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Nuclear Fuel Cycle Simulation System (VISTA)

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FOREWORD

As early as the 1970s, the International Atomic Energy Agency has seen the need to be able to estimate nuclear energy and its correlated needs for uranium and services required for different nuclear fuel cycle strategies. The early tools were able to provide estimates on uranium and fuel cycle service requirements, but were limited to the open nuclear fuel cycle strategy.

It was the international symposium Nuclear Fuel Cycle and Reactor Strategies: Adjusting to New Realities, held in 1997 (IAEA-TECDOC-990), which required additional estimates. Those were based on different reactor and fuel cycle strategies; most important is the inclusion of the reprocessing-recycling strategies. A new model has been developed and the Nuclear Fuel Cycle Simulation System (VISTA) was established.

The models and computer tools analyzing the nuclear fuel cycle in its different strategies and options, share the same basic information: the isotopic composition of spent nuclear fuels. One of the purposes of this publication is to describe the method used by the IAEA in obtaining this basic data. Isotopic composition in spent nuclear fuel is calculated by a module called Calculating Actinide Inventory (CAIN). The module is a simple fuel depletion code which requires a small number of input parameters to achieve the requested results.

The VISTA model will be disseminated through the internet as a standalone PC application to enable interested Member States to use it for their analysis. This publication will provide an introduction to the simulation system by giving the technical description of the model and its fuel depletion module CAIN. This publication also gives selected example scenarios and the comparative results for those scenarios in order to demonstrate the capabilities of the VISTA code to interested parties.

The IAEA wishes to thank the experts who took part in the preparation of this publication for their valuable contribution, especially R. Yoshioka from Japan for providing the CAIN code to the IAEA. The IAEA is also grateful to Member States and individual organizations for their generous support in providing experts to assist in this work. The IAEA officer responsible for this publication was M. Ceyhan of the Division of Nuclear Fuel Cycle and Waste Technology.

EDITORIAL NOTE

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1. INTRODUCTION

1.1. Background

The international symposium on Nuclear Fuel Cycle and Reactor Strategies: Adjusting to New Realities was held in Vienna 3–6 June 1997 [1]. For the preparation of this symposium, an international steering group with representatives from twelve countries and three international organizations (IAEA, OECD/NEA and WNA) coordinated, from 1995, the work of six working groups. They studied different scenarios of energy consumption including nuclear electricity production. Nuclear electricity production and the associated nuclear fuel cycle requirements should then to be estimated.

Working Group 2 did a comparison of the existing calculation tools for that purpose. At that time, none of them were able to give simple and accurate estimations. Working Group 2, then asked the IAEA to adapt its old CYBA calculation database to take into account the two options for nuclear fuel back end strategy: direct disposal and reprocessing & recycling.

A new simulation system, named VISTA, was developed in 1996. It was then intensively used to quantify the different scenarios fixed by the Working Groups of the conference.

The VISTA model needs isotopic composition of spent nuclear fuel in order to make estimations of the material arisings from the nuclear reactor operation. For this purpose, in accordance with the requirements of the VISTA code, a new module called Calculating Actinide Inventory (CAIN) was developed. CAIN is a simple fuel depletion model which requires a small number of input parameters and gives results in a very short time.

VISTA has been used internally by the IAEA for the estimation of: spent fuel discharge from the reactors worldwide, Pu accumulation in the discharged spent fuel, minor actinides (MA) accumulation in the spent fuel, and in the high level waste (HLW) since its development. The IAEA decided to disseminate the VISTA tool to Member States using internet capabilities in 2003. The improvement and expansion of the simulation code and the development of the internet version was started in 2004. A website was developed to introduce the simulation system to the visitors providing a simple nuclear material flow calculation tool. This website has been made available to Member States in 2005 [2]. The development work for the full internet version is expected to be fully available to the interested parties from IAEA Member States in 2007 on its website.

Appendix I gives more information about the VISTA internet site.

1.2. Objective

VISTA is able to calculate, year by year over a long period, nuclear fuel cycle requirements for all types of reactors. Calculations are performed for a reactor, reactor park in a country or a worldwide nuclear power plant park. Natural uranium, conversion, enrichment and fuel fabrication requirements can be estimated. Furthermore, the quantities and qualities (isotopic composition) of discharged and/or stored fuels can be evaluated to let the user apply a recycling strategy if desired.

Data inputs are reduced to a few basic data in order to let non-nuclear fuel specialists develop different energy scenarios. The calculation speed of the system is fast enough to enable making comparisons of different scenarios in a considerably short time.

So the simulation system is designed to be an optimum mixture of accuracy, simplicity and speed.

1.3. Scope

VISTA calculations can cover the period ranging from the beginning of nuclear energy production to 2050 or 2100. Calculations can be done for a specific reactor, reactor park in a country or worldwide nuclear reactor park.

In order to support estimations for the future term, VISTA needs data on historical operations of nuclear power plants. Historical data mainly come from the existing IAEA databases such as the Power Reactor Information System (PRIS) [3]. Other authoritative publications and consultant reports are also sources for historical data. Future projection data can be calculated by using publications from different institutions. The IAEA's Energy, Electricity and Nuclear Power Estimates up to 2030 (2005 edition) [4] is one of the authoritative publications which was used to calculate future nuclear power projection data in VISTA.

The existing VISTA database has global average data for input parameters which are available for all users, but the tool itself can be used for a specific country if the user provides the historical data and future predictions for the selected country.

Fresh fuel requirements and spent fuel isotopic composition are then automatically calculated from a set of internal parameters that have been selected by the user and introduced in the program. The user may then choose to use spent fuel stockpiles to develop a recycling strategy. The estimation of accumulation of actinides including minor actinides is one of the capabilities of the simulation. Those accumulation estimations might be used to compare any future fuel cycle options for transmutation of minor actinides.

2. VISTA MODELLING

2.1. General

There are a number of models and computer tools available for calculating uranium and fuel cycle service requirements [5]. These models are based on sophisticated databases that include information on each nuclear power reactor in the world. Such databases are useful for portraying the history and short term nuclear power projections. It is however very difficult to build such databases with a view toward the far future such as 30 to 100 years. The incentive for developing the new scenario-based model was to simplify long term estimations [6].

There are similar other tools which have been used by some organizations. These include:

• DANESS: Dynamic Analysis of Nuclear Energy System Studies (DANESS) is a software code that permits the integrated process modelling of nuclear energy systems for parameter studies, economic analysis, and for variations in the fuel cycle. The software can currently describe 10 nuclear reactor types and 10 fuel types with a crossflow of fissile material. The reactor and fuel types are stored in a library that can be updated as necessary. The nuclear reactor and fuel type history can be traced as an operating facility to determine the cost of energy generation per reactor and for the total nuclear system. The model has been developed by Argonne National Laboratory [7].

- DESAE: Dynamic of Energy System Atomic Energy (DESAE) is an interactive computer tool which has a potential to become a useful tool to perform energy planning studies. i.e:
	- o simulating future energy scenarios (not only nuclear energy);
	- o predictive analysis of resource consumption and waste;
	- o management of nuclear energy systems;
	- o predicting economics of nuclear energy systems along with other alternative energy options.

DESAE has been developed by the IAEA to be used in INPRO assessment works.

There are other tools which are used by many organizations for their internal purposes. Most of them are specifically designed for the organization's specific purpose and not suitable for general use.

2.2. VISTA information flow

VISTA can be described as a simulation tool which makes calculations using a set of input parameters to produce a set of output parameters. The input parameters used in the model may be divided into three groups:

- **Strategy parameters** nuclear capacity variants and reprocessing-recycling strategies, reactor-type mixture and load factors, all on an annual basis;
- **Fuel parameters** average discharge burnup, average initial enrichment and average tails assay on an annual basis;
- **Control parameters** share of mixed-oxide fuel in the core of reactors using this type of fuel, lead and lag times for different processes, process loss coefficients, use of depleted or enriched uranium and the number of reprocessing cycles.

The results are divided into the following groups:

- **Front End:** Natural uranium requirements, conversion requirements, enrichment service requirements and fresh fuel requirements
- **Back End:** Spent fuel arising, total individual nuclides arising including Uranium, Plutonium and Minor Actinides, reprocessing requirements.

The illustration of inputs and outputs of the simulation system is given in Figure 1. The left side of the sketch gives the input parameters whereas the right side shows the list of output parameters.

Fig. 1. VISTA information flow.

2.3. Nuclear fuel cycle

Nuclear fuel cycle can be defined as the set of processes to make use of nuclear materials and to return it to final state. It starts with the mining of unused nuclear materials from nature and ends with the safe disposal of used nuclear materials in the nature. All the elements of a commercially available nuclear fuel cycle options are described in this section. See Figure 2 for a simplified nuclear fuel cycle diagram showing main processes in a recycle mode.

Fig. 2. Simplified diagram of the nuclear fuel cycle in recycle mode.

Mining & milling: Uranium is an element that is widely distributed within the earth's crust as ores. Its principal use is as the primary fuel for nuclear power plants. The uranium ore needs to be mined and then processed (milled) before being usable. Uranium ore is mined by openpit or underground mining methods and the uranium is extracted from the crushed ore in processing plants or mills using chemical methods. Sometimes it is possible to pass chemical solutions to the ore beds and dissolve the uranium from the ore directly. This process is known as in situ leaching. This is the first step in a nuclear fuel cycle. The feed for mining $\&$ milling process is uranium ore and the product is U_3O_8 concentrate, which is mostly called yellowcake due to its color and shape.

Conversion: The term conversion refers to the process of purifying the uranium concentrate and converting it to the chemical form required for the next stage of the nuclear fuel cycle. There are three such forms in common usage: metal, oxide $(UO₂$ or $UO₃)$ and uranium hexafluoride (UF₆). UF₆ is the predominant product at this stage of the nuclear fuel cycle since it is easily converted to a gas for the enrichment stage, as employed in world's most common reactor type (LWRs). For the PHWR fuel cycle, which generally uses natural uranium oxide as the fuel, conversion to the 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 metal form. The feed for this stage is U_3O_8 concentrate, and the products are UF₆, oxide (UO₂ or $UO₃$) or metal, in applicability order.

Enrichment: Uranium naturally consists of about 0.7% of ²³⁵U isotope which is the main energy source in thermal reactors which are only commercially existing nuclear power plants in significant amounts. 99.3% of the natural uranium is 238 U isotope. For LWR technology which is the most common reactor type in the world, it is impossible to build a LWR with the natural occurrence of ^{235}U , so the ^{235}U content should be increased with a special process. This process is called enrichment. There are two commercially available enrichment technologies: gaseous diffusion and centrifuge. Both techniques are based on the slight mass difference between 235 U and 238 U. So the enrichment is defined as the process of increasing the amount of 235U contained in a unit quantity of uranium. The feed for this stage is natural $UF₆$ and the product is enriched UF₆. The other output of the process is the uranium which has lower ²³⁵U content than the natural uranium. It is known as enrichment tail or depleted uranium.

Fuel fabrication: Enriched uranium in UF_6 form is converted to UO_2 powder to make fuel for LWR technology. This powder then is formed 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, which are 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. The similar procedure is adopted for natural uranium oxide fuel for some reactor types. The feed of this process is enriched or natural uranium oxide powder and the product is fuel assembly. The feed for Magnox fuel is uranium metal.

Reactor: The reactor itself is irradiator for nuclear fuel. It burns the fuel, produces energy and spent fuel. There are currently 7 commercially available reactor types in the world (classification is based on VISTA assumptions): PWR, BWR, PHWR, RBMK, GCR, AGR and WWER. The feed for reactor is fresh fuel containing uranium or uranium/plutonium, in case of mixed oxide (MOX) fuel, for existing nuclear fuel cycle options. The product is the spent fuel consisting of newly generated nuclides such as fission products (Cs, I, ...), minor actinides (Np, Am, Cm) and plutonium as well as the uranium. The biggest part of the spent fuel is still uranium (more than 95% for the most reactor types).

Reprocessing: The spent nuclear fuel still consists of significant amount of fissile material that can be used to produce energy. The considerable amount of ^{235}U is still contained in the spent fuel and there are new fissile nuclides that were produced during normal operation of nuclear reactor such as ²³⁹Pu. Some nuclear fuel cycle options consider taking out those fissile material from the spent fuel, refabricating it as fuel and burning in the reactor. MOX fuel is the most common fuel that uses reprocessed material. Reprocessing process is based on chemical and physical processes to separate the required material from spent nuclear fuel. The feed of this process is spent fuel and the products are reusable material and high level wastes (HLW).

Spent fuel storage: The spent fuel, which is not reprocessed, could be stored temporarily for future use or could be stored indefinitely. Spent fuel could be stored in pools (wet type, temporarily) or in silos (dry type).

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

2.4. VISTA nuclear material flow model

VISTA simulation code is a two layer computer model to calculate the overall nuclear material flow in a nuclear fuel cycle option as well as the individual nuclide discharge and accumulation in the spent nuclear fuel. This section explains the overall nuclear material flow model of the VISTA whereas Section 2.5 explains the fuel depletion model which calculates individual nuclide discharge and accumulation in the spent nuclear fuel.

Overall material flow for a nuclear fuel cycle can be sketched by tracking the nuclear materials in each of the processes in the cycle. VISTA is capable of simulating different nuclear fuel cycle models with different reactor types and fuel types including non-existing fuel types (i.e. fuels with MA content) with the introduction of necessary libraries and data. For the purpose of this publication commercially existing nuclear fuel cycle options were simulated. These options are once through fuel cycle and U and Pu recycling in LWRs in the form of MOX fuel. Figure 3 shows the overall material flow diagram of the nuclear fuel cycle which is simulated in VISTA for this publication. Multi-recycling is possible in the system but the second fuel type must always have the same initial nuclide content as the fresh (first generation) MOX fuel.

The first fuel type in the model is uranium fuel from unused material whereas the second fuel type is the fuel from reprocessed material. The second fuel type in the system is MOX fuel type for the purpose of this publication since it is the only commercially available fuel from reprocessed material. Other fuel types such as fuels containing MA content could also be used to investigate future options.

Fig. 3. Overall material flow diagram simulated in VISTA.

2.4.1. Process losses

In each stage of the nuclear fuel cycle, the materials are processed in a facility. There are chemical and physical processes involved in those stages. Each stage has some losses in processed material. This should be taken into account when simulating the real situation. The VISTA simulation code is capable of having individual process loss coefficients in terms of percentage of processed material amount for each stage of the nuclear fuel cycle.

2.4.2. Process lead and lag times

Process lag time is defined as the time necessary to produce the output from the input of the process. Process lead time is defined as the time between the two processes. For example reprocessing can be done only after waiting certain period of time following the discharge of spent fuel from the reactor.

2.4.3. Calculation model

The VISTA fuel cycle simulation system is designed for estimating fuel cycle material and service requirements and material arisings year by year. The model calculates also, whenever relevant, cumulative amounts by summing annual amounts. All annual results represents yearly average amounts. The calculation method and algorithms are described in Appendix II in details.

