAL CORE LOADING AND FINAL CORE DISCHARGE

The NFCSS is a simulation system which tries to represent the travel of nuclear material in the real world. In order to do that, like in every other simulation systems, there are assumptions to enable simulation models to run. One of the assumptions of the NFCSS model was about initial core loading and the final core discharge.

In NFCSS's previous status, initial core loading for a new power added to the reactor type (basically adding a new reactor to the electricity grid) had been calculated using the Residence Time parameter which is given in scenario input parameters in whole years (etc. 4 years, 5 years). This has an effect in the resulting initial core loading depending on how the actual residence time differs from the whole integer. For example, if the real residence time is 4.65 years then we should enter Residence Time as 5 (nearest integer).

In real operation of a nuclear power plant, loading and unloading of the fuels performed according to scheme which is given in Fig.II-22. Upper part of the figure shows the fuel types in the reactor core (initial core fuel or equilibrium core fuel) for whole life of the reactor. Cycle (1) is initial loading and Cycle (n) is the final discharge. Middle part shows the loadings to the reactor at every cycle. In the first cycle, only initial core fuel type is loaded into the reactor. In the following cycles, equilibrium fuel type is loaded. The lower part of the figure shows the discharges from the reactor. In the first cycle there is no discharge from the reactor. In the following cycles, first initial core fuel type is discharged and then equilibrium fuel type is discharged. In the final cycle full core containing equilibrium fuel is discharged from the reactor.

The NFCSS model has been modified to reflect the real situation of refuelling scheme of the reactors. The NFCSS first calculates the material flow and then calculates the composition in each stage (beginning of cycle and end of cycle stages).

The NFCSS calculations are based on annual estimations, not cycle-wise estimations, so that the initial core loading and final core discharge must be estimated different than the equilibrium loading and discharge. Initial core loading is calculated using the Irradiation Time which is defined as the full-power irradiation time in the reactor. The equations used for calculating loadings are:

$$\textit{Irradiation Time (yr)} = \textit{Burnup (yr)} \times 1000 / (\textit{Power density (yr)} \times 365)$$

$$\textit{Initial Core Loading (yr)} = \textit{Irradiation Time (yr)} \times \textit{Added Capacity (yr)} \times 365 / (\textit{Thermal Efficiency (yr)} \times \textit{Burnup (yr)} \times 1000)$$

$$\textit{Equilibrium Core Loading (yr)} = \textit{Load Factor (yr)} \times \textit{Existing Capacity (yr)} \times 365 / (\textit{Thermal Efficiency (yr)} \times \textit{Burnup (yr)} \times 1000)$$

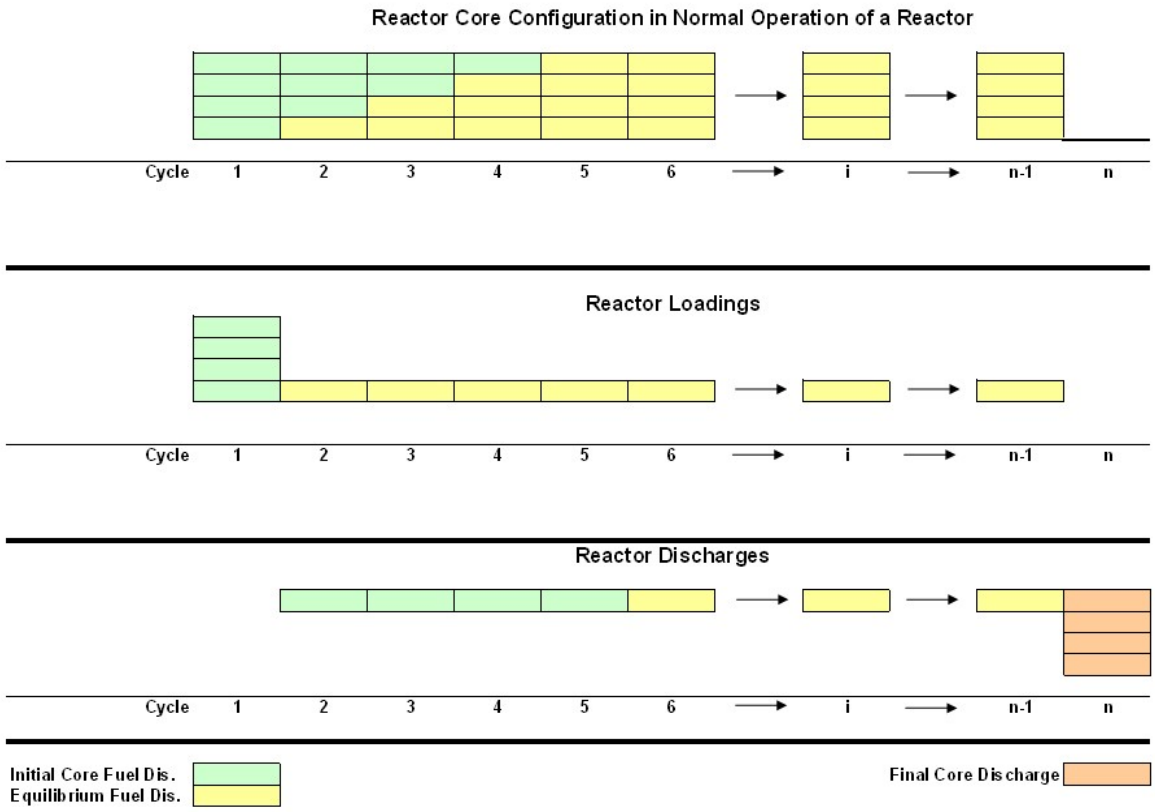


FIG.II-22. Schematic illustration of loadings in and discharges from the reactor.

The discharges are calculated using below formula:

$$\textit{Equilibrium Core Discharge (t)} = \textit{Existing Capacity (yr)} \times (\textit{Load Factor (yr)} - \textit{Residency Time (yr)}) \times 365 / [(\textit{Thermal Efficiency (yr)} - \textit{Residence Time (yr)}) \times (\textit{Burnup (yr)} - \textit{Residence Time (yr)}) \times 1000]$$

$$\textit{Final Core Discharge (t)} = \textit{Removed Capacity (yr)} \times \textit{Total Fuel In Core (yr-1)} / \textit{Total Capacity (yr-1)}$$

Units are:

Burnup:	MW·d/kgU,
Power Density:	kW/kg,
Irradiation Time:	year,
Capacity:	MW(e),
Loading Discharge:	tonnes,
Residence Time:	year.

One assumption is made in this calculation. Although we load the fuel into the reactor in its every operation cycle in real life, we assume that the fuel is loaded and discharged every year. Since we are using Irradiation Time parameter in initial core loading and final core discharge calculations, annual loading is not exactly the same as full core amount divided by Residence Time defined by integer number mentioned previously.

Another important assumption is made in the calculation of isotopic composition of discharged fuel. Although the composition of initial core fuel is different than the equilibrium fuel, we assume that the composition of the discharged fuel is the same in the initial core and the equilibrium core. Similarly, although the average burnup level of the final core discharge is usually lower than the equilibrium fuel, we assume the composition of the final core discharge is the same as the one of the discharged fuel in equilibrium core.

REFERENCES TO ANNEX II

[II-1] International Atomic Energy Agency, Nuclear Fuel Cycle Simulation System (VISTA), IAEA-TECDOC-1535, IAEA, Vienna (2007).

ANNEX III: BURNUP MODEL FOR UO_2 AND MOX FUEL CYCLES

III-1 GENERAL

This Annex describes the burnup model of the CAIN (Calculation of Actinide INventory) module in the NFCSS for UO_2 and MOX fuel cycles. It draws relevant information from TECDOC-1535 [III-1] and incorporates additional information on cross section data and its verification, relation between specific power and neutron flux, effect of operation mode, initial core loading and final core discharge, clarification on Am-241 cross section.

III-2 CAIN MODULE

The CAIN is a subprogram to calculate actinide inventory in the spent fuel. The module uses Bateman's equation, a one group neutron energy and cross sections based burnup solution for a point reactor [III-2]. Since the transmutation of all actinides starts from U-235 and U-238 for UO_2 fuels, initial enrichment and corresponding discharge burnup values are needed as input.

III-3 BATEMAN'S EQUATION AND ITS SOLUTION

A simplified diagram of nuclide transmutation is shown in Fig.III-1.

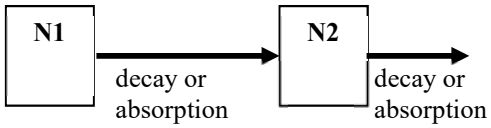


FIG.III-1. Simple diagram of nuclide transmutation.

Bateman's equation of nuclide-1 is given below:

$$dN_1/dt = -\lambda_1 N_1$$

If transmutation is caused by neutron absorption (capture + fission), this equation is modified as follows and assumes constant cross section and neutron flux throughout burnup:

$$dN_1/dt = -\sigma_1 \phi N_1$$

where,

N_1 : atomic concentration of nuclide-1,
λ_1 : decay constant of nuclide-1, 1/sec ($\lambda = 0.693/T_{1/2}$, where $T_{1/2}$ is half-life in sec),
σ_1 : absorption cross section of nuclide-1, 10^{-24} cm^2(=1barn),
ϕ : average neutron flux, n/cm^2/sec.

