FICST: A Tool for Sensitivity Analysis of SCWR Fuel Isotopic Composition to Nuclear Data

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FICST: A TOOL FOR SENSITIVITY ANALYSIS OF SCWR FUEL ISOTOPIC COMPOSITION TO NUCLEAR DATA

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ABSTRACT

With an ever-increasing population both in Canada and globally, an improved quality of life will depend on having access to energy. The non-renewable, carbon-based, sources of energy that presently provide a major amount of the world's energy supply are depleting and therefore will be expensive in the future. Nuclear technology is a relatively new technology which can fulfill future energy needs but requires highly specialized skills and knowledge to continue to make it safer, cleaner, more reliable, and more affordable. Thus the nuclear industry puts lots of efforts to develop and improve the next generation of nuclear power plants. The Supercritical Water Reactors (SCWRs) are one of the Generation IV nuclear-reactor systems.

The SCWRs, to a large extent, are very similar to light water reactors, but with a simpler design. The main advantage of SCWRs is their higher thermal efficiency. The Canadian SCWR has adopted an innovative fuel concept which is a mixture of plutonium and thorium oxides (Th, Pu) O_2.

The role of nuclear data in fuel development and reactor-physics analysis is quite significant. With the development of nuclear data files over the years, nuclear cross sections and other parameters are widely available, but their accuracy is still a concern. Also the accuracy of nuclear data is more reliable for uranium-based fuels than for thorium-based fuels. It is not known how the uncertainties in the nuclear data will impact the fuel depletion in a SCWR. Thus a sensitivity analysis tool has been developed to evaluate the impact of uncertainties in the neutron cross-sections of the actinides present in SCWR fuel. This document provides the details on the theory and methodology used to develop this tool (FICST). The objective of this work is to develop a code, not any specific calculation done with it.

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Chapter 1:
Introduction and Problem Statement

For an increasing world population and an increasing population in Canada, an improved quality of life will depend on having access to affordable and reliable electricity. The non-renewable, carbon-based sources of energy that presently produce most of the world's electricity are being depleted, and consequently the electricity produced from these sources will become increasingly expensive. Nuclear power is a relatively new technology which can fulfil future electricity needs but will require highly specialized skills and knowledge to continue to make it cheap, safe, clean, reliable, and socially acceptable. Thus the nuclear industry has invested resources to develop and improve the next generation of nuclear power plants. The Supercritical Water Reactor (SCWR) is one design of these "Generation IV" nuclear reactor systems.

The first chapter starts with an overall introduction to generation IV reactors and specifically to SCWRs followed by a problem statement and a brief explanation about FICST. Chapter two focuses on the literature review and provides a brief explanation of the commercial codes available for the depletion analysis and explains why FICST was developed. Chapter 3 will focus on the methodology used in developing this tool. Chapter 4 will outline code description followed by results in Chapter 5. Conclusion and the future work will be discussed at the end of this thesis, Chapter 6.

1.1 Available Sources of Energy

The non-renewable sources of energy in the world are coal, oil, natural gas, and nuclear. "Coal is relatively cheap, with large deposits left that are reasonably easy to

obtain. It is relatively easy to transport because it is a solid. However some sources of coal are deep below the ground, as in the UK. They can be difficult, costly and dangerous to mine. Besides, burning coal contributes to global warming, as well as to the production of smog (smoke and fog), which is harmful to health. It is a finite resource and will eventually run out."[1]

The renewable sources of energy, such as solar energy, are not cheap. Large facilities are required for the collection of solar energy and the storage of the electricity is also a problem. [2]

Another option is wind power, and the footprint for "wind farms" is smaller than for the solar energy. However, it has been proven that the turbines have negative environmental impacts in terms of avian mortality and noise. In addition, solar and wind power are intermittent forms of power. Hydroelectricity is an exception and, nowadays, is the main source of electricity supply in Canada. However hydroelectricity may - not be sufficient in the future.

The hydraulic fracturing of gas-bearing rock formations and the development of oil-bearing tar sands are providing new sources of power. In addition, the efficiency of solar cells is improving, and the cost of solar cells is dropping. Thus one expects the electricity market throughout the world to change dramatically in the future.

In the meantime, the use of carbon-based fuel-sources is increasing the concentrations of carbon dioxide in the atmosphere and in the oceans. While the contribution of this greenhouse gas to climate change is unclear at present, that contribution may become more evident in the future. Thus, the environmental issues associated with the emission of greenhouse gases from burning fossil fuel may become a fundamental concern.

Against that background nuclear power is a relatively new technology which can fulfill future energy needs and is a viable option to minimize the production of greenhouse gases. Nuclear energy is a possible replacement for the other sources of energy and will be available with reasonable cost. [3] However, like other technologies, specialized skills and knowledge are required to continue to make it safer, cleaner, more reliable and more affordable.

These considerations led to the establishment of several international organizations, including the Generation IV International Forum (GIF), "the International Nuclear Energy Research Initiative (INERI), the Euratom Project on Reactor for Process Heat and Electricity (RAPHAEL) and the IAEA-coordinated International Project on Innovative Nuclear Reactors and Fuel Cycles (INPRO)."[2]

1.2 Generation III and III+ Nuclear Power Plants

As is stated by the World Nuclear Association, the designs of nuclear power plants have been constantly improved during the past fifty years. The first generation of commercial power reactors was developed in the 1950 and 1960s. The second-generation commercial reactors were largely French and US reactors, reactors which have now reached the end of their design life. Most of the currently operating reactors are generation III designs. PWR, BWR and CANDU reactors are some of the generation III reactors. The next generation of reactors is generation (3+).

The generation (3+) of the reactors such as ESBWR, EPR, AP-1000 and ACR-1000 are the evolutionary designs of generation III reactors. The generation (3+) design was developed to make these reactors safer and easier to operate and maintain, and to

increase the operating life (to about 60 years), to increase the burnup and fuel efficiency, to reduce the capital cost and construction time and to make them easier to license. [4]

The next generation of nuclear power reactors is Generation IV, which is in the conceptual stage of design. Figure 1 presents different generations of nuclear power plants.

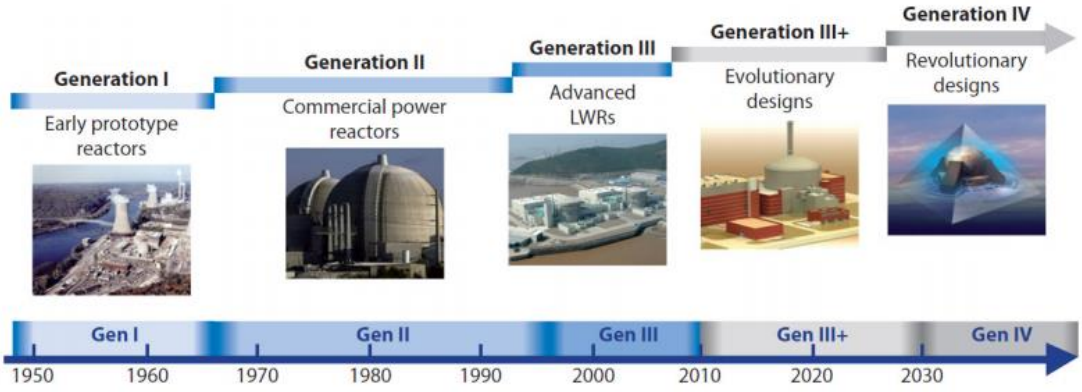


Figure 1: Generations of nuclear power: Time ranges correspond to the design and the first deployments of different generations of reactors [5]

1.3 Review of Global Roadmap for Generation IV Nuclear Energy

The design of Generation IV reactors was promoted by the establishment of the Generation-IV International Forum (GIF) in 2009 to promote international cooperation in the necessary research and development. GIF was created with a nine-country membership, which has gradually increased to 13 countries today. The goals of the GEN-IV are to improve:

1. Sustainability
    - By generating energy sustainably and promoting the long-term availability of nuclear fuel
    - By effective fuel utilization and minimization of waste

2. Economics
    - Mainly by competitiveness with respect to other energy sources in terms of financial risk
    - By having a lifecycle cost advantage over other energy sources

3. Safety and reliability
    - By excelling in safety and reliability
    - Having a very low likelihood and degree of core damage, exemplified by the lack of need for off-site emergency response

4. Proliferation resistance and physical protection
    - Being a very unattractive route for diversion or theft of weapons or usable materials
    - Preventing terrorist acts by providing increased physical protection [6]

The objective of the Generation IV International Forum (GIF) is to have the GEN-IV available for international deployment in about the year 2030, when many of the world's currently operating nuclear power plants will be at or near the end of their operating licenses. [7]

The "Technology Roadmap for Generation IV Nuclear Energy Systems" [2] has divided the GEN IV reactors into the following six groups:

- GFR: Gas Cooled Fast Reactors: "Fast neutron spectrum, reactor helium cooled. pressure 7 MPa and Temperature 480-850 $^{\circ}$C
- LFR: Lead Alloy Cooled Fast Reactors: A fast spectrum, cooled by lead or lead/bismuth eutectic, temperature 550-800 $^{\circ}$C
- MSR: Molten Salt Reactors: an epithermal-spectrum reactor, sodium-fluoride salt cooled, temperature 700-800 $^{\circ}$C.
- SCWR: Supercritical Water Cooled Reactors: thermal spectrum, supercritical water cooled, pressure 25 MPa, temperature up to 625 $^{\circ}$C

- SFR: Sodium Cooled Fast Reactors: A fast spectrum, sodium cooled, temperature (520-550 $^{\circ}$C)
- VHTR: Very High Temperature Reactors: A graphite moderator, thermal cycle. Helium Cooled, pressure 9 MPa and temperature (500-1000 $^{\circ}$C)"[7]

Canada is mainly focused on developing the SCWR. Canada's interest in SCWRs is mainly due to the following two factors:

- "Merging proven advanced fossil and nuclear technologies
- Many utilities operate both nuclear and supercritical fossil plants" [7]

1.4 SCWR in Canada

The idea of a high temperature water and steam cooled reactor is not completely new to the nuclear industry. According to OKA, during the 1950's and 60's, the idea of a steam cooled reactor was considered as an alternative for the liquid metal cooled fast breeder reactor, and even years before that the commercial power plants put this technology into operation. [9] However, still R&D is required to develop new SCWR concepts. The thermalhydraulics of fossil supercritical plants has been studied in detail, and this information can be used in studying the thermalhydraulics of SCWRs to some extent. However, the nuclear supercritical-water-cooled reactors have a different core condition. The reduction of the coolant density in SCWRs results in changes in the neutron spectrum, which leads to changes in the reactivity of the core. "Supercritical water coolant density variations for many cycles can be large, particularly if the water temperature crosses the critical point in the core. Such a density change complicates flux gradients and flux shaping requirements."[11] Thus, further studies are necessary to have

a better understanding of the SCWR's performance. The focus of this thesis is to develop a tool to help the reactor designers to study the behavior of Canada's new SCWR fuel concept.

The R&D Activities for the Development of the SCWR in Canada are planned by NRCan's Ottawa Office; Figure 2 shows the main areas of focus in Canada.

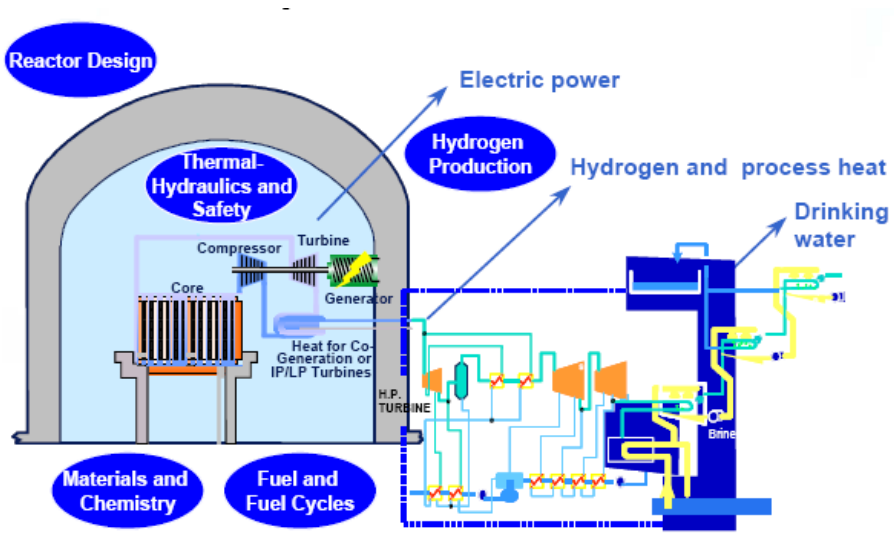


Figure 2: SCWR R&D Areas [10]

The Canadian SCWR satisfies the goals of the Generation IV initiative by combining some of the features of the CANDU system and the Light Water Reactors in a new design. The SCWR features a heavy-water moderator with a direct-cycle light-water coolant passing over the fuel loaded in an array of pressure tubes before being fed to the turbine-generator.

1.4.1 Sustainability

The design of SCWR preserves much of the neutron economy of the CANDU system by using heavy water as the principal moderating material, and this design permits the adoption of a thorium fuel cycle.

In addition, the pressure tube is a fabrication of a zirconium alloy with a wall thickness almost four times thicker than that of the pressure tube of a CANDU plant. This heavier pressure tube allows a substantial increase in coolant pressure (inlet/outlet) from 11/10 MPa (a) for CANDU to 26/25 MPa (a) for SCWR. It is intended that, the temperature of the coolant be increased to (inlet/outlet) 350˚C /625˚C in SCWR compared to 277˚C /312˚C in CANDU. At this outlet temperature, the experience with conventional fossil-fired steam generating equipment can be applied because the superheated coolant is fed directly to the steam turbine. In addition, the higher outlet temperature means the overall efficiency of the nuclear power plant is raised. For example, if the processes within the nuclear power plant represented a perfect Carnot cycle, then for a heat sink at 30˚C the efficiency increases from (585K-303K)/(585K) = 48% under CANDU operating conditions to (898K-303K)/(898K) = 66% for SCWR operating conditions.

In practice the efficiencies of the SCWR and CANDU are lower than these theoretical limiting values because of losses within the plant such as the nuclear energy lost in the moderator system, the overall turbine efficiency and the internal demands of the plant such as the primary pumps. Thus, the overall thermal efficiency of SCWRs is about 45% compared to those of the advanced LWRs and ACR-1000 with efficiencies of about 35%.[12]

The SCWR also uses thorium as a fuel. Thorium is a naturally occurring element. It is present in the earth's crust as thorium-232 which has a half-life of $1.4x10^{10}$ years; other isotopes of thorium have half-lives of less than $1.0x10^{5}$ years, and so have small concentration on the earth's crust. Thorium is more abundant than uranium, and thorium-232 is similar to uranium-238 because both nuclides are fertile. That is, during irradiation in a neutron flux, these nuclides absorb a neutron to form daughter isotopes, which decay to fissile isotopes, uranium-233 and plutonium-239.

For thorium-232, the sequence is Th-232 + n → Th-233 → Pa-233 + e^- → U-233 + $2e^-$ and for uranium-238, the sequence is U-238 + n → U-239 → Np-239 + e^- → Pu-239 + $2e^-$. Thus the SCWR satisfies the first requirement of sustainability of the Generation IV systems; it exploits an element that is more abundant than the uranium of current reactor types.

The production of the fissile uranium-233 also satisfies the second requirement of sustainability - namely, effective fuel utilization and minimization of waste.

Irradiation of Th-232 produces virtually no transuranic (Pu, Am or Cu) compared to irradiation of U-238. Thus thorium is one the best candidate for waste reduction.

On the other hand, in order to use thorium fuel, one has to "top up" with U-235, U-233 or Pu-239. The first option results in using up uranium reserves, while the other two options require reprocessing the irradiate fuel. There is no certain indication that the use of plutonium is more cost effective compare to the used uranium.

This treatment is an over-simplification since many other processes are competing for the 2.3 fission neutrons from the second absorption in what was, initially, a thorium-232 nucleus. These competing processes include neutrons leaking from the reactor and

absorption of the fission products formed in the fission process as well as absorption in structural materials and absorption at epithermal neutron energies, and finally absorption in the moderator and coolant.

For these reasons reactors using a thorium fuel cycle invariably use uranium or plutonium as an immediately fissile component of the fuel. For the Canadian SCWR, plutonium has been chosen as the fissile component. Thus, the SCWR consumes plutonium generated in uranium fuelled reactors; that is, the SCWR reduces one of the long-lived radioactive wastes from reprocessing spent fuel from the uranium fuel cycle, thereby satisfying the second requirement of sustainability, the minimization of waste.

1.4.2 Economics

Ultimately the economics of a plant that generates electricity will depend on the capital costs of that plant, the operating costs of the plant, and the prevailing interest rates on any debt issued to build the plant over the lifetime of the plant. These are beyond the scope of this thesis.

The direct-cycle of SCWR simplifies the design of the nuclear power plant, because no secondary side equipment between the reactor core and the turbine is present. Significant differences in the fuel channels and safety systems could lead to big differences in capital costs. Thus, the other capital costs need to be comparable in order for the SCWR to be competitive with the current designs.

The operating costs have two principal components: labour and fuel costs. The proposed SCWR concept adopts a batch refuelling scheme. Consequently, fewer operating staff would be required compared with the staff in a CANDU plants, because on-power refuelling demands a large staff to service the refuelling system and to plan the weekly

refuelling schedule. In addition, the batch refuelling system eliminates a complex on-power refuelling system and the process systems needed to support on-power refuelling. With SCWR, staffing levels would rise during periods of batch refuelling as with LWR. So operating costs of labour should be comparable with those of other reactor types.
The fuel costs would depend on the commitment by any country to the thorium fuel cycle.

At the same time, the plutonium fissile component of the fuel would involve fresh costs. However, the extraction of plutonium from spent uranium fuel also involves chemical processes rather than costly enrichment. One needs to keep in mind that extraction of plutonium from the spent fuel is always accompanied by the proliferation issue.
Thus, at this stage of the design one cannot really conclude that the fuelling costs of SCWR will be lower than those of uranium-fuelled reactors.

Finally, the increase in overall efficiency of the SCWR over CANDU and other operating light-water reactors such as Pressurized Water Reactors (PWR) and Boiling Water Reactors (BWR) suggests a significant economic advantage over current reactor designs.
The costs of comparable fossil-fuelled electricity plants are more difficult to anticipate when carbon taxes are a possibility or even a probability. Those same intangible costs must be associated with some forms of renewable power sources since gas-fired power plants are needed as standby plants when the sun does not shine or the wind does not blow or blows in non-steady manner.
Hence, one may conclude that the costs of SCWR are more certain than those of competing sources of electricity except for the costs of hydroelectric power, and the SCWR can fulfil the need for low cost energy. [2]

1.4.3 Safety and Reliability

It is ensured that in any loss-of-coolant event, the SCWR reactor-power coefficient is negative. This design feature will add to the safety of the reactors. However, since SCWRs are in the conceptual design phase, it is hard to make a comparison about reliability. Without a detailed assessment of the unavailability of different reactors and the cause of unavailability, it is difficult to comment on the reliability of the SCWR, particularly when the fuel channel components are fabricated from new materials with no performance data.