2.5. Fuel depletion model

2.5.1. Need to track actinides

The actinide group includes elements from Th $(Z=90)$ to Lr $(Z=103)$, however major interest is given to the different isotopes of U and Pu (major components of fresh and spent nuclear fuel) and so-called minor actinides (MA - Np, Am and Cm) with extremely long life, high alpha (with energy of alpha-particles of 4-6 MeV, major contributors to the residual heat of spent fuel) and gamma radioactivity.

Assessment of the worldwide inventories of these elements/isotopes in spent fuel is important due to non-proliferation issues (for fissile isotopes of U and Pu) and radiotoxicity of long lived MAs. The latter relates to open fuel cycle, when the safety of spent fuel storage and further final disposal should be justified and guaranteed, and to closed fuel cycle, when the same is applicable to immobilized high level waste (HLW) containing MAs.

Characteristics of major actinides (half life, mode of decay, presence of gamma-radiation, total and alpha activities) are presented in TABLE 1. Concentration of actinides and their specific activities are given for $UO₂$ fuel with initial enrichment of 3.2% after irradiation in 900 MWe PWR until burnup of 33 MW·d/kg U and 5 years storage in the table.

It could be seen from TABLE 1 that about 90% of alpha-radioactivity of discharged spent fuel, or HLW in case of reprocessing, i.e. potential radiotoxicity, is contributed by 238 Pu, ²⁴¹Am and ²⁴⁴Cm (spent fuel) or ²⁴¹Am and ²⁴⁴Cm (HLW).

During irradiation actinides migrate in Z+N (Z and N-number of protons and neutrons respectively) space due to competing processes: radioactive decay and neutron capture. Figure 4 shows the transmutation chain of actinides. Radioactive decay impacts on residual concentration of MAs and respectively - on potential radiotoxicity.

Potential radiotoxicity of actinides may be defined, without taking into account any barriers, by calculating a "source term" obtained by weighting the activity of each radionuclide by its specific toxicity coefficient (by ingestion or inhalation) and then by summing up the resulting values. TABLE 2 shows the evolution of the potential radiotoxicity of spent fuel and the contribution of each long lived actinide and total of FP (in Sieverts per ton of $UO₂$ spent fuel or by TWh_e produced). It could be seen that after decay of highly radioactive FPs $(^{137}Cs$ and 90 Sr) during ~ 300 years, the major contribution is dealt with Pu, up to 10⁶ years. Americium has a predominant position among the MAs between 10^2 and 10^5 years, Np - after 10^5 years, and Cm - before 10^4 years [8]. Uranium is predominant after 10^6 years.

For the long term storage or disposal of spent fuel or HLW the potential release of activity to the biosphere could be evaluated as consequence of degradation of engineering barriers and transfer of radionuclides through geological environment. With taking into account the solubility of actinides, the permissible concentrations in water and solids, the actinide hazard factors in spent fuel /HLW may be ranged as [8]:

²⁴¹
$$
Am \rightarrow ^{240}Pu \rightarrow ^{239}Pu \rightarrow ^{243}Am \rightarrow ^{242}Pu \rightarrow ^{237}Np \rightarrow Cm
$$
 (spent fuel)
²⁴¹ $Am \rightarrow ^{243}Am \rightarrow ^{240}Pu \rightarrow ^{239}Pu \rightarrow ^{237}Np \rightarrow Cm$ (HLW)

In late 70s vast R&D programmes to increase fuel burnup were initiated in several countries in order to reduce uranium and separative work requirements, fuel cycle cost and the amount of discharged spent fuel. At present the reduction of the amount of discharged spent fuel and the nuclear fuel cycle costs are seen as major results of burnup extension programmes. The historical design batch average burnup of LWRs, around 30 MW·d/kg U, have been increased now up to 40-45 MW·d/kg U for PWRs and 36-42 MW·d/kg U for BWRs. Economic incentives exist for extending burnup even further, to at least ~ 60 MW·d/kg U batch average.

However, burnup increase has also resulted in an increase in specific actinide content and alpha-activity in spent fuel or MAs in HLW. The growth of actinide's alpha radioactivity is faster than linear, also the contribution of each actinide changes with burnup increase (TABLE 3). This should be taken into account in the safety assessment of spent fuel or HLW storage or disposal facilities.

Also, assessment of actinide inventories in spent fuel or HLW is a first step in the P&T (Patitioning and Transmutation) programmes initiated in several countries in the beginning of the 1990s'.The OECD/NEA is coordinating the R&D activities in the area [9]. Since there are activities in this area outside the OECD, the Department of Nuclear Energy of the IAEA carried out P&T related activities by coordinating the programmes of mainly non-OECD countries. Thus, several technical committee meetings have been conducted [10][11][12] and a coordinated research programme to evaluate safety, environmental and non-proliferation aspects of P&T of actinides and fission products was initiated in 1994 upon recommendation of the technical committee meeting held in 1993 [11].

TABLE 1. CHARACTERISTICS OF MAJOR ACTINIDES [8][9][13][14]

^a Spontaneous Fission

^b Isomeric Transition

Time, years	10 ²	10 ³	10 ⁴	10 ⁵	10 ⁶	10 ⁷
Total, Sv/TWhe	$1.1x10^{9}$	$3.1x10^{8}$	$7.7x10^7$	$4.2x10^6$	$5.2x10^5$	$1.4x10^5$
Components,%						
Rep U	-	$\overline{}$	0.1	6	29	79
Pu	85	90	97	88	50	17
Np	-	۰		1.3	13	3
Am	10	9.2	2,5	2.7	6.8	1.4
Cm	0.4	0.3	0.4	$\overline{}$		-
FP	4.2	$6x10^{-4}$	$2.4x10^{-3}$	3.2×10^{-2}	$9.6x10^{-2}$	$1.4x10^{-1}$

TABLE 2. SOURCE TERM (ACTINIDES AND LONG-LIVED FISSION PRODUCTS — FP) AND ITS COMPONENTS — VARIATION WITH TIME (Sv/TWhe) [8]

TABLE 3. ALPHA-ACTIVITY OF SPENT FUEL OF THERMAL REACTORS (Ci/t HM) AS A FUNCTION OF BURNUP [9]

2.5.2. Selection of actinides

The following criteria were applied to select actinides to be calculated by the VISTA code:

- Short lived actinides or actinides of very small concentrations were excluded as unimportant for spent fuel/HLW in a long run term;
- Long lived actinides (half-life > 400 years) are assumed as stable.
- Only 235 U and 238 U are considered as the initial nuclides in fresh uranium fuel. 234 U is ignored because its transmutation into 235U is small.

Thus the following 14 nuclides have been selected and transmutation chain, which is given in Figure 4, has been obtained:

235U, 236U, 238U, 238Pu, 239Pu, 240Pu, 241Pu, 242Pu, 237Np, 241Am, 242mAm, 243Am, 242Cm and 244 Cm.

Fig. 4. Actinide transmutation chain. Fig. 4. Actinide transmutation chain.

2.5.3. Methods available

2.5.3.1. Introduction

There are several computer programs available for the calculation of nuclide inventories in spent fuel. The overall procedure for the calculation is common to all. The programs differ in the detail with which each step in the calculation is carried out.

In general, actinide inventories are calculated by solving the equation that is obtained by taking a nuclide balance. This equation consists of terms that represent the production rate and removal rate of the nuclide. For the actinides, production consists of neutron capture or decay of a precursor nuclide. Removal may consist of neutron induced or spontaneous fission, neutron capture and radioactive decay.

The calculation of the reaction rates requires nuclide concentration and cross section data, the neutron flux level and energy spectrum in the fuel. As the energy spectrum in the fuel is dependent on the lattice structure and composition, such calculations involve repeated iterative solutions for the spectrum and cross sections. The extent to which this is carried out depends on the accuracy required of the final solution. After each burnup interval, the converged spectrum is used to obtain the neutron cross sections which are subsequently used for the calculation of the nuclide reaction rates.

The points to be considered in making an evaluation of the available methods are:

- nuclide cross section data
- energy spectrum calculation
- calculation of neutron flux level during irradiation, and
- numerical solution of the burnup equations.

The treatment of these quantities in the several alternative codes has been examined. They are WIMS, ORIGEN and VISTA module CAIN. Each of the codes is described below.

2.5.3.2. The WIMS Code

WIMS [15] is a lattice code that uses neutron transport theory to solve the multienergy group neutron balance equations in one or two dimensions. Several cross section libraries are available as input. The current popular choice seems to be the ENDF/B libraries. The data in this library is condensed to 69 energy groups for use in WIMS.

The code includes the effect of the temperature of the lattice components (especially those with significant neutron scattering rates) on the neutron spectrum and subsequently on the nuclide inventories.

In order to make a meaningful comparison to ORIGEN and CAIN, the following features of WIMS should be noted:

Since the cross section library has data for 69 energy groups, the option is available to calculate the nuclide reaction rates for each of these groups. (usually, between 14 to 33 energy groups are used, depending on the special requirements of the problem). The enrichment level affects the neutron spectrum; the detailed calculation of the neutron spectrum for a given reactor type, takes this into account.

- The shift in neutron spectrum due to the change in the fuel composition as burnup proceeds is accounted for. Consequently the change in actinide cross sections due to the spectral shift is included before the nuclide balance equations are solved for the following burnup interval.
- WIMS calculates the nuclide inventories separately for each fuel pin in the assembly. The pins operate at different power levels and consequently have different nuclide concentrations and reaction rates. This is significant as the nuclide reaction rates are not linear functions of flux or power level.
- Several isotopes with high mass number (curium and above) are not included in the burnup chain solved by WIMS.
- In WIMS the nuclide balance equations may be solved separately for annular regions within each fuel pin. This results in a distribution of nuclide concentration along the pin radius. The calculation of the neutron flux distribution within the pin (for each energy group) is therefore based on a realistic distribution of nuclides. This is especially relevant to the effect that the plutonium isotopes have on flux and the power density.
- The numerical solution of the transport equation in WIMS is carried out by an iterative process that is designed in such a way that the user can control the order of the convergence.

The above features of the WIMS code are emphasized to support its role as a benchmarking code for ORIGEN and subsequently for CAIN.

2.5.3.3. The ORIGEN code

The ORIGEN code [16] solves the nuclide balance equations as in WIMS but for an expanded set of nuclides. A large number of fission products and transuranic actinides are included which are absent in the WIMS code. A major difference between the two codes is that ORIGEN treats the fuel assembly as a point lattice, i.e. it solves a single set of equations that represent the assembly. This simplified representation is achieved by pre-calculating the neutron cross sections and energy spectrum for the assembly by using a code such as WIMS, and then averaging the reaction rates to obtain a single set of cross sections to be used in ORIGEN for each burnup interval. A set of such time dependent cross sections are needed for each reactor type and fuel cycle.

The point assembly representation in ORIGEN makes it practical to use a desktop PC to calculate a large number of nuclide concentrations for various reactor and fuel cycle types. The error introduced by the point representation in ORIGEN can be controlled by adjusting the number of cross section sets. As an example, a unique set can be used for each enrichment level within a given fuel type; or a specific fuelling strategy may require its own cross section set. On the other hand, a single set of cross sections for each reactor type may be sufficient to meet the accuracy requirements.

The cross section data library that is generally used in ORIGEN is one of the versions of the ENDF/B library. The neutron spectrum is implicit in the set of cross sections that are input to the code. Stepwise integration of the nuclide balance equations is carried out. Analytical expressions are used for the solution at each step. This allows the user to choose whether the neutron flux level or the power density be kept constant during burnup.

Compared with WIMS and CAIN, ORIGEN has a larger number of nuclides in its database.

2.5.3.4. The CAIN code

The CAIN Code was written to meet the special requirements of the Nuclear Fuel Cycle Simulation System being developed at the IAEA [5]. It solves, essentially, the same equations as ORIGEN for a point assembly. The neutron spectrum is implicit in the set of cross sections that the user inputs to the code. Analytical expressions are available for the solution of the equations. This makes the code computationally very efficient. As with ORIGEN, the accuracy of the calculated nuclide inventories can be improved in CAIN by using cross sections that are pre-calculated by a lattice code that models the complete assembly and accounts for the detailed neutron spectrum in obtaining the nuclide cross sections. The number of cross section sets to be used is based on the user's judgment to meet the accuracy requirements. At present, the code uses a set of cross sections for each reactor and fuel type.

2.5.4. Criteria for model selection

2.5.4.1. Accuracy requirements

Since the objective of VISTA is to predict for example the global amount of actinides in the discharged fuels from all civilian power reactors, it is not required to evaluate the actinides inventory for each specific reactor. Therefore, all power reactors are categorized to seven reactor types, which are PWR, BWR, PHWR, RBMK, AGR, GCR and WWER. These types represent almost all of the commercially existing reactor types in significant amounts.

Considering the future capability to implement the "CAIN" depletion model to VISTA, the CAIN model should be simple. But it should be accurate enough compared with other verified codes. Therefore, the Bateman's Equation is adopted, because it is a theoretical burnup solution for a point reactor with one group neutron cross section.

Also, it is not required to calculate the inventory for short lived actinides or the actinide of very small concentration, because we are considering the actinide inventory of spent fuels in the long term. Therefore, the following 14 actinides are calculated: 235 U, 236 U, 238 U, 238 Pu, 239 Pu, 240 Pu, 241 Pu, 242 Pu, 237 Np, 241 Am, 242 mAm, 243 Am, 242 Cm and 244 Cm.

The detailed model of the CAIN code is explained in Section 2.5.5. Regarding the accuracy of the CAIN code, the results of validation and benchmarks are shown in Section 2.6.

2.5.4.2. Computational requirements

The computer software to develop the VISTA simulation system has been chosen in order to comply with the following requirements:

- Experts studying the global nuclear materials flow deduced from electricity generation capacity scenarios want to have on their personal computer a user-friendly tool to quickly test their hypotheses.
- The tool must be in accordance with nuclear physics principles and reflect nuclear industry realities.
- Data to be inputted by user should be kept to a minimum unlike the more sophisticated models.

• Formulae giving the isotopic composition of the different nuclear fuels, both before and after irradiation must be incorporated into the program. This will allow the size of the program to be reduced hence speeding up the calculation and also limit the amount of data to be inputted in order to evaluate the nuclear material flows and isotopic compositions.

2.5.5. CAIN model

2.5.5.1. Introduction

The calculation model of the actinide inventory in the discharged fuel which is described below is programmed as a computer code "CAIN" (Calculation of Actinide INventory). The data inputs for the CAIN (cross sections and other reactor constants) are explained in Section 2.5.7 and Section 2.5.8. The calculated isotopic compositions by the CAIN code are mentioned in Section 2.5.9. The results of verification for the CAIN code are discussed in Section 2.6.

2.5.5.2. Bateman's Equation and its solution

The Bateman's Equation is adopted to be used in CAIN model. It is a theoretical burnup solution for a point reactor with one group neutron cross section, as explained below. In order to solve the Bateman's Equation several parameters are needed to be known. Those parameters are listed in below sample solution.