The solution of the Bateman's equation is given below:

$$N_1 = N_1^0 \cdot \exp(-\lambda_1 t)$$

or

$$N_1 = N_1^0 \cdot \exp(-\sigma_1 \phi t)$$

where,

N_1^0 : atomic concentration of nuclide-1 at time zero,
t : irradiation or cooling period (sec).

For nuclide-2 which transmutes only by decay, the equation is given as

$$dN_2/dt = -\lambda_2 N_2 + \lambda_1 N_1$$

If transmutation occurs only by neutron reaction, the equation is then

$$dN_2/dt = -\sigma_2 \phi N_2 + \sigma_1 \phi N_1$$

where,

σ_1 : Capture cross section of nuclide-1, 10^{-24} cm^2(=1barn). If nuclide-1 has a capture reaction and a fission reaction, N_1 decreases by both reactions but N_2 increases only by capture reaction of nuclide-1,
σ_2 : Absorption (capture + fission) cross section of nuclide-2, 10^{-24} cm^2 (=1barn).

Here, the first term is annihilation of nuclide-2, and second term is generation of nuclide-2 from nuclide-1.

The solution of the above equation is as follows, using the initial condition if nuclide-2 does not exist at time zero;

$$N_2 = N_1^0 \cdot \lambda_1/(\lambda_2-\lambda_1) \cdot [\exp(-\lambda_1 t) - \exp(-\lambda_2 t)]$$

or

$$N_2 = N_1^0 \cdot \sigma_1/(\sigma_2-\sigma_1) \cdot [\exp(-\sigma_1 \phi t) - \exp(-\sigma_2 \phi t)]$$

If there exists nuclide-2 at time zero, the solution (N_2) is modified as follows;

$$N_2' = N_2 + N_2^0 \cdot \exp(-\lambda_2 t)$$

or

$$N_2' = N_2 + N_2^0 \cdot \exp(-\sigma_2 \phi t)$$

That is, the second term is added as decrease for the initial nuclide-2, and, N_2^0 is an atomic concentration of nuclide-2 at time zero.

The generic form of Bateman's equation is as follow:

$$\frac{dN_i}{dt} = -\sum_{j \neq i}\left[\lambda_{ji} + \sigma^{tr}_{ji}\varphi\right]N_i + \sum_{j \neq i}\left[\lambda_{ij} + \sigma^{tr}_{ij}\varphi\right]N_j$$

where,

N_i : atomic content of nuclide-i,
N_j : atomic content of nuclide-j,
λ_{ji} : decay constant from nuclide-i to nuclide-j, 1/sec,
λ_{ij} : decay constant from nuclide-j to nuclide-i, 1/sec,
σ^{tr}_{ji} : transmutation cross section from nuclide-i to nuclide-j, 10^{-24} cm^2(=1barn),
σ^{tr}_{ij} : transmutation cross section from nuclide-j to nuclide-i, 10^{-24} cm^2(=1barn),
ϕ : average neutron flux, n/cm^2/sec.

If cross sections and neutron flux are constant throughout the entire period, then the above Bateman's equation has an analytical solution, which is given below, with a diagram of nuclide transmutation in Fig.III-2. Here, it is assumed that only the first nuclide-1 exists and other nuclides do not exist at time zero. As explained above, if other nuclides exist at time zero, solution should be modified.

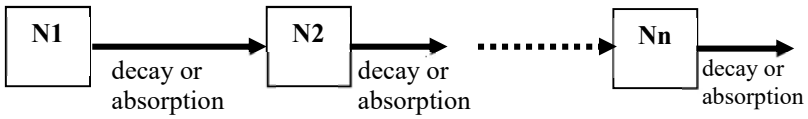


FIG.III-2. Generic diagram of nuclide transmutation.

$$N_n = C_1 \exp(-\lambda_1 t) + C_2 \exp(-\lambda_2 t) \cdots + C_n \exp(-\lambda_n t)$$

where;

$$C_1 = N_1^0 \cdot [\lambda_1\lambda_2 \cdots \lambda_{n-1}] / [(\lambda_2-\lambda_1)\cdot(\lambda_3-\lambda_1)\cdots(\lambda_n-\lambda_1)]$$
$$C_2 = N_1^0 \cdot [\lambda_1\lambda_2 \cdots \lambda_{n-1}] / [(\lambda_1-\lambda_2)\cdot(\lambda_3-\lambda_2)\cdots(\lambda_n-\lambda_2)]$$

As for the decrease by neutron absorption, the solution is give below:

$$N_n = C_1 \exp(-\sigma_1 \phi t) + C_2 \exp(-\sigma_2 \phi t) \cdots + C_n \exp(-\sigma_n \phi t)$$

where;

$$C_1 = N_1^0 \cdot [\sigma_1\sigma_2 \cdots \sigma_{n-1}] / [(\sigma_2-\sigma_1)\cdot(\sigma_3-\sigma_1)\cdots(\sigma_n-\sigma_1)]$$
$$C_2 = N_1^0 \cdot [\sigma_1\sigma_2 \cdots \sigma_{n-1}] / [(\sigma_1-\sigma_2)\cdot(\sigma_3-\sigma_2)\cdots(\sigma_n-\sigma_2)]$$

If there are two nuclides in the initial fuel, for example [U235+U238] fuel case, conversion from enrichment (WF235 in wt.%) to atomic fraction (AF235 in at%) is required as follows:

AF(U235) = [WF(U235) 235] / [235·WF(U235)+238·WF(U238)]·100
AF(U238) = [WF(U238) 238] / [235·WF(U235)+238·WF(U238)]·100

An example of using Bateman's equation to solve the chain starting from U-238 up to Pu-240 is shown below

$$^{238}U \rightarrow {}^{239}Pu \rightarrow {}^{240}Pu$$

$$AF_1 \cdots\cdots AF_2 \cdots\cdots AF_3$$

$$AF_1 = AF_1(initial) \cdot e^{(-\Sigma_{t1} \cdot \Phi \cdot T \cdot 10^{-24})}$$

$$AF_2 = AF_1(initial) \cdot \left[\left(\frac{\Sigma_{c1}}{\Sigma_{t2} - \Sigma_{t1}}\right) \cdot e^{(-\Sigma_{t1} \cdot \Phi \cdot T \cdot 10^{-24})} + \left(\frac{\Sigma_{c1}}{\Sigma_{t1} - \Sigma_{t2}}\right) \cdot e^{(-\Sigma_{t2} \cdot \Phi \cdot T \cdot 10^{-24})} \right]$$

$$AF_3 = AF_1(initial) \cdot \left[\begin{array}{l} \left(\frac{\Sigma_{c1} \cdot \Sigma_{c2}}{(\Sigma_{t2} - \Sigma_{t1}) \cdot (\Sigma_{t3} - \Sigma_{t1})}\right) \cdot e^{(-\Sigma_{t1} \cdot \Phi \cdot T \cdot 10^{-24})} \\ + \left(\frac{\Sigma_{c1} \cdot \Sigma_{c2}}{(\Sigma_{t3} - \Sigma_{t2}) \cdot (\Sigma_{t1} - \Sigma_{t2})}\right) \cdot e^{(-\Sigma_{t2} \cdot \Phi \cdot T \cdot 10^{-24})} \\ + \left(\frac{\Sigma_{c1} \cdot \Sigma_{c2}}{(\Sigma_{t1} - \Sigma_{t3}) \cdot (\Sigma_{t2} - \Sigma_{t3})}\right) \cdot e^{(-\Sigma_{t3} \cdot \Phi \cdot T \cdot 10^{-24})} \end{array} \right]$$

where

AF_i = Atomic content of nuclide(i) in the chain.

Σ_c = Capture cross section, 10^{-24} cm^2 (=1barn)

Σ_f = Fission cross section, 10^{-24} cm^2 (=1barn)

Σ_{n2n} = (n,2n) cross section, 10^{-24} cm^2 (=1barn)

Σ_{ex} = Excited cross section, 10^{-24} cm^2 (=1barn)

Σ_t = Total cross section (barns)

$$\Sigma_{decay} = \frac{0.693}{T_{1/2} \cdot 365 \cdot 24 \cdot 3600 \cdot 10^{-24} \cdot \Phi}$$

$$\Sigma_t = \Sigma_c + \Sigma_f + \Sigma_{ex} + \Sigma_{decay}$$

$T_{1/2}$ = Half-life (years)

Φ = Average flux (n/cm^2/sec), (0 to 10MeV total flux)

T = Irradiation time (sec)

$$T = \frac{E_d \cdot 1000 \cdot 24 \cdot 3600}{KWKG}$$

E_d = Discharge burnup (GW·d/t)

$KWKG$ = Specific power (kW/kg or MW/ton)

At the end of calculation for Bateman's equation, the atomic fraction should be converted to the weight fraction of the initial fuel weight.

$$WF(i) = [AF(i)\ Mass(i)]/[235 \cdot AF(U235)+238 \cdot AF(U238)] \cdot 100$$

where,

Mass(i): Atomic Mass of nuclide(i).

III-4 ASSUMPTIONS IN CAIN

This section describes CAIN assumptions for UO_2 and MOX fuel cycles, and the summary is shown below. The errors due to these assumptions are small and explained in the reference [III-1]. As for the specific assumptions for Th fuel cycle, they are described in Section 5.1.7.