1.4.4 Proliferation Resistance and Physical Protection

The use of thorium fuel in the Canadian SCWR has two other benefits from a radioactive waste and non-proliferation viewpoint. The SCWR consumes rather than generates plutonium. In addition, because the amount of plutonium present in the fuel initially is 13-15%, the buildup of higher actinides is implicitly reduced from that of a uranium-fuelled reactor where the uranium-238 provides an almost constant feed for the higher actinides. Indeed, those higher actinides, -americium, curium, berkelium and californium- will build up with irradiation time so the higher burnup of the fuel will increase their abundances in the spent fuel. However, the half-lives of the more abundant of these higher actinides will be substantially shorter than the half-life of plutonium-239. Consequently, the radio-toxicity of the spent fuel from SCWR is expected to be smaller than that from LWR spent fuel.

Finally, under irradiation the thorium fuel also forms uranium-232 which undergoes successive alpha decays through Th-228, Ra-244, Rn-220, and Po-216 to Pb-212. That last daughter undergoes beta decay to Bi-212, which undergoes alpha decay to Tl-208 and then beta decay to Pb-208. Some of the gamma radiations emitted in these decays are

very energetic, so the decay radiation presents an inherent radiation hazard demanding special equipment for handling the fuel which should be considered during the estimation of the fuel cost. The following shows the decay chain of U-232 and the gamma energy associated with it:

"U-232 (α, 68.9 years)→ Th-228 (α, 1.9 year)→ Ra-224 (α, 3.6 day, 0.24 MeV)→ Rn-220 (α, 55 s, 0.54 MeV)→ Po-216 (α, 0.15 s)→ Pb-212 (β−, 10.64 h)→ Bi-212 (α, 61 m, 0.78 MeV)→Tl-208 (β−, 3 m, 2.6 MeV) (35.94% branching ratio)→ Pb-208 (stable)"1

1.4.5 The use of Thorium/Plutonium Fuel

The generation 3 and 3+ are using mostly uranium fuel, which is either with the natural abundance of U-235 (CANDU reactors) or to some level of enrichment of U-235 (PWR and most of Generation III+). In recent years there have been some developments to use uranium-thorium fuel in the CANDU reactors.

As has been discussed above, thorium fuel has advantages over the fuel types of current nuclear power plants in that a mixture of thorium and plutonium has been selected as the reference fuel of Canadian SCWRs. The main advantages of this new fuel can be summarized as below:

1. The abundance of thorium is much higher than that of uranium in nature.
2. The plutonium in spent fuel from the thermal reactors and in weapons can be recycled and used in this fuel.
3. The use of thorium fuel as an alternative to uranium results in significantly less plutonium and other higher actinides in the spent fuel, thus reducing the

[1] This can be derived from table of isotopes or any other book. This specific format was taken from http://en.wikipedia.org/wiki/Uranium-232 and compared against Table of Isotopes for verification.

long term decay heat and radio-toxicity of the irradiated spent fuel compared to uranium fuels.

However, the new fuel requires further research and developments.

1.5 The Objective of this Study

As discussed, the Canadian SCWR has adopted a new fuel concept. The new fuel many benefits compare to the current fuel used in the nuclear power plants; however further research and development is required.

In fuel development and reactor physics analysis, the role of nuclear data is quite significant. With the development in recent years of modern data files, most nuclear data are widely available, but their accuracy is still a major concern. It is also expected that the accuracy of nuclear data is more reliable for uranium-based than for thorium-based fuels, because of the greater widespread use of the former. It is not known how the uncertainties in the nuclear data impact the fuel depletion, which in turn impacts the accuracy of fuel recycling calculations, and radio-toxicity and decay heat from spent fuel. Thus, a sensitivity analysis tool is needed to evaluate the impact of uncertainties in the nuclear data. This work is a contribution to the reactor physics concept proposed for the Canadian SCWR.

This study focuses on developing a tool that can be used to determine the impact of nuclear data uncertainties on the irradiated fuel isotopic composition of Canadian

SCWR fuel. The Simulink/MATLAB computer language has been used to develop this tool.[2] (See Figure 3)

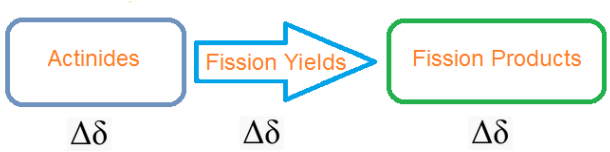


Figure 3: Schematic Diagram of the Matlab Model

The SCWR irradiated Fuel Isotopic Composition Sensitivity Tool, (FICST), makes it possible for the user to compute the time-dependent concentration of a large number of nuclides that are produced in the Canadian SCWRs irradiated fuel and to determine the impact of nuclear data uncertainties on the irradiated fuel isotopic composition. These isotopes are simultaneously produced or/and lost through activation, fission, capture, and radioactive decay.

FICST provides the user with an option of inputting multi-group cross sections of different nuclear data such as the ENDF/B data base and corresponding neutron fluxes with the variable level of uncertainties to calculate the reaction rates.

The initial fuel concentration can be put in as number of atoms; thus by having an average thermal, epithermal, and fast flux, a crude simulation of the irradiation of the fuel can be developed. Also, by having a detailed flux map, it is possible to develop a model for a small segment of the fuel.

Chapter 2 of this thesis will focus on the literature study and the other commercial codes that can potentially be used for sensitivity analysis.

[2] MATLAB® is a high-level language and interactive environment that enables the performance of computationally intensive tasks faster than with traditional programming languages such as C, C++, and FORTRAN. http://www.mathworks.com/products/matlab/

Chapter 2:
Literature Review

As discussed in the previous chapter, the Generation IV reactors are mainly focused on the following goals to meet the global energy demands: 1) improving safety and reliability 2) building an effective fuel cycle and minimizing the waste, 3) increasing the efficiency and 4) reducing the cost. SCWR is one of the six Generation IV reactors, which are mainly under research and development in Canada By providing up to 45% efficiency, the Canadian SCWR is significantly improved compared to its ancestors. Also, SCWRs have adopted a new fuel design with a mixture of thorium/plutonium oxide.

The library data available for analysis have been verified for the operating conditions of the current reactors. Not only the new fuel design, but also the huge differences in the operating condition of SCWR compared to current reactors demand more research and development. This thesis project aims to develop a tool for the sensitivity analysis of the new fuel to the uncertainties that might exist in the library data.

The main focus of this chapter is to provide a review of the commercial tools which are currently available and can be used for the sensitivity analysis of SCWR fuel and compare them against FICST code.

2.1 Similar Analysis Tools

For fuel and core design, several nuclear codes have been developed which are mostly focused on the following issues [13]:

- neutron multiplication factor,
- neutron and gamma-ray source terms,
- decay-heat source terms,

- radiological and chemical toxicity composition of the fuel.

The main focus of this thesis is determining the isotopic composition of the irradiated fuel.

The current, commercially available computer codes are mainly used for the uranium fuel used in LWR or MOX fuel. Thus, to use these codes, one would need to extract or develop the specific library for the SCWR Pu/Th fuel. The following subchapters provide a brief overview of the available commercial codes that potentially can be used for depletion analysis and eventually for the uncertainty analysis of SCWR new fuel.

2.1.1 FISPIN

FISPIN is a point depletion code. FISPIN calculates the numbers of atoms as a function of irradiation time. Besides actinides and fission products, FISPIN also includes structural or activation materials. "The whole sample of nuclear fuel element is subject to the same irradiation conditions. Usually, the sample of reactor fuel initially contains atoms of a few uranium and plutonium isotopes and, optionally, atoms of some structural material such as pin clad, graphite moderator or impurities in the fuel pin. The atomic number densities of the various actinides, fission products and structural material nuclides are of interest in themselves." [14]

FISPIN can potentially be used for sensitivity analysis. The main concern will be providing the proper input data to the code. As it is stated in the code description, FISPIN needs several input data, such as cross-sectional data: "other class of nuclear data required by FISPIN is the cross sections for various neutron induced reactions in the various nuclides. For example, many of the actinides undergo fission, (n, 2n) reactions and neutron capture (n, γ), sometimes to several distinct states of the daughter product

nuclide. These cross section data changes markedly between different types of reactor fuel and can also change with burnup, due to changes in neutron spectrum and to changes in resonance shielding." [14]

FISPIN is usually coupled with the CASMO lattice physics code for modelling PWR and BWR fuel. The CASMO code is a multi-group two-dimensional transport code which is used for burnup calculations of BWR and PWR reactors assemblies or pin cells. The code can model cylindrical fuel rods in a square lattice pitch.[15] However, adaptation of the code to model SCWR fuel could be challenging due to the differences in the fuel lattice.

2.1.2 DRAGON4-DONJON4

DRAGON and DONJON are used to perform full-core calculations. DRAGON is a lattice code which generates multi-parameter reactor databases which are used by DONJON, which is a diffusion code. These codes can be used to compute the fluxes over the reactor using a diffusion approximation. In this case, the fuel depletion in the core is derived by the computation of new burnup. There is a relatively new feature added to DRAGON/DONJON code which is called the micro-depletion method. The Micro-depletion method is based on the numerical solution of the depletion equations, also called the Bateman equations. In each bundle, isotopic concentrations are available to compute the reaction rates and perform the depletion. At each burnup step, these concentrations are updated with the aid of a depletion equations solver. [16] DRAGON/DONJON can potentially be used for sensitivity analysis of SCWR fuel. One needs to set the proper lattice cell for the new fuel design, which might be a challenge.

2.1.3 SCALE

The computer program which is most widely used to look at the spent or irradiated fuel isotopic content of the fuel is called SCALE (Standardized Computer Analyses Licensing Evaluation). Irradiated fuel isotopic compositions are calculated using the two-dimensional isotope depletion models and ENDF/B-V-based cross sections.[17]

"SCALE is a computer code developed at Oak Ridge National Laboratory (ORNL) since the 1970s". [18] The SCALE code system can be used to determine the isotopic concentration of the irradiated fuel using its depletion module TRITON and ORIGEN-S, which allows a depletion simulation of fuel assembly configurations [18]

SCALE is the best available commercial code for conducting this type of sensitivity analysis. However, a user needs to use TRITON and ORIGEN-S to develop a model for the SCWR specific conditions.

ORIGEN (Oak Ridge Isotopic Generation) is a point depletion, radioactive decay and burnup code that is one part of the SCALE package. "TRITON (Transport Rigor Implemented with Time Dependent Operating for Neutronic depletion) is a control module developed to enhance the depletion calculation by coordinating interactive calls between a neutron transport solver and ORIGEN." [19]

In short, SCALE is a flexible tool that can be used for the sensitivity analysis of SCWR fuel. However, since it is not a tool designed specifically for this purpose, it can be time consuming to change all the input parameters to include the desired variation, such as the changes in fission yield uncertainties, the cross sections uncertainties, or the changes in the moderator or coolant temperature.

2.1.4 MONTEBURNS 1.0 (MCNP+ORIGEN-2)

"MONTEBURNS is a fully automated tool that links the Monte Carlo transport code MCNP with the radioactive decay and burnup code ORIGEN2. MONTEBURNS produces a large number of criticality and burnup results based on various material feed/removal specifications, power(s), and time intervals" [21] a brief description of MCNP is given in the following section.

2.1.4.1 MCNP

"Monte Carlo N-Particle Transport Code "MCNP6™ is a general-purpose, continuous-energy, generalized-geometry, time-dependent, Monte Carlo radiation-transport code designed to track many particle types over broad ranges of energies. The code uses a library of differential or fine group cross sections as a user option.

A Monte Carlo code generates a statistical history for a particle based on random samples from probability distributions. These distributions are then used in calculations to determine the type of interaction the particle undergoes at each point of life, the resulting energy of the particle if it scatters, the number of particles that "leak" from the system because of geometry constraints, and the number of neutrons produced if the neutron causes fission. The probability of the particle to behave in a certain manner (to scatter, to absorb, to fission) can be obtained from the cross-section values of the material(s) with which the particle will interact. Thus, a Monte Carlo code can model the series of events that occur in the lives of a large number of particles to determine the flux of different types of particles in various regions in a system. These fluxes can then be used to tally a wide variety of information (reaction rates, heating rates, doses, etc.) for the system. Additionally, the value of the effective multiplication factor, k_{eff}, for a system (the ratio of

the number neutrons in the system with respect to the number of neutrons that existed in the previous generation) can be calculated using MCNP."[20]

MCNP can handle a material burnup. However, running a Monte Carlo calculation is relatively time consuming. Also, to complete the sensitivity analysis, one needs to have a huge number of the same run with a small change in one number.

Compared to MCNP, ORIGEN is a far better tool for this type of analysis; however, to run ORIGEN, one needs to have the proper fluxes and cross-sections. This is where MONTEBURNS becomes helpful. "The primary function of MCNP is to calculate one-group cross-sections and fluxes that are used by ORIGEN2 in burnup calculations as well as provide, if requested, criticality and neutron economy information. After performing burnup calculations using ORIGEN2, MONTEBURNS passes isotopic compositions of materials back to MCNP to begin another burnup cycle. The Figure below shows how MONTEBURNS interacts with MCNP and ORIGEN2."[21]

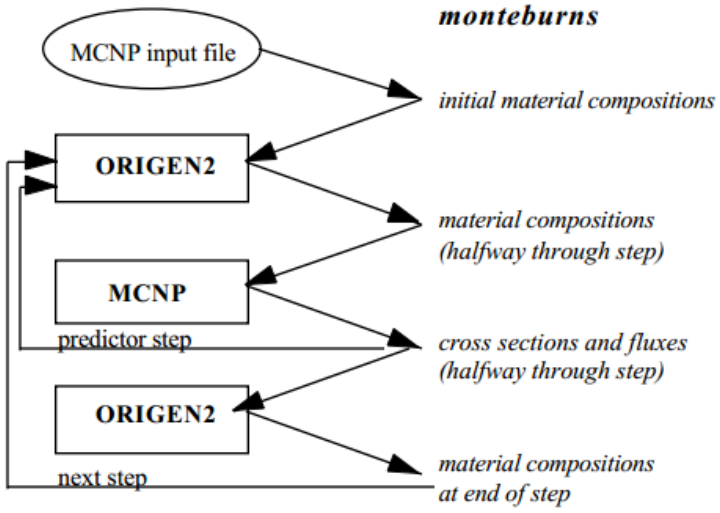


Figure 4: Interaction of MONTEBURNS with MCNP and ORIGEN [21]

MONTEBURNS consists of 15 different parts as listed below (from [21]):

1 Read input parameters

2 Create basic ORIGEN2 input files for each main burn step based on continuous feed/removal information

3 Put the user's MCNP input file into MONTEBURNS format

4 Create tally requests for MCNP

5 Write ORIGEN2 composition input file, separating natural elements into individual isotopes

6 Update the MONTEBURNS input file to indicate the current step number and to update the list of isotopes being tracked

7 Determine which material is located in each region

8 Add discrete feed to ORIGEN2 composition input file (if requested by the user)

9 Modify the previous MCNP input file with new material compositions

10 Modify ORIGEN2 input files for predictor steps to calculate compositions halfway through each burn step

11 Modify ORIGEN2 libraries with cross-sections calculated by MCNP and ORIGEN2 input files with fluxes from MCNP

12 Calculate the recoverable energy per fission based on the actinide distribution

13 Perform discrete removal in the ORIGEN2 composition input file

14 Output results of ORIGEN2

15 Calculate the amount of material burned and produced based on feed and inventory information

16 MONTEBURNS combines the best part of MCNP and ORIGEN and, moreover, provides the user with a reliable tool. Many modifications are needed to prepare

the MONTEBURNS model for SCWR core. For example, it can be a challenge to manually access the library data and vary the uncertainties for one isotope while keeping the rest unchanged.

2.1.5 TRIPOLI-4

TRIPOLI-4 is a depletion code which was developed by Commissariat à l'Energie Atomique for the design of the gas-cooled fast reactors. This code was developed for the equivalent homogeneous model of fuel rods in a hexagonal mesh assembly. TRIPOLI-4 has been also used for depletion calculation for PWR high-burnup UO2 and MOX spent fuel.[22]. "A new TRIPOLI-PEPIN coupled code, (TR4PEP) combines the continuous-energy Monte Carlo transport code, TRIPOLI-4.3 and the point depletion code, PEPIN-2, to perform the burnup dependent material data evaluation and to provide information for the validation of cell codes."[23]

This program is also capable of calculating the Keff calculations as well as burnup dependency. The TR4PEP is mainly used, developed, and validated for PWR high burnup UO2 and MOX fuel applications.[23] Thus, modeling the SCWR new fuel itself can be challenging.

2.1.6 MVP-BURN

"MVP-BURN is a coupling code of a continuous-energy Monte Carlo code MVP and a burn-up calculation module BURN which solves a depletion equation analytically". [24] The MVP-BURN code performs the burn up calculations using Monte Carlo Code MVP and a buildup and decay of nuclide code, called BURN. By coupling these two codes it becomes possible to perform the microscopic reaction calculation. Since the

Monte Carlo method is very time consuming, the MVP-BURN employs two kinds of time period. One is a burnup step, and the MVP step is carried out at the start point of each burnup step. The figure below shows the time steps used in MVP-BURN calculations.[24]

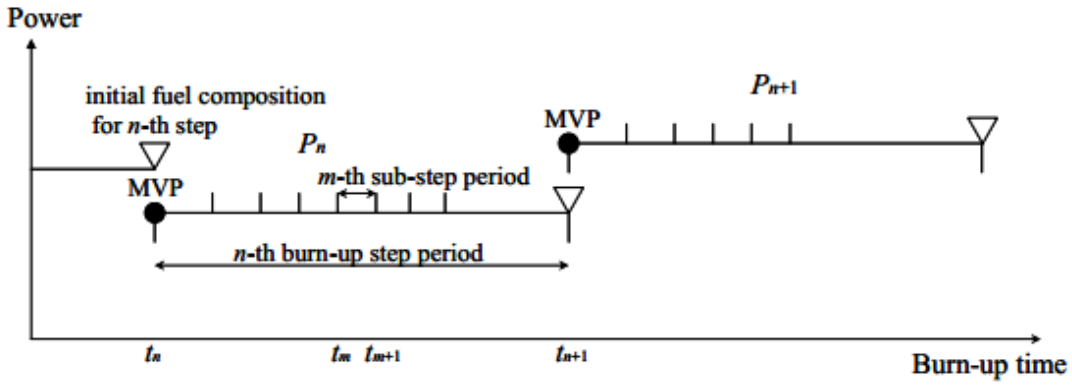


Figure 5: Burnup Steps and Sub-steps in MVP-BURN Calculations [24]

The chain model for the burnup calculation can be easily changed according to reactor types and computer resources. This code has been developed by Japan Atomic Energy Research Institute (JAERI). The library data used in this code is based on JENDL-3.2 for all nuclides (energy range from 1.0E-5eV to 20MeV) [25] As for the other commercial code discussed above, even though MVP-BURN can be used for burnup calculations, performing sensitivity analysis for the SCWR new fuel might be challenging and time consuming using MVP-BURN.