The main expression for Bateman's equation is given below:

$$
\frac{dN_i}{dt} = -\sum_{j\neq i} \biggl[\lambda_{ji}^d + \overline{\sigma}_{ji}^{\text{tr}}\overline{\phi} \biggr] N_i + \sum_{j\neq i} \biggl[\lambda_{ij}^d + \overline{\sigma}_{ij}^{\text{tr}}\,\overline{\phi} \biggr] N_j
$$

where

$$
N_i
$$
 - atomic content of isotope (*i*);

$$
\lambda_{ji}^d
$$
 - decay constant, 1/s;

- σ_{ii}^{ν} transmutation cross section from isotope *i* to isotope *j*, barn;
- $\sigma_{ii}^{\prime\prime}$ transmutation cross section from isotope *j* to isotope *i*, barn;
- φ average neutron flux, n/(s⋅cm²);
- N_i atomic content of isotope (*j*).

If the neutron flux and cross sections are constant on a time interval, the equation has a simple analytical solution.

An example to solve the transmutation chain starting from 238 U up to 240 Pu is shown below, using Bateman's Equation.

$$
^{238}U \rightarrow ^{239}Pu \rightarrow ^{240}Pu
$$
\n
$$
AF_1 \cdots .AF_2 \cdots .AF_3
$$
\n
$$
AF_l = AF_l (initial) \cdot e(-\sigma_{t1} \cdot \Phi \cdot T \cdot l0^{-24})
$$
\n
$$
AF_2 = AF_l (initial) \cdot \left[\left(\frac{\sigma_{cl}}{\sigma_{t2} - \sigma_{t1}} \right) \cdot e^{(-\sigma_{t1} \cdot \Phi \cdot T \cdot l0^{-24})} + \left(\frac{\sigma_{cl}}{\sigma_{t1} - \sigma_{t2}} \right) \cdot e^{(-\sigma_{t2} \cdot \Phi \cdot T \cdot l0^{-24})} \right]
$$
\n
$$
AF_3 = AF_l (initial) \cdot \left[\left(\frac{\sigma_{cl} \cdot \sigma_{c2}}{(\sigma_{t2} - \sigma_{t1}) \cdot (\sigma_{t3} - \sigma_{t1})} \right) \cdot e^{(-\sigma_{t1} \cdot \Phi \cdot T \cdot l0^{-24})} \right]
$$
\n
$$
AF_3 = AF_l (initial) \cdot \left(\frac{\sigma_{cl} \cdot \sigma_{c2}}{(\sigma_{t3} - \sigma_{t2}) \cdot (\sigma_{t1} - \sigma_{t2})} \right) \cdot e^{(-\sigma_{t2} \cdot \Phi \cdot T \cdot l0^{-24})} + \left(\frac{\sigma_{cl} \cdot \sigma_{c2}}{(\sigma_{t1} - \sigma_{t3}) \cdot (\sigma_{t2} - \sigma_{t3})} \right) \cdot e^{(-\sigma_{t3} \cdot \Phi \cdot T \cdot l0^{-24})}
$$

where

 AF_i = Atomic content of isotope(i) in the chain

- σ_c = Capture cross section (barns)
- σ_f = Fission cross section (barns)

 σ_{n2n} = (n,2n) cross section (barns)

 σ_{ex} = Excited cross section (barns)

 σ_t = Total cross section (barns)

$$
\sigma_{decay} = \frac{0.693}{T_{1/2} \cdot 365 \cdot 24 \cdot 3600 \cdot 10^{24} \cdot \phi}
$$

$$
\sigma_t = \sigma_c + \sigma_f + \sigma_{ex} + \sigma_{decay}
$$

$$
T_{1/2} = \text{Half life (years)}
$$

- Φ = Average flux (n/cm/cm/sec), (0 to 10MeV total flux)
- $T =$ Irradiation time (sec)

$$
T = \frac{E_d \cdot 1000}{KWKG \cdot 24 \cdot 3600}
$$

 E_d = Discharge burnup (GW·d/t)

KWKG = Specific power (KW/Kg or MW/tonne)

The equation solver first calculates the isotopic composition in atomic fraction. The obtained atomic fractions then are converted to the weight fractions.

2.5.5.3. Assumptions in CAIN model

There are several assumptions in this fuel depletion model in order to achieve the functional and computational requirements of the model. The assumptions are listed below:

- (1) Only 235 U and 238 U are considered as the initial nuclides in the fresh uranium fuel, and the descending nuclides are analytically calculated by Bateman's equation. Although natural uranium includes 234 U (<0.01%), this nuclide is ignored, because the transmutation from 234 U to 235 U is small.
- (2) The existing chains are selected to be suitable for fresh fuels containing any of the 14 nuclides of the CAIN library.
- (3) CAIN is capable of handling variable neutron flux and cross sections throughout the irradiation. In order to do this the flux and cross sections should be entered as different values for different burnup steps. Otherwise, both cross sections and neutron flux are assumed to be constant throughout the burnup period.
- (4) Short life nuclides (half life ≤ 8 days) are skipped. That is, ²³⁷U (7 days), ²³⁸Np (2 days), ²⁴³Pu (5 hrs), ²⁴²Am (16 hrs), ²⁴⁴Am (10 hrs) and ²⁴⁴Am (26 min) are assumed to decay and go to next nuclide simultaneously.
- (5) On the other hand, long life nuclides (half life > 400 years) are assumed as stable for the irradiation period. For example, 24 Am (432 yr) are treated as stable. For decay (cooling) period after discharge, all nuclides are treated by their actual decay scheme.
- (6) Therefore, 14 nuclides are calculated based on the chains shown in Figure 4. Among 14 nuclides, decays of ²³⁸Pu (87.7 yr), ²⁴¹Pu (14.4 yr), ²⁴²Cm (0.447 yr) and ²⁴⁴Cm (18.1 yr) are considered during irradiation.
- (7) Transmutation is terminated for certain nuclides (shown as mark "x"). For example, 238 Pu decreases by neutron capture, but the decrease of 238 Pu is not added to 239 Pu. This treatment is imposed in order to stop endless calculation of Bateman's equation. This assumption is reasonable, because the contribution due to these transmutations is very small.

The full transmutation chain (Figure 4) is simplified (Figure 5) based on the above assumptions. This simplified chain has been implemented in CAIN to calculate isotopic composition of spent fuel after irradiation period and after cooling/storage period. The list of all chains is given in Appendix III.

2.5.6. Inclusion of MOX recycling in VISTA

In the first development phase of VISTA, MOX fuel was handled in a simple way. The composition of spent MOX fuel had been calculated by introducing a factor to composition of spent uranium fuel. This simplification was mainly due to the assumption of ignorance of MOX fuel reprocessing. But with the increased use of MOX fuel in several countries and with the concerns of radiotoxicity of spent nuclear fuel the multirecycling option became more possible. This brought a need for more accuracy in calculation of composition of spent MOX fuel. In order to do so, VISTA was expanded to handle MOX fuel to PWR, BWR and WWER. There are several modifications on VISTA, which are described in this section.

2.5.6.1. Chains for MOX

For uranium fuel, the initial nuclides are 235 U and 238 U only (VISTA assumption). But, for MOX fuel, there are more initial nuclides such as $^{238}Pu^{239}Pu^{240}Pu^{241}Pu^{242}Pu$. In some MOX fuel, there may exist 241 Am, which decays from 241 Pu with 14 years half-lifetime. So, new chains starting from the above Pu nuclides are necessary.

Also, in some countries, reprocessed uranium is used occasionally. This reprocessed $UO₂$ includes 236 U, which does not exist in the natural uranium, and it becomes necessary to include 236 U as an initial nuclide for this fuel.

Finally, in order to handle the future fuels, which includes MA isotopes such as Np/Am/Cm, new chains starting from $^{237}Np^{241}Am^{242m}Am^{243}Am^{242}Cm^{244}Cm$ are necessary. In here, 242m Am comes from neutron capture of 241 Am, and goes to 243 Am by another neutron capture. (Also, 242m Am decays to 242 Cm, but its half-life is as long as 141 years.)

The new chains, added for MOX fuel modelling in CAIN, are listed in Appendix III.

2.5.6.2. Pu content for fresh MOX

In order to perform burnup calculation for MOX fuel in VISTA, we have to assume the initial composition of Pu in the fresh MOX fuel. The contents of each Pu isotope in the total Pu amount is often called "Pu Vector". Pu vector which is used in VISTA is given in the first column of TABLE 4. This vector is calculated assuming that Pu comes from reprocessing of 3.3% enriched PWR fuel with 33 000 MW·d/t discharge burnup after 7 years of cooling and reprocessing time. If we assume the source fuel is 4.0% enriched PWR fuel at 45 000 MW·d/t discharge burnup after 7 years of cooling and reprocessing time the Pu vector becomes slightly different and this affects the fissile content in the total Pu. Current VISTA assumption is acceptable for the historical calculations since the most of the fuels which have already been reprocessed are in the first case (3.3%, 33 000 MW·d/t). But VISTA allows using of different Pu vectors. Figure 6 shows the Pu vector in the fresh MOX fuel for the above two cases.

	Fresh MOX used in VISTA ¹ $(\%)$	Discharged UO ₂ at 45GW·d/t, and 7 years cooling + reprocessing (%)
238 Pu	1.4	2.6
^{239}Pu	60.0	54.5
240 Pu	21.7	28.1
241 Pu	11.8	8.0
242 \mathbf{p}_1	5.2	6.8

TABLE 4. PERCENT FRACTION OF EACH PU NUCLIDE IN FRESH MOX AND DISCHARGED UO₂

Fig. 6. Percent fraction of Pu nuclides in fresh MOX and discharged UO₂.

2.5.6.3. Pu Generation effect (multiple recycling)

One more assumption in VISTA/MOX calculation is that we assume the above Pu vector is constant, even in the second or third generation MOX. When the fresh MOX is discharged, there exist higher fractions in 241 Pu or 242 Pu than the fresh MOX. This effect is shown in Figure 7. In this figure, "2nd generation MOX" is the discharged MOX at 45 GW·d/t with 7 years cooling, calculated by VISTA.

This effect is neglected in VISTA calculation, because second generation MOX is expected to be mixed with fresh MOX, and therefore the generation effect would be small. Of course, if we need higher accuracy in MOX calculation, it would be necessary to include this effect.

 \overline{a}

¹ It is calculated by using 33 MW·d/kg Burnup, 3.3% Enriched PWR fuel after 7 years of cooling and reprocessing time.

Fig. 7. Percent fraction of Pu nuclides in fresh MOX and 2nd generation MOX.

2.5.6.4. Total Pu amount for fresh MOX

VISTA user can specify the burnup trend and corresponding enrichment trend as the future prediction, for both $UO₂$ fuel and MOX fuel respectively. For the convenience to the user, corresponding sets of burnup and enrichment are supplied for both $UO₂$ and MOX, which are described as follows.

Conversion factor from 235U enrichment to total Pu amount

Below equation is used in VISTA to calculate initial total plutonium amount in fresh MOX fuel. The equation is proposed by a French consultant for VISTA, based on their experience.

Initial Total Pu = 235 U_{enr} * $(1.6 + 0.23*(BU - 33)/10)$

where 235 U_{enr} is the enrichment of uranium fuel for the same discharge burnup, and BU is the discharge burnup.

This equation is verified by another approach. There is an open report from JAERI [17], which provides the Pu composition at the initial and discharge burnup of $33/45/60$ GW·d/t uranium fuel.

Unfortunately, this MOX calculation assumes that the initial Pu vector is constant for any burnup. It assumes the Pu vector from 33 GW·d/t U fuel. So, it is assumed that 45 GW·d/t MOX uses discharged Pu from 45 GW·d/t U fuel. Also, for 60 GW·d/t MOX, Pu from 60 GW·d/t U fuel is used. Then, a little bit higher Pu-total enrichment for 45/60 GW·d/t MOX fuel is estimated. Using this corrected Pu-total, the ratio of Total Pu to 235 U enrichment (Conversion Factor from 235 U to Pu-total) is calculated. These values are shown in TABLE 5 and Figure 8.

TABLE 5. CONVERSION FACTOR FROM 235U ENRICHMENT TO TOTAL Pu IN FRESH MOX

Burnup $(GW \cdot d/t)$	JAERI report $[17]$	VISTA
33	1.72	1.60
45	1.85	1.88
60	198	2.22

Fig. 8. Conversion factor from 235U enrichment to Total-Pu.

Even after the above correction, there is some difference between VISTA and current verification study. But, the difference is 10% or so in 60 GW·d/t. That JAERI report does not perform full core calculation for MOX. It uses assembly calculation, and estimates full core design, and there may be some error, especially for high burnup point. If the VISTA user has more accurate design value, it is possible to input that value, anytime. So, it is concluded that VISTA assumption is acceptable as an initial estimation or just a recommended value.

Figure 9 shows the relation between Pu-total content and burnup for MOX fuel. Also, the relation between ²³⁵U enrichment and burnup for $UO₂$ is shown. Of course, these data are just the recommended values, and user can specify their own values.

Fig. 9. Pu-total and 235U enrichment vs. burnup.

2.5.7. Cross-sections used

The CAIN code needs various inputs to evaluate the actinide inventory in the discharged fuel. They are cross sections and reactor constants such as specific power or neutron flux.

Appendix IV gives one group cross section data for 14 nuclides of current concern. The origins of the cross sections used for the 7 existing reactor types which are included in this study are described below:

- PWR, BWR and PHWR uranium fuel cross section data are identical to the ORIGEN library (PWR-UO2-33G library for PWR and BWR-UO2-27.5G library for BWR).
- RBMK uranium fuel cross sections were calculated by the Japanese consultant using a similar code to WIMS. 242m Am cross sections are extrapolated from PHWR library.
- AGR uranium fuel cross sections were calculated by the Canadian consultant using the WIMS code. Am and Cm cross sections were copied from RBMK data, because their neutron spectrums are similar. 242m Am cross sections are extrapolated from PHWR library.
- 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. Am and Cm cross sections were copied from PHWR data, because both reactors are using natural uranium fuel. ^{242m}Am cross sections are identical from PHWR library.
- 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 ORIGEN library (PWR-PuPu library for PWR-MOX and BWR-PuPu library for BWR-MOX).

2.5.8. Other constants

Other constants, which CAIN code requires are the specific power and the neutron flux and so on. The list of all constants which are required input parameters for CAIN code is given in TABLE 6.

The specific power (kW/kg) was calculated using the data in the Directory of Nuclear Power Plants in the World [18]. It may vary plant by plant, so the typical plant was selected. This constant is used to convert the discharge burnup to the irradiation time.

The neutron fluxes for PWR/BWR/PHWR are identical to the ORIGEN 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.

One more constant is reference enrichment. Since single cross section set is applied for different enrichment fuels, actual neutron flux can be modified in the CAIN code using the following formula. Although this adjustment has a very small effect on the results it might increase the speed of the calculation.