(a) Normally U-235 and U-238 are considered as the initial nuclides in the fresh uranium fuel, and the descending nuclides are analytically calculated using Bateman's equation. Although natural uranium includes U-234 (<0.01%), this nuclide can be ignored because the transmutation from U-234 to U-235 is small. But, U-234 can be also included as initial nuclides in the CAIN;

(b) The existing chains are selected to be suitable for fresh fuels containing any of the following 18 nuclides for UO_2, MOX and Th fuels: Th-232, Pa-233, U-233, U-234, U-235, U-236, U-238, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Np-237, Am-241, Am-242m, Am-243, Cm-242 and Cm-244;

(c) CAIN adopts analytical solution of the Bateman's equation, and assumes that both cross sections and neutron flux are constant throughout the burnup period;

(d) Short life nuclides (half-life < 8 day) are skipped. That is, Th-233 (22.3 min.), Pa-234 (1.17m/6.69h), U-237 (7 day), Np-238 (2 day), Pu-243 (5 hr), Am-242 (16 hr), Am-244 (10 hr) and Am-244 (26 min) are assumed to decay and go to next nuclide simultaneously;

(e) On the other hand, long life nuclides (with half-life > 400 years) are assumed as stable through the irradiation period. For example, Am-241 (432 years) is treated as stable. Other nuclides such as Th-232, U-233, U-234, U-235, U-236 and Np-237 are also treated as stable. But, for decay (cooling) period after discharge, all nuclides are treated by their actual decay scheme;

(f) Based on the above two assumptions, decays of Pa-233 (27.0 day), Pu-238 (87.7 year), Pu-241 (14.4 year), Cm-242 (0.447 year) and Cm-244 (18.1 year) are considered during irradiation, among the above 18 nuclides;

(g) Transmutation is terminated for certain nuclides (shown as 'x'). For example, Pu-238 decreases by neutron capture, but the decrease of Pu-238 is not added to Pu-239. This to terminate the calculations of Bateman's equation after nonconverging terms in the decay chain. Because the contribution due to these transmutations is very small, this assumption is reasonable and simplifies the calculations.

Based on the above assumptions, the full transmutation chain shown in Fig.III-3 is simplified to Fig.III-4. The 14 nuclides are calculated in the CAIN model for UO_2 and MOX fuels based on the chains shown in Fig.III-4.

This simplified chain has been implemented in the CAIN to calculate isotopic composition of spent fuel within the irradiation period and the cooling or storage period.

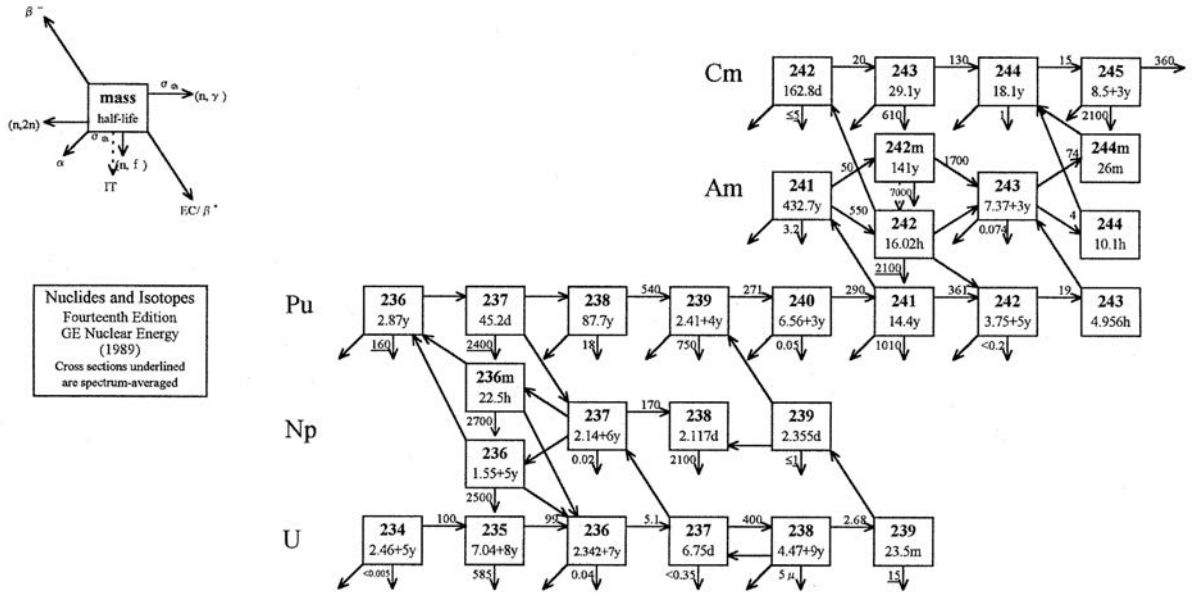


FIG.III-3. Actinide transmutation chains for UO_2 and MOX fuel (detail).

III-5 CROSS SECTIONS FOR UO_2 FUEL AND MOX FUEL

The CAIN module needs various inputs to evaluate the actinide inventory in the discharged fuel. They include cross sections and reactor constants such as specific power or neutron flux for 7 reactor types, which are PWR, BWR, PHWR, RBMK, AGR, GCR and WWER.

One group cross section data for 14 nuclides considered in CAIN are shown in p.59-63 of [III-1]. A user can also input and override these built-in cross section data. Also, if users can prepare the necessary inputs, examining other reactors such as FR or FBR are also possible.

PWR and BWR uranium fuel cross section data are identical to the ORIGEN2 library (PWR-UO_2-33G library, BWR-UO_2-27.5G library) [III-3]. PHWR uranium fuel cross section data are also identical to the ORIGEN2 library (CANDU-NatU library) [III-4]. RBMK uranium fuel cross sections were calculated by a Japanese consultant using a similar code to WIMS. AGR uranium fuel cross sections were calculated by a Canadian consultant using the WIMS code. GCR uranium fuel (0.71% enrichment) cross sections were linearly extrapolated by the above AGR cross sections of 1.6% and 2.6% enrichment at 0 to 4 GW·d/t range. WWER cross sections (both uranium fuel and MOX fuel) were calculated by the Russian consultant.

PWR and BWR MOX fuel cross sections are identical to ORIGEN2 library, that is PWR-PuPu library (211 library) for PWR-MOX, and BWR-PuPu library (258 library) for BWR-MOX) [III-3].

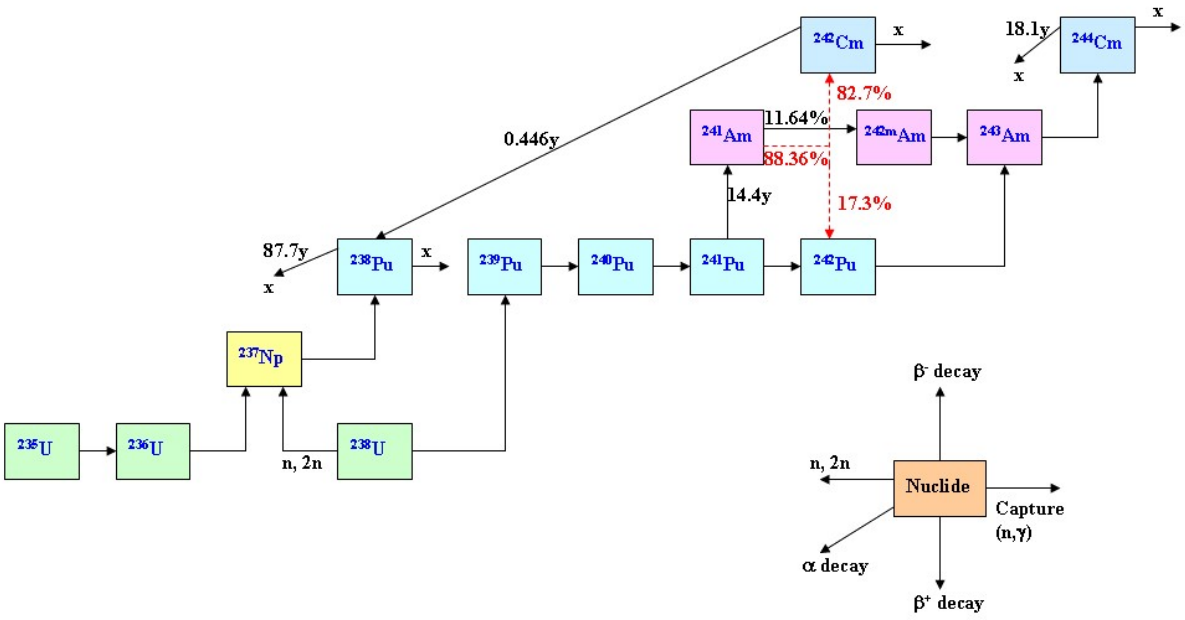


FIG. III-4. Simplified transmutation model in CAIN for UO_2 and MOX fuel.

III-6 OTHER CONSTANTS

Other constants, which the CAIN code requires, are the specific power and the neutron flux and so on. These are summarized in Table III-1.

The specific power (kW/kg or MW/ton) was calculated using the data from the Directory of Nuclear Power Plants in the World. It may vary across plants, so a typical plant was selected. PHWR data is derived from the old Pickering-A plant and may require an update. This constant is used to convert the discharge burnup to the irradiation time.