2.1.7 CESAR

Simplified Evolution Code Applied to Reprocessing (CESAR) is a depletion code developed by Commissariat à l'Energie Atomique. CESAR has developed significantly

during the past years and the current version of the code has the library for more than 100 heavy nuclides and 200 fission products and is providing depletion calculation for many different nuclear fuels. [26] Around 2005 a new application was added to CESAR which makes it capable of depletion calculations and it uses the JEF2.2 nuclear data. CESAR also has developed into a much more user friendly code due to its Graphical User Interface. CESAR is usually coupled with the APOLLO2, which is a 2D lattice physics code. It collapses all the obtained cross-sectional groups into one energy group before completing the depletion analysis.[27] As well, CESAR is compatible with DARWIN, a fuel-cycle code that models depletion and mainly focuses on the characteristic of the burn-up fuels from reactors exploiting experimental data. To perform sensitivity analysis for SCWR fuel, one needs to manipulate manually the library data to impose the uncertainties of interest.

2.1.8 FICST CODE

The objective of this thesis project as stated in chapter one was to develop a code to be used as an SCWR irradiated Fuel Isotopic Composition Sensitivity Tool, (FICST). FICST, like FISPIN, is a 'point' code.

FICST completes the analysis by treating the fuel element, fuel bundle, fuel channel or core as one point, (i.e. the same irradiation condition). As a result, it can be used to perform detailed analysis for a small part of the fuel pin, say with $1cm^3$ volume, or it can be generalized to perform a whole core analysis. FICST input can be altered so that one can change densities of the nuclides in the fuel. Thus, one can study the sensitivities of fuel performance having different isotopic compositions such as slightly higher plutonium oxide content or different isotopic compositions of the plutonium. If

one is interested, besides the isotopic composition of the atoms, it is also possible to extract the radioactivity in becquerels or curies.

To make FICST user friendly, the radioactive decay constants were added to the library in an Excel file. The decay paths and the branching ratios for the various actinides and fission products have been embedded in the code. If an isotope of interest is not included in the current library of FICST, one can easily modify the library and include this data. The library data is saved in Microsoft EXCEL; it is easy to understand and alter.

In order to calculate the depletion and generation rates, there is also a library of the cross sections for many actinides and fission products in the model. This information can be readily changed to simulate reaction rates with different flux data, e.g., time dependent flux data and more detailed neutron flux spectra. In its present form, FICST assumes neutron fluxes are available in three energy ranges. These energy ranges are referred to as thermal; epithermal and fast neutrons and the library of cross sections were assembled in these energy groups.

The accumulative and indirect fission yields of several fission products created by the fission of the actinides which undergo significant amounts of fission are also included in the library of the code, which can be altered if necessary to simulate different types of fuel which may contain either other fissile isotopes or higher atomic number actinides.

In short, the main purpose of FICST is to project the concentrations of the actinides and fission products in the fuel sample chosen as a function of time. FICST provides the user with a tool to perform the sensitivity analysis of those time dependent concentrations to any uncertainties in the nuclear data such as cross section parameters. FICST allows one to simulate changes in reactor power. By introducing a power-generator or a step function, the average flux values can be changed at different time

steps. This modification allows the user to keep track of actinide and fission product inventories during maintenance outages and during refuelling outages when the fuel is exchanged or moved. The latter demands further design detail and can be further exploited in the next stage of the design.

The main advantages of FICST over the other codes stated in this chapter are as follows:

- It is specifically developed to handle the Canadian SCWR fuel.
- It is user friendly; little or no alteration is needed from the user.
- The libraries are available in EXCEL and Matlab, and the code can be run in WINDOWS.
- This code is specific for sensitivity analysis and the run time is very short; that makes it perfect for preliminary design analysis, whereas more complicated code such as Monte Carlo codes need much longer run time and more complicated model.
- There are specific blocks developed in the code that will allow the user to simply change the properties of one the isotopes while keeping the rest un-changed, and thereby undertake a sensitivity analysis.
- The code automatically saves the output data into an EXCEL file, which makes it much easier to report.

2.1.9 Comparison of Available Codes

Table 1 summarizes the information about the codes that potentially can be used for sensitivity analyses of SCWRs irradiated fuel. In total, seven main commercial codes were identified and compared with FICST.

Table 1: List of Potential Codes for Performing on Uncertainty Analysis

DEPLETION CODES	DATA LIBRARY	GEOMETRY MODELLING	METHOD USED FOR CALCULATIONS
FISPIN	"JEF-2.2: The Joint Evaluated File (JEF-2.2) is an evaluated library produced via an international collaboration of Data Bank. The JEF-2.2 library comprises several sub libraries; incident neutron data (general purpose library), radioactive decay data, fission yields data and thermal scattering law data. It is in ENDF-6 format and contains data for 313 materials"[28]	point calculations	FISPIN is usually coupled with CASMO lattice physics code for modeling PWR and BWR fuel however optimization of the code to model SCWR fuel could be challenging due to the differences in the fuel designs.
DRAGON-DONJON 4	ENDF	2D modeling	It has its limitation in modeling the lattice pitch for SCWRs
SCALE	ORLIBJ33 (based on JENDL3.3)	2D calculation	SCALE is best available commercial code for conducting this type of sensitivity analysis. However user needs to use TRITON and ORIGEN to develop a model for the SCWR specific conditions. Thus not the best to be used at preliminary design stage
MONTBURNS (MCNP+ORIGEN)	JENDL3.2	2D and 3D calculation	longer computational time and detailed design information is required to develop the model

TRIPOLI-4	ENDF format continuous energy cross-sections, from various international evaluations including JEFF-3.1.1, ENDF/B-VII.0, JENDL4 and FENDL2.1[30]	3D calculation	The TR4PEP is mainly used and developed to validity for PWR high burnup UO2 and MOX fuel applications. Some modification is required to be able to use it for SCWRs fuel
MVP-BURN	JENDL-3.2	2D calculation	longer computational time and detailed design information is required to develop the model
CESAR	JEF2.2	point calculations	-
FICST	ENDF/B-VII.0	point calculations	it is specifically developed for the Canadian SCWRs fuel, fast computation time and easy to use

In short, as L.Blomeley and J. Pencer have stated, [31] most of the nuclear data are developed for the current reactors and based on the current operating conditions. However, the Canadian SCWRs like other Generation-IV reactors have significantly different operating condition and materials.[31] Thus the current data may not be accurate enough to be used for the SCWR analysis. It is important to conduct sensitivity analysis, to understand how sensitive the result of our analysis is to the library data that were used for the analysis. FICST is a code developed specifically for this purpose. FISCT provides the user with the option to study the effect of every single change, such as the uncertainties in cross sectional data, the fission yields, and the concentration of original atoms. The sensitivity analysis can be perform relatively simple via FISCT user interface, where in other available codes significant effort is required in order to perform perturbations to cross sections. This is an important and unique contribution.

The next chapter focuses on the theory used to develop FICST.

Chapter 3:
Theory

To determine the impact of nuclear data uncertainties on the irradiated-fuel isotopic-composition, one must start by determining the time dependent nuclide concentrations by solving the following first-order differential equation:

$$\frac{dN_i(t)}{dt} = Production\ Rate - Loss\ Rate \qquad (3-1)$$

To solve this first-order differential equation for each of the nuclides of interest, a large set of mathematical equations, which describe the production rate (i.e. fission/capture/decay process), and the loss rate (i.e. capture and decay), with initial conditions and a specified time frame ,was developed using the MATLAB/ Simulink computer code[3]. The following sections provide a brief description of neutron absorption, reaction rate, and decay which are essential to developing and using this tool.

In this section the theoretical background of the project is reviewed.

3.1 Neutron absorption (fission and capture)

Neutron absorption is the process in which neutron radiation induces radioactivity in materials, and occurs when atomic nuclei capture free neutrons. The absorption of a neutron can split the nucleus into two smaller nuclei (nuclear fission); the nuclei also can become heavier and enter an excited state (capture). The excited nucleus often decays

[3] Simulink® is an environment for multidomain simulation and Model-Based Design for dynamic and embedded systems. It provides an interactive graphical environment and a customizable set of block libraries. (http://www.mathworks.com/products/simulink)

immediately by emitting particles such as neutrons, protons, or alpha particles and at marginally longer decay times by emitting beta particles.

An example of nuclear fission is the absorption of a thermal neutron by U-235 in the reactors. This process can lead to production of fission products, such as rubidium, cesium, tellurium and others. An example of nuclear capture is the production of cobalt-60 when cobalt-59 absorbs a neutron.

In this study one would be interested in studying how fission products are produced from irradiation of the different actinides present in the fuel in the core.

3.2 Reaction Rate

If a substance with the macroscopic cross section of $\sum(E)$ is placed in a neutron flux the number of reactions /cm3/s is called the reaction rate, which can be used in the specific depletion and generation calculations. The reaction rate (reaction/cm3/s) is given by: [42]

$$\psi = \int_0^\infty \sum(E)\Phi(E)d(E) \qquad (3-2)$$

ψ =reaction rate (reaction/cm^3/s)

$\sum(E)$ =cross section

$\Phi(E)$ =neutron flux

This reaction rate can be written as:$\psi = \bar{\bar{\sum}}\Phi$ product of average cross-section and the total neutron flux where:

$$\bar{\bar{\sum}} = \int_0^\infty \sum(E)\frac{E}{E_T}e^{-E/E_T}\frac{dE}{E_T} \qquad (3-3)$$

Where $EE_T = kT = \frac{1}{2}mv_T^2$ and v_T is the most probable velocity for Maxwell Distribution of Energies.

For the special case of a 1/v absorber in a neutron flux that can be characterized by a Maxwellian distribution:

$$\sum_a = \sqrt{\frac{\pi}{4}}\sum_a(E_T) \qquad (3-4)$$

and average neutron velocity $\bar{v} = \sqrt{\frac{4}{\pi}}v_T$

Thus, it can be concluded that:

$$\psi = \bar{\sum}_a \Phi = \bar{\sum}_a(\bar{v})n\bar{v} \qquad (3-5)$$

Equation (3-5) can be solved by having the corresponding flux and cross-sections in multi-groups.

The neutron flux distribution over the energy range in most of the thermal reactors can be divided into these three groups. (See Figure 6)

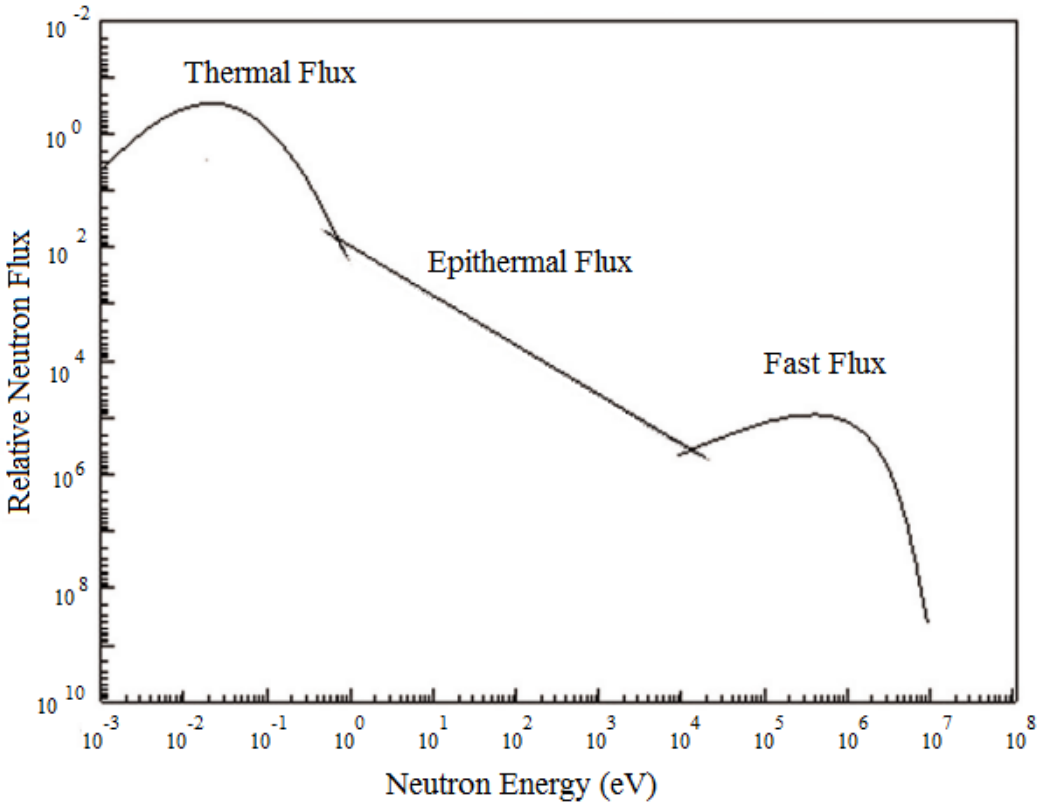
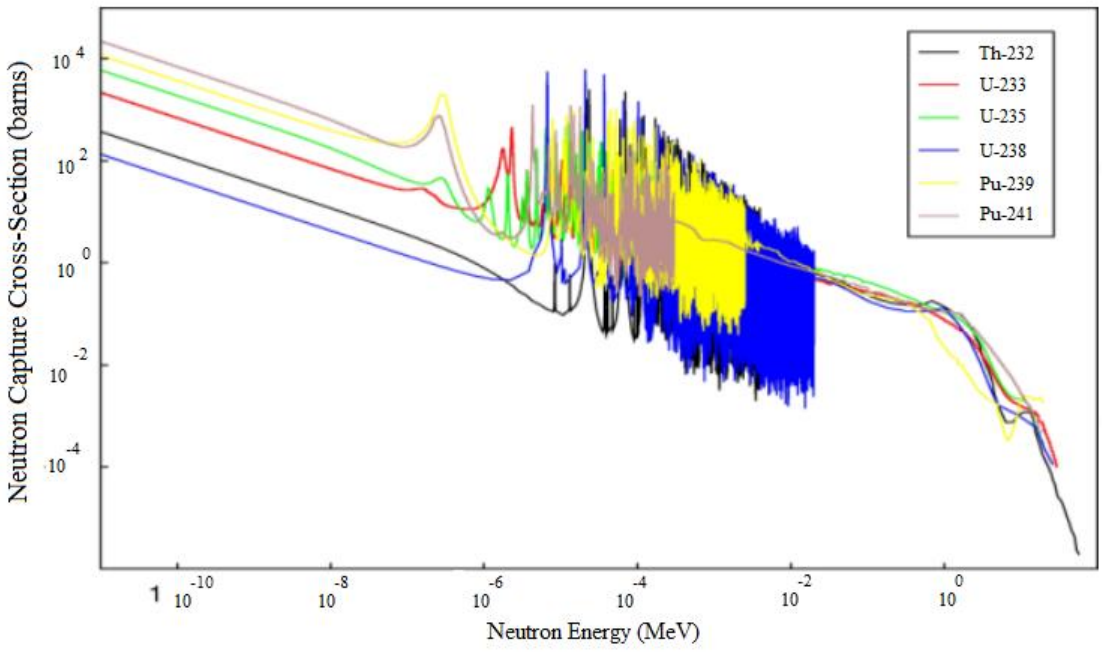


Figure 6: A Typical Reactor Neutron Energy Spectrum and the Three Energy Groups [29]

The fast flux is very similar to the fission neutron spectrum. The epithermal neutron component consists of neutrons (energies from 0.5 eV to 100 keV). The thermal neutrons (energies below 0.5eV) are in thermal equilibrium with the moderating material(s).[4] The energy spectrum of thermal neutrons at room temperature is best described by a Maxwell-Boltzmann distribution with a mean energy of 0.025 eV and a most probable velocity of 2200 m/s. Figure 7 shows the relationship between neutron cross-section and neutron energy for the major actinides.[29] It can be observed that for the intermediate group it is a straight line.



[4] These group boundaries are based on the neutron cross sections and resonance integral and fast group defined in the "Chart of the Nuclides" data. The reason to choose these boundaries is discussed in more details in Section 4.3.3 and Appendix C.

Figure 7: Neutron Cross-section vs. Neutron Energy for Major Actinides

Hence the equation (3-5) can be derived for the three energy-groups as discussed above.

$$\psi = \psi_{th} + \psi_{epi} + \psi_{fast} \qquad (3-6)$$

Where

$$\psi_{th} = \Phi_{th}\sigma\sqrt{\frac{\pi}{4}\times\frac{T_0}{T}} \qquad (3-7)$$

ψ_{th}= Reaction rates due to thermal neutron interactions

Φ_{th}= Thermal neutron flux (n/cm^2/s)

σ= Thermal neutron microscopic cross-section;

$$\psi_{epi} = \Phi_{epi}RI\frac{1}{ln\frac{E_u}{E_l}} \qquad (3-8)$$

ψ_{epi}= Reaction rates due to neutron interactions in the resonance range

Φ_{epi}= Epithermal neutron flux (n/cm^2/s)

RI = Resonance integral (cm^2)

E_u = 0.821 MeV (upper energy limit)

E_l = 0.414 eV (lower energy limit)

$$\psi_{fast} = \Phi_{fast}\sigma F_{fast} \qquad (3-9)$$

ψ_{fast}=Reaction rate due to fast neutron interactions

Φ_{fast}= Fast neutron flux (n/cm^2/s)

σ = Fast neutron microscopic cross-section

F_{fast} = Correction factor = $\frac{1}{0.755}$ where 0.755 is calculated from the distribution of neutrons over the whole fission neutron spectrum.[5]

[5] These correction factors are derived from the information obtain from "K.H. Beekurt, K. Writz, Neutron Physics, translated by L. Dresner. Springer-Verlag New. York Inc. (1964)" and also national Physics Laboratory, http://www.npl.co.uk/

3.3 Neutron absorption model

The fission, neutron capture, and decay processes of the nuclides can be modelled in Simulink using combinations of first-order differential equations.

The atomic populations of existing actinides[6] in the SCWR or those produced via neutron absorption and/or decay can be modelled and tracked FICST. The fission yields of the fission materials such as thorium, plutonium and uranium are included in the code so the fission products atomic populations can be tracked. Also, tracking the concentration of the daughter products of these isotopes (such as Xe-132 from the decay of I-132) is included in the model.

3.4 Activation of actinides

Activation of actinides can be calculated using the following:

$$\frac{dN_a(t)}{dt} = -\lambda_a N_a(t) - \psi N_a(t) - \gamma N_a(t) \qquad (3-10)$$

$N_a(t)$ total number of atoms
λ_a the decay constant
ψ the reaction rate
γ the fission rate

The model for the rest of the fission products:

$$\frac{dN_i(t)}{dt} = fission\ yield - decay - capture \qquad (3-11)$$

$$\frac{dN_i(t)}{dt} = \gamma N_i(t) - \lambda_i N_i(t) - \psi N_i(t) \qquad (3-12)$$

Where:

N_i number of fission product atoms of the i^{th} species
λ_i the decay constant
ψ the reaction rate

[6]Actinide: series of fifteen metallic chemical elements with atomic numbers from 89 to 103

γ the fission rate

The production of the daughter products is determined by the decay term of the parent products.

$$\frac{dN_j(t)}{dt} = \lambda_i N_i(t) - \psi N_j(t) - \lambda_j N_j(t) \qquad (3-13)$$

And for the isotopes produced during the neutron capture reactions

$$\frac{dN_k(t)}{dt} = \psi N_j(t) - \lambda_k N_k(t) - \psi N_k(t) \qquad (3-14)$$

3.5 Decay

One of the mechanisms for production and removal of a nuclide is the radioactive decay. Radioactive decay is a process by which an unstable nucleus loses energy. This decay, or loss of energy, results in an atom of one type (called the parent nuclide) transforming into an atom of a different type, (named the daughter nuclide). The decay is a loss from the inventory of the parent isotope and a creation or generation event for the daughter nuclide. The effect of radioactive decay is modelled by the following equation for the parent nuclide:

$$\frac{dN_i(t)}{dt} = -\lambda_i N_i(t) \qquad (3-15)$$

$N_i(t)$ number of atoms of the i^{th} species or nuclide

λ_i The decay constant for the i^{th} species, the decay constant (λ) of radioactive decay is equal to the reciprocal value of the average lifetime (τ).