 Φ (a) = Φ (r) x ($ENR(r)$ / $ENR(a)+1$) / 2

where

Φ**(a): Actual neutron flux**

Φ**(r):Reference neutron flux**

ENR(r):Reference enrichment

ENR(a): Actual enrichment

2.5.9. Isotopic composition of spent fuels

Isotopic composition in the discharged spent fuel is calculated by the CAIN code using the above model and constants. In these calculations, initial enrichments which were supplied by the IAEA (Figure10) are used for corresponding discharge burnups. Since initial 235 U burns and lower Pu saturates at discharged burnup, high accuracy for this relation is not required for burnup calculation. The isotopic composition results are given in Appendix V.

Fig. 10. Discharge burnup vs. enrichment.

2.6. Validation and benchmarking

Validation and benchmarking of VISTA simulation system with its reactor depletion model CAIN was performed in two steps. The first step involves the validation of reactor depletion model CAIN and the second step involves the validation of overall material flow model.

2.6.1. Validation of reactor model, CAIN

Validation of CAIN model was carried out separately for uranium fuels and MOX fuels. CAIN results were compared to the results of other well known computer programmes such as ORIGEN and WIMS and to the actual measurement results wherever possible. The details of the validation studies and the results are given in Appendix VI.

The results show that the results of CAIN model fits very well with the results of ORIGEN code. CAIN results show good agreement with also actual measurements. The CAIN results agree very well with WIMS code except some higher actinides. Considering that the CAIN is one group model and WIMS is multi-group model, the results are acceptable.

From the results of validation and benchmarking studies, it can be concluded that CAIN code can be used in VISTA simulation system in order to estimate the isotopic composition of spent nuclear fuel in discharge time and after cooling.

2.6.2. Validation of overall nuclear material flow calculations

There is not publicly available and commonly accepted nuclear fuel cycle simulation code which can easily be used to validate VISTA nuclear material flow calculations. But there are published reports such as Interdisciplinary Study on the Future of Nuclear Energy by Massachusetts Institute of Technology (MIT) in 2003 [19]. The study calculates the fuel cycle material flow for different fuel cycle options for the predicted future nuclear power plant capacity. The VISTA has been used to calculate the same requirements using the same assumptions. The assumptions and input parameters are given in TABLE 7. The results from both studies are displayed in TABLE 8. The results show that the overall nuclear material flow calculations fit very well with the values reported by MIT.

TABLE 7. ASSUMPTIONS FOR THE OVERALL MATERIAL FLOW CALCULATIONS

TABLE 8. COMPARISON OF THE RESULTS OF THE OVERALL MATERIAL FLOW CALCULATIONS

3. EXAMPLE SCENARIO WITH INPUT AND OUTPUT PARAMETERS

In order to demonstrate the capabilities of the VISTA simulation code to the readers, a sample study was performed and a result set was obtained. The available scenarios, selection of scenarios, input parameters and outputs for the selected scenarios are given in following sections.

3.1. Input parameters

The VISTA input parameters contain datasets which are combination of historical actual data and estimations for future projections. The simulation system database contains historical data from the beginning of the commercial nuclear activities. The historical data has been retrieved from the actual reported data wherever possible. The data sources are usually well known databases such as IAEA PRIS database [3]. The other data sources include reports which are generated by consultant companies such as NAC International's Nuclear Industry Status Report [20]. The data reported to the IAEA conferences or publications are also used in some cases.

For the purpose of this publication the simulation system has been used for the estimation of the world needs of fuel cycle material and services associated with several nuclear energy programmes and spent fuel policies up to 2050. The different reactor and fuel cycle characteristics and their evolution over the period up to 2050 were used in this simulation system. Although the raw database has reactor by reactor data for most of the input parameters, all datasets used in this study are realistic mean values for each reactor type worldwide. They do not reflect any country specific characteristics, or performance of reactors and fuel cycle facilities.

Scenario selection for this TECDOC is also described at the end of this section.

3.1.1. Nuclear power

Historical nuclear power data comes from IAEA PRIS database [3]. PRIS is one of the most comprehensive and commonly used databases on nuclear power plants and their operating experience in the world. Future nuclear power projection is based on the IAEA Energy, Electricity and Nuclear Power Estimates for the Period up to 2030, 2005 Edition [4]. Estimations from the publication are based on many factors and reflect the most realistic situation for the period that it covers. The publication provides estimations until year 2030. VISTA then extrapolates the estimations up to the year 2050 by linear extrapolation technique.

The publication gives two variants for the nuclear power evolution. One is low and the other is high variant. VISTA uses those two variants as well as their arithmetic averages. The low nuclear power capacity case is called **P0**, and the medium case is called **P1** and the high case is called **P2** in VISTA. The variation of the parameters is displayed in Figure 11.

Fig. 11. The projection of installed nuclear capacity in the world.

3.1.2. Reactor type mixture

At present there are a number of commercially available reactor types in the world. All those types are actually grouped into 7 main groups based on their nuclear characteristics in order to reduce the data requirements in VISTA as given in Chapter 2.

The share of each reactor type in the total nuclear reactor park is represented in this data set. The historical data comes from the IAEA's PRIS database [3] and the future projection is based on consultants' recommendations. Presently about 57% of the operating reactors are PWR, 22% are BWR, 5% are PHWR, 3% are RBMK, 2% are AGR, 1% are GCR and 9% are WWER in terms of installed capacity. Figure 12 displays the evolution of the reactor types.

Fig. 12. Reactor type shares.

3.1.3. Load factors

Load factor is defined as the ratio of the electricity generated in a given year to the total electricity to be generated if the facility is operated whole year in 100% capacity. Historical load factor values come from IAEA PRIS database [3] and the future projection is based on the trends in operating experience and performance of the current reactor park. Figure 13 shows average annual load factors.

Fig. 13. Average annual load factors.

3.1.4. LWR reprocessing scenario

Different countries chose different alternative fuel cycle options based on their specific policies and goals, taking into account the balance between their domestic energy resources and industrial capabilities. The choice also depends on the nuclear electricity generation growth. For some countries there would be incentives to reprocess spent fuel to recover and recycle fissile nuclear materials as a means of reducing natural uranium requirement. The recycling option can also be chosen as a means to address issues related to management of the back-end of the fuel cycle. This scenario assumes only uranium fuel from natural material is reprocessed although the VISTA is capable of having multi-cycling options with the introduction of proper data.

In the view of existing alternative fuel cycle options, VISTA has an input parameter to determine the amount of reprocessed material for each reactor type. The reprocessing ratio is defined as the ratio of the spent fuel to be reprocessed after a period of cooling time to the total spent fuel discharged in a given year. VISTA assumes that the reprocessing ratio for PWR and BWR types are same due to the lack of data for individual types. All GCR fuel is assumed to be reprocessed. There is no reprocessing for PHWR and RBMK in the selected scenario. Reprocessing data for AGR fuels were calculated from the historical reported values. Reprocessing ratio for WWER fuel is selected similar to PWR and BWR case for future projection.

VISTA has four different reprocessing scenarios in its database. First scenario assumes that reprocessing will decrease in time and there will be no reprocessing after year 2030 (**R0** case). The second scenario assumes that the current reprocessing ratio will be kept at steady value through the period of calculation (**R1** case). The third and the fourth scenario assume that more part of the spent fuel will be reprocessed in the future (**R2** and **R3** cases). The scenario chart is presented in Figure 14. The figure only shows the reprocessing ratio for PWR and BWR.

Fig. 14. Reprocessing ratio for PWR and BWR types.

3.1.5. MOX fuel ratio in LWR

Reprocessed material has already been used in some countries in the form of mixed oxide (MOX) fuel since 1980s. This scenario assumes that only PWR and BWR type reactors are using and will use MOX fuel type. The MOX fuel ratio input parameter is defined as the ratio of the MOX fuel amount to the total fuel amount used in the reactor type to generate electricity. The same ratio is used for PWR and BWR types. This assumption is made based on the lack of data for individual types. The historical data is derived from the reported values of MOX fuel fabrication amounts in the fuel fabrication facilities.

VISTA has 5 MOX fuel scenario in its database starting from low case (**M0**) to very high case (**M4**). Variation is displayed in Figure 15.

Fig. 15. MOX fuel ratio in PWR and BWR.

3.1.6. Discharge burnups

VISTA can use different burnup values for UOX and MOX fuel types (first and second fuel type in the fuel cycle model). However, due to the lack of historical information and simplicity of the calculation, we assumed both fuels have the same average discharge burnups. Average discharge burnup values for historical operations are calculated from the reactor by reactor data which is provided in NAC International reports [20]. The burnup projection is based on consultants' recommendations and reflects the latest developments in fuel performance and power reactor operating experience [21][22]. Discharge burnup values are displayed in Figure 16.

Fig. 16. Average discharge burnups.

3.1.7. Initial enrichments

Average initial enrichment values for UOX fuels are calculated by using the relation between the discharge burnup and initial enrichment. This assumption is valid if the reactor fuel is burned effectively. In some cases, for some reasons, the fuel is discharged before its nominal burnup value but these are not significant amount and do not change worldwide averages so much. Calculated initial enrichment values are displayed in Figure 17. Total Pu amount for MOX fuel is calculated using the relation between the initial enrichment of UOX fuel and the total Pu amount in the same loading Figure 9.

Fig. 17.Initial enrichment values for uranium fuels.

3.1.8. Enrichment tail assay

Average enrichment tail assay is another parameter which can be selected from different options. VISTA has three scenarios for average tail assay values. **T0** is the high case and assumes that the long-term average value will be kept constant in its 2000 value (=0.30%). **T1** assumes that the average tail assay will drop to 0.25% in 2025 and will be constant at that level. **T2** assumes that the average tail assay will drop to 0.20% in 2025 and will be constant afterwards. T2 scenario reflects the latest rapid increase in natural uranium prices. Figure 18 shows average enrichment tail assay values.

Fig. 18. Average enrichment tail assay.

3.1.9. Process losses and process lag times

In reality all processes have some material losses. VISTA has input parameters for conversion, enrichment, fuel fabrication and reprocessing loss coefficients. But this study assumes that the process loss coefficients are 0 (zero-loss) for all processes due to the lack of actual data.

All processes are assumed to occur in real time with no lags except the cooling period between the reactor discharge and reprocessing time and manufacturing of MOX fuel. For PWR and BWR spent uranium fuel, cooling time is assumed to be 6 years, reprocessing time is 1 year and the MOX fuel manufacturing time is assumed to be 1 year.

3.1.10. Fuel residence times

VISTA requires fuel residence times in terms of year due to the calculation procedure. The values could be given in year by year values. However, for the purpose of this study, and due to the fact that VISTA ignores the effect of full core loading and unloading for the time being, fixed residence times are assumed for each reactor type. This eliminates the possibilities of getting discrepancy in the result set. In the long run, this assumption does not affect the results such as inventory of actinides or cumulative spent fuel discharges. The selected values are: 4 years for PWR and BWR; 3 years for WWER, RBMK and AGR; and 1 year for PHWR and GCR.

Fig. 19. Fuel residence times in the reactor.

3.2. Scenario selection

In order to demonstrate the capabilities of the VISTA simulation system, three example scenario datasets have been selected. The realistic cases have been tried to be selected for each of the parameters in the scenario category. The selection of the example scenario is just based on the consultants' recommendations and does not reflect any official declaration from the IAEA or its Member States. It should also be noted that this is a theoretical calculation and might not reflect technically or practically possible options in any way.

The description of the selected example scenario data sets is below:

- *Low scenario:* Low scenario is combination of low power capacity projection (**P0**), low reprocessing ratio (**R0**) and low MOX use ratio (**M0**). The scenario code is **P0-R0-M0**.
- *Medium scenario:* Medium scenario is combination of medium power capacity projection (**P1**), medium reprocessing ratio (**R1**) and medium MOX use ratio (**M1**). The scenario code is **P1-R1-M1**.
- *High scenario:* High scenario is combination of high power capacity projection (**P2**), high reprocessing ratio (**R2**) and high MOX use ratio (**M2**). The scenario code is **P2-R2-M2**.
- *Enrichment tail assay:* Low case has been selected (**T2** in Figure 18) for all scenarios.
- All the other parameters use the basic data set, which is described in Section 3.1 of this TECDOC.

3.3. Output parameters

Several results have been selected out of complete result set from the VISTA simulation system. These results are believed to provide good overview of the capabilities of the VISTA. The results presented here focus on the material and service requirements for the main stages of the nuclear fuel cycle and total Pu discharge from the reactors. More results from the VISTA for different scenarios are presented in other publications such as [23][24][25] and [26].

Only cumulative results are presented in this TECDOC but annual results for all of the output parameters could be obtained from the VISTA code.

3.3.1. Electricity generation

First of all, the nuclear electricity generation will increase faster than the installed nuclear capacity (Figure 11) in the near future due to the better performance of the power plants. Average annual load factors have been increasing for almost all of the reactor types in the world for recent years (Figure 13). This trend is expected to continue, and the multiplication result of Figure 11 and Figure 12 is shown in Figure 20.

*Fig. 20.*Cumulative nuclear electricity production*.*

3.3.2. Natural uranium requirements

Estimated annual and cumulative natural uranium requirements are shown in Figure 21. Annual natural uranium requirement will increase until 2010 and then reach a plateau on about 70 000 t U in medium case. After year 2030 the requirement will start increasing again. Natural uranium requirement calculation is matched with the requirements published in IAEA-OECD/NEA joint publication Uranium 2003: Resources, Production and Demand (Red Book) which gives 70 605 t and 73 820 for low and high cases in 2010 [27].

Fig. 21.Cumulative natural uranium requirements.

3.3.3. Conversion requirements

Conversion requirement shows the same progress as the natural uranium requirement. The results show any conversion requirement from natural uranium to UF_6 or UO_2 or U metal for different types of reactor fuels. Figure 22 shows the result for annual and cumulative conversion requirements.

Fig. 22.Cumulative conversion requirements.

3.3.4. Enrichment requirements

Enrichment is required to increase fissile content of $UF₆$. Annual enrichment requirement is expected to be increased significantly until 2025 due to the increasing share of the reactor types which uses enriched uranium for their fuels (mainly LWRs). After year 2025, this increase will be slower because the share of the LWRs will reach to its maximum value. The result is shown in Figure 23.

Fig. 23.Cumulative enrichment requirements.

3.3.5. Fresh fuel fabrication requirements

Annual fresh fuel fabrication requirement is expected to increase until year 2010 and then decrease (Figure 24). This decrease is explained by increase in discharge burnup value and decrease in share of the GCR, AGR and RBMK which basically require more amount of fuel in terms of tonnage than the PWR, BWR and WWER types.

Fig. 24.Cumulative fresh fuel requirements.

3.3.6. LWR MOX fabrication requirements

Figure 25 displays the annual and cumulative LWR MOX fuel fabrication requirements for the selected scenarios.

Fig. 25.Cumulative LWR MOX fuel fabrication requirements.

3.3.7. Spent fuel discharge amount

Discharged amount of spent fuel looks similar to the fresh fuel requirement with some lag time which actually equals to the fuel residence time in the reactor. The result is displayed in Figure 26.