The neutron fluxes for PWR/BWR/PHWR are identical to the ORIGEN2 code. The neutron flux for RBMK was estimated using a similar code to WIMS by the Japanese consultant. The neutron fluxes for AGR/GCR are estimated to be proportional to kW/kg, using the proportional constant derived from PWR/BWR cases.

The neutron flux input is mandatory, but it is an initial guess, and the final neutron flux corresponding to specific power is calculated in NFCSS by the iterative procedure. This procedure and the reason why both specific power and neutron flux are required are described in Section III-8.

TABLE III-1 REACTOR CONSTANTS FOR CAIN

Reactor Type	*Specific Power (kW/kg)*	*Reference Neutron Flux ($n/cm^2/sec$)*	*Reference Enrichment (wt%)*
PWR	37.5	2.99×10^{14}	4.0
BWR	25.9	1.997×10^{14}	4.0
PHWR	18.8	1.85×10^{14}	0.71

Reactor Type	*Specific Power (kW/kg)*	*Reference Neutron Flux (n/cm²/sec)*	*Reference Enrichment (wt%)*
RBMK	15.75	1.48×10^{14}	1.8
AGR	10.9	8.75×10^{14}	2.6
GCR	3.33	2.66×10^{14}	0.71
WWER	45.8	3.747×10^{14}	4.36

One more constant is reference enrichment. Since single cross section set is applied for different enrichment fuels, actual neutron flux can be modified in CAIN using the following formula, which was derived from ORIGEN2 calculations for PWR and BWR fuels. This formula for PWR UO_2 fuel is shown in the following Fig.III-5**.**

$$\Phi(a) = \Phi(r) \times (ENR(r) / ENR(a) + 1) / 2$$

where,

φ(a): Actual neutron flux (n/cm^2/sec),
φ(r): Reference neutron flux (n/cm^2/sec),
ENR(a): Actual enrichment (wt.%),
ENR(r): Reference enrichment (wt.%).

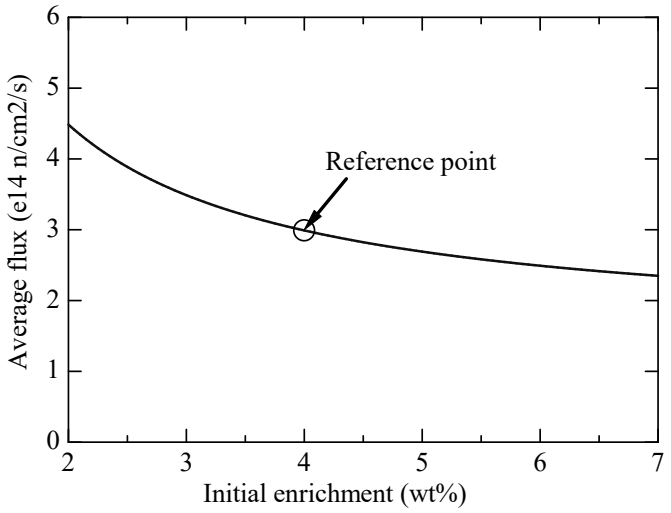


FIG.III-5. Average neutron flux vs. Initial enrichment for UO_2 fuel.

III-7 INITIAL ENRICHMENT AND DISCHARGE BURNUP

In the NFCSS, initial enrichment and discharge burnup are required as input data. Since these combined data are the output of reactor design codes and may not be available for NFCSS users. Therefore, the relation between initial enrichment and discharge burnup are provided in Fig.III-6.

Similar relation is used for MOX fuel in CAIN, as shown in Fig.III-7. Here, plutonium content is determined as follow:

As described in [III-1], the following formula is used in the NFCSS in order to estimate the initial plutonium content in fresh MOX fuel. This formula was proposed by a French consultant,

based on their experience. Plutonium content can be estimated by U-235 enrichment and its burnup value and this relation is shown in Fig.III-7.

$$\text{Initial Total Pu} = {}^{235}\text{U} \times (1.6 + 0.23 \times (\text{BU} - 33)/10)$$

Here, [^{235}U] is the initial ^{235}U enrichment in wt.%, and [BU] is the corresponding discharge burnup in GW·d/t. For example, 7.50% Pu-total content is assumed as equivalent to 4.00% enriched UO_2 fuel for 45 GW·d/t discharge burnup.

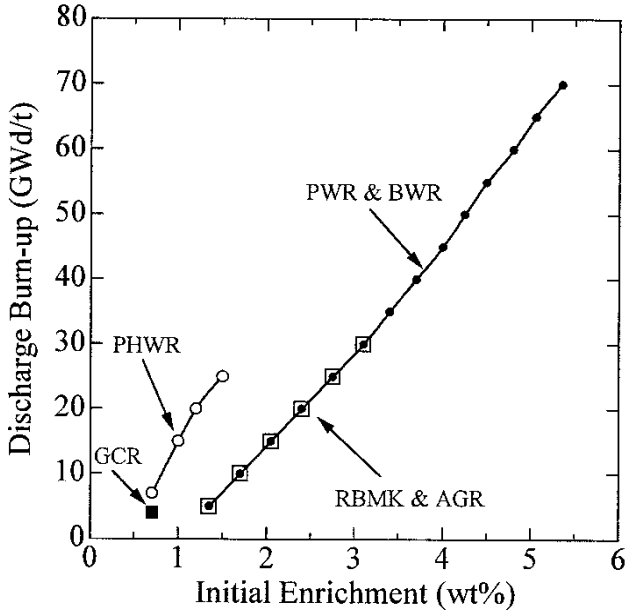


FIG.III-6. Discharge burnup vs. enrichment (reproduced from [III-1]).

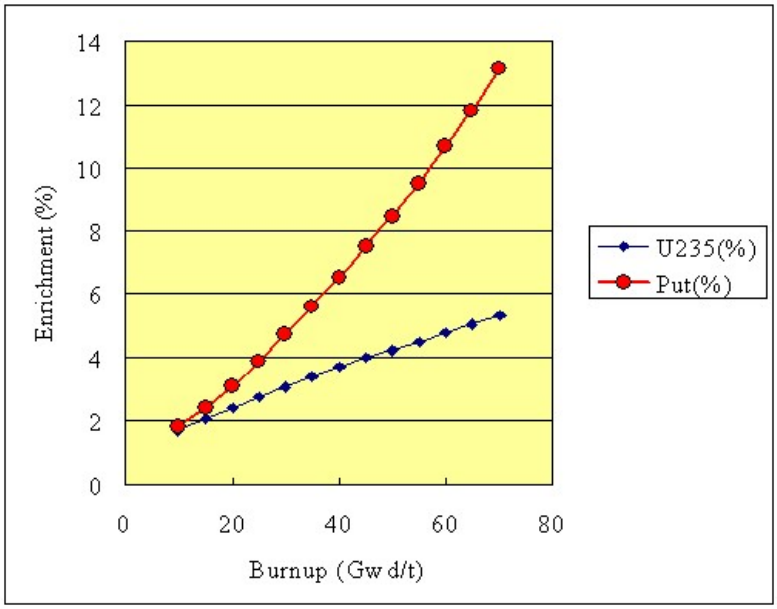


FIG.III-7. Pu-total and U-235 enrichment vs. burnup (PWR&BWR) (reproduced from [III-1).

Each Pu nuclide fraction (Pu vector) before burnup is shown in the Table III-2 (reproduced from Table-4 of [III-1]).

TABLE III-2 PLUTONIUM NUCLIDE FRACTION IN FRESH MOX (wt.%)

Nuclide	*MOX-1 (Discharged UO_2 at 33GW·d/t, and 7 years cooling+reprocessing)*	*MOX-2 (Discharged UO_2 at 45GW·d/t, and 7 years cooling+reprocessing)*
Pu-238	1.4	2.6
Pu-239	60.0	54.5
Pu-240	21.7	28.1
Pu-241	11.8	8.0
Pu-242	5.2	6.8

III-8 RELATION BETWEEN SPECIFIC POWER AND NEUTRON FLUX

Both specific power (power density) and neutron flux are required as input. In most burnup codes such as ORIGEN2, neutron flux is calculated within the code based on power density. There is a correlation between power density and neutron flux. For example, ORIGEN2 adopts the following formula for specific power (MW/ton or kW/kg) [III-3].

$$SP = 1.602\times10^{-19} \times \varphi\times\Sigma(N_i \cdot \sigma_i \cdot R_i)$$

where,

SP : Specific Power (MW/ton),
φ: Neutron flux (n/cm^2/sec),
N_i : Number of nuclide-i (in 1-ton fuel),
σ_i: Fission cross section of nuclide-i (10^{-24} cm^2),
R_i: Fission energy of nuclide-i (typically 200 MeV/fission),
1.602×10^{-19}: Conversion factor from MeV/sec to MW.

Then, neutron flux can be derived by the inverse formula as follows, and thus, it may be unnecessary to input neutron flux in the NFCSS. This formula can also be solved arithmetically if cross sections and neutron flux are constant.

$$\varphi = SP / [1.602\times10^{-19} \times\Sigma(N_i \cdot \sigma_i \cdot R_i)]$$

In the ORIGEN2 burnup calculation, neutron flux (φ) increases with burnup because fissile material amount (N_i) decreases, under constant power density. A result from ORIGEN2 is shown in Fig.III-8 for neutron flux. For U-233 content in PWR thorium fuel up to 45 GW·d/t with 37.5 MW/t specific power results are shown in Fig.III-9.