The effect of radioactive decay is modelled by the following equation for daughter nuclide:

$$\frac{dN_j(t)}{dt} = \lambda_i N_i(t) \qquad (3-16)$$

$N_j(t)$ At t=0 is equal to the initial number of daughter nuclide atoms of the j^{th} species

$N_i(t)$	number of active atoms of the ith species
λ_i	The decay constant for the ith species, the decay constant (λ) of radioactive decay is equal to the reciprocal value of the average lifetime (τ).

The theory discussed in Chapter 3 was used to solve a series of first order differential equations, using MATLAB/Simulink. Chapter 4 will provide a brief explanation about how FICST was developed.

Chapter 4:
SCWR Irradiated Fuel Isotopic Composition Sensitivity Tool (FICST)

The purpose of this chapter is to provide an explanation of how FICST was developed based on theory explained in chapter 3.

4.1 SCWR Fuel Compositions – Initial Number of Atoms

As discussed in chapter 2, FICST is a point code. The user can decide to model a fuel element, fuel bundle, fuel channel or the whole core. The irradiation conditions in terms of neutron fluxes and duration of the irradiation are the same for the whole sample. The current model of SCWRs has input data for one fuel bundle; however, the input can be easily modified. More than 82 actinides and 84 fission products nuclides have been included in the library of this code. The initial inventories of these atoms are set to zero except for the following nuclides: Th-232, Pu-238, Pu-239, Pu-240, Pu-241, and Pu-242. The number of atoms of these actinides in the fresh fuel bundle is calculated using the given data in the Canadian SCWR concept. (See Appendix A for more details)

The fission products are produced as a result of fuel irradiation. The reaction-rate-chain was developed for each of the actinides stated above, considering the capture, fission, and decay process. The original numbers of atoms are zero for all other nuclides except the actinides stated above.

4.1.1 Initial Number of Atoms Sensitivities

The initial numbers of atoms that are currently used in developing FICST are based on the current anticipated fuel composition. These numbers can easily be modified

and assembled as FICST input data to accommodate any changes to the fuel or alternative fuel compositions. Also, a vector has been developed in which the user can change the concentration of each nuclide in the fuel by an arbitrary percentage. For example, one can study the effect of increasing the concentration of plutonium by 0.1% on the overall concentration of fission and fissile products in the irradiated fuel after the desired irradiation time. Sensitivity analysis due to uncertainties in the cross-sectional data is also an option which is discussed in more detail in 4.3.5

4.2 Burnup Chain Model

The burnup chain model used for modelling the depletion and production paths of SCWRs irradiated fuel is shown in Figure 8. The FICST library has the information for many actinides, and the chain model can be modified based on the reactor type. The chain model illustrated below is demonstrating the SCWRs fuel main burnup reactions. This model will be different for CANDU-6 fuel. An example of a chain model for some of the fission products is also shown in Figure 9. The Burnup Chain model was verified against the information available in the literature. (Appendix B)

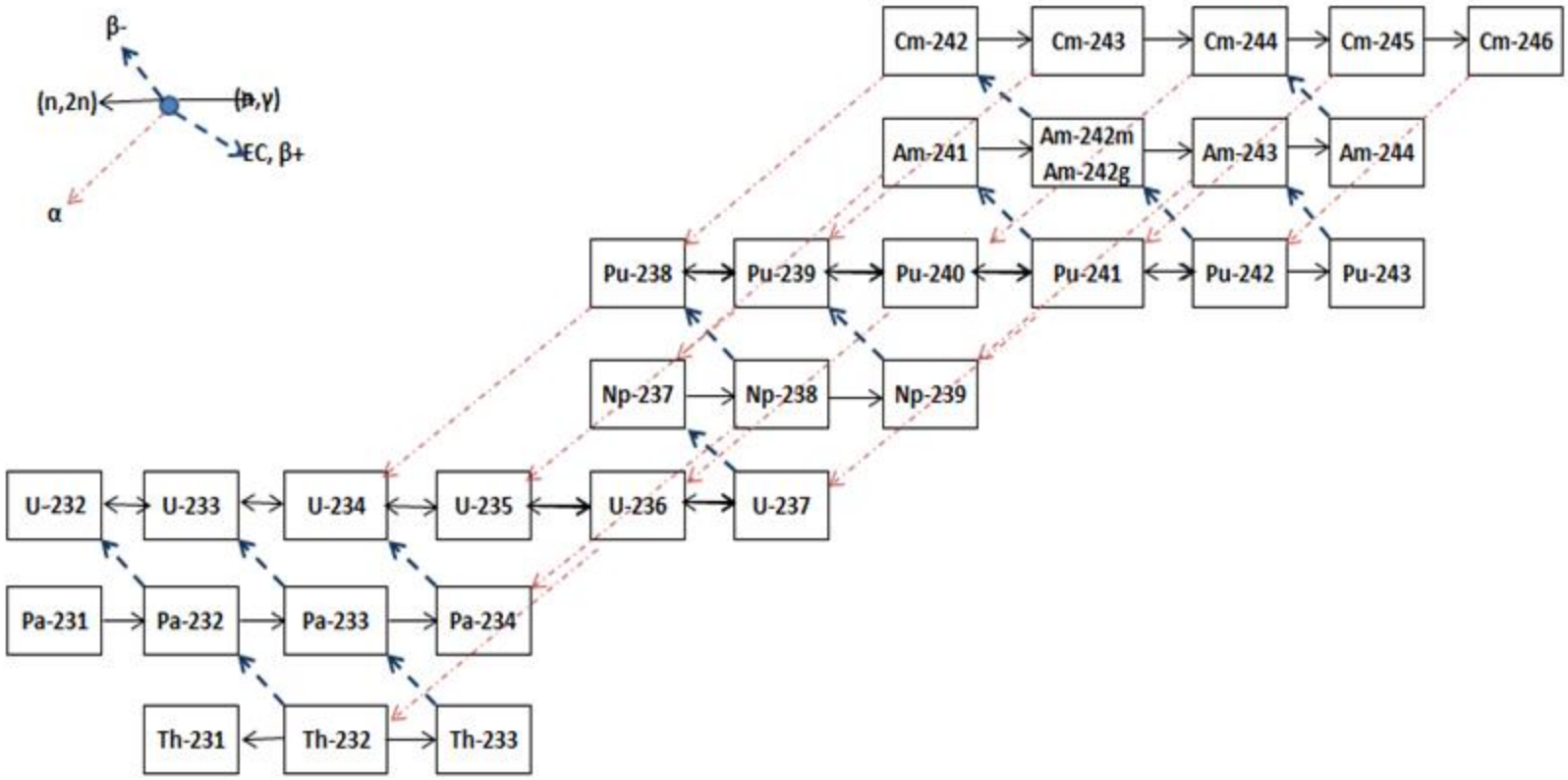


Figure 8: Canadian SCWRs Fuel Burn-up Chain Model

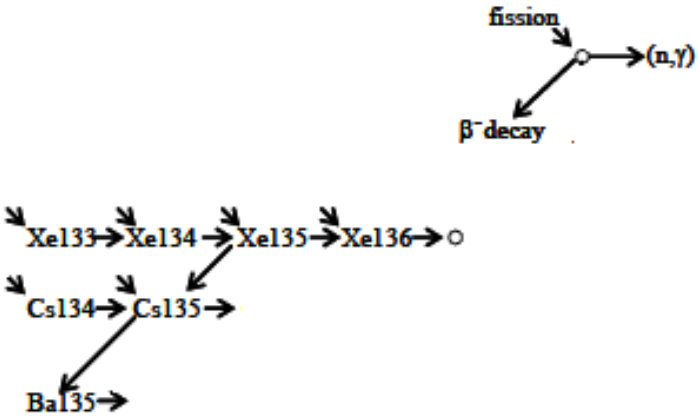


Figure 9: Canadian SCWRs Example of Fission Products Chain Model [24]

4.3 Reaction Rates

To complete the reaction rate calculation in the MATLAB model the following information was gathered:

- Fluxes
- The half-life (lambda) for both fissile and fission material
- Cross-sectional libraries for (capture and fission)
    - Cross-sectional data sensitivities factor
- The correction factors for the cross-sections
- Reaction rates-matrix multiplications
- Fission yields
    - Fission yields sensitivities factor

The requirement listed above will be explained in the following sections.

4.3.1 Fluxes

To illustrate the application of the FICST Tool, a simple treatment was applied to estimate the fluxes in the following three energy groups as described in the section 3.2: [7]

- Thermal energy which includes any neutron with an energy below 0.5 eV
- Epithermal or intermediate energy which is between 0.5 eV and 0.821 MeV
- And fast energy group which includes any neutron with energies above 0.821 MeV.

4.3.2 Decay constant

The half-life of a nuclide is defined as the period of time taken until half of the initial radioactive nuclide has disappeared or decayed away. And the lambda or radioactive decay constant is equal to the natural logarithm of 2 over the half-life value.

$$t_{1/2} = \frac{\ln(2)}{\lambda}$$

The half-life values of each of the actinides and the fission product`s model are extracted from "Chart of the Nuclides and Isotopes" [32] and saved as an Excel worksheet. Also, an extra utility was added which allows the information in the corresponding unit: i.e. second, minute, day or years. This utility automatically converts the half-life value of the desired time unit for the calculation. Thus, no unit conversion is required. The advantages of the"Unit" utility are easier verification of the data and reduction of probability of error in unit conversion.

[7] These group boundaries are based on the neutron cross sections and resonance integral and fast group defined in the "Chart of the Nuclides" data. The reason to choose these boundaries is discussed in more details in Section 4.3.3 and Appendix C.

4.3.3 Neutron Cross-sections and Resonance Integrals

The cross-section of a nuclide is defined as the probability of interaction of a neutron with that nuclide, and it is a function of neutron energy. Several types of reactions are possible as the neutron reacts with the nuclide: e.g. scattering, absorption and fission. [32]

The Canadian SCWR concept, like other thermal reactors, has a wide spectrum of neutron energies, which for the purpose of this study has been collapsed in the following three groups: thermal, intermediate (epithermal) and fast energy ranges. (See Chapter 3 for more information).

"When neutrons reach equilibrium with the moderator their energies are determined by the thermal energy distribution of the moderating atoms and the neutron energy spectrum becomes a Maxwellian distribution at the temperature of the moderator material."[31] The data given in the chart of nuclides for the thermal energy group are for a moderator at room temperature (20 °C); this neutron speed is 2200 m/s and the corresponding energy of 0.0253 eV. Thus, one needs to correct the Chart of Nuclide values to get the corresponding thermal cross sections for the current SCWR concept based on the formulas discussed in chapter 3. In the thermal region the absorption cross section of many materials varies as square route of 1/E, where E is the neutron energy. These materials are called 1/v absorbers. When a material such as U238 (n, γ) and U235 (n, f), does not follow $E^{-1/2}$, a correction factor is applied to correct this discrepancy. (Table B-1, Appendix B)

In the Chart of Nuclides, "the cross-sections given for the intermediate energy range are based on resonance integral. Where the resonance absorption peak occurs, a 1/E

function is used to represent the neutron spectrum. The resonance integral is the reaction rate integral over a broad energy range. To derive an average cross section for the energy range the resonance integral is divided by the integral of dE/E over the same energy range."[31] These values are based on the diluted quantities where there is no self-shielding factored in. Thus, there is no neutron flux depression in the neutron spectrum despite the presence of strong resonance absorption. And the infinite dilute resonance integral is a reaction rate integral over a broad energy range above 0.5 eV. The average cross section of this energy range is obtained from the following formulas.

$$EI = \int_{E_{0\max}}^{E} \sigma(E)\frac{dE}{E} \qquad (4\text{-}1)$$

$$\overline{e_{res}} = \frac{RI}{\int_{E_0}^{E_{max}} \frac{dE}{E}} \qquad (4\text{-}2)$$

Other methods such as the Bondarenko model can be used to derive a better value for the resonance regions for certain materials such as thorium and uranium if required and when a final flux distribution is available. However, at this stage of the design these values have not been included in the code. Note, when a small volume of fuel is modeled, self-shielding isn't an issue. Thus, the most accurate results of FICST can be obtained when the fluxes used in FICST is obtained for a small volume of fuel.

And finally, the values used for the fast cross-sections are taken from Appendix C.

4.3.4 The correction factors for the cross-sections

In thermal reactors a wide spectrum of neutron energies exists, because neutrons are slowed down when colliding with the moderator atoms. Three different correction

factors are used for the cross-sectional data in the three regions. These correction factors are discussed in Chapter 3. The moderating environment temperature is an important factor in calculating the correction factor for the thermal energy group. The neutrons released in the fuel have interaction with the fuel, the cladding, the pressure tube material, the heavy water moderator, and the light-water coolant. However, the interaction with the cladding and the pressure tube can be considered negligible.

To have a better understanding of how moderator, coolant, and fuel affect the neutron thermalization, one needs to study the elastic and the absorption cross sections of these materials. Figures shown in Appendix C were studied to determine the probability that the neutrons bounce around, are absorbed, or slowed downed in the coolant, moderator, and the fuel.

It can be observed that hydrogen, deuterium, and oxygen have a bigger elastic cross section in the thermal region than thorium and plutonium. Thus, most of the moderation is happening in the moderator and coolant rather than in the fuel.

In short, the fission in the fuel is caused by neutrons that were slowed down by the moderator and coolant. In the fuel, the neutrons are generally fast neutrons, since the neutrons generated in the fuel have high energies. The moderator and the coolant temperature determine the neutron temperature. Coolant also moderates neutrons, so its temperature plays a role.

The neutron temperature was calculated by a mass-weighted average of coolant and moderator temperature.

4.3.5 Cross Sections Sensitivities

One component of the input data that is very important for sensitivity analysis is the cross-sectional data. The objective of the cross sections sensitivities option, in FICST is to provide the user with an option to vary the cross-sectional data used in the library and to study the sensitivity of the results to those changes. For example, if there is a 1% uncertainty in the absorption cross-sectional value of Th-232, how does the xenon isotopic concentration change? To reach this goal, a cross section perturbation vector was developed that is multiplied by the original set of cross-sectional data used for the analysis.

The current value of the cross section perturbation vector for each of the actinide and fission products is equal to one (i.e. no perturbation from the library values). The user has the option of simply changing any of these numbers for the nuclides of interest. In the example above, the value used for Th-232, is changed from 1 to 1.01. Since the data is saved in an Excel-input file, no special skill is required to use this program. However, it is recommended that the original set of input files be saved separately, to track the changes made.

4.3.6 Decay Matrix Multiplications

The objective of the decay matrix is to take into account the production of the daughter products after the decay of a parent product. The decay constant is modelled using a gain block which is connected to a sum block to account for the loss of the different nuclides through decay. See Table 2 for a description of the gain and sum blocks. The decay constant -gain block- is connected to the decay matrix. The decay matrix

essentially represents the decay of one fission product into a daughter nuclide. If a fission product decays into a daughter nuclide, which is one of the n nuclides being modeled by FICST, a value of 1 (or the associated branching ratio) is inserted in the corresponding element of the (n x n) matrix.

4.3.7 Capture Matrix Multiplications

The loss of a nuclide through the capture process means that it contributes to the gain of another radioisotope. This production is accounted for in the "capture matrix". The capture matrix determines the formation of a radionuclide through the capture process. A (n x n) matrix determines which radionuclide is formed when another radionuclide undergoes the capture process. As for the decay matrix, a value of 1 is placed in an element located in a row that represents the nuclide formed through the capture process and a column which represents the radionuclide that underwent the capture process.

This information is explained in more detail in the Simulink Model, and Table 2.

4.4 Fission Yields

To determine the number of atoms of each fission product, one needs to decide which fission products need to be modelled. FICST outputs more than eighty fission product concentrations as a result of fuel irradiation. Most of the fission products that have not been included have very short half-lives. Because of their short half-lives the

probability of their transmutation through neutron capture is low, if the daughter products of these isotopes were of an interest, they have been included in the FICST library.

The other factor that was taken into account for calculating the fission products of interest was the fission yield. To find the production rate of fission products in equilibrium, one can use the yield data and fission rate of actinides. Some of the fission yields are zero or near to zero, so the production rate is small and negligible.

In order to determine accurately the fission yields and the mode of decay, the table of nuclides and the chart of nuclides were consulted to determine the branching ratios of the various isotopes. These branching ratios were then used to determine the number of atoms of the various isotopes that were decaying to subsequent daughter products. The direct fission yields or cumulative fission yields were extracted and used for each of the fission products based on their modeled decay chain.

To obtain the fission yield data, the Los Alamos National Library[8], Data Centre, National Nuclear Data Center, Evaluated Nuclear Data File (ENDF) [9] and the Nuclear Data Center at Japan Atomic Energy Agency[10] were studied. These libraries were saved in an EXCEL file, in a matrix format, which makes them easily accessible and facilitated verification of the data.

[8] http://t2.lanl.gov/nis/data.shtml[46]

[9] http://www.nndc.bnl.gov/exfor/endf00.jsp[47]

[10] http://wwwndc.jaea.go.jp/[38]

4.4.1 Fission Yields Sensitivities

The fission yield data are always accompanied by some uncertainties. Despite the improvements to JEFF fission-yields data, there is still some discussion on how these numbers can be improved. "Fission-yields data depend on the proton and neutron number of the target nucleus as well as on the incident neutron energy. Evaluated nuclear data on fission product yields are available for all relevant target nuclides in Gen IV reactor applications. However, the description of their energy dependence in the evaluated data is still rather elementary, which is due to the lack of experimental fission data and reliable physical models."[33]

Thus, the capability to perform sensitivity analysis based on the uncertainties of the fission yield data can be important for the conceptual design of SCWRs.

FICST provides a very simple tool to perform sensitivity analysis based on the uncertainties in the fission yields data. For example, if the user wants to study the effect of 2% uncertainty in the recorded fission yield of one of the actinides, this number can be easily accessed and changed within the "fission yield sensitivity" vector. The default setting of "fission yield sensitivity" vector (the same as the "cross section sensitivity" vector) is one; however, the user has the option of simply changing any of the parameters for the isotopes of interest and study the sensitivity of isotopic concentration to a change in the fission yield data.

4.5 The Simulink Model

FICST was developed using MATLAB/Simulink.[34] Other possible programming languages and software applications such as C++ or Microsoft Excel were

also an option. However, due to the flexibility offered by Simulink and its compatibility with EXCEL, MATLAB was adopted as the computer language for FICST. Some calculations were done in EXCEL to cross check the results of analysis in MATLAB.

MATLAB/ Simulink has an advantage over other available languages. It can be easily modified in a very time efficient manner. It also allows for some simple quality assurance procedures to be incorporated in the development of this tool. The Simulink part of FICST can be used to inspect visually the behavior of each isotope and the connections between them. Appendix D provides a brief discussion of Simulink and its features.