Fig. 26.Cumulative spent fuel discharge amounts.

3.3.8. Reprocessing requirements

Reprocessing requirement heavily depends on the recycling strategies of the countries. For the medium case (R1), the annual reprocessing requirement will decrease until the year 2020 and then steadily increase (Figure 27). This is explained by the phase out of the GCR and AGR reactors in time. The amount of reprocessed fuel is estimated about 3 000 tonnes in year 2050 which is 30% of the total discharged spent fuel assigned as **R1** scenario.

Fig. 27.Cumulative reprocessed spent fuel amount.

3.3.9. Spent fuel storage requirements

Amount of spent fuel stored in interim storage facilities or reactor pools are displayed in Figure 28. The annual spent fuel storage requirement will increase until the year 2015 due to the decreased amount of reprocessing for **R1** case. But after that, with the recovery of the reprocessed amount and due to the decrease in amount of discharged spent fuel, annual spent fuel storage requirement will decrease slightly and then keep steady trend. The results for fresh fuel loading and spent fuel discharge, storage and reprocessing are in agreement with each other which validates the material flow calculation.

Fig. 28.Cumulative stored spent fuel amount (excluding storage for reprocessing).

3.3.10. Total plutonium discharge

Figure 29 shows the amount of total plutonium which will be discharged from the commercial nuclear power plants. The content of Pu in spent fuel increases with the increase in discharge burnup. This effect can be seen in the figure. The rate of increase in total Pu discharge is higher than the rate of increase in spent fuel discharge.

Fig. 29.Cumulative total Pu discharge from the reactors.

3.3.11. Separated Pu stocks

Figure 30 shows the annual and cumulative amount of separated total Pu stocks. It can be seen that the amount of separated Pu stocks will be increased if the current trend in LWR reprocessing (**R1**) and LWR MOX use (**M1**) continue. If the MOX use is increases (**M2**) the amount of separated Pu stock will start decreasing after reaching its maximum values about 2015.

Fig. 30.Cumulative separated Pu stocks.

3.3.12. Minor Actinide discharge

Figure 31 displays the amount of total minor actinides (Am, Cm, Np) which will be discharged from the reactors in the next years.

Fig. 31.Cumulative total MA discharge from the reactors.

3.3.13. Minor Actinide accumulation

Figure 32 displays the amount of total minor actinides (Am, Cm, Np) which will be discharged from the reactors in the next years.

Fig. 32. Accumulated amount of MA at the end of 2005. This calculation considers the decay of all discharged material during the cooling and storage period.

4. SUMMARY AND CONCLUSIONS

4.1. Summary

The Nuclear Fuel Cycle Simulation System (VISTA) was developed by the IAEA to support The International Symposium on Nuclear Fuel Cycle and Reactors Strategies: Adjusting to New Realities held in Vienna, 3–6 June 1997. The objective of the code is to calculate for a period of year the nuclear fuel cycle material and service requirements and material arisings for the different fuel cycle options.

It was used by the IAEA intensively for its internal purposes since then. Starting year 2003, the IAEA decided to enable interested parties from Member States to use VISTA tool through a user interface which is accessible through the internet. For this purpose, the tool was expanded to include new and future reactor and fuel types.

VISTA consists of two modules. First one is the overall nuclear material flow module which is the main part of VISTA calculation and the second one is the fuel depletion module CAIN which calculates the spent fuel composition in discharge time and after a cooling period.

VISTA and CAIN has been validated against other available and well accepted codes such as ORIGEN and WIMS as well as the measurement results. Overall nuclear material flow was also compared with the reported values from other organizations.

As a result, we can summarize VISTA as:

- A series of algorithms linking electricity generation and nuclear fuel operating data to nuclear fuel cycle material and service requirements and spent fuel arisings;
- A simplification to nuclear fuel cycle requirements modelling, by not reflecting the actual fuelling pattern reactor by reactor. VISTA does not take into account commissioning and shutdown schedules for each reactor;
- A method to calculate reactor type average requirements. For this purpose existing nuclear power reactors are grouped into 7 types as explained in Section 2.4
- A system capable of simulating the evolution of key fuel cycle features for given parameters, e.g. load factors, fuel burnup and enrichment, tails assay, reprocessing fractions, and recycling related parameters. All parameters can be changed from reactor type to reactor type and from time period to time period.
- A tool to track the individual actinide content in any stage of the nuclear fuel cycle including in the discharged and stored spent fuel even after a period of time. So it can be used to evaluate different fuel cycle options in terms of their effectiveness in reducing the radiotoxicity of the spent fuel or reducing the natural nuclear material requirements.
- A tool designed for being an optimum mixture of accuracy, simplicity and speed.

The VISTA simulation system is available in the Integrated Nuclear Fuel Cycle Information Systems web site (*http://www-nfcis.iaea.org/)* [2]. Appendix I gives more information about the VISTA website.

4.2. Conclusions

In its current status, VISTA is capable of evaluating the reactor parks with commercially existing reactor and fuel types. If the study is to be done for about or less than 30 years this is acceptable. In order to make analysis beyond 30 years, new fuel and reactor types should be introduced into the system. This is actually in progress by investigating the inclusion of the most probable fuel and reactor types. Currently, new reactors such as fast reactor types, high temperature gas cooled reactor types, and high conversion reactor may be considered. As for a new fuel cycle, thorium fuel cycle, molten salt reactors or ADS types may be considered.

In parallel to the development work of the internet version of the software, new fuel and reactor types have been introduced to the system including Pebble Bed Modular Reactor (PBMR), Gas Cooled (GTMHR), Pebble Bed Gas Cooled Fast Reactor (PBGCFR), European Fast Reactor (EFR) and Liquid Metal Cooled Fast Reactor (LMFR). The work for the other fuel cycle options with new fuel types including thorium fuel cycle and DUPIC fuel cycle is also underway. All of these new developments will be available in the full internet version.

The current VISTA version ignores the effect of commissioning of new reactors or shutdown of existing reactors (full core loading or full core unloading). This has no effect on a long run in cumulative amounts. But in order to increase the accuracy in annual requirements full core loading or full core unloading should be implemented in VISTA.

One of the purposes of the VISTA is to evaluate the radiotoxic impacts of the different nuclear fuel cycle options. Currently radiotoxicity can be calculated using isotopic contents from VISTA and their individual radiotoxic contribution. Direct calculation of radiotoxicity of fuel cycles is not available in VISTA. One of the improvements of the system might be to introduce the calculation of radioactivity and radiotoxicity of the spent fuel and high level wastes from different fuel cycle options directly in VISTA.

Appendix I VISTA WEBSITE

A web site has been developed to disseminate the VISTA to the Member States. The first phase of the web site included a detailed description of the simulation system including its fuel depletion model CAIN. A simple material flow calculation tool was also implemented in the first phase of the development.

The second phase of the VISTA web site development aimed at having an internet version of the VISTA tool with all capabilities: allowing users to create their own scenarios with their own data, creating the combination of the scenarios, selecting the requested result set. The web site is planned to have all the tools necessary to create and edit scenarios including data entry, chart displays.

The main internet address of the web site is http://www-nfcis.iaea.org/ which hosts actually more than VISTA. Some other IAEA databases which are related to the nuclear fuel cycle are also published in the same web site. The web site requires simple registration and login procedure only for statistical purposes. Everybody who has a valid email address can register and then use the system freely.

I.1.First phase of the development

The main purpose of the first phase of the VISTA web site development was to announce the system to interested parties. The development included the background information, the description of the model, an example study with inputs and outputs and a simple calculation tool which enables users to select their own fuel cycle parameters and make material flow calculation for a given year. Figure 33 shows web page which illustrates the information flow in the VISTA simulation system.

Figure 34 displays the page which is used for parameter entry by the users of the calculation tool. The form is filled with some default entries when it is first visited. The users, then, can either use those default data or freely enter the input parameters such as the nuclear capacity, or reactor type, or reprocessing ratio. After the selection and entrance of the material flow calculation is one-click away. When the user click the calculate button in just a few seconds, based on the speed of the internet connection of course, the results are displayed in diagram form in Figure 35.

Fig. 33. Description page from the VISTA web site.

A F A	nternational Atomic Energy Agency	NFCIS				Home Logout Feedback Disclaimer		NFCIS UDEPO PIE VISTA MADB Projects
	$\mathbb A$ Nuclear Fuel Cycle Simulation System							
Background	Description	Modeling	Example	Calculation	Full Version	Help		User Mehmet Ceyhan
	VISTA Calculation VISTA Equilibrium Core Annual Material Flow Calculation Calculation Model							
Fuel Cycle Option	UOX + MOX in LWR		\checkmark	Click to see the fuel cycle diagram.				Basic Calculation
			Reactor					
Reactor Type		PWR		Fuel Type 1		$UOX \times$		
				Fuel Type 2		$MOX-C$ \vee		
				Scenario Parameters (Default numbers are typical values for the selected option)				
Nuclear Power (MWe)		1000		Load Factor (%)		85		
Thermal Efficiency (%)		32.6		Tails assay from enrichment (%)		0.3		
				Fuel Parameters (Default numbers are typical values for the selected option)				
Fuel Type 1				Fuel Type 2 (share %)		5		
Mine Grade (% U)		$\mathbf 1$						
Enrichment (%)		3.968		Total Pu Content(%)		7.23		
Burnup (GWD/t)		45		Burnup (GWD/t)		45		
Reprocessing ratio (%)		33		Reprocessing ratio (%)		o		
Cooling Time before Reprocessing (y)		5	(v)	Cooling Time before Reprocessing		$\overline{7}$		
Rep U Use		$No \vee$		Uranium Source		DepU V		
Calculate	Hide Calculation							

Fig. 34. Data entry part of the simple material flow calculation too from VISTA web site.

The requirements and arisings for the above inputs

Fig. 35. Material flow result for the selected parameters from the VISTA web site.

I-1. Second phase of the development: Full internet version

After completing the first phase of the web site development, studies have been started to enable interested people to get benefit from the full capabilities of the VISTA simulation system. Hence, the second phase of the development work has focused on the development of a web based application which provides all features of the VISTA tool to the visitors of the web site. The development work is still ongoing and the prototype version is ready by the time of drafting of this TECDOC. The full version is expected to be completed and published by the time of the actual publication of this TECDOC.

Figures 36–41 show several screenshots from the prototype full version.

AEA	INFEIS		Home Logout Feedback Disclaimer			
ational Atomic Energy Agency					NFCIS UDEPO PIE VISTA MADB Projects	
$\mathbb A$ Nuclear Fuel Cycle Simulation System						
Background Description	Modeling Example	Calculation	Full Version	Help	User Mehmet Ceyhan	
Scenario List Fuel List Selected Scenario ()						
	List of Available VISTA Scenarios for User : Mehmet Ceyhan					
Create New Scenario						
Scenario Code	Scenario Explanation				Scenario Reference	
Scenario 2	Scenario 2			Scenario 2		
Test for a completely new scenario Scenario MC Test						
This page was retrieved on 2006-04-03.						
Send your comments to responsible officer. @ 2003 International Atomic Energy Agency.						

Fig. 36. Main entry to the full version: Scenario selection page.

Fig. 37. Description of the scenario and the selection of scenario parameters.

Fig. 38. Entering reactor types for the selected scenario.

Fig. 39. Entering the fuel details.

Fig. 40.Calculation page.

Fig. 41. Some results from the simulation.

Appendix II VISTA CALCULATION MODEL

The VISTA calculates annual average fuel cycle material and service requirements and material arisings and, whenever relevant, cumulative amounts by summing annual amounts. The mathematical model of the fuel cycle calculations has been developed by tracking the nuclear material from the beginning of the cycle to the end of cycle based on material balance principle.

The formulas which are given below in details are limited to the model used for this publication. Calculations are performed separately for each reactor type. The MOX fuel is produced by using the plutonium separated by reprocessing spent fuel and the depleted uranium from enrichment facilities. The lead times between fuel discharges, reprocessing and MOX fuel fabrication are taken into account in the calculations. Use of reprocessed uranium in uranium fuel is also eliminated from the calculation.

II.1. Definition of parameters (*variable***):**

- *Year* : Calculation year
- **Type** : Reactor type
- *Ft* : Fuel type
- *NuclearCapacity(year)* : Total nuclear capacity by year
- *ReactorMix(type,year)*: Ratio of nuclear power by reactor type and year
- *LoadFactor(type, year)* : Average load factor by reactor type and year
- *Efficiency(type,year)* : Average thermal efficiency by reactor type and year
- *Burnup(type, year,ft)* : Average discharge burnup by reactor type, year and fuel type
- *Share2Type(type,year,ft) :* Ratio of second fuel type *(ft=2 in all cases)*
- *Reprocessing(type, year,ft)*: Reprocessing ratio by reactor type, year and fuel type
- *Type2Uranium(type,year)* : Uranium source for second type fuel (DepU, RepU or NatU) by reactor type and year (for this publication, uranium source for second fuel type is limited to DepU from enrichment process)
- *Enrichment(type,year,ft)*: Initial enrichment in fresh fuel by reactor type, year and fuel type *(it is the amount of total Pu in case of U-Pu MOX fuel)*
- *Multirecycling* : Multirecycling parameter; 0 for no-multirecycling, 1 for multirecycling.
- *Residence(type,year,ft)* : Fuel residence time in core by reactor type, year and fuel type
- *TailsAssay(year) :* Average enrichment tails assay by year
- *EnrichmentLoss, FabricationLoss, ReprocessingLoss, ConversionLoss* : Process loss coefficients for each of the respective processes
- *ReprocessingCooling(type,year,ft):* Cooling time before reprocessing by reactor type, year and fuel type
- *FabricationTime(type,year,ft)*: Fuel fabrication times by reactor type, year and fuel type
- *ReprocessingTime(type,year,ft) :* Reprocessing time by reactor type, year and fuel type

II.2. Mathematical Model

The calculation steps are given below and follow the order of actual algorithm for each reactor type. Process losses are ignored in the formulas for easy reading.

Net nuclear capacity by reactor type (GWe)

TypeCapacity(type, year) = *ReactorMix(type, year)* TotalCapacity(year)*

Equilibrium core (tHM)

(Efficiency(type, year) (Burnup(type, year)) TypeCapacity(type, year)* 365* Residence(type, year)* LoadFactor(type, year) FullCore(type, year)* ⁼

Annual fresh fuel requirements (tHM)

FreshFuelT otal(type, year) = *FullCore(t ype, year) / Residence(type, year)*

Annual fuel loading (tHM)

Two categories of fuel have to be considered to calculate annual fuel loading in reactors. Index $f\hat{t}$ in below formulas corresponds to the fuel types in the material flow model. 2 and 1 refers to fuel type 2 and fuel type 1 respectively (ft=2, ft=1).