The above formula suggests that if number densities of all fissile materials are known at each burnup point, then neutron flux can be solved. But, this is impossible before burnup behaviour is calculated. Actually, ORIGEN2 adopts the prediction of burnup behaviour using Taylor series expansion, and ordinary design codes adopt short time steps where neutron flux can be assumed as constant. In reality, cross sections would not be constant throughout the burnup period. But this influence in actual reactor conditions is not discussed here.

Regarding this issue, after the original publication [III-1] was issued, an improved method was installed by the IAEA. This improvement was not described in the original publication.

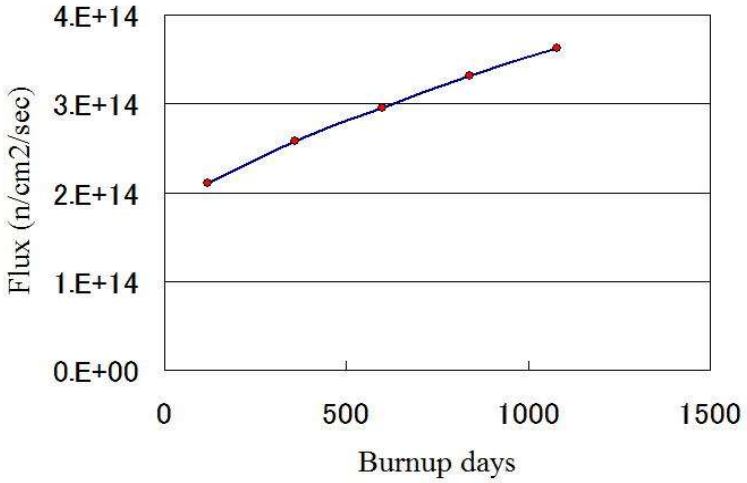


FIG.III-8. Neutron flux vs. burnup for PWR [^{232}Th+ ^{233}U 4w/o] fuel.

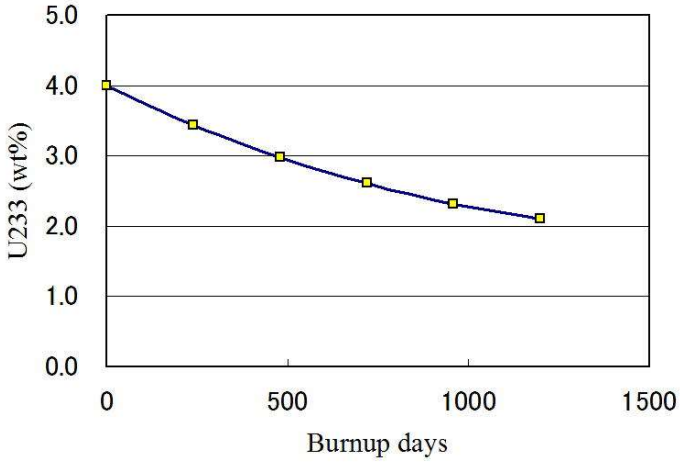


FIG.III-9. U-233 content vs. burnup for PWR Th fuel.

The improved method in the NFCSS would be as follows:

(a) Neutron flux input is used as an initial guess;
(b) Actinide inventory at discharged burnup (say, 50 GW·d/t) is calculated by the CAIN;
(c) Decrease of Actinide inventory is calculated as follows

DA = [InitialHM – DischargedActinides] / InitialHM (say, 0.05 or 5%)

where,
InitialHM = Heavy Metal weight at BU=0, equals to actinides inventory at BU=0;

(d) Roughly speaking, 5% decrease of actinides means 50 GW·d/t burnup, because 1 gram fission generates 1 MW·d thermal energy;

(e) If the above equivalence is not proved, then the initial neutron flux is adjusted, and the above process is repeated. It is not sure what adjustment is applied, but, possible adjustment may be as follows.
⇒ For example, if DA=0.045, it means that input neutron flux is too low, then initial neutron flux is multiplied by 1.1 (=0.050/0.045), and CAIN is repeated using this adjusted neutron flux. It is not sure how many iterations are repeated.

In the above study, emission energy for one nuclide fission (MeV/fission) is calculated by the following formula shown in ORIGEN2 (p.44 of [III-3]). Then, the exact value of MW·d/gram-fission can be calculated by the following formula, and the result is shown in Table III-3.

$$\text{MeV/fission} = 0.00129927 \times Z^2 \times A^{0.5} + 33.12$$

$$\text{MW·d/g-fission} = 0.6023\text{x}10^{24} \times [\text{MeV/fission}] \times 1.602\text{x}10^{-19} / A / 24 / 3600$$

In CAIN, constant value of 0.97 MW·d/g-fission is applied for all nuclides, and the error due to this assumption is about 1% as is shown in Table III-3.

TABLE III-3 MW·d/g-FISSION FOR MAJOR FISSILE NUCLIDES

Nuclide	*Z*	*A*	*MeV/fission*	*MW·d/g-fission*	*Error to 0.97*
U-233	92	233	201.0	0.963	-0.7
U-235	92	235	201.7	0.959	-1.2
Pu-239	94	239	210.6	0.984	1.5
Pu-241	94	241	211.3	0.979	1.0

Based on the comparison with other burnup codes, the above procedure in the NFCSS looks reasonable, and a final neutron flux is added in the output. Then, users can understand that this neutron flux input is an initial guess and the final neutron flux is derived in the NFCSS by the iterative procedure described in Annex I-2.1.

III-9 EFFECT OF OPERATION MODE

III-9.1. Overview

Current NFCSS can input Load Factor (LF), for example, 80%, in order to evaluate the actual fuel requirement corresponding to the generated energy (as electricity and thermal output). The load factor here is defined as the ratio of the electricity generated in a given year to the total electricity that will be generated if the facility is operated whole year at its full rated capacity.

The NFCSS assumes 100% power operation in the CAIN burnup calculation as follows (p.16 of [III-1]). That is, the CAIN does not include LF.

$$T = \text{Irradiation time (sec)} = BU \times 24 \times 3600 / SP$$

where,

BU: Discharge burnup (MW·d/t),
SP: Specific power (MW/t or kW/kg).

Therefore, there is a concern that this assumption may cause some error in the fuel cycle evaluation. As described above, current NFCSS considers actual LF in power generation, and decays of 14 nuclides are calculated by decay-chain equations for their cooling period after spent fuel is discharged (p.56-57 of [III-1]).

The nuclide of greatest concern is Pu-241 because its half-life is 14.4 years. Besides that, inventories of Am-241 (daughter of Pu-241) and Am-242m (neutron capture to Am-241) are affected due to this assumption.

III-9.2. Calculation procedure

ORIGEN2 code was used for PWR-UO_2 fuel with 220-library (PWR high burnup fuel library). Initial enrichment is 4.0%, and comparison is made at 45 GW·d/t for the assumed operation mode as shown in Fig.III-10:

- Case-1A: 100% power operation for 1168 days (power density of 38.53 kW/kg);
- Case-1B: After [100% power operation for 1168 days], decay calculation up to 1460 days;
- Case-2: 80% power operation for 1460 days (power density of 30.82 kW/kg), that is LF=80%.

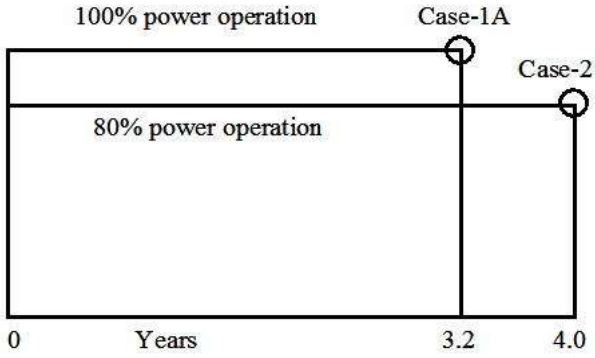


FIG.III-10. Assumed operation mode.

III-9.3. Calculated results

Comparison is shown in the following Table III-4 for 14 nuclides between Case-1A and Case-2. It is shown that the difference is big at Am-241 and at the following daughter nuclide such as Am-242m.

TABLE III-4. ACTINIDE INVENTORY AT 45 GW·d/t

Nuclide	*Case-1A(wt.%)*	*Case-2(wt.%)*	*% Difference*
U-235	0.793400	0.797500	0.5
U-236	0.519400	0.519000	-0.1
U-238	92.900000	92.910000	0.0
Np-237	0.068130	0.068240	0.2
Pu-238	0.024590	0.025340	3.1
Pu-239	0.538700	0.540300	0.3
Pu-240	0.211200	0.211000	-0.1

Nuclide	*Case-1A(wt.%)*	*Case-2(wt.%)*	*% Difference*
Pu-241	0.187000	0.185400	-0.9
Pu-242	0.078670	0.078040	-0.8
Am-241	0.005547	0.006986	25.9
Am-242m	0.000224	0.000279	24.8
Am-243	0.018360	0.018160	-1.1
Cm-242	0.002006	0.002111	5.2
Cm-244	0.006459	0.006333	-2.0
Total	95.353686	95.368689	0.0

Since Pu-241 decays to Am-241 with half-life of 14.4 years, both nuclides data are shown in the following Table III-5 for the above three cases.