There are three parts to FICST as shown in Figure 10. The first part was used to simulate the irradiation of actinides in the SCWR fuel (the blue block); the yellow block represents the fission yield calculations, followed by the fission products in the green block. Under each of these subsystems, there are sets of blocks which are used to simulate the decay, capture, and fission. Two different integrators are used for the calculation of the actinide and the fission products population. The populations of thorium and plutonium atoms in the fresh fuel were put in as the initial condition of the actinide integrator used in the blue block, whereas the initial populations of fission products were set to zero. The yellow block takes care of the fission yield and the sensitivity vectors which produce the feed for the fission products. The subsystems under each of these blocks are shown in Figure 11, Figure 12, and Figure 13. The separation of actinides from the fission products and the vectorization of the model provide FICST with the ability to be used for sensitivity analysis of re-irradiated fuel besides the fresh fuel. The

user would need to change the initial condition in each of these integrators to present the initial number of atoms in the irradiated fuel.

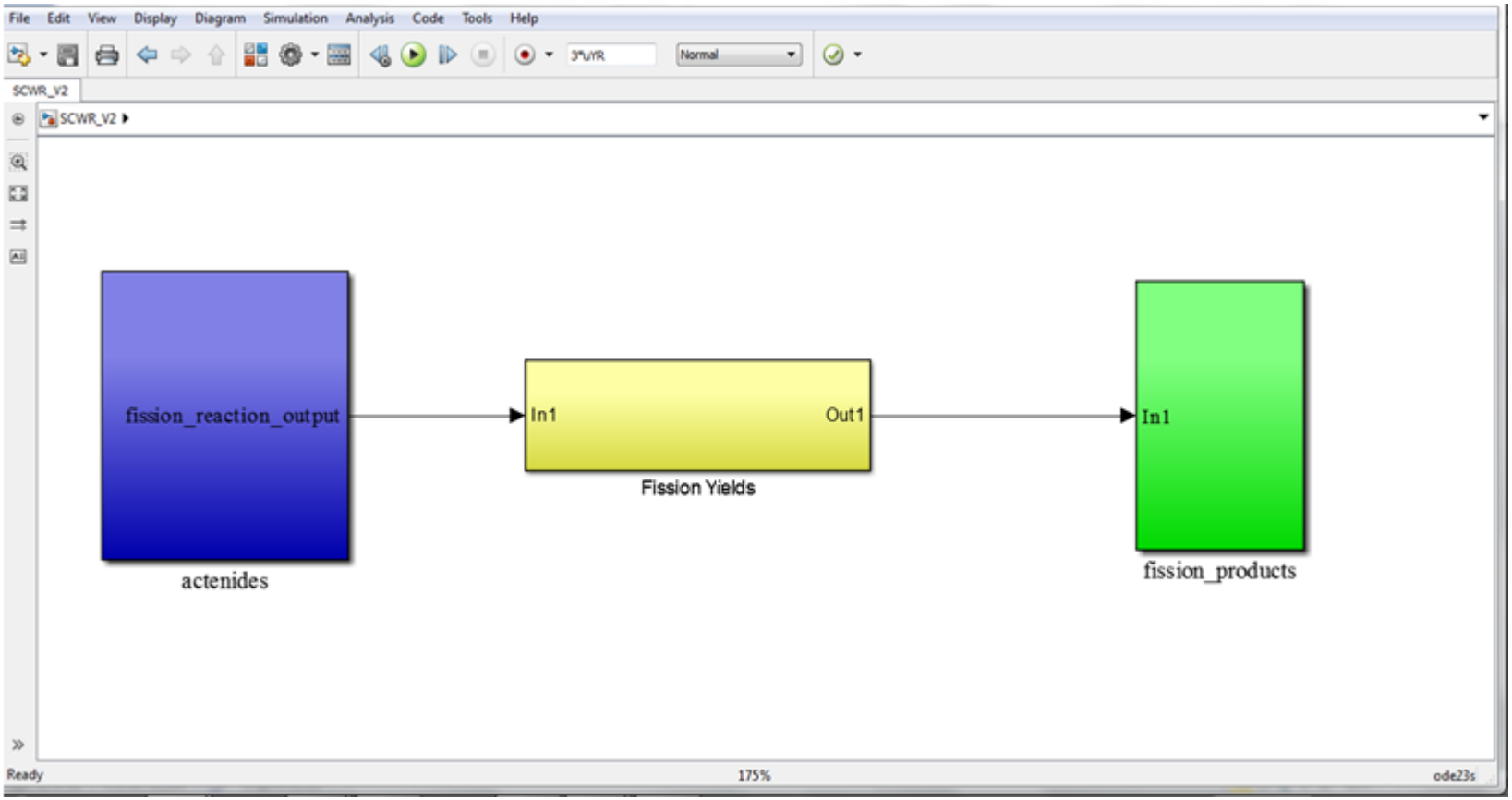


Figure 10: FICST Simulation Tool and the Three Outer Layers

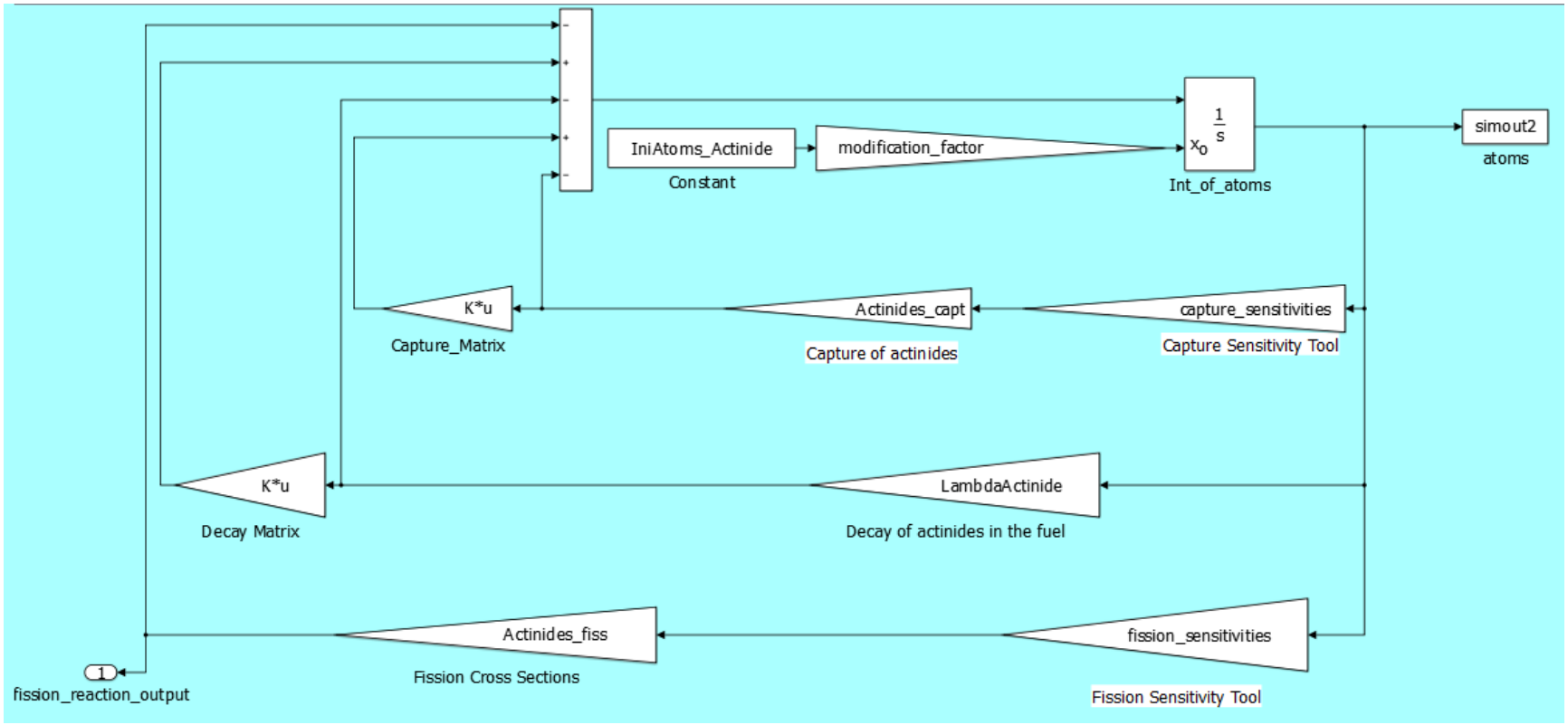


Figure 11: Actinide Simulation Tool

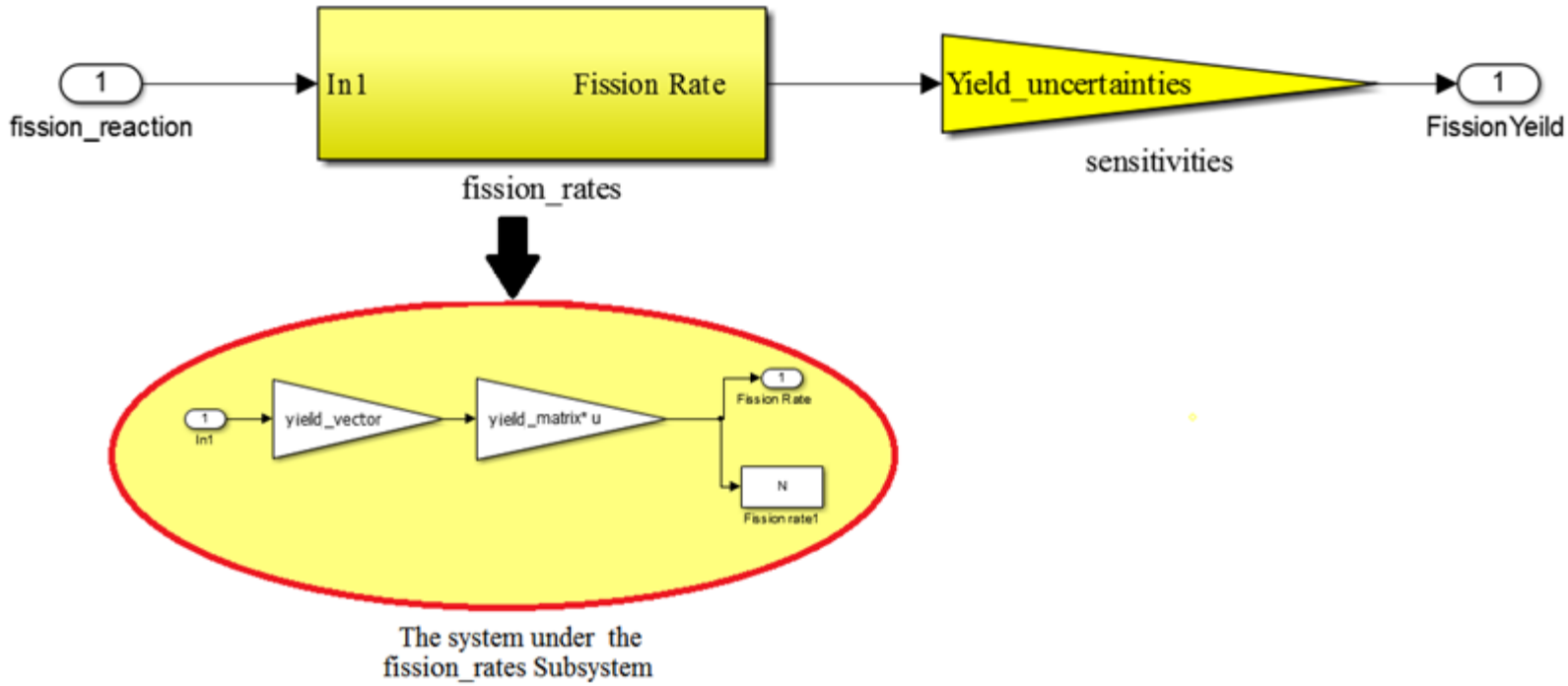


Figure 12: Fission Yield Simulation Tool and its Subsystem

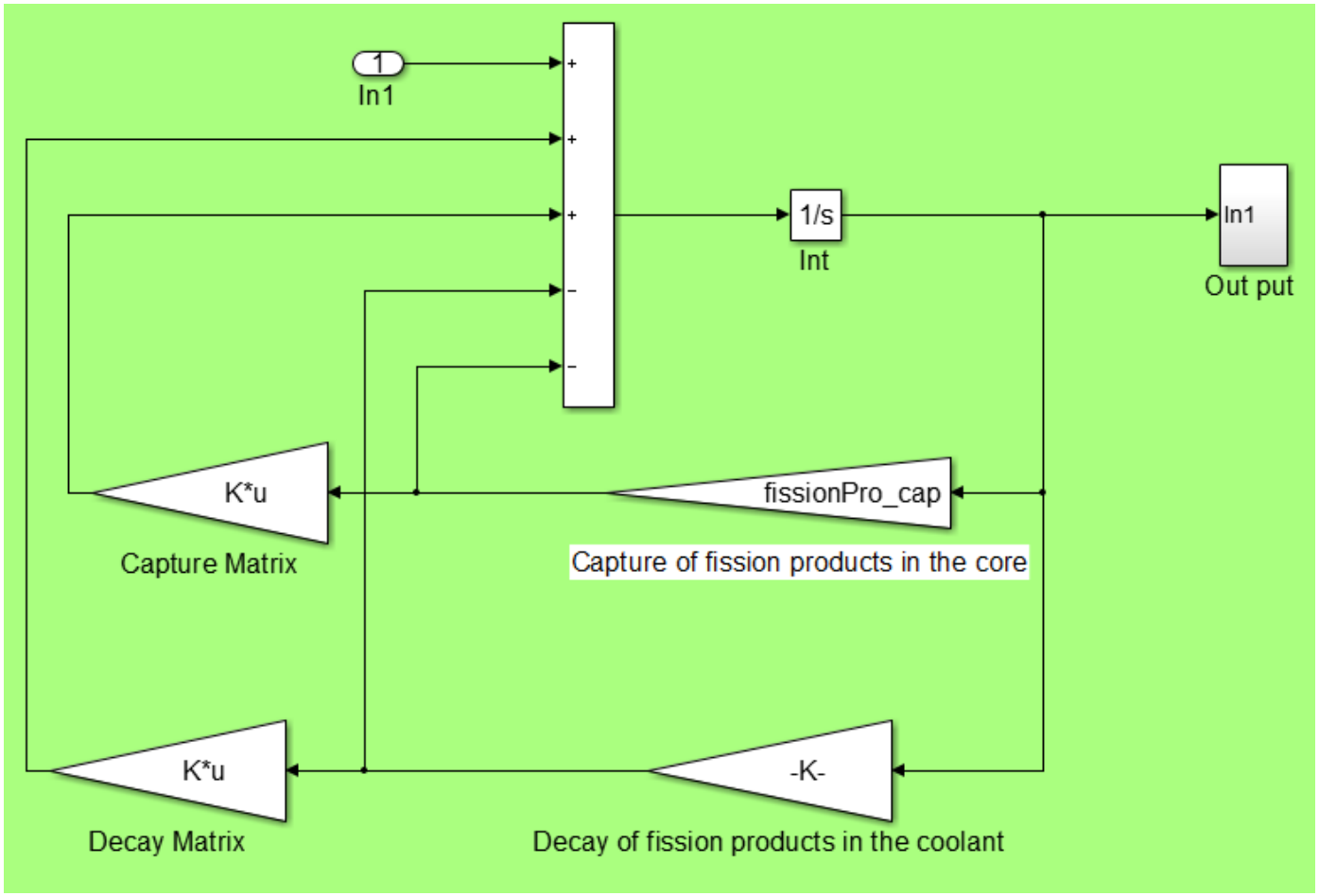
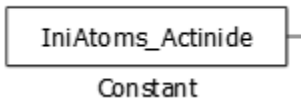
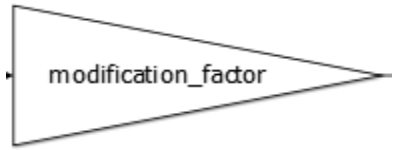
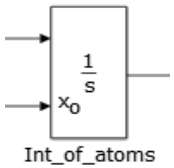
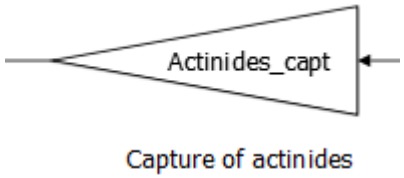
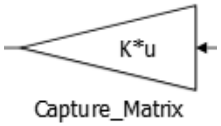
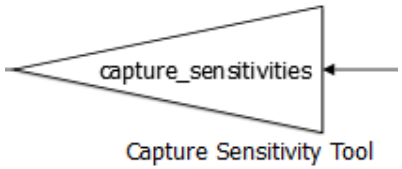
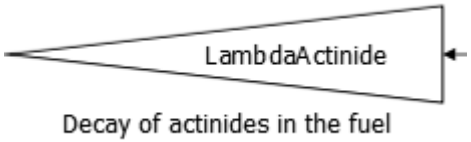
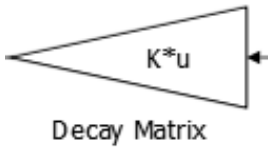
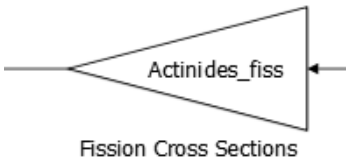


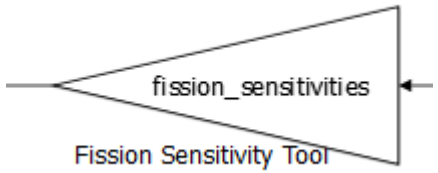
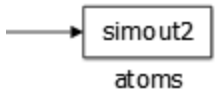
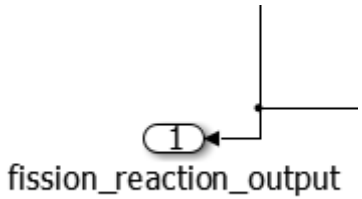
Figure 13: Fission Product Simulation Tool

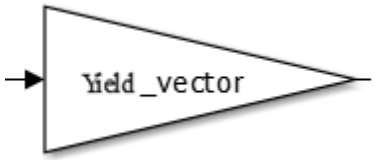
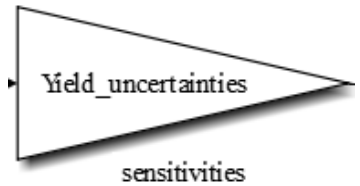
Table 2: Simulation Blocks Details and Descriptions [35]

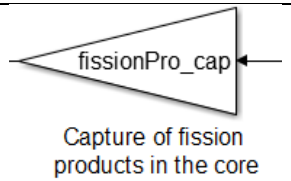
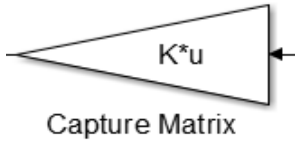
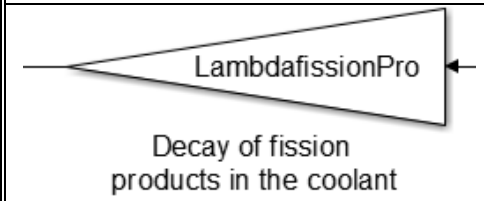
SIMULATION BLOCKS	SIMULINK LIBRARY BLOCK NAME	DESCRIPTION
	Constant	Constant number, which in this model refers to the initial number of atoms in the fresh SCWR fuel. This number can be modified if one is interested for example to look at the CANDU-6 fuel.
	Element-wise Gain block	A gain block which provide the user with the opportunity to change the % of initial number of atoms (i.e. increase the Th-232 by 0.1%
	Integrator with external initial condition	The integrator block. The initial conditions are fed in externally. The initial condition is the initial number of atoms in the fresh fuel.