If there is enough reprocessed material in the stockpile

FreshFuel(type, year,2) = *FreshFuelT otal(type, year)* Share2Type (type, year,2)*

else

FreshFuel(type, $year, 2) = 0$

FreshFuel(type, year,1) = *FreshFuelT otal(type, year) - FreshFuel(type, year,2)*

Annual fuel unloading (tHM)

Annual fuel unloading is calculated for each fuel type taking into account the residence time of fuels in reactor. It means any fuel is discharged after burning in reactor for its residence time.

 $SFD(type, year, ft) = FreshFuel(type, year - Residence(type, year, ft), ft)$

 $=$ $\sum_{\rm ft}$ $SFDTotal(t$ ype, year) = \sum SFD(type, year, ft)

Spent fuel route (tHM)

Unloaded spent fuel can be either reprocessed or disposed of directly, depending on the type of reactor and fuel, and on the strategy considered. Spent fuel of all reactor types except LWRs is never reprocessed according to the simulation. The shares of LWR fuels that are reprocessed vary depending on the strategy considered. Simulation considers that the initial content of the second fuel type is same and the fuel can be recycled unlimited times.

Spent fuel to be stored for recycling (tHM)

 SFRS(type, year, ft) = *SFD(type, year, ft)* Reprocessi ng(type , year, ft)* $SFRSTotal$ (type,year) = Σ *ft* $SFRSTotal(type, year) = \sum SFRS(type, year, ft)$

Spent fuel to be stored for future use (or for disposal) (tHM)

SFS(type, year, ft) = *SFD(type, year, ft) - SFRS(type, year, ft)*

 $SFSTotal(t$ ype, year) = \sum_{ft} *SFSTotal(t ype, year) SFS(type, year, ft)*

Reprocessing (tHM)

SFR(type, year, ft) = *SFRS(type, year1, ft)*

where

year2(ft) = *Reprocessi ngCooling(type, year, ft)* + *Reprocessi ngTime(typ e, year, ft)*

 $\text{year1}(ft) = \text{year} - \text{year2}(ft)$

 $=\sum_{ft}$ *SFRTotal(t ype, year) SFR(type, year, ft)*

Availability of reprocessed material for fuel type 2 (Pu in case of MOX fuel) (tHM)

The availability of reprocessed material is calculated by calculating the isotopic content of spent fuel. The fuel depletion code CAIN is used to calculate isotopic content of spent fuel. There is also possibility to use actinide tables from other authoritative depletion codes such as ORIGEN. CAIN calculates isotopic composition of spent nuclear fuels for different initial fissile content, different discharge burnup and different cooling times.

NucStock(*type*, *year*, *n*) =
$$
\sum_{f}
$$
 SFR(*type*, *year*, *ft*) * *NucContent*(*type*, *year1*(*ft*), *ft*, *n*, *year2*(*ft*)))

where

NucStock(type, year,n) is the available isotope n amount from reprocessing

NucContent(type, year1, ft,n, year2(ft)) is the content of isotope *n* in spent fuel type \hat{f} after cooling time *year2*

year2(ft) = *Reprocessi ngCooling(type, year, ft)* + *Reprocessi ngTime(typ e, year, ft)*

 $\text{year1}(ft) = \text{year} - \text{year2}(ft)$

Used nuclear material (tHM)

 $=\sum_{ft}$ *UsedNuc(type, year,n)* = \sum *FreshFuel(type, year, ft)** *NucContent (type, year, ft,n,0))*

Natural uranium savings due to recycling of Pu (in MOX) (tHM)

0.00711 -TailsAssay(type, year) Enrichment(type, year)-TailsAssay(type, year) K(type, year) ⁼

NatUSavingPu(type, year) = *K* FreshFuel(type, year,2)*

Annual plutonium arising in discharged spent fuel

 $=$ \sum_{ft} \sum_{n} \sum_{p} $\text{AnnualTotP } u(\text{type}, \text{year}) = \sum \sum \text{SFD}(\text{type}, \text{year}, \text{ft})^* \text{Nu } c\text{Content}(\text{type}, \text{year}, \text{ft}, n, 0)$

Annual enrichment service requirements (MTSWD)

 ** FreshFuel(type, year) SWURequirement(type, year)*= *{Ve(type, year)*+ *(K(type, year)- 1)* Vt(type, year)- K(type, year)* Vn(type, year)}*

⎩ ⎨ \int $\text{EnrichedU(type, year)} = \begin{cases} \text{FreshFuel(type, year,1)} & \text{if enrichment(type, year,1) > 0.711} \\ 0 & \text{if enrichment(type, year,1) < = 0.711} \end{cases}$

DepletedU(type, year) = *EnrichedU(type, year)* (K(type, year)- 1)*

where

$$
K(type, year) = \frac{Enrichment(type, year) - TailsAssay(type, year)}{0.00711 - TailsAssay(type, year)}
$$

 $Ve(type, year) = \{2 * Enrichment(type, year)/100 - 1\} * LN\{\frac{Enrichment(type, year)/100}{I - Enrichment(type, year)/100}\}$

 $Vt(type, year) = \{2 * TailsAssay(type, year)/100 - 1\} * LN\left\{\frac{TailsAssay(type, year)/100}{1 - TailsAssay(type, year)/100}\right\}$

 $Vn(type, year) = {2 * 0.00711 - 1} * LN{ \frac{0.00711}{1 - 0.00711} }$

Annual conversion requirements (tHM)

FreshFuel(type,year,1) if Enrichment 0.711 EnrichedU(type,year) DepletedU(type,year) if Enrichment 0.711 ConvRequirement(type, year) \overline{a} ⎨ \int $=\begin{cases} EnrichedU(type, year) + DepletedU(type, year) & if Enrichment > 0 \\ FreshFuel(type, year, 1) & if Enrichment < 1 \end{cases}$

Annual natural uranium requirements (tHM)

NatURequirement(type, year)= *ConvRequirement(type, year)*

Appendix III REACTION AND DECAY CHAINS

The following list gives the reaction chains used in CAIN to calculate the changes in isotopic calculations during the irradiation period. The decay of each nuclide is also taken into consideration during the irradiation period.

CHAIN 0 (Decay and capture of initial *238Pu* during irradiation)

 238 *Pu* $\frac{(87.7 \text{ y})}{x}$ *x* $^{238}Pu \xrightarrow{(n,\gamma)} x$ **CHAIN** 1 ** $\frac{(n,\gamma)}{2^{35}U}$ $\frac{(n,\gamma)}{2^{36}U}$ $\frac{(n,\gamma)}{2^{37}Np}$ $\frac{(n,\gamma)}{2^{38}Pu}$ **CHAIN** 2 ** $U \xrightarrow{(n,2n)} 237 \text{ Np} \xrightarrow{(n,\gamma)} 238 \text{ P} u$ **CHAIN** 3 ** $^{238}U^{(n,\gamma)}$ $^{239}Pu^{(n,\gamma)}$ $^{240}Pu^{(n,\gamma)}$ $^{241}Pu^{(n,\gamma)}$ $^{242}Pu^{(n,\gamma)}$ $^{242}Pu^{(n,\gamma)}$ $^{243}Am^{(n,\gamma)}$ ^{244}Cm **CHAIN** 4 ** $^{238}U^{-(n,y)}\rightarrow ^{239}Pu^{-(n,y)}\rightarrow ^{240}Pu^{-(n,y)}\rightarrow ^{241}Pu^{-(14.4y)}\rightarrow ^{241}Am^{-(n,y)(88.36\%)+decay(82.7\%)}\rightarrow ^{242}Cm^{-(0.446y)}\rightarrow ^{238}Pu^{-(0.446y)}$ **CHAIN** 5 ** $^{238}U^{-(n,y)}\rightarrow ^{239}Pu^{-(n,y)}\rightarrow ^{240}Pu^{-(n,y)}\rightarrow ^{241}Pu^{-(144y)}\rightarrow ^{241}Am^{-(n,y)(8836\%) \text{H}decay (17.3\%)}\rightarrow ^{242}Pu^{-(n,y)}\rightarrow ^{243}Am^{-(n,y)}\rightarrow ^{244}Cm^{-(n,y)}$ **CHAIN** 6 ** $^{238}U^{-(n,y)}\rightarrow ^{239}Pu^{-(n,y)}\rightarrow ^{240}Pu^{-(n,y)}\rightarrow ^{241}Pu^{-(144y)}\rightarrow ^{241}Am^{-(n,y)(11.64\%)}\rightarrow ^{242m}Am^{-(n,y)}\rightarrow ^{243}Am^{-(n,y)}\rightarrow ^{244}Cm$ **CHAIN** (ignored for irradiation period (half life = 432 year)) $^{238}U^{(n,y)}\rightarrow ^{239}Pu^{(n,y)}\rightarrow ^{240}Pu^{(n,y)}\rightarrow ^{241}Pu^{(14.4y)}\rightarrow ^{241}Am^{(432y)}\rightarrow ^{237}Np^{(n,y)}\rightarrow ^{238}Pu^{(n,y)}$ **CHAIN** (ignored for irradiation period (half life = 6560 year)) $^{238}U^{(n,\gamma)}\rightarrow ^{239}Pu^{(n,\gamma)}\rightarrow ^{240}Pu^{(6560y)}\rightarrow ^{236}U^{(n,\gamma)}\rightarrow ^{237}Np^{(n,\gamma)}\rightarrow ^{238}Pu$ **CHAIN** 7 ** ^{239}Pu $\xrightarrow{(n,\gamma)}$ ^{240}Pu $\xrightarrow{(n,\gamma)}$ ^{241}Pu $\xrightarrow{(n,\gamma)}$ ^{242}Pu $\xrightarrow{(n,\gamma)}$ ^{243}Am $\xrightarrow{(n,\gamma)}$ ^{244}Cm

CHAIN 8 **

 $^{239}Pu \xrightarrow{(n,y)} ^{240}Pu \xrightarrow{(n,y)} ^{241}Pu \xrightarrow{(14.4y)} ^{241}Am \xrightarrow{(n,y)(88.36\%)+decay (82.7\%)} ^{242}Cm \xrightarrow{(0.446y)} ^{238}Pu$ **CHAIN** 9 **

 $^{239}Pu \xrightarrow{(n,r)} ^{240}Pu \xrightarrow{(n,r)} ^{241}Pu \xrightarrow{(14.4y)} ^{241}Am \xrightarrow{(n,r)} ^{(88.36\%) \text{H}decay (17.3\%)} ^{242}Pu \xrightarrow{(n,r)} ^{243}Am \xrightarrow{(n,r)} ^{244}Cm$

CHAIN 10 ***

 ^{239}Pu \rightarrow $^{(n,r)}$ \rightarrow ^{240}Pu \rightarrow ^{241}Pu \rightarrow $^{(144y)}$ \rightarrow ^{241}Am \rightarrow $^{(n,r)(11.64\%)}$ \rightarrow ^{242m}Am \rightarrow $^{(n,r)}$ \rightarrow ^{243}Am \rightarrow ^{244}Cm

CHAIN (ignored for irradiation period (half life = 432 year))

 $^{239}Pu \xrightarrow{(n,y)} ^{240}Pu \xrightarrow{(n,y)} ^{241}Pu \xrightarrow{(144y)} ^{241}Am \xrightarrow{(432y)} ^{237}Np \xrightarrow{(n,y)} ^{238}Pu$

CHAIN (ignored for irradiation period (half life = 6560 year))

 $^{239}Pu \xrightarrow{(n,\gamma)} ^{240}Pu \xrightarrow{(6560y)} ^{236}U \xrightarrow{(n,\gamma)} ^{237}Np \xrightarrow{(n,\gamma)} ^{238}Pu$

CHAIN 11 ***

 ^{240}Pu \longrightarrow ^{241}Pu \longrightarrow $^{(n,\gamma)}$ \longrightarrow ^{242}Pu \longrightarrow $^{(n,\gamma)}$ \longrightarrow ^{243}Am \longrightarrow $^{(n,\gamma)}$ \longrightarrow ^{244}Cm

CHAIN 12 ***

 $^{240}Pu \xrightarrow{(n,y)} ^{241}Pu \xrightarrow{(14.4y)} ^{241}Am \xrightarrow{(n,y)(88.36\%)+decay (82.7\%)} ^{242}Cm \xrightarrow{(0.446 y)} ^{238}Pu$

CHAIN 13 ***

 $^{240}Pu \xrightarrow{(n,y)} ^{241}Pu \xrightarrow{(144y)} ^{241}Am \xrightarrow{(n,y)(88.36\%) \text{H} decay(17.3\%)} ^{242}Pu \xrightarrow{(n,y)} ^{243}Am \xrightarrow{(n,y)} ^{244}Cm$

CHAIN 14 ***

 ^{240}Pu \longrightarrow ^{241}Pu \longrightarrow $^{(14.4y)}$ \longrightarrow ^{241}Am \longrightarrow $^{(n,y)(11.64\%)}$ \longrightarrow ^{242m}Am \longrightarrow $^{(n,y)}$ \longrightarrow ^{243}Am \longrightarrow ^{244}Cm

CHAIN (ignored for irradiation period (half life = 432 year))

 $^{240}Pu \rightarrow ^{241}Pu \rightarrow ^{241}Pu$ $(14.4y) \rightarrow ^{241}Am \rightarrow ^{232}Np \rightarrow ^{237}Np \rightarrow ^{238}Pu$

CHAIN (ignored for irradiation period (half life = 6560 year))

 $\frac{p_u - (6560y)}{236}$ \rightarrow $\frac{(n,y)}{237}$ \rightarrow $\frac{(n,y)}{238}$ \rightarrow $\frac{p_u - (6560y)}{236}$

CHAIN 15 ***

 $\frac{241}{P_u} - \frac{(n,y)}{242} P_u - \frac{(n,y)}{243} A_m - \frac{(n,y)}{244} C_m$

CHAIN 16 ***

 ^{241}Pu \longrightarrow ^{241}Am \longrightarrow ^{241}Am \longrightarrow $^{(n,y)(88.36\%)+decay(82.7\%)}$ \longrightarrow ^{242}Cm \longrightarrow $^{(0.446\ y)}$ \longrightarrow ^{238}Pu

CHAIN 28 **

 $\mu^{236} U \xrightarrow{(n,\gamma)} {}^{237} Np \xrightarrow{(n,\gamma)} {}^{238} P u$

The following 14 chains are used to calculate the changes in the isotopic composition of spent fuel during the cooling/storage period after the discharge from the reactor. The period assumes there is no neutron in the medium and there is no fission occurred. The only reaction is the radioactive decays of the nuclides. The end nuclide of each decay chain is out of the calculation and shown as *x*.