TABLE III-5 Pu-241 and Am-241 INVENTORY AT 45 GW·d/t

	Case-1A	*Case-1B*	*Case-2*
Pu-241 (wt.%)	0.187000	0.180000	0.185400
Am-241 (wt.%)	0.005547	0.012600	0.006986

Comparison between Case-1A and Case-2, Case-2 (4-years operation) shows more decays from Pu-241, and then production of Am-241 is larger than Case-1A.

Case-1B is a calculation for 1168 days of operation at its full rated capacity with a cooling period of up to 1460 days. Case-1B shows a large reduction of Pu-241. This is because large amount of Pu-241 decays during the cooling period. Am-241 generation is also larger than Case-2. The difference is almost two times, although the absolute value is small in both cases.

The actual reactor operation would operate as shown in the Fig.III-11, and the true answer will be known if the following operation mode is simulated using ORIGEN2. But this simulation would be complicated.

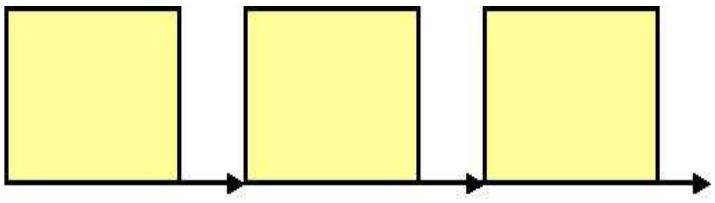


FIG.III-11. Actual operation mode.

As shown above, the Am-241 difference is large, and the true answer is not known. But if long-term evaluation is required, this difference will be small. That is, the difference of Pu-241 is only 0.8% between Case-1A and Case-2, which is the final difference for Am-241 nuclide. For example, inventories of Pu-241 and Am-241 are shown in the following Table III-6 after 14.4 years cooling period, where half of Pu-241 decays to Am-241, assuming one ton of initial fuel. As shown in Table III-6, the differences in Am-241 and Pu-241 are 3% between these two cases. This difference will be smaller for long cooling periods.

TABLE III-6 Pu-241 AND Am-241 INVENTORY AFTER 4.4 YEARS

	Case-1B	*Case1B+14.4years*	*Case-2*	*Case2+14.4years*
Pu-241 (g)	1800	900	1854	927 (+3%)
Am-241 (g)	126	1026	70	997 (-3%)

III-9.4. Summary

The NFCSS can input Load Factor (LF) but assumes 100% power operation in the CAIN burnup calculation. The influence of this assumption was investigated. Nuclides of concern are mainly Pu-241, Am-241 and Am-242m.

For long term evaluation, say more than a decade, the above error decreases as small as 2-3%, and then current NFCSS can be applied for most of the fuel cycle evaluations.

But, if a user wants to use NFCSS for a single reactor simulation for a shorter time period, some error may occur in the inventory of Am-241 and Am-242m by as large as 20–30%.

Therefore, it is recommended to include LF in the CAIN burnup calculation. Or, at least, the above influence should be described in the user manual.

III-10. INITIAL CORE LOADING AND FINAL CORE DISCHARGE

The original publication for the NFCSS does not describe how to simulate initial core loading and final core discharge. In general, a reactor requires 3-4 times large volume of fuels as an initial core than that in equilibrium cycles, and all fuels in the core are discharged together at the end of plant lifetime.

Regarding this issue, after the publication of IAEA-TECDOC-1575 in 2007, an improved method was installed by the IAEA. This improvement was later described in the NFCSS user manual (see Annex II). Since the improved method is described in its manual, a sample calculation result is shown in this section.

One clarification regarding this method is that only HM (Heavy Metal) weight of initial core is roughly estimated by the following formula, and the CAIN burnup calculation is not performed. Also, Final core discharge is estimated by an identical formula.

Initial Core HM (ton) = [MW(th)] / SP
Final core discharged HM (ton) = [MW(th)] / SP

where,

[MW(th)]: Thermal power output of the reactor (= MWe / Thermal efficiency),
SP: Specific Power of the reactor (MW(th)/ton).

Also, an initial enrichment can be given as input to the NFCSS as percentage to that of reload fuels. This is because in general designs an initial enrichment would be lower than that of reload fuels. This lower enrichment is used for front-end calculations such as natural uranium requirement, enrichment, and SWU. Regardless of this treatment, actual CAIN burnup

calculation is not performed for initial enrichment fuel, and equilibrium fuel result is used for initial fuel.

The following sample calculation assumes 1GW(e)-PWR with 4% enrichment and 45 GW·d/t burnup fuel, and specific power of 37.5 MW/t for 10 years operation periods. An initial enrichment ratio of 70% to reload fuel is specified, which means 2.8% as an initial enrichment.

As explained in Section 3.1.10 of [III-1], the NFCSS requires an input of RT (Residence Time). In this sample calculation, RT=4 is used. This RT input is mandatory, although it does not affect the output of the NFCSS. This is not described in the original publication. RT input must be positive and an integer. Meanwhile, a theoretical RT input can be calculated by the following formula. Therefore, a user can input 1,2,3,4,5 or use the following formula for RT input. Either input gives the identical result.

RT (years) = integer value of [BU / SP / 365 / LF]

Here,

BU: Discharge burnup (MW·d/t),
SP: Specific Power (MW/t).
LF: Load Factor (fraction).

In the actual calculation of the NFCSS, RT is calculated by the following formula, which does not include LF:

RT = BU / SP / 365

Numerical results of sample NFCSS calculation is shown in Fig.III-12. Initial core loading is shown as 80.81 tons, which is calculated by the above formula.

For the equilibrium cycle, annually loaded HM and annually discharged HM are calculated by the following formula, which is 19.66 tons in this case.

Annually loaded HM (ton) = Annually discharged HM (ton) = MW(th) × LF × 365 / BU

Here,

MW(th): Thermal output of the reactor (MW),
LF: Load Factor (fraction),
BU: Discharge burnup (MW·d/t).

Since an initial enrichment of 2.8% is assumed, natural uranium requirement is not large as initial core loading and is shown in Fig.III-13.

Discharged fuel weight is shown in Fig.III-14. Final core discharge is 80.81 tons, which is calculated by the above formula.

NFCSS Nuclear Material Flow Result

Reactor Type :PWR-45GWd/t-4%

General | Front End | Back End | Nuclide Groups

Year	NatU (tHM)	ConversionUF6 (tHM)	ConversionUO2 (tHM)	ConversionUMet (tHM)	ConversionTot (tHM)	ENR_In (tHM)	SWU (MT SWU)	Enr_DepU (tHM)	ENR_U (tHM)	FF_1 (tHM)
2015	491.53	491.53	0.00	0.00	491.53	491.53	247.79	410.73	80.81	80.81
2016	177.02	177.02	0.00	0.00	177.02	177.02	103.75	157.35	19.66	19.66
2017	177.02	177.02	0.00	0.00	177.02	177.02	103.75	157.35	19.66	19.66
2018	177.02	177.02	0.00	0.00	177.02	177.02	103.75	157.35	19.66	19.66
2019	177.02	177.02	0.00	0.00	177.02	177.02	103.75	157.35	19.66	19.66
2020	177.02	177.02	0.00	0.00	177.02	177.02	103.75	157.35	19.66	19.66
2021	177.02	177.02	0.00	0.00	177.02	177.02	103.75	157.35	19.66	19.66
2022	177.02	177.02	0.00	0.00	177.02	177.02	103.75	157.35	19.66	19.66
2023	177.02	177.02	0.00	0.00	177.02	177.02	103.75	157.35	19.66	19.66
2024	177.02	177.02	0.00	0.00	177.02	177.02	103.75	157.35	19.66	19.66

FIG.III-12. Sample output for front-end requirement.

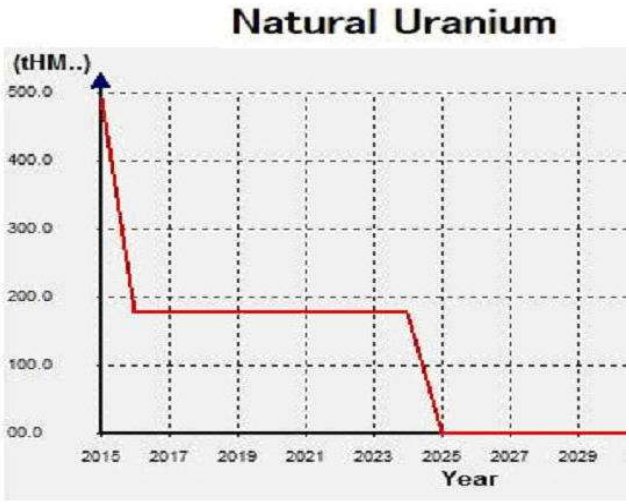


FIG.III-13. Natural uranium requirement.

III-11. CONCERN ON AM-241 CROSS SECTION

III-11.1. Overview

The NFCSS and its burnup model were verified against ORIGEN2 code [III-1]. But recently, when a verification study was performed using cross sections in ORIGEN2 PWR-50GW·d/t library [III-3], it was found that all data showed good agreement except for Am-242. The NFCSS value for this nuclide was almost half of ORIGEN2 value. Although its absolute value is only in the order of grams in 1-ton of spent fuel, it is necessary to confirm the validity of the NFCSS.

III-11.2. Study on Am-241 cross section

The NFCSS recommends using one group cross section data in ORIGEN2 libraries, although users can generate any data set and provide them as input in the NFCSS.