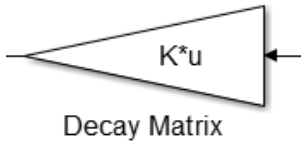
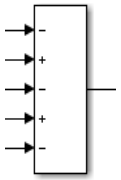
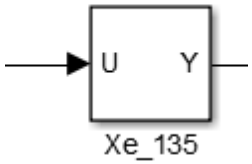
SIMULATION BLOCKS	SIMULINK LIBRARY BLOCK NAME	DESCRIPTION
	Element-wise Gain block	A gain block, represent the capture cross- sections for the actinides
	Matrix Gain block	The gain block, a the matrix multiplication , representing the neutron capture inside the fuel and the production of second nuclide
	Element-wise Gain block	A vector which provide the user with the opportunity to perform sensitivity analysis by changing the % of the given cross-section for an specific actinide

SIMULATION BLOCKS	SIMULINK LIBRARY BLOCK NAME	DESCRIPTION
	Element-wise Gain block	A matrix representing the decay constant of isotopes
	Matrix Gain block	A matrix representing the decay of isotopes inside the system to the daughter products
	Element-wise Gain block	A gain block, representing the fission cross- sections for the actinides

SIMULATION BLOCKS	SIMULINK LIBRARY BLOCK NAME	DESCRIPTION
	Element-wise Gain block	A gain block (vector) that provides the user with the opportunity to perform sensitivity analysis by changing the given fission cross section of specific isotope(s).
	Sim block (it is a Sink block)	"This block is used to put the output to the work space. For menu-based simulation, data is written in the MATLAB base workspace. Data is not available until the simulation is stopped or paused. For command-line simulation using the sim command, the workspace is specified using DstWorkspace field in the option structure."[34]
	Output block (it is a Sink block)	"Provide an output port for a subsystem or model. The 'Output when disabled' and 'Initial output' parameters only apply to conditionally executed subsystems. When a conditionally executed subsystem is disabled, the output is either held at its last value or set to the 'Initial output'."[34]

SIMULATION BLOCKS	SIMULINK LIBRARY BLOCK NAME	DESCRIPTION
	Element-wise Gain block	A vector providing the user with the option, to select the actinide that one wants to include its fission.
	Matrix Gain block	A matrix that represents the fission yield data of each of the actinides to the each of the fission products.
	Element-wise Gain block	A vector which provides the user with the opportunity to perform sensitivity analysis by changing the % of the given cross-section for a specific actinide

SIMULATION BLOCKS	SIMULINK LIBRARY BLOCK NAME	DESCRIPTION
	Element-wise Gain block	A gain block representing the fission products capture cross-sectional data
	Matrix Gain block	A gain block, the matrix multiplication , representing the neutron capture inside the fuel and the production of second nuclide
	Element-wise Gain block	A matrix representing the decay constant of fission products

SIMULATION BLOCKS	SIMULINK LIBRARY BLOCK NAME	DESCRIPTION
	Matrix Gain block	A matrix representing the decay of fission products inside the system to the daughter products
	Sum block	"Add or subtract inputs"[34]
	Selector	"Select or reorder specified elements of a multidimensional input signal. The index to each element is identified from an input port or this dialog. You can choose the indexing method for each dimension by using the "Index Option" parameter."

SIMULATION BLOCKS	SIMULINK LIBRARY BLOCK NAME	DESCRIPTION
	Floating scope	Provides a graph for a specific isotope selected by the Select block. X-axis is the time in (defined unit of time (i.e. Sec) and Y axis provides the number of atoms (in this application)

4.1 The m-File

"An m-file, or script file, is a simple text file where you can place MATLAB commands. When the file is run, MATLAB reads the commands and executes them exactly as it would if you had typed each command sequentially at the MATLAB prompt."[34] The m-file used for FICST, reads all the input data from the EXCEL file, submits the data to the Simulink model and runs the Simulink model for three years of operation and outputs the data into an excel file. The time intervals used in the output data can be reduced to decrease the computation time or increased to have more detailed data. The m-file of FICST is shown in Appendix E.

Chapter 5:
Results

The objective of this thesis project is to develop a tool for performing uncertainty analysis for the SCWR fuel. Chapter 4 provided a detailed explanation of how this tool was developed. In this chapter a series of examples are given to demonstrate how this code works.

FICST allows the user to determine the impact of uncertainties in the nuclear data on the irradiated-fuel isotopic composition by: studying the sensitivities to the uncertainties in the cross-sectional data, the fission yield data, the neutron temperature or the initial fuel composition. In this chapter, the first three scenarios are studied to demonstrate how FICST can be used. These examples are based on the isotopic composition of a three-year-irradiated fuel.

5.1 Cross-sectional Data Sensitivity

Thorium-232 capture cross-section is selected as an example to demonstrate how FICST can be used to study the sensitivity of the isotopic concentration of the fuel to the uncertainties in one piece of cross-section data.

According to K. Kobayashi in his article in the "Journal of Nuclear Science and Technology", the uncertainty of Th-232 capture cross-section is around 1% near 400 keV and 0.5% near 1 keV.[36]. B.Burris and R. Morehouse [37] have also indicated Th(n,γ) cross-sections uncertainties are about 2% within the energy range of 3 to 3000 keV; [37] which is also in agreement with the findings of K. Kobayashi (More details are provided in Appendix F)

In ENDF/B-VII-1 libraries, the neutron cross section data recorded is associated with 1% uncertainty for the calculated data and 0.2% for the measured data.

The mixture of the experimental data and the calculated data was constructed by assuming the following uncertainties: [38]

Table 3: Th-232 Cross-sectional data uncertainties (ENDF library) [38]

TH-232	UNCERTAINTIES RANGE	
	resonance	non-resonance
total cross section:	1.50%	0.50%
capture cross section	1.50%	

After determining the uncertainties in thorium cross sectional data, a large number of the same run were conducted, and the only difference between these runs was the changes made on the Th-232 absorption cross section value within the boundaries obtained from the literature. A similar method is described by D. Cruz. [39]

As expected and explained in the chain reactions in Chapter 4, not all the actinides are affected by the thorium concentration. Table 4 shows the actinides affected by the uncertainties in the Th-232 absorption cross section.

The isotopic concentrations of plutonium and americium are independent of the isotopic concentration of thorium or its cross-sectional data as results no sensitivity to the changes in Th-232 absorption cross sections is observed, whereas a visible change in the isotopic concentration of protactinium, uranium, neptunium and the thorium isotopes is shown (See Table 4).

Table 5 and Figure 14 show the sensitivity of isotopic concentration of xenon isotopes to the uncertainties of Th-232 cross sections. In most cases a small variation of the isotopic concentration of xenon is observed.

Table 4: An example of sensitivity analysis of actinides isotopic concentration to the uncertainties in cross sectional data obtained with FICST

		UNCERTAINTIES IN Th -232 ABSORPTION CROSS SECTION (%)								
		1.0%	1.5%	2.0%	2.5%	3.0%	3.5%	4.0%	4.5%	5%
% EACH OF ACTINIDES ARE AFFECTED BY THE UNCERTAINTIES IN TH-232	238Np	0.991%	1.486%	1.982%	2.477%	2.973%	3.468%	3.964%	4.459%	4.954%
	237Np	0.991%	1.486%	1.982%	2.477%	2.973%	3.468%	3.964%	4.459%	4.954%
	237U	0.990%	1.485%	1.981%	2.476%	2.971%	3.466%	3.961%	4.456%	4.951%
	236U	0.990%	1.485%	1.980%	2.476%	2.971%	3.466%	3.961%	4.456%	4.951%
	235U	0.989%	1.484%	1.978%	2.473%	2.967%	3.462%	3.956%	4.451%	4.945%
	234U	0.987%	1.481%	1.975%	2.468%	2.962%	3.456%	3.949%	4.443%	4.936%
	233U	0.985%	1.477%	1.969%	2.462%	2.954%	3.446%	3.938%	4.430%	4.922%
	234Pa	0.977%	1.465%	1.953%	2.441%	2.929%	3.417%	3.905%	4.393%	4.881%
	233Pa	0.977%	1.465%	1.953%	2.441%	2.929%	3.417%	3.905%	4.393%	4.881%
	234Th	0.977%	1.465%	1.953%	2.441%	2.929%	3.417%	3.905%	4.393%	4.880%
	233Th	0.976%	1.464%	1.952%	2.440%	2.927%	3.415%	3.903%	4.390%	4.877%
	232Th	-0.018%	-0.027%	-0.036%	-0.045%	-0.054%	-0.063%	-0.071%	-0.080%	-0.089%

Table 5: An example of sensitivity analysis of fission products isotopic concentration to the uncertainties in cross sectional data obtain from FICST

		UNCERTAINTIES IN Th-232 ABSORPTION CROSS SECTION (%)								
		1.0%	1.5%	2.0%	2.5%	3.0%	3.5%	4.0%	4.5%	5%
% Xenon isotopes are affected by the uncertainties in Th-232	Xe 129	0.00007%	0.00010%	0.00014%	0.00017%	0.00020%	0.00024%	0.00027%	0.00031%	0.00034%
	Xe 311m	0.20422%	0.30632%	0.40841%	0.51048%	0.61255%	0.71461%	0.81666%	0.91870%	1.02073%
	Xe 131	0.08445%	0.12668%	0.16890%	0.21112%	0.25333%	0.29554%	0.33776%	0.37996%	0.42217%
	Xe 132	0.05799%	0.08698%	0.11597%	0.14496%	0.17394%	0.20293%	0.23191%	0.26089%	0.28987%
	Xe 134	0.04872%	0.07308%	0.09744%	0.12180%	0.14615%	0.17050%	0.19486%	0.21921%	0.24355%
	Xe 135	0.11614%	0.17420%	0.23225%	0.29030%	0.34835%	0.40639%	0.46442%	0.52245%	0.58047%
	Xe 136	0.05757%	0.08636%	0.11514%	0.14392%	0.17270%	0.20148%	0.23026%	0.25903%	0.28780%

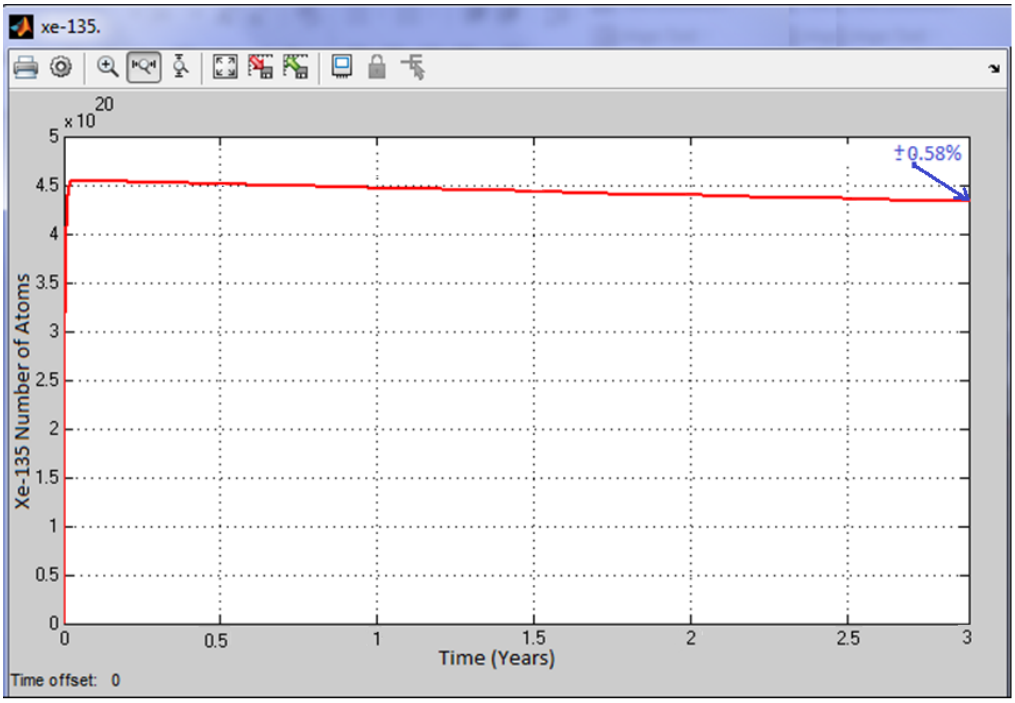


Figure 14: Sensitivity of xenon isotopic concentration to Th-232 cross sectional data uncertainties

5.2 Fission Yield Sensitivity

The independent fission yields are hard to measure, and there are few measurements available; as a result there are bigger uncertainties in the nuclear data for the independent yields compared to the cumulative yields. On the other hand, cumulative yields are easy to measure and fit the empirical models well; as a result the cumulative yields have smaller uncertainties compared to the independent yields.[40] The major actinides independent and cumulative fission yield graphs are provided in Appendix G.

The uncertainties of the independent fission yields of Th-232, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242 for Xe-131 and their effect on Xe-131 concentration are shown in Table 6. The sensitivity analysis for Xe-132 and Xe-135 concentrations based on the

uncertainties in the cumulative yields of stated actinides are shown in Table 7 and Table 8.

Please note: the fission yields and the uncertainties associated with this fission yields data were obtained from JAEA nuclear data center [41]. FICST was used to obtain the sensitivity of the isotopic concentration of different Xenon isotopes to the uncertainties existing in the fission yields data. The purpose of this analysis was to demonstrate an example on how FICST is used to perform sensitivity analysis.

Table 6: Sensitivity of Xe-131 Concentration to Uncertainties in Fission Yield Data

XE-131		
Actinides	Independent Yield	Independent dY
Th232	2.28E-12	1.46E-12
238Pu	1.11E-07	7.13E-08
239Pu	1.24E-07	7.93E-08
240Pu	1.22E-08	7.82E-09
241Pu	2.35E-09	1.50E-09
242Pu	2.50E-10	1.60E-10
Total Effect On the Xe-131 Isotopic Concentration		58.51%

Table 7: Xe-132 Isotopic Concentration Sensitivity to Uncertainties in Fission Yield Data

XE-132		
actinides	Cumulative yield	Cumulative dY
Th232	2.97E-02	4.17E-04
238Pu	5.30E-02	8.49E-03
239Pu	5.41E-02	2.70E-04
240Pu	4.81E-02	7.70E-03
241Pu	4.57E-02	6.40E-04
242Pu	3.97E-02	6.35E-03

Total Effect On the Xe-132 Isotopic Concentration	0.97%

Table 8: Xe-135 Isotopic Concentration Sensitivity to Uncertainties in Fission Yield Data

XE-135		
Actinides	Cumulative yield	Cumulative dY
Th232	5.46E-02	1.28E-03
238Pu	6.72E-02	1.08E-02
239Pu	7.60E-02	7.65E-04
240Pu	7.22E-02	1.16E-02
241Pu	7.16E-02	1.44E-03
242Pu	7.46E-02	1.20E-02
Total Effect On the Xe-135 Isotopic Concentration		1.32%

5.3 Thermal Neutron Temperature Sensitivity

As discussed in chapter 3 and 4 of this document, the thermal cross-section used in the library of FICST is based on the data available in Chart of Nuclides. These data are based on the moderator (i.e. neutron temperature) of 20°C or 293.15K. In order to calculate the thermal reaction rates, these cross-sections are multiplied by a mass averaged temperature between the moderator and the coolant temperature. Since this is an approximation of the real thermal neutron energy, here a sensitivity analysis is performed on the effects of neutron temperature on the isotopic concentration of more than eighty fission products. (See Figure 15) Also, the sensitivity of isotopic concentration of several actinides was studied. (See Figure 16)

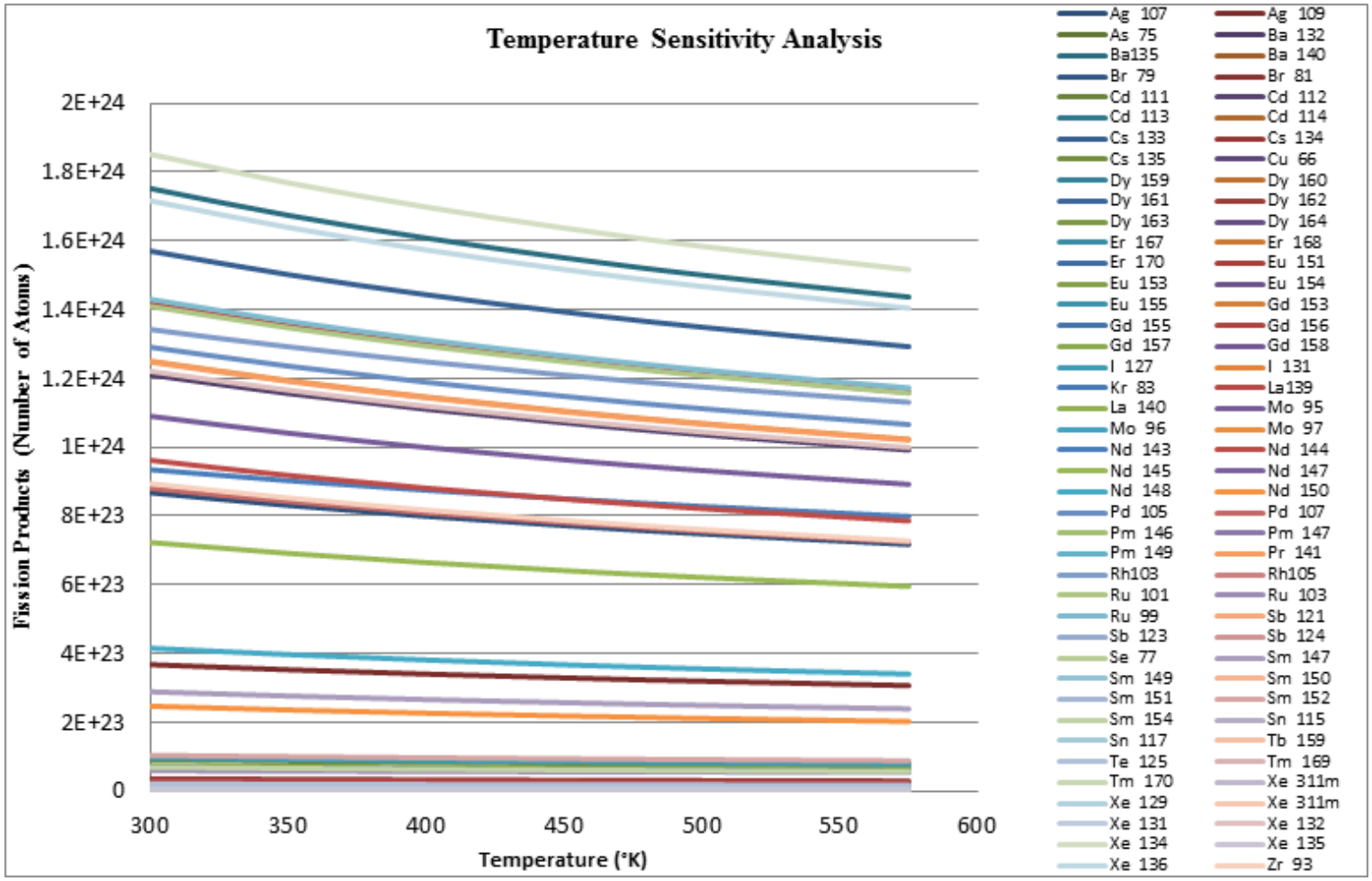


Figure 15: Example of Temperature Sensitivity Analysis (Fission Products Isotopic Concentrations)

As expected, the concentration of fission product reduces as the temperature of the moderator material (in this case the averaged temperature of the coolant and moderator) increases. This phenomenonon can be explained by looking at the following formula as described in Chapter 3.

$$\psi_{th} = \phi_{th}\sigma\sqrt{\frac{\pi}{4}\times\frac{T_o}{T}}$$ [42]

ψ_{th} = Reaction rates due to thermal neutron interactions

ϕ_{th} = Thermal neutron flux (n/cm^2/s)

σ = Thermal neutron microscopic cross-section

T_o =293.15 °K

As the temperature increases, the correction factor used in calculating the thermal reaction rate decreases; as a result the thermal fission and capture rate drops. A smaller fission rate is equvalenti to the fewer fission products.