DECAY CHAIN 11 **

 $2^{42m}Am - \frac{(141y)}{2^{42}Cm - \frac{(0.446y)}{2^{38}Pu - \frac{(87.7y)}{2}}x}$

DECAY CHAIN 12 **

 $\frac{(7.37 \cdot 10^3 y)}{243}$ $\frac{239}{9}$ $\frac{p_u - (2.41 \cdot 10^4 y)}{235}$ $\frac{(7.04 \cdot 10^8 y)}{x}$ $\frac{x}{24}$

DECAY CHAIN 13 **

 $2^{42}Cm \xrightarrow{(0.446y)} 2^{38}Pu \xrightarrow{(87.7y)} x$

DECAY CHAIN 14 **

 $2^{44}Cm \xrightarrow{(18.1y)} 2^{40}Pu \xrightarrow{(6.56 \cdot 10^3 y)} 2^{36}U \xrightarrow{(2.34 \cdot 10^7 y)} x$

Appendix IV CROSS-SECTIONS USED IN CALCULATIONS

VISTA is capable of using any reactor and fuel type if one group neutron cross sections are provided. For the purpose of this publication, 7 reactor types with 9 fuel types (7 uranium fuels and 2 MOX fuels) were introduced to the system. One group neutron cross sections of those 9 fuel types are given in TABLES 9–17.

Nuclide	σ_c (inc σ_{ex})	σ_{f}	σ_{n2n}	$T_{1/2}(y)$
235 U	10.4600	46.7100	0.002696	$7.04E + 08$
236 U	7.5410	0.1975	0.002644	$2.34E + 07$
238 U	0.9021	0.1004	0.005525	4.47E+09
237 Np	32.1200	0.5244	0.000275	$2.14E + 06$
^{238}Pu	34.6700	2.4650	0.000167	$8.77E + 01$
239 Pu	58.6100	106.2000	0.001120	$2.41E + 04$
240 Pu	104.0000	0.5840	0.000448	$6.56E + 03$
241 Pu	38.6800	118.1000	0.007518	$1.44E + 01$
242 Pu	31.7200	0.4146	0.002307	$3.75E + 05$
241 Am	118.8000	1.1230	0.000328	$4.33E + 02$
$242m$ Am	98.0400	466.2000	0.005670	$1.41E + 02$
243 Am	49.4870	0.3959	0.000207	$7.37E + 03$
242 Cm	5.8010	0.5591	0.000053	4.46E-01
244 Cm	13.8200	0.8746	0.001048	$1.81E + 01$

TABLE 9. ONE GROUP NEUTRON CROSS-SECTIONS FOR PWR URANIUM FUEL (BARN)

TABLE 10. ONE GROUP NEUTRON CROSS-SECTIONS FOR BWR URANIUM FUEL (BARN)

Nuclide	σ_c (inc σ_{ex})	$\sigma_{\scriptscriptstyle{f}}$	σ_{n2n}	$T_{1/2}(y)$
235 U	11.21000	50.00000	0.001969	$7.04E + 08$
236 U	8.24900	0.16480	0.001935	$2.34E + 07$
238 U	0.91900	0.08083	0.004039	$4.47E + 09$
237 Np	34.07000	0.46150	0.000210	$2.14E + 06$
238 Pu	37.27000	2.48800	0.000123	$8.77E + 01$
239 Pu	63.07000	114.10000	0.000818	$2.41E + 04$
240 Pu	111.10000	0.52660	0.000328	$6.56E+03$
241 Pu	41.51000	126.30000	0.005496	$1.44E + 01$
242 Pu	33.07000	0.40380	0.002245	$3.75E + 05$
241 Am	121.30000	1.12500	0.000319	$4.33E+02$
$242m$ Am	234.2638	1210.7879	0.004338	$1.41E + 02$
243 Am	51.58100	0.38520	0.000202	$7.37E + 03$
242 Cm	6.03300	0.55540	0.000052	4.46E-01
244 Cm	14.39000	0.87090	0.001019	$1.81E + 01$

Nuclide	σ_c (inc σ_{ex})	σ_{f}	σ_{n2n}	$T_{1/2}(y)$
235 U	28.6400	159.10000	0.001391	$7.04E + 08$
236 U	5.6590	0.10750	0.001487	$2.34E + 07$
238 U	1.1650	0.05424	0.002779	$4.47E + 09$
237 Np	58.6300	0.29150	0.000046	$2.14E + 06$
238 Pu	142.5000	5.08700	0.000109	$8.77E + 01$
239 Pu	123.1000	267.30000	0.000587	$2.41E + 04$
240 Pu	144.5000	0.33290	0.000268	$6.56E+03$
241 Pu	115.6000	339.40000	0.003755	$1.44E + 01$
242 Pu	23.8100	0.25170	0.001105	$3.75E + 05$
241 Am	393.37000	2.19100	0.000069	$4.33E + 02$
$242m$ Am	849.4000	4166.0000	0.000658	$1.41E + 02$
243 Am	76.274	0.06523	0.000045	$7.37E + 03$
242 Cm	12.1400	1.67700	0.000010	4.46E-01
244 Cm	23.1900	1.03790	0.000217	$1.81E + 01$

TABLE 11. ONE GROUP NEUTRON CROSS-SECTIONS FOR PHWR URANIUM FUEL (BARN)

TABLE 12. ONE GROUP NEUTRON CROSS-SECTIONS FOR RBMK URANIUM FUEL (BARN)

Nuclide	σ_c (inc σ_{ex})	σ_f	σ_{n2n}	$T_{1/2}(y)$
235 U	17.9000	93.0000	$\boldsymbol{0}$	$7.04E + 08$
236 U	5.6900	0.0920	$\boldsymbol{0}$	$2.34E + 07$
238 U	0.8670	0.0452	0.00226	$4.47E + 09$
237 Np	41.9000	0.2610	$\boldsymbol{0}$	$2.14E + 06$
238 Pu	74.9000	3.0500	$\boldsymbol{0}$	$8.77E + 01$
^{239}Pu	113.0000	210.0000	$\boldsymbol{0}$	$2.41E + 04$
240 Pu	122.0000	0.3040	$\boldsymbol{0}$	$6.56E + 03$
^{241}Pu	79.9000	238.0000	$\boldsymbol{0}$	$1.44E + 01$
^{242}Pu	24.7000	0.2210	$\boldsymbol{0}$	$3.75E + 05$
241 Am	179.9000	1.4600	$\boldsymbol{0}$	$1.41E + 02$
$242m$ Am	432	2775	$\boldsymbol{0}$	$4.33E + 02$
243 Am	42.4200	0.1680	$\mathbf{0}$	$7.37E + 03$
242 Cm	2.6400	0.8310	$\mathbf 0$	4.46E-01
244 Cm	10.6000	0.9780	$\boldsymbol{0}$	$1.81E + 01$

Nuclide	σ_c (inc σ_{ex})	σ_{f}	σ_{n2n}	$T_{1/2}(y)$
235 U	19.0000	84.0000	$\boldsymbol{0}$	$7.04E + 08$
236 U	6.1700	0.1200	$\boldsymbol{0}$	$2.34E + 07$
238 U	1.0600	0.05640	0.00226	$4.47E + 09$
237 Np	52.0400	0.3060	$\boldsymbol{0}$	$2.14E + 06$
^{238}Pu	118.4000	4.4200	$\boldsymbol{0}$	$8.77E + 01$
^{239}Pu	125.0000	240.0000	$\boldsymbol{0}$	$2.41E + 04$
240 Pu	142.0000	0.3526	$\boldsymbol{0}$	$6.56E + 03$
241 Pu	101.000	319.0000	$\boldsymbol{0}$	$1.44E + 01$
^{242}Pu	31.2000	0.2650	$\boldsymbol{0}$	$3.75E + 05$
241 Am	179.9000	1.4600	$\boldsymbol{0}$	$4.33E + 02$
$242m$ Am	432	2775	$\boldsymbol{0}$	$1.41E + 02$
243 Am	42.4200	0.1680	$\boldsymbol{0}$	$7.37E + 03$
242 Cm	2.6400	0.8310	$\boldsymbol{0}$	4.46E-01
244 Cm	10.6000	0.978	$\boldsymbol{0}$	$1.81E + 01$

TABLE 13. ONE GROUP NEUTRON CROSS-SECTIONS FOR AGR URANIUM FUEL (BARN)

TABLE 14. ONE GROUP NEUTRON CROSS-SECTIONS FOR GCR URANIUM FUEL (BARN)

Nuclide	σ_c (inc σ_{ex})	σ_{f}	σ_{n2n}	$T_{1/2}(y)$
235 U	19.0000	96.0000	$\boldsymbol{0}$	$7.04E + 08$
236 U	6.3000	0.13000	$\boldsymbol{0}$	$2.34E + 07$
238 U	0.8800	0.06000	0.00278	$4.47E + 09$
237 Np	48.0000	0.30000	$\boldsymbol{0}$	$2.14E + 06$
^{238}Pu	118.0000	4.00000	$\boldsymbol{0}$	$8.77E + 01$
239 Pu	139.0000	249.00000	$\boldsymbol{0}$	$2.41E + 04$
240 Pu	185.0000	0.38000	$\boldsymbol{0}$	$6.56E+03$
^{241}Pu	107.0000	255.00000	$\boldsymbol{0}$	$1.44E + 01$
242 Pu	25.0000	0.30000	$\boldsymbol{0}$	3.75E+05
241 Am	391.7000	2.19100	$\boldsymbol{0}$	$4.33E+02$
$242m$ Am	849.4	4166	$\boldsymbol{0}$	$1.41E+02$
243 Am	75.8140	0.06523	$\boldsymbol{0}$	$7.37E + 03$
242 Cm	12.1400	1.67700	$\boldsymbol{0}$	4.46E-01
244 Cm	23.1900	1.03790	$\boldsymbol{0}$	$1.81E + 01$

Nuclide	σ_c (inc σ_{ex})	σ_{f}	$\sigma_{\scriptscriptstyle n2n}$	$T_{1/2}(y)$
235 U	8.1400	35.1100	0.00430	$7.04E + 08$
236 U	6.4000	0.2100	0.00270	$2.34E+07$
238 U	0.9600	0.1000	0.00570	$4.47E + 09$
237 Np	29.7400	0.5300	0.00150	$2.14E + 06$
238 Pu	25.2100	2.4100	0.00014	$8.77E + 01$
239 Pu	49.2000	86.5700	0.00150	$2.41E + 04$
240 Pu	153.0700	0.5800	0.00140	$6.56E + 03$
241 Pu	30.9200	92.4900	0.00310	$1.44E + 01$
242 Pu	29.8700	0.4200	0.00200	$3.75E + 05$
241 Am	95.7900	1.0200	0.00076	$4.33E + 02$
$242m$ Am	130.4300	564.78000	0.00071	$1.41E + 02$
243 Am	49.0300	0.4500	0.00150	$7.37E + 03$
242 Cm	4.2800	1.3500	0.00046	4.46E-01
244 Cm	15.4400	0.8200	0.00110	$1.81E + 01$

TABLE 15. ONE GROUP NEUTRON CROSS-SECTIONS FOR WWER URANIUM FUEL (BARN)

TABLE 16. ONE GROUP NEUTRON CROSS-SECTIONS FOR PWR-MOX FUEL (BARN)

Nuclide	σ_c (inc σ_{ex})	σ_{f}	σ_{n2n}	$T_{1/2}(y)$
235 U	6.3980	22.6900	0.0032	$7.04E + 08$
236 U	8.4870	0.2166	0.0031	$2.34E + 07$
238 U	0.8718	0.1105	0.0064	4.47E+09
237 Np	24.2300	0.5713	0.0004	$2.14E + 06$
^{238}Pu	15.2600	2.0330	0.0002	$8.77E + 01$
239 Pu	26.0400	46.4500	0.0013	$2.41E + 04$
240 Pu	43.8800	0.6222	0.0005	$6.56E + 03$
241 Pu	16.7200	54.5200	0.0087	$1.44E + 01$
242 Pu	25.5600	0.5354	0.0024	$3.75E + 05$
241 Am	64.3940	0.8959	0.0004	$4.33E + 02$
$242m$ Am	45.8400	224.4000	0.0066	$1.41E + 02$
243 Am	41.9900	0.4455	0.0003	$7.37E + 03$
242 Cm	5.3410	0.4676	0.0001	4.46E-01
244 Cm	13.8400	0.9332	0.0012	$1.81E + 01$

Nuclide	σ_c (inc σ_{ex})	σ_{f}	σ_{n2n}	$T_{1/2}(y)$
235 U	8.131000	32.0200	0.002190	$7.04E + 08$
236 U	8.624000	0.1792	0.002159	$2.34E + 07$
238 U	0.871900	0.0881	0.004502	$4.47E + 09$
237 Np	27.960000	0.4995	0.000230	$2.14E + 06$
^{238}Pu	22.650000	2.1590	0.000137	$8.77E + 01$
^{239}Pu	38.520000	69.2000	0.000910	$2.41E + 04$
240 Pu	52.630000	0.5540	0.000366	$6.56E + 03$
241 Pu	25.010000	78.7700	0.006098	$1.44E + 01$
^{242}Pu	26.200000	0.4607	0.001722	$3.75E + 05$
241 Am	86.790000	0.978	0.004741	$4.33E + 02$
$242m$ Am	66.720000	321.6000	0.000218	$1.41E + 02$
243 Am	46.200000	0.4163	0.000056	$7.37E + 03$
242 Cm	5.767000	0.4963	0.001102	4.46E-01
244 Cm	14.520000	0.9094	0.000419	$1.81E + 01$

TABLE 17. ONE GROUP NEUTRON CROSS-SECTIONS FOR BWR-MOX FUEL (BARN)

The results of CAIN code for 9 different fuel types are presented in Tables 18-26. The tables give isotopic compositions at the time of discharge from the reactor. However CAIN is capable of calculating isotopic calculatio The results of CAIN code for 9 different fuel types are presented in Tables 18–26. The tables give isotopic compositions at the time of discharge from the reactor. However CAIN is capable of calculating isotopic calculations after a waiting period following the discharge.

TABLE 18: ISOTOPIC COMPOSITION OF SPENT URANIUM FUEL (%) - PWR TABLE 18: ISOTOPIC COMPOSITION OF SPENT URANIUM FUEL (%) - PWR

TABLE 19: ISOTOPIC COMPOSITION OF SPENT URANIUM FUEL (%) - BWR TABLE 19: ISOTOPIC COMPOSITION OF SPENT URANIUM FUEL (%) - BWR

3.10 30.00 0.492498 0.397423 95.441165 0.021962 0.005895 0.256750 0.190159 0.060766 0.032101 0.003342 0.000385 0.003308 0.000723 0.000483

0.000483

TABLE 23: ISOTOPIC COMPOSITION OF SPENT URANIUM FUEL $(\%)$ — GCR TABLE 23: ISOTOPIC COMPOSITION OF SPENT URANIUM FUEL (%) — GCR

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Appendix VI VALIDATION AND BENCHMARKING OF CAIN MODEL

In order to use CAIN code in the VISTA simulation system, one needs to validate the CAIN code against the other available well known codes and measurement results. The validation study was performed for uranium fuels and MOX fuels separately since handling MOX fuels was added to the system later on.

VI.1. Validation of CAIN code for uranium fuels

Different methods and sources were used to validate CAIN code for uranium fuels. For PWR, BWR and PHWR uranium fuels CAIN results were compared with those given by ORIGEN code (Section VI.1.1). Both calculations used the same cross section set which is available in ORIGEN standard library. For AGR, GCR, RBMK and PHWR uranium fuels, validation against WIMS code was performed (Section VI.1.3). In addition, CAIN results are compared with available measurements (Section VI.1.2).