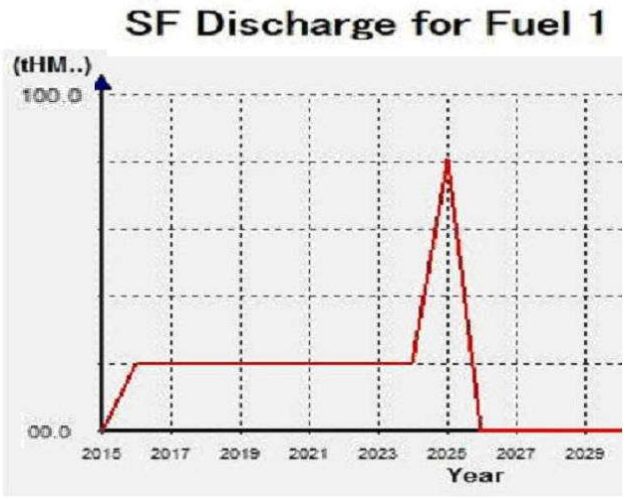


FIG.III-14. Discharged fuel weight.

Among nuclide burnup chains, as is shown in Fig.III-15, when Am-241 captures a neutron, there are two reactions, which go to;

- Ground-state Am-242 (σ_c=106 barns in ORIGEN2-205-library);
- Meta-stable Am-242m (σ_{ex}=13 barns).

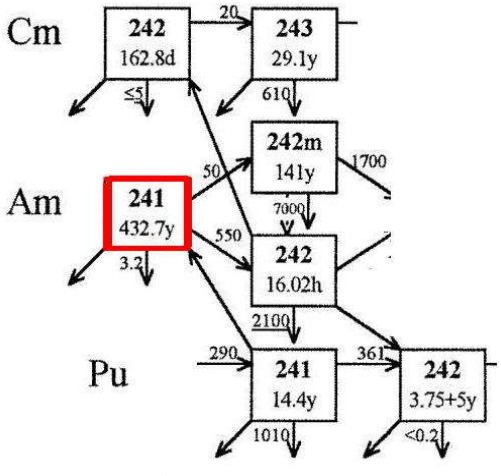


FIG.III-15.Am-241 burnup chains.

Ground-state Am-242 decays to Cm-242 with half-life of 16.0 hour. Also, almost all meta-stable Am-242m decays to Cm-242, but its half-life is 141 year. Meanwhile, absorption cross section of Am-242m is very large, then, Am-242m can be regarded as a stable nuclide.

Since the NFCSS assumes that a nuclide of short half-life decays to its daughter nuclide directly, it can be assumed that Am-241 captures a neutron with σ_c (106 barns) and becomes Cm-242 directly. But, another branch, which decays to Am-242m, must be handled separately.

Usually a Branch Fraction (BF241) is defined as follows.

$$BF_{241}=\sigma_c / (\sigma_c + \sigma_{ex})$$

As shown in Fig.III-16, BF_{241} is constant at thermal neutron energy, and then BF_{241} would be almost constant for different fuel designs of thermal neutron reactors such as PWR, BWR, and so on. But, BF_{241} decreases 5–10% at fast neutron energy, and it may be required to adopt a different value for FBR.

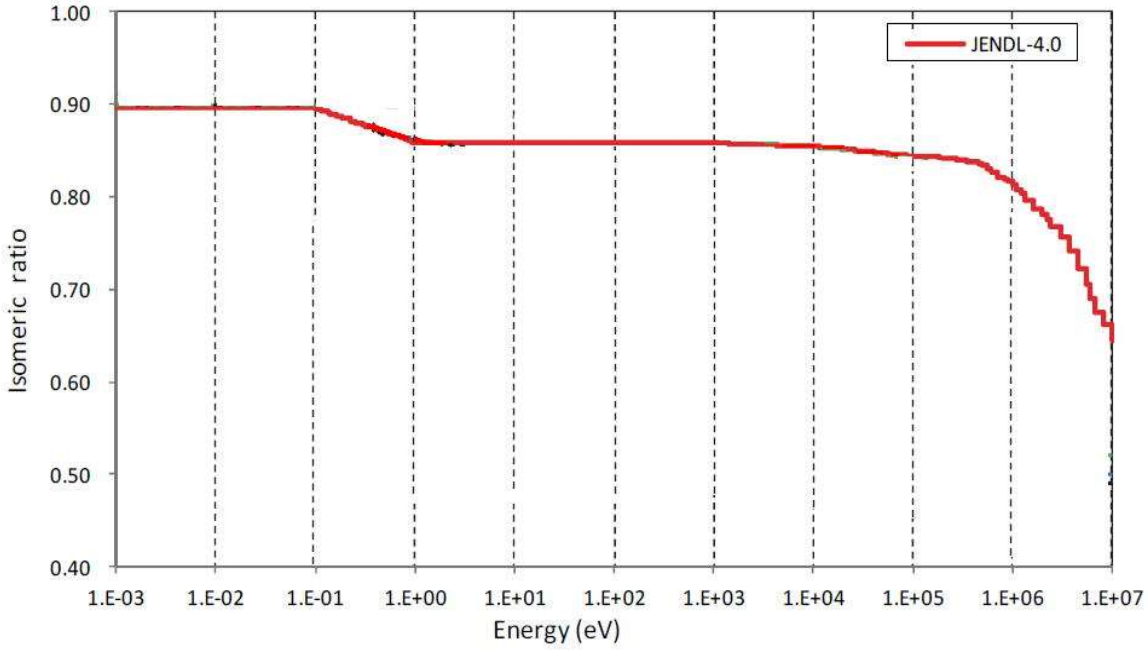


FIG.III-16. Branch Fraction to ground-state Am-242 from Am-241 (reproduced courtesy of JAEA [III-5]).

The NFCSS adopts a constant value of 0.8836 for BF241, which is fixed in the programme, and users cannot change this value (p.18 of [III-1]).

BF_{241} value has been checked in all available ORIGEN2 libraries and several JENDL-4.0 data. The comparisons are shown in the following Table III-7. Most BF_{241} values are in the range of 0.88 to 0.89, except several low values as 0.80 (shown by ★ in the table). As explained above, this low value is inappropriate for thermal neutron reactors. Meanwhile, the FBR-312-library in ORIGEN2 gives σ_c=1.32 (barn) and σ_{ex}=0.33, that is BF_{241}=0.80, which is reasonable from the Fig.III-16. Based on these considerations, the value of 0.80 for thermal neutron reactor is not correct.

TABLE III-7 CROSS SECTION OF Am-241 AND ITS BRANCH FRACTION ($BF_{241}=\sigma_c / (\sigma_c + \sigma_{ex})$)

Library		σ_c	σ_{ex}	$\sigma_c + \sigma_{ex}$	BF_{241}	
ORIGEN205	PWR-UO2-33GW·d/t	105.800	13.070	118.8700	0.8900	
ORIGEN208	PWR-Pu	95.020	11.740	106.7600	0.8900	
ORIGEN211	PWR-PuPu	57.310	7.084	64.3940	0.8900	
ORIGEN214	PWR-ThO2	97.500	12.100	109.6000	0.8896	
ORIGEN217	PWR-PuTh	31.280	7.821	39.1010	0.8000	★
ORIGEN220	PWR-UO2-50GW·d/t	83.250	20.810	104.0600	0.8000	★
ORIGEN223	PWR-U235-Th	81.650	20.410	102.0600	0.8000	★

Library		σ_c	σ_{ex}	$\sigma_c + \sigma_{ex}$	BF_{241}	
ORIGEN226	PWR-U233-Th	77.580	19.400	96.9800	0.8000	★
ORIGEN252	BWR-UO2	108.300	13.390	121.6900	0.8900	
ORIGEN255	BWR-Pu	100.800	12.460	113.2600	0.8900	
ORIGEN258	BWR-PuPu	77.240	9.546	86.7860	0.8900	
JENDL4.0	PWR-UO2-4.1%U235	94.536	13.136	107.6721	0.8780	
JENDL4.0	PWR-UO2-4.7%U235	90.029	12.511	102.5398	0.8780	
JENDL4.0	PWR-MOX-10%Put	35.588	4.946	40.5340	0.8780	

Therefore, it is recommended to apply 0.89 to all BF_{241} values in ORIGEN2 libraries, and revised cross sections are proposed in the following TABLE III-8, where other cross sections such as fission and n2n are not shown, because they are not changed. Since the measurement of total capture cross section ($\sigma_c + \sigma_{ex}$) would be more reliable than each component, it is assumed that the original [$\sigma_c + \sigma_{ex}$] value is fixed, and it is re-balanced to σ_c and σ_{ex}, using a fixed BF_{241} value of 0.89.

Hence there is no need to revise the NFCSS because it already uses [$\sigma_c + \sigma_{ex}$] values with correct BF_{241} value, which is fixed as 0.8836 in the programme code. This observation will be useful to users when comparing the NFCSS results with ORIGEN2 code. If users want to run ORIGEN2 with the following libraries, $\boldsymbol{\sigma_c}$ and $\boldsymbol{\sigma_{ex}}$ must be revised using the data in Table III-8.