This situation can be more complicated for the original actinides in the fuel. The increase in temperature means a reduction in the thermal reaction rate; however, this means fewer actinides undergo fission and capture, and as a consequence the isotopic concentration of these actinides is expected to increase.

Despite this expectation, after running the analysis, it was observed that among, Th-232, Pu-238, Pu-239, Pu-240, Pu-241and Pu-242 only the isotopic concentrations of Th-232, Pu-238, Pu-239 and Pu-241 were increasing and the number of atoms of Pu-240 and Pu-242 were decreasing as the temperature was increasing. (See Table 9 and Figure 16)

Table 9: Isotopic Concentration of Some Actinides as Function of Thermal Neutron Temperature Variation

	TH-232	PU-238	PU-239	PU-240	PU-241,	PU-242
300	3.52E+26	8.66E+23	9.89E+24	5.20E+24	7.43E+24	6.01E+24
350	3.52E+26	8.97E+23	1.06E+25	5.20E+24	7.76E+24	5.88E+24
400	3.52E+26	9.24E+23	1.13E+25	5.20E+24	8.04E+24	5.77E+24
450	3.52E+26	9.47E+23	1.18E+25	5.19E+24	8.28E+24	5.68E+24
500	3.52E+26	9.66E+23	1.23E+25	5.18E+24	8.49E+24	5.60E+24
575	3.53E+26	9.91E+23	1.29E+25	5.16E+24	8.76E+24	5.49E+24

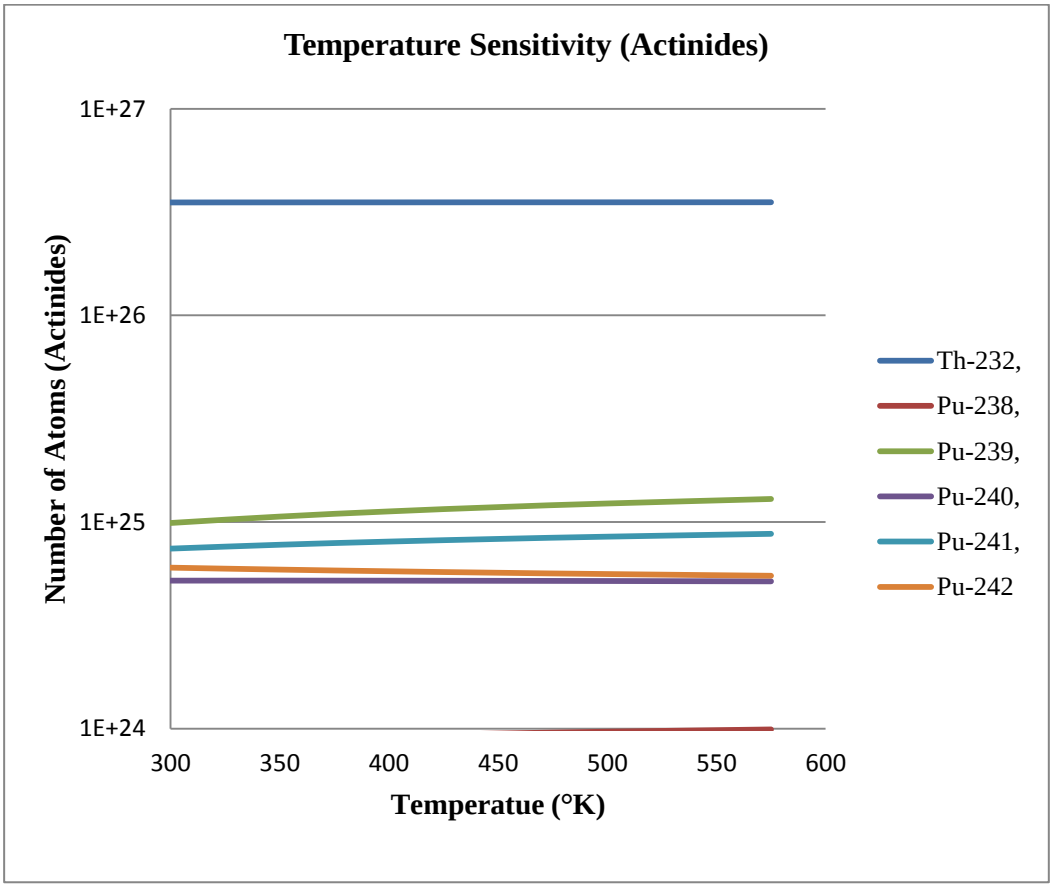


Figure 16: Example of Temperature Sensitivity Analysis (Actinides Isotopic Concentration)

This phenomenon can be explained by looking at the thermal and epithermal fission and capture cross sections. Pu-238, Pu-239 and Pu-240 have relatively large thermal absorption cross-sections compared to their epithermal absorption cross-sections; thus, when the thermal reaction rate decreases, the isotopic concentration of these isotopes increases. Whereas Pu-240, Pu 242 and Th-232 have relatively small thermal absorption cross-section compared to their epithermal cross sections, thus their isotopic concentration is not expected to be affected by changes in thermal reaction rate.

This occurrence is true for Th-232; however, the Pu-240 and Pu-242 concentrations dropped as the temperature increased. This decrease can be explained by the reduction of the capture reaction rate of Pu-239 and Pu-241, which are relatively significant source of Pu-240 and Pu-242, respectively. Table 10 shows the ratio between the thermal and epithermal cross-section for the main actinides.

Table 10: Thermal and Epithermal Capture and Fission Cross Sections Ratios

ACTINIEDS	THERMAL/EPITHERMAL (CAPTURECROSS-SECTION)	THERMAL/EPITHERMAL (FISSION CROSS-SECTION)
Th-232	0.09	N/A
242Pu	0.02	0.87
241Pu	2.35	1.84
240Pu	0.04	0.02
239Pu	1.53	2.65
238Pu	2.59	0.52

The thermal neutron energy (i.e. the moderating environment temperature) is about 574.5 K, and during normal operation it is not expected to see such a huge temperature variations. This example demonstrates the ability of FICST to undertake sensitivity analysis based on the temperature changes.

Chapter 6:
Discussion and Future Work

Microsoft EXCEL was used to perform some spot checks and verifications; however, FICST, like any other code, needs to be verified by an independent verifier. The nuclear data used in the code can be changed easily and replaced by the most updated information as it becomes available. It is possible to change the number of energy groups used in the calculations; however, as the discussion in the methodology, a three-group calculation is sufficient for these calculations, unless one is concerned with the resonance cross-sections data used for some of the actinides. Even then, FICST can handle changes in the resonance cross section data successfully once the detailed flux distributions are available for the different resonance data.

FICST can be further developed to estimate the following quantities:

- Fission Power (The heat generated by fission)
- Changes in the reactivity of the core during a shutdown
- Changes in the inventories of relevant fissile species and strong neutron absorbing fission products during maintenance or shutdowns
- Tracking the isotopic concentration of spent fuel and the radioactive releases from the reactor
- Adding a flux calculator, to vary the flux information based on $\frac{1}{\sigma}$ information

Even though FICST is a user friendly code, it is beneficial to add a graphical user interface (GUI) to the code. Most of the commercial code such as ORIGEN has already included this feature into their codes. A GUI is available within the MatWorks products

and it is easy to develop and work with. The GUI can be exploited to allow the user to pick a different energy group, different uncertainties data, and different fission products or actinides to perform sensitivity analysis on.

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Appendix A:
Canadian SCWRs Core Physics Concepts

The current design of Canadian SCWR has 336 vertical fuel channels; each channel is 5 m long. It contains heavy water moderator surrounding 336 fuel channels and light water coolant. The fuel assembly has two rings of fuel element and a central flow tube [43]. "The fuel assembly has a two-pass counter-flow configuration, where the coolant flows downwards through a central flow tube and up through fuel elements."[44]

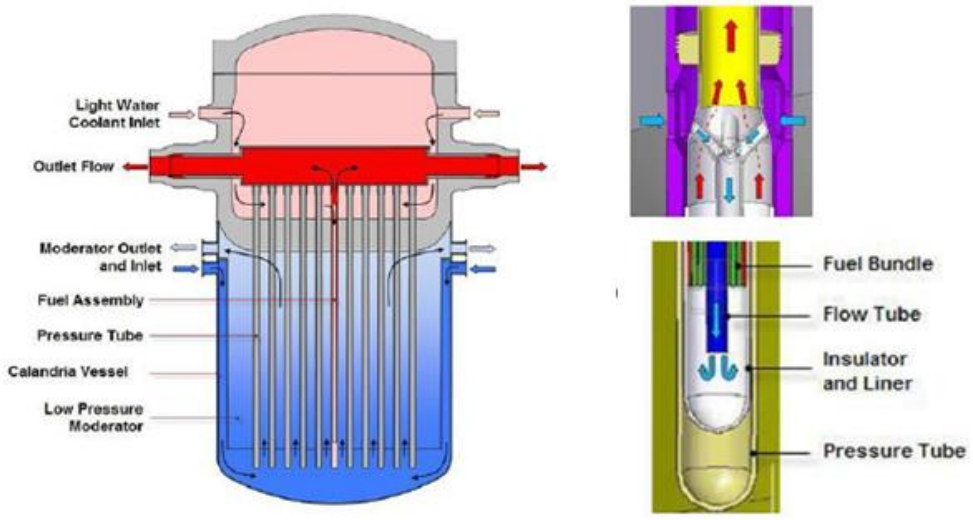


Figure A- 1: Canadian SCWR Core Layout and Redirection of the Coolant Flow

The inlet temperature of the coolant is approximately 350ºC and inlet pressure is about 26 MPa. Coolant exits the central flow tube below the critical temperature of 374ºC and changes its direction. While the coolant flows up through the fuel elements it is heated again to above the supercritical temperature. [45] "The supercritical water exiting the fuel channels combines and mixes in the outlet plenum, which is located inside the

inlet plenum, at an average target temperature of up to 625ºC and at a pressure of 25 MPa. The key parameters for the SCWR core are provided in Table A-1."[43]

Table A- 1: Canadian SCWR Core Specifications

PARAMETERS	VALUES
Thermal Power	2540 MW
Electric Power	1200 MW
Inlet Temperature	350 C
Outlet Temperature	625 C
Inlet Pressure	26 MPa
Outlet Pressure	25 Mpa
Number of Channels	336
Lattice Pitch	25 cm
Core radius (including the radial reflector)	355 cm
Core Hight (including the axial reflector)	650 cm
fuel assembly lenghth 500	500 CM
fuel batches	3
target exit burnup	40 MWD/kg

Figure A-2 illustrates the cross sectional view of the fuel bundle and the high-efficiency re-entrant channel (HERC). The pressure tube is made of zirconium-based alloy which is in direct contact with the moderator. However, the direct contact of pressure tube with the high temperature coolant is avoided by the solid encapsulated zirconia insulator which is located directly inside the pressure tube. The coolant enters the central coolant tube from the top and flows down the channel; after reaching the bottom of the channel, it is directed upwards into the outer fuel-containing annulus where it is

heated up by the fuel. “The central flow tube is a solid tube of zirconium hydride clad on the inner and outer surfaces with zirconium-modified stainless steel. The tube acts as a physical barrier to prevent mixing of the downward flowing coolant with the upward flowing coolant.”[43]

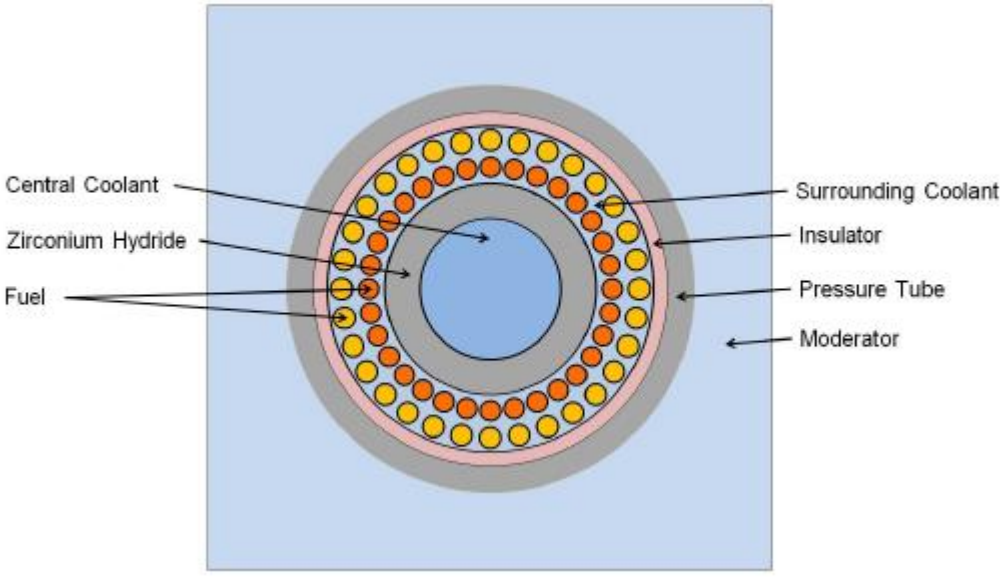


Figure A- 2: Cross-sectional view of the 64-element Canadian SCWR fuel bundle concept, channel, and lattice cell.[43]

The SCWR fuel bundle has two fuel rings, each ring has 32 elements. The fuel elements cladding are made of 0.6mm thick zirconium-modified 310 stainless steel, filled with a mixtures of thorium dioxide and plutonium dioxide. The PuO_2 is assumed to be obtained from used light-water reactor-fuel. The thorium is assumed to be isotopically pure Th-232. “The theoretical densities of pure PuO_2 and ThO_2 used for this study were 10.0 g/cm^3 and 11.5 g/cm^3, respectively, For the $(Pu\ Th)O_2$ mixtures, it was assumed that the densities of the mixtures were simply the volume weighted averages of the

components. It was further assumed that the fuels in pellet form had densities equal to 97% times the theoretical density." [43] Table A-2

Table A- 2: Specifications for the 64-Element Fuel Assembly and Channel

Component	Dimension	Material	Composition (wt%)	Density (g/cm3)
Central Coolant (inside flow tube)	3.6 cm radius	light water	100% H2O	variable
flow Tube Inner Cladding	3.6 cm inner radius (IR) 0.05 cm Thick	Zr- modified 310 Stainless Steel (zr-mod SS)	C:0.034, Si: 0.51, Mn:0.74, P:0.016, S:0.0020, Ni: 20.82, Cr: 25.04, Fe: 51.738, Mo: 51, Zr:0.59	7.9
flow Tube Inner Cladding	3.65 cm IR 1cm thick	Zirconium Hydride	Zr:98.26, H:1.74	5.64
Flow Tube Outer Cladding	4.65 cm IR 0/05 cm thick	Zr-mod SS	Zr:98.26, H:1.74	7.9
Inner Pins (32)	0.415 cm radius 5.4 cm pitch circle radius no displacement angle	15 wt% PuO2/ThO2	Pu:13.23, Th: 74.70, O:12.07	9.91

Outer Pins (32)	0.440 cm radius 6.575 cm pitch circle radius no displacement angle	12 wt% PuO2/ThO2	Pu:10.59, Th:77.34, O:12.08	9.87
Cladding	0.06 cm thick	Zr-mod SS	Pu:10.59, Th:77.34, O:12.08	7.9
Coolant	n/a	light water	100% H2O	variable
Liner Tube	7.20 cm IR 0.05 cm thick	Zr-mod SS	100% H2O	7.9
Insulator	7.25 cm IR 0.55 cm thick	Zirconia (ZrO2)	zr:66.63, Y:7.87, O:25.5	5.83
Outer Liner	7.8 cm IR 0.05 cm thick	Excel (Zirconium Alloy)	Sn:3.5, Mo:0.8, Nb:0.8; Zr:94.9	6.52
Pressure tube	7.85 cm IR 1.2 cm thick	Excel (Zirconium Alloy)	Sn:3.5, Mo:0.8, Nb:0.8; Zr:94.9	6.52
Moderator	25 cm square lattice pitch	D2O	D2O: 99.8333, H2O: 0.167	variable (1.0851 nominal)
N/A	N/A	Rg-Ru	Pu-235:2.75, Pu-239:51.96, Pu-240:22.96, Pu-241:15.23, Pu-22:7.10	

Appendix B:
CROSS SECTIONAL DATA CONCEPT

"When neutrons reach thermal equilibrium with the moderator, their energies are determined by the thermal energy distribution of the moderator atoms, and the neutron energy spectrum becomes a Maxwellian distribution at the temperature (T in °K) of the moderator material. Setting the kinetic energy of neutron motion equal to the thermal energy of the moderator, one can obtain the most probable speed (magnitude of the velocity) of the neutrons in thermal equilibrium. For a moderator at room temperature (20°C), this neutron speed is 2200 meters per second and the energy corresponding to it is 0.0253 eV. To obtain a reaction rate, one forms the product of the density of neutrons, this most probable speed of 2200 meters/second and the neutron cross section corresponding to this speed or 0.0253 eV. The thermal neutron absorption cross section is the sum of the cross sections for all reactions except scattering of the neutron. For many materials, it is inversely proportional to the speed of the neutron. These materials are called 1/v absorbers. A correction function, g (kT) is used to describe the departure of the cross section from the 1/v law for certain materials. The function g (kT) is defined as the ratio of the reaction rate in a Maxwellian flux at the temperature T to the reaction rate at 2200 meter/sec. Isotopes known to have cross sections that deviate from 1/v behavior by more than 3% (i.e., $g > 1.03$ or $g < 0.97$) are listed in Table A-1 along with the g values at T = 20°C.

Table B- 1: Non 1/v cross sections for nuclides of interest to reactor technology; g values

Nuclides	Gγ	Gf
113Cd	1.33	-
135Xe	1.16	-
149Sm	1.71	-
151 Eu	0.9	-
152 Eu	0.9	-
153Eu	0.97	-
154Eu	0.9	-
155Gd	0.84	
157Gd	0.85	-
176Lu	1.74	-
182Ta	1.64	-
233U	0.05	-
237Np	-	0.96
238Pu	0.96	0.96
239Pu	1.13	1.06
241 Pu	1.04	1.04
241 Am	1.05	-
242mAm	1.11	1.1
245Cm	0.95	0.95
249Bk	1.47	-

For a neutron slowing down in a moderating medium without absorption, the flux can be shown to be inversely proportional to the energy. Between 1 eV and a few keV (1E3 eV), especially for elements with intermediate and high mass numbers, there are often particular energies for which the rate of interaction is exceptionally high. A curve of the cross section versus energy in this region shows narrow peaks called resonances. The rate of occurrence of a particular reaction in this resonance region is proportional to the integral of the cross section as a function of neutron energy multiplied by the flux density, which is called a resonance integral. The resonance integral assumes that the flux density has a 1/E dependence that is not disturbed by the absorbing isotope; i.e., extreme dilution

of the absorber in the moderator is assumed. Integrals of this type are called infinite dilution resonance integrals. The measurement of the reaction rate in a reactor neutron spectrum produces contributions from intermediate neutrons with a 1/E shape and from thermal neutrons with a Maxwellian distribution of energies. To distinguish between these two contributions, a cadmium cover is often used. Cadmium filters do not curtail the intermediate neutron spectrum sharply, but a sharp (effective cadmium cutoff energy,)" E_{Cd}, can be defined for a 1/v absorbers. E_{Cd} is the energy associated with a perfect filter under which irradiated cadmium cover. Suitable cadmium filters terminate the intermediate neutron energy spectra at approximately 0.5 eV. This energy is sufficiently high to exclude most of the low-energy deviations of the flux from a 1/E shape."[11]

[11] "Nuclides and Isotopes" Revised by E William Walker, Josef R. Parrington and Frank Feiner. Copyright General Electric Company.

Figure B-1 shows the burn-up Chain model that was used for verification of the chain model used in FICST.

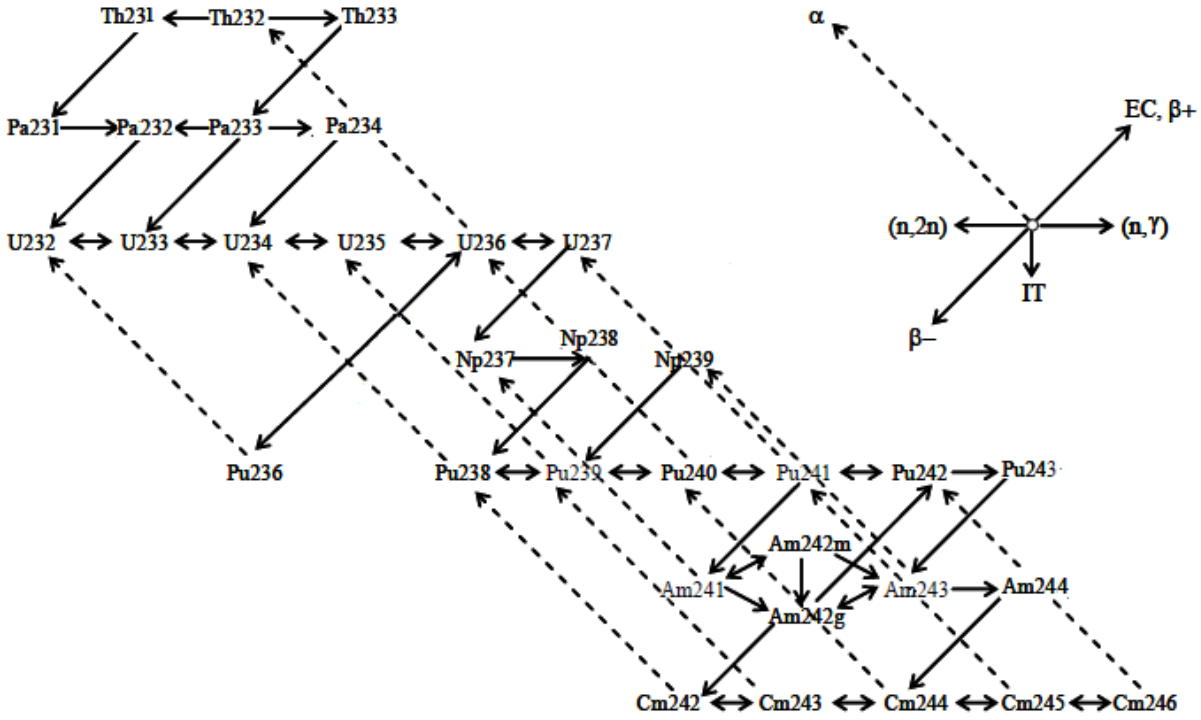


Figure B-1: Burn-up Chain Model Available in Literature [24]

Appendix C:
CROSS SECTIONAL DATA OF THREE MAIN MODERATING MATERIALS IN THE CORE

The following figures are obtained from reference [46]. The total, absorption and elastic cross section of hydrogen, Oxygen and Pu-242 and Th-232 are shown in Figures C-1 to C-4 respectively.

Figure C-1: H-2 Cross Section Data

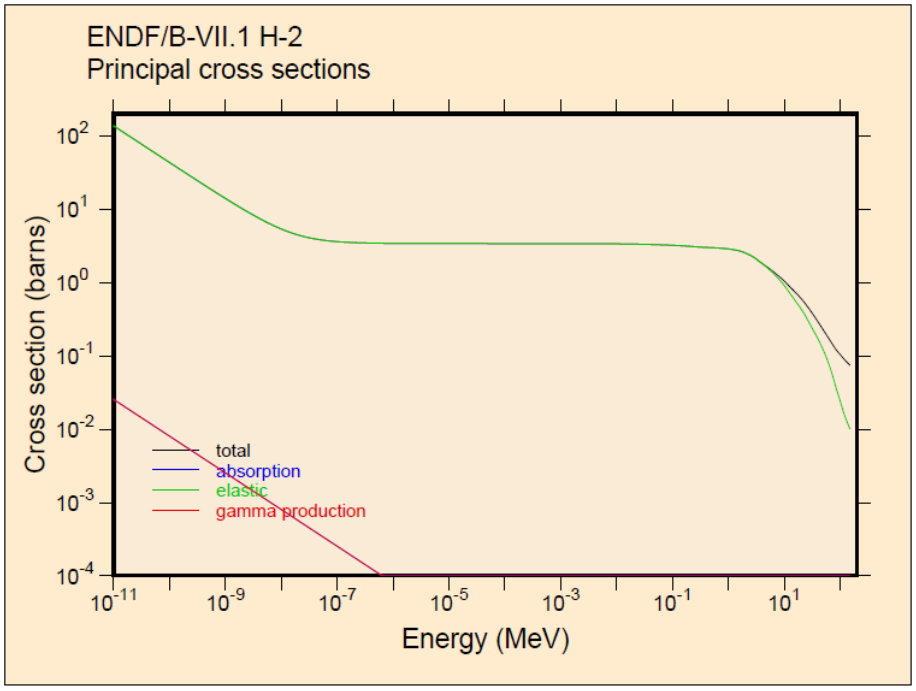


Figure C-2: O-16 Cross Section Data

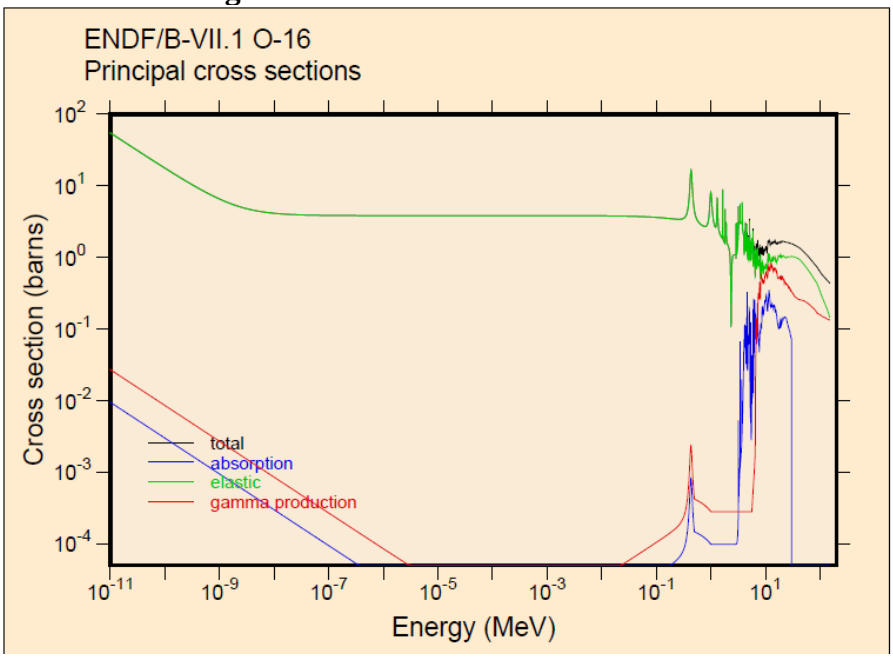


Figure C-3: Pu-242 Cross Section Data

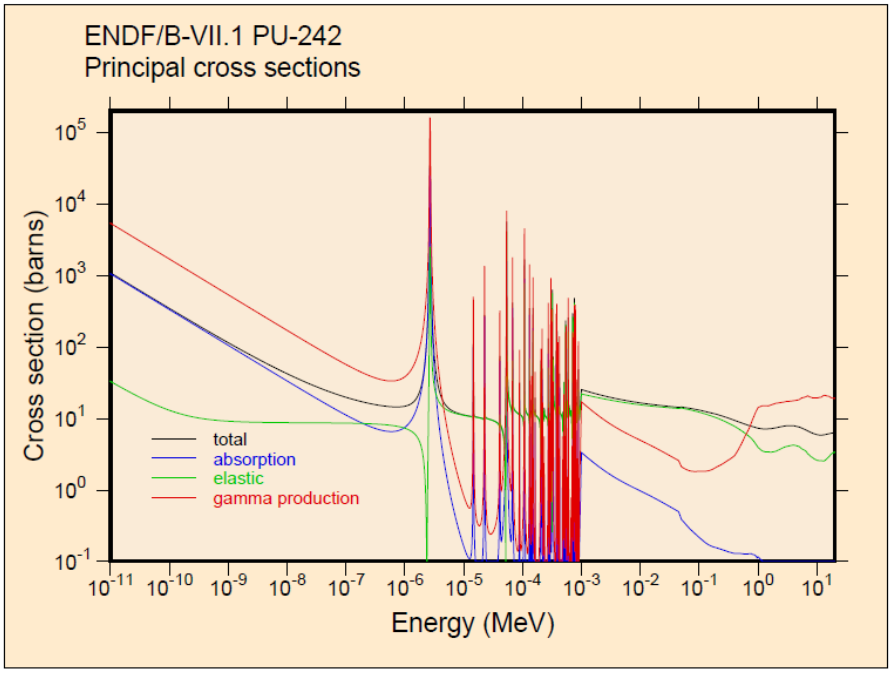
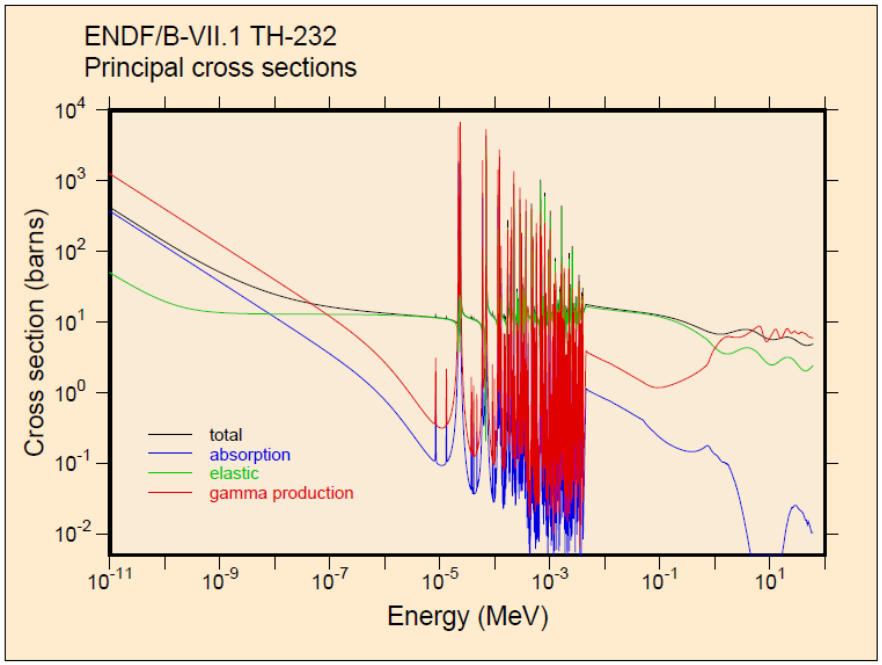


Figure C-4: Th-232 Cross Section Data



Appendix D:
MATLAB/SIMULINK DESCRIPTION

"Simulation and Model-Based Design Simulink® is a block diagram environment for multi-domain simulation and Model-Based Design. It supports system-level design, simulation, automatic code generation, and continuous test and verification of embedded systems. Simulink provides a graphical editor, customizable block libraries, and solvers for modeling and simulating dynamic systems. It is integrated with MATLAB®, enabling you to incorporate MATLAB algorithms into models and export simulation results to MATLAB for further analysis.

Key Features:

- Graphical editor for building and managing hierarchical block diagrams
- Libraries of predefined blocks for modeling continuous-time and discrete-time systems
- Simulation engine with fixed-step and variable-step ODE solvers
- Scopes and data displays for viewing simulation results
- Project and data management tools for managing model files and data
- Model analysis tools for refining model architecture and increasing simulation speed
- MATLAB Function block for importing MATLAB algorithms into models
- Legacy Code Tool for importing C and C++ code into models"[34]

Appendix E:
FICST M-FILE

The following is the m-file developed for FICST. The purpose of m-file is to call all the input data and transfer thesis data to the workplace, then run the Simulink model and finally output the results.

Content

The SPWRs irradiated fuel Model, 2013/2014

This program is developed for studying the uncertainties of available libraries on the concentration of the atoms in the irradiated fuel. It is assumed in here that all of the fuel bundles see the same flux, but the user can modify the flux by changing the flux input. If the half-life of an isotopes is longer than 30 yrs in this calculation the lambda of that isotope is assumed to be zero. The vectors defined here to identify the uncertainties and the isotopes modeled can be easily modified in the provided excel files. Since this model is vectorized to make it user friendly. Acknowledgment to: Adriaan Buijs, Jeremy Pencer, Charles Boss, Glenn Gomes

```
clear all;clc

warning ('off');

GL_UNITS; % Unit function

UNITS('SI','YR');

%%----initial atoms: Th-232            Pu-238  Pu-239  Pu-240   Pu-241        Pu-242

% the number atoms are calculated for one fuel bundle

% the modification factor provide the user with the option to change the
```

```
% concetration of the fuel (i.e. increase the Pu by 5% or reduce the Th by

% 2%

Inner_fuel_ring =[1.93E26;7.08E23; 1.33E25;5.86E24; 3.87E24; 1.80E24];

Outer_fuel_ring =[1.66E26;7.90E23; 1.49E25;6.54E24;          4.32E24; 2.00E24];

Total_Initial_atoms= Inner_fuel_ring+Outer_fuel_ring;

IniAtoms_Actinide=xlsread('actinides_Inp_v33','initialAtoms','E2:CG2');

modification_factor=xlsread('actinides_Inp_v33','initialAtoms','E4:CG4');

size(IniAtoms_Actinide);

% The info used to calculated the initial number atoms:

%Outer Ring                :                 Inner Ring

%number of elements                  32        number of elements                        32

%radius of elements                  0.44cm    radius of elements                        0.415cm
```

---------Temperature calculated for reaction rates ----------

```
Temp =574.44;

Temp1 = 293.15;

Temp2 = Temp;
```

----------Fluxes ----------

Average Fluxes in fuel assumed, the number can be modified as more info become available

```
Ther_flux = 1.1E+13*uCM^-2*uSEC^-1;

Int_flux = 2.28E+13*uCM^-2*uSEC^-1;
```

```
Fast_flux = 8.15E+12*uCM^-2*uSEC^-1;

CF = 1.00; %capacity factor, assumed that the reactor will run at 100%,

%not realistic but conservative
```

----------Lambda and Xsections ----------

The half-lives or better say the Lambdas and cross-sections are defined in the input excel file for actinides and the fission products. To make it easier for the user, a utility was developed that defines the units. Please note this is not one part of MATLAB and it was code developed and called GL_UNITS. for example: Lambda_Th232 = log(2)/(1.4E10*uYR);

```
%sig_fist_Th232 = 0*MICRO*uBARN;

%sig_capt_Th232 = 7.37*uBARN;
```

----------Actinides Input Data from the Excel file----------

```
[num1, ActinideHalfLives] = xlsread('actinides_Inp_v33','actinide','B5:B85');

LambdaActinide = zeros(length(ActinideHalfLives),1);

for j = 1:length(ActinideHalfLives)

   LambdaActinide(j)=log(2)/(eval(ActinideHalfLives{j}));

    if LambdaActinide(j)< (7.32E-10*uSEC)

      LambdaActinide(j)=0;

   end

end



Therm_cap_Actinide=xlsread('actinides_Inp_v33','actinide','G5:G85')*uBARN;
```

```
Therm_fiss_Actinide=xlsread('actinides_Inp_v33','actinide','H5:H85')*uBARN;

Int_cap_Actinide=xlsread('actinides_Inp_v33','actinide','I5:I85')*uBARN;

Int_fiss_Actinide=xlsread('actinides_Inp_v33','actinide','J5:J85')*uBARN;

fast_cap_Actinide=xlsread('actinides_Inp_v33','actinide','K5:K85')*uBARN;

fast_fiss_Actinide=xlsread('actinides_Inp_v33','actinide','L5:L85')*uBARN;
```

---------- Reaction Rates----------

In the MATLAB model the reaction rates were calculated using the following equation: RR = RRthermal + RRintermediate + RRfast

Where thermal energy is below 0.5 eV, intermediate energy is between 0.5 eV and 0.821 MeV and fast energy is above 0.821 MeV.

RRthermal = Φ(thermal)σF(thermal), where Fthermal is the correction factor for the cross section in the thermal energy range.

Fthermal = and To = 293 K and T = K

RRintermediate = Φintermediate σ Fintermediate, where Fintermediate is the correction factor for the cross section in the intermediate energy range.

Fintermediate = and Eu = 0.821 MeV and Eo = 0.5 eV

RRfast = Φfast σ Ffast, where Ffast is the correction factor for the cross section in the fast energy range.

Ffast = where 0.755 is calculated from the distribution of neutrons over the whole energy spectrum.

---------- calculation of reaction rates - matrix multiplication-------

```
% -------------------- correction factors -------------------------------

Ther_fac = ((pi/4)*(Temp1)/(Temp2))^(1/2);

Int_fac = 1/(log(0.821/0.000000625));

fast_fac = (1/0.755);
```

```
% -------------------- reaction rate calculations-------------------------

Actinides_capt=
(Ther_flux*Ther_fac*Therm_cap_Actinide)+(Int_flux*Int_fac*Int_cap_Actinide)+(Fast_flux*fast_fac*fast_cap_Actin
ide);

Actinides_fiss=
(Ther_flux*Ther_fac*Therm_fiss_Actinide)+(Int_flux*Int_fac*Int_fiss_Actinide)+(Fast_flux*fast_fac*fast_fiss_Actin
ide);

sum= Actinides_capt+Actinides_fiss;

Actinides_decay_matrix=xlsread('actinides_Inp_v33','decay_mat','B2:CD82');

Actinides_capture_mat=xlsread('actinides_Inp_v33','capture_mat','B2:CD82');

size(Actinides