VI.1.1. CAIN vs. ORIGEN

The CAIN burnup calculation was compared with the ORIGEN code for 3 reactor types, which are PWR, BWR and PHWR. Since cross sections and the neutron flux are identical for both CAIN and ORIGEN, these two results should be identical except the small influence due to the assumptions listed in Section 2.5.5.3.

TABLES 27–29 show the comparisons of CAIN and ORIGEN results. The results show that the CAIN code agrees very well to the ORIGEN, and the errors are less than 1–2% for PWR and BWR cases. For PHWR case, the CAIN code also agrees very well to the ORIGEN within 1-5% error except 238 Pu. 238 Pu concentration calculated by the ORIGEN is 10% smaller, and this may be due to an inappropriate large 237 U cross section in the ORIGEN.

Based on these results, it is concluded that the CAIN model gives essentially identical results to the ORIGEN.

Isotope	$CAIN(wt\%)$	ORIGEN (wt%)	Error $(\%)$
235 U	0.679918	0.679800	0.02
236 U	0.524208	0.524400	-0.04
238 U	93.046956	93.050000	0.00
237 Np	0.068681	0.068590	0.13
^{238}Pu	0.024492	0.024040	1.88
^{239}Pu	0.511364	0.518300	-1.34
240 Pu	0.263429	0.265100	-0.63
241 Pu	0.150552	0.151300	-0.49
242 Pu	0.064934	0.065110	-0.27
241 Am	0.004761	0.004772	-0.23
$242m$ Am	0.000108	N/A	N/A
243 Am	0.014612	0.014530	0.56
242 Cm	0.001791	0.001801	-0.53
244 Cm	0.004835	0.004832	0.06
Total	95.360641	95.372575	-0.01

TABLE 27: CAIN AND ORIGEN COMPARISON (PWR WITH 4.0% ENRICHMENT AT 45 MW $\cdot d/kg$)

TABLE 28: CAIN AND ORIGEN COMPARISON (BWR WITH 4.0% ENRICHMENT AT 45 MW·d/kg)

Isotope	$CAIN(wt\%)$	ORIGEN (wt%)	Error $(\%)$
235 U	0.626722	0.625100	0.26
236 U	0.527411	0.527700	-0.05
238 U	93.125703	93.120000	0.01
237 Np	0.070138	0.070180	-0.06
^{238}Pu	0.026709	0.026630	0.30
^{239}Pu	0.485480	0.491600	-1.24
^{240}Pu	0.255193	0.256800	-0.63
241 Pu	0.146241	0.146800	-0.38
242 Pu	0.067542	0.067850	-0.45
241 Am	0.006797	0.007037	-3.42
$242m$ Am	0.000155	N/A	N/A
243 Am	0.015633	0.015590	0.27
242 Cm	0.001981	0.002015	-1.69
244 Cm	0.005273	0.005264	0.18
Total	95.360977	95.362566	0.00

Isotope	$CAIN(wt\%)$	ORIGEN (wt%)	Error $(\%)$
235 U	0.236956	0.232600	1.87
236 U	0.071047	0.071830	-1.09
238 U	98.583303	98.570000	0.01
237 Np	0.002596	0.002576	0.76
^{238}Pu	0.000333	0.000303	9.81
^{239}Pu	0.265876	0.270100	-1.56
240 Pu	0.095796	0.097760	-2.01
^{241}Pu	0.018118	0.018670	-2.96
242 Pu	0.003937	0.004132	-4.72
241 Am	0.000183	0.000187	-2.37
$242m$ Am	0.000002	N/A	N/A
243 Am	0.000123	0.000130	-4.82
242 Cm	0.000060	0.000055	8.32
244 Cm	0.000010	0.000011	-7.02
Total	99.278338	99.268354	0.01

TABLE 29: CAIN AND ORIGEN COMPARISON (PHWR WITH 0.71% ENRICH. AT 7 MW·D/KG)

VI.1.2. CAIN vs. measurement

Direct verification of the CAIN model was performed by comparing its results with the measurement on discharged fuels for PWR and BWR fuels.

There is one report of 220 pages [28], which compiles the results of the open data on the actinide measurement of the discharged fuels from both PWRs and BWRs. This report contains PIE (post irradiation experiment) data for the spent fuels from 7 PWRs and 6 BWRs. Unfortunately, most of the data are shown in the format of tables, and the only available graphs on ^{235}U and Pu composition are shown here. Figures 42–48 are the comparison between CAIN results and the measured data for 235 U, total Pu, and each Pu $(^{239}$ Pu, 240 Pu, 241 Pu, 242 Pu, 238 Pu) composition.

In order to verify the CAIN model, two calculations were performed for the 3% enrichment of PWR and BWR fuel. Based on the report, the actual enrichments vary from 2.5% to 3.4%, and this would affect the result slightly. But, in general, the CAIN model agrees very well with the measurement. As can be seen in the figures, there is very little difference between PWR and BWR. Actually, because of the similar neutron spectrum for both reactors, isotopic composition would become similar. Usually, PWR is using smaller fuel rod, and this will cause a little bit higher amount of plutonium due to larger resonance absorption for the same enrichment.

Regarding other actinides such as Np/Am/Cm, another report is available [29]. The comparison between the CAIN model and the PIE data is shown in Figures 49–51 on 237 Np, 241 Am, 243 Am, 242 Cm and 244 Cm. The CAIN model also agrees well for these actinides. As for the content of 241 Pu or 242 Cm, the measurement may include the effect of the decay,

meanwhile the calculation does not include the effect of the decay of 14.4 years half life of 241 Pu and 0.446 year of 242 Cm. the CAIN calculation is done by assuming zero cooling time. If the PIE has been done after short cooling time, this factor would not affect the results.

Fig. 42.CAIN vs. Measurement (235U).

Fig. 43.CAIN vs. Measurement (Pu total).

Fig. 44.CAIN vs. Measurement (239Pu).

Fig. 45. CAIN vs. Measurement $\binom{240}{ }$ *Pu*).

Fig. 46.CAIN vs. Measurement (241Pu).

Fig. 47.CAIN vs. Measurement (242Pu).

Fig. 49.CAIN vs. Measurement (237Np).

Fig. 51. CAIN vs. Measurement ℓ^{242} *Cm and* ℓ^{244} *Cm).*

VI.1.3. CAIN vs. WIMS

For other reactors such as RBMK, GCR and AGR, verification was performed against the WIMS results, which have been provided by the Canadian consultant. The WIMS calculations were carried out in 33 energy groups. Also, just for confirmation, same comparison was done for PHWR. In these CAIN calculations, cross sections given in TABLE 30–TABLE 33 were used in order to keep consistency with the WIMS library. Also, the power density is set to 25 kW/kg for PHWR, 16 kW/kg for RBMK and 15 kW/kg for AGR in order to keep consistency with WIMS inputs. The results are shown in TABLES 34–37.

TABLE 30: CROSS SECTIONS (BARNS) AT MID-BURNUP

AGR, 24 MW·d/kg - 2.6% Fuel

TABLE 31: CROSS SECTIONS (BARNS) AT MID-BURNUP

GGR, 4 MW·d/kg - 0.71% Fuel

TABLE 32: CROSS SECTIONS (BARNS) AT MID-BURNUP

PHWR, 7 MW·d/kg - 0.71% Fuel

TABLE 33: CROSS SECTIONS (BARNS) AT MID-BURNUP

RBMK, 18.5 MW·d/kg - 1.8% Fuel

Isotope	$CAIN(wt\%)$	WIMS $(wt\%)$	Error $(\%)$
235 U	0.240804	0.242000	-0.49
236 U	0.068596	0.070500	-2.70
238 U	98.605267	98.630000	-0.03
237 Np	0.001220	0.001240	-1.65
^{238}Pu	0.000177	N/A	N/A
239 Pu	0.245007	0.252000	-2.78
240 Pu	0.090768	0.092300	-1.66
241 Pu	0.021008	0.018200	15.43
242 Pu	0.005116	0.004670	9.55
241 Am	0.000188	0.000163	15.38
$242m$ Am	0.000002	N/A	N/A
243 Am	0.000151	0.000152	-0.35
242 Cm	0.000043	N/A	N/A
244 Cm	0.000010	N/A	N/A
Total	99.278356	99.311225	-0.03

TABLE 34: CAIN AND WIMS COMPARISON (PHWR WITH 0.71% ENRICHMENT AT 7 MW·D/KG)

TABLE 35: CAIN AND WIMS COMPARISON (RBMK WITH 1.8% ENRICHMENT AT $18 MW \cdot D/KG$

Isotope	$CAIN(wt\%)$	WIMS (wt%)	Error $(\%)$
235 U	0.445671	0.441000	1.06
236 U	0.217093	0.213000	1.92
238 ^U	96.936072	97.020000	-0.09
237 Np	0.009102	0.008490	7.20
^{238}Pu	0.002792	N/A	N/A
^{239}Pu	0.288814	0.281000	2.78
^{240}Pu	0.152649	0.157000	-2.77
241 Pu	0.060783	0.051700	17.57
242 Pu	0.026245	0.024500	7.12
241 Am	0.002014	0.001540	30.76
$242m$ Am	0.000031	N/A	N/A
243 Am	0.002157	0.002140	0.78
242 Cm	0.000537	N/A	N/A
244 Cm	0.000293	N/A	N/A
Total	98.144252	98.200370	-0.06

Isotope	$CAIN(wt\%)$	WIMS $(wt\%)$	Error $(\%)$
235 ^U	0.700327	0.687000	1.94
236 ^I J	0.324978	0.312000	4.16
238 U	96.023271	96.140000	-0.12
237 Np	0.013680	0.012200	12.13
238 Pu	0.004585	N/A	N/A
239 Pu	0.289806	0.279000	3.87
240 Pu	0.173623	0.185000	-6.15
241 Pu	0.064404	0.052100	23.62
242 Pu	0.027288	0.026500	2.98
241 Am	0.002786	0.002090	33.28
$242m$ Am	0.000050	N/A	N/A
243 Am	0.002790	0.002850	-2.11
242 Cm	0.000663	N/A	N/A
244 Cm	0.000486	N/A	N/A
Total	97.628738	97.698740	-0.07

TABLE 36: CAIN AND WIMS COMPARISON (AGR WITH 2.6% ENRICHMENT AT 23 MW \cdot D/KG)

TABLE 37: CAIN AND WIMS COMPARISON (GCR WITH 0.71% ENRICHMENT AT $4 MW \cdot D/KG$

Isotope	$CAIN(wt\%)$	WIMS $(wt\%)$	Error $(\%)$
235 U	0.417815	0.401000	4.19
236 U	0.047706	0.051000	-6.46
238 U	98.859341	98.878000	-0.02
237 Np	0.001839	N/A	N/A
^{238}Pu	0.000224	N/A	N/A
^{239}Pu	0.187812	0.181000	3.76
240 Pu	0.057494	0.052000	10.57
241 Pu	0.012865	0.011000	16.95
242 Pu	0.001962	0.001700	15.39
241 Am	0.000442	N/A	N/A
$242m$ Am	0.000023	N/A	N/A
243 Am	0.000049	N/A	N/A
242 Cm	0.000068	N/A	N/A
244 Cm	0.000003	N/A	N/A
Total	99.5876	99.5757	0.01

As it can be seen from the tables, the CAIN code agrees very well with WIMS code except several higher actinides. Considering that the CAIN is a one group and one point model, it is concluded that the CAIN code has enough accuracy to meet the requirements of VISTA simulation model.

VI.2. MOX fuels

VI.2.1. Benchmark of PWR-MOX fuel

In the ORIGEN, there is only one PWR-MOX library. Cross sections used in VISTA which is given in TABLE 16 are identical to ORIGEN code. In the ORIGEN manual, minor modification to U/Pu cross sections due to burnup is proposed. But this modification is complex, and its effect on the isotopic concentration is in the order of several percent. So, the original library cross sections can be used in VISTA.

In order to compare the VISTA and ORIGEN results , constant flux is used in ORIGEN, that is, IRF=2.42E14 is used, instead of IRP=39.2 kW/kg. Also, in order to adjust to 45 GW·d/t, 1 155 days is used instead of 1 148 days as irradiation time.

The result is shown in TABLE 38. The maximum error is in 238 Pu (5.3%), but this nuclide is the end of long chain, and the error is acceptable.

$BU=0$		$BU=45$ GW \cdot d/t		
	gram	ORIGEN	VISTA	$Error(\%)$
235 U	2 7 8 0	1 3 8 0	1 3 6 2	-1.3
236 U	$\boldsymbol{0}$	282	274	-2.8
238 U	924 421	902 600	902 272	$\boldsymbol{0}$
237 Np	$\boldsymbol{0}$	131	132	0.8
^{238}Pu	924	925	974	5.3
239 Pu	43 672	16 800	16 5 12	-1.7
240 Pu	15 765	14 800	14 677	-0.8
241 Pu	8 5 5 8	9 100	9 0 5 0	-0.5
242 Pu	3 8 2 1	4 8 6 0	4870	0.2
241 Am	0	700	719	2.7
$242m$ Am	$\overline{0}$	17	19	(2g)
243 Am	0	1720	1750	1.7
242 Cm	$\boldsymbol{0}$	140	142	1.4
244 Cm	$\boldsymbol{0}$	826	851	3
Total	999 941	954 281	953 604	-0.1

TABLE 38: COMPARISON BETWEEN ORIGEN AND VISTA/CAIN FOR PWR-MOX

VI.2.2. Benchmark of BWR-MOX Fuel.

In the ORIGEN2, there is only one BWR-MOX library. Cross sections used in VISTA are identical to ORIGEN code TABLE 17.

In order to compare the VISTA and ORIGEN results, constant flux is used in ORIGEN, that is, IRF=1.21E14 is used, in stead of IRP=24.6 kw/kg. The result is shown in TABLE 39. The maximum error is in 241 Am (-5.5%).

In the above study, it became necessary to recognize the difference on the number-of-fission to energy conversion. In the ORIGEN [16], emission energy for one nuclide fission is calculated by the following formula.

MeV/fission = $0.00129927 * Z^2 * A^{0.5} + 33.12$

Some typical values are shown in TABLE 40. Since MW·d/gram-fission is proportional to MeV/fission, and in-proportional to the atomic-mass, MW·d/gram-fission value varies between 235 U and 239 Pu, which are also shown in the table.

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TABLE 40: MW·D/GRAM-FISSION ESTIMATION

Of course, even in $UO₂$ fuel, there exists Pu fission. So, it is difficult to include this effect exactly in CAIN. Current CAIN uses 0.97 MW·d/gram-fission value for all fuel types. This value may increase 1 or 2 % for MOX fuel, and this will improve the general tendency between current ORIGEN and VISTA. But, this improvement is small, and will not affect the total result so much. As a conclusion, we can use 0.97 value for MOX.

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GLOSSARY

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