TABLE III-8 RECOMMENDED CROSS SECTIONS FOR Am-241

Library		*new-*σ_c	*new-*σ_{ex}	$\sigma_c + \sigma_{ex}$	BF_{241}
ORIGEN217	PWR-PuTh	34.800	4.301	39.1010	0.8900
ORIGEN220	PWR-UO2-50GW·d/t	92.613	11.447	104.0600	0.8900
ORIGEN223	PWR-U235-Th	90.833	11.227	102.0600	0.8900
ORIGEN226	PWR-U233-Th	86.312	10.668	96.9800	0.8900

Current NFCSS is primarily meant for performing fuel cycle calculations for thermal neutron reactors. But, if users can prepare cross sections for FR or FBR, it is possible to include this option in the NFCSS as described in Section 9. Since Branch Fraction of Am-241 for FBR is different from current NFCSS value, calculated inventory in the burnup chains after Am-241 should be modified.

III-11.3. Other meta-stable nuclides

There are two other nuclides besides Am-241, which have a branch to a meta-stable daughter. They are Pa-233 and Am-243.

III-11.3.1. Pa-233

When Pa-233 captures a neutron (Fig.III-17), it goes to;

(a) Ground-state Pa-234 (σ_c=11.2 barns in ORIGEN2-214-Th-library);
(b) Meta-stable Pa-234m (σex=11.2 barns).

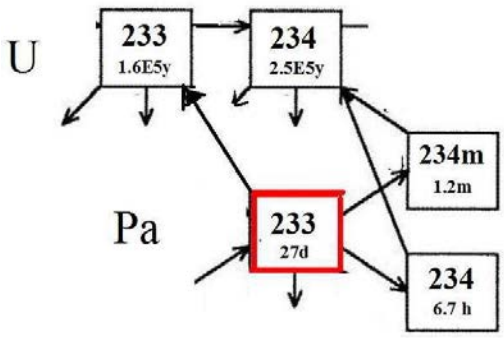


FIG.III-17. Pa-233 burnup chains.

Ground-state Pa-234 decays to U-234 with half-life of 6.70 hours. Also, almost all meta-stable Pa-234m decays to U-234 with half-life of 1.17 minutes, that is the destinations of the above two paths are identical.

Since NFCSS assumes that a nuclide of short half-life decays to its daughter nuclide directly, it can be assumed that Pa-233 captures a neutron and generates U-234 directly without an intermediate branching step. NFCSS assumes that Pa-233 captures a neutron and becomes U-234 directly as described in Section 5.

III-11.3.2. Am-243

When Am-243 captures a neutron (Fig.III-18), it goes to;

(a) Ground-state Am-244 (σ_c=2.5 barns in ORIGEN2-205-library);
(b) Meta-stable Am-244m (σ_{ex}=47.3 barns).

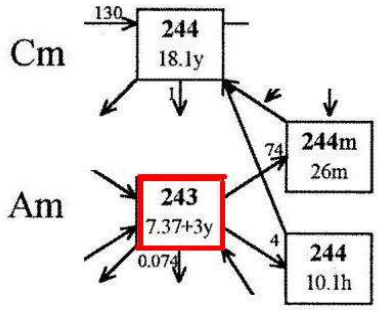


FIG.III-18. Am-243 burnup chains.

Ground-state Am-244 decays to Cm-244 with half-life of 10.1 hours. Also, almost all meta-stable Am-244m decays to Cm-244 with half-life of 26 minutes, that is the destinations of the above two paths are identical.

Since the NFCSS assumes that a nuclide of short half-life decays to its daughter nuclide directly, it can be assumed that Am-243 captures a neutron and generates Cm-244. Therefore, it is not necessary to consider this branch.

III-11.4. Am-241 cross section

Based on the study of Am-241 cross section, there is no revision required for the NFCSS. If a user wants to run ORIGEN2 with certain specified libraries in order to compare the NFCSS or wants to use certain specified ORIEN2 library cross sections for the NFCSS, however, σ_c and σ_{ex} of Am-241 in its ORIGEN2 library should be revised as shown in Table III-6.

Pa-233 and Am-243 also have a branch to a meta-stable daughter nuclide, and this is correctly processed in current NFCSS. In order to use the NFCSS for FBR, the calculated inventory in the burnup chains after Am-241 should be modified because Branch Fraction of Am-241 for FBR is different from the value provided in the NFCSS.

REFERENCES TO ANNEX III

[III-1] INTERNATIONAL ATOMIC ENERGY AGENCY, Nuclear Fuel Cycle Simulation System (VISTA), IAEA-TECDOC-1535, IAEA, Vienna (2007).

[III-2] BATEMAN, H., "Solution of a System of Differential Equations Occurring in the Theory of Radio-active Transformations", Proc. Cambridge Philosophical Society, IS (1910) P.423-427.

[III-3] CROFF, A. G., ORIGEN2 - A Revised and Updated Version of the Oak Ridge Isotope Generation and Depletion Code, ORNL-5621, Oak Ridge National Laboratory (1980).

[III-4] CROFF, G. et al., Once-Through CANDU Reactor Models for the ORIGEN2 Computer Code ORNL/TM-7177, Oak Ridge National Laboratory (1980).

[III-5] OKUMURA, K. et al., A Set of ORIGEN2 Cross Section Libraries Based on JENDL-4.0: ORLIBJ40, JAEA-Data/Code 2012-032, Japan Atomic Energy Agency (2013).

ANNEX IV: ERRATA IN IAEA-TECDOC-1535

IV-1. ERRATA AND CORRECTIONS

IV-1.1. Errata 1

The following formula in P.16 of [IV-1] is incorrect (due to typographical error):

$$T = \frac{E_d \cdot 1000}{KWKG \cdot 24 \cdot 3600}$$

It needs to be corrected to:

$$T = \frac{E_d \cdot 1000 \cdot 24 \cdot 3600}{KWKG}$$

where

E_d = Discharge burnup (GW·d/t),

$KWKG$ = Specific power (kW/kg or MW/t).

IV-1.2. Errata 2

Capture cross section and fission cross section of Am-242m for BWR-UO_2 fuel (Table 10 of [IV-1]) are incorrect. Since the calculated content of Am-243 by the CAIN code agrees very well to ORIGEN2 code as shown in Table 28 of [IV-1], this would be a typographical error.

TABLE IV-1 CORRECTED CORSS SECTIONS

	σ_{cap} *of Am-242m*	σ_{fis} *of Am-242m*
Reference [IV-1] (incorrect)	234.2638	1210.7879
Correct value (ORIGEN2, 252-library)	**100.1000**	**476.1000**

IV-1.3. Errata 3

Neutron flux input is only for an initial guess, and final neutron flux corresponding to specific power is calculated in NFCSS by the iterative procedure. In order to clarify this procedure, final neutron flux is added in the output of current NFCSS.

IV-1.4. Errata 4

In Table 6 of [IV-1], the Specific Power (SP) of PHWR is given as 18.8 kW/kg. This value is derived from Pickering A plant, but recent data shows it to be 24.5 kW/kg.

IV-1.5. Errata 5

Description in Section 3.1.10 of [IV-1] suggests that the NFCSS ignores initial core loading and final core discharge. This is not correct. After the publication of [IV-1], an improvement

procedure was installed in order to handle this issue. Details are described in Section III-10 of Annex III.

IV-1.6. Errata 6

In Section 2.5.7 of [IV-1], PHWR cross section is not referenced. Cross section data itself is shown in Table 34 of [IV-1], and this data is from the ORIGEN2 code provided by ORNL. Its original source is shown in [IV-2].

REFERENCES TO ANNEX IV

[IV-1] INTERNATIONAL ATOMIC ENERGY AGENCY, Nuclear Fuel Cycle Simulation System (VISTA), IAEA-TECDOC-1535, IAEA, Vienna (2007).
[IV-2] CROFF, G. et al., Once-Through CANDU Reactor Models for the ORIGEN2 Computer Code, ORNL/TM-7177, Oak Ridge National Laboratory (1980).

ABBREVIATIONS

ADS	Accelerator driven system
AGR	Advanced gas cooled reactor
ALWR	Advanced light water reactor
ASP	Active server pages
BAU	Business as usual
BNFL	British Nuclear Fuel Limited
BWR	Boiling water reactor
CAIN	Calculation of actinide inventory (a subroutine name in the NFCSS)
DCF	Dose conversion factor
EFPD	Effective full power day
FP	Fission product
JAEA	Japan Atomic Energy Agency (former Japan Atomic Energy Research Institute)
FR	Fast reactor
GAINS	Global Architecture of Innovative Nuclear Energy Systems Based on Thermal and Fast Reactors Including a Closed Fuel Cycle
GCR	Gas cooled reactor
GUI	Graphical user interface
HLW	High level waste
HM	Heavy metal
HTGR	High temperature gas reactor
IAEA	International Atomic Energy Agency
INPRO	International project on innovative nuclear reactors and fuel cycles
LEU	Low enriched uranium
LWR	Light water reactor
MA	Minor actinide
MOX	Mixed oxide
MSR	Molten salt reactor
NES	Nuclear energy system
NFCSS	Nuclear Fuel Cycle Simulation System
NPP	Nuclear power plant
OECD/NEA	Organization for Economic Co-operation and Development/Nuclear Energy Agency
ORNL	Oak Ridge National Laboratory
PHWR	Pressurized heavy water reactor
PRIS	Power Reactor Information System
PWR	Pressurized water reactor
RBMK	High power channel type reactor (derived from Russian)
SWU	Separative work unit
VISTA	Former name of NFCSS
WNA	World Nuclear Association
WWER (VVER)	Water-water energetic reactor (derived from Russian)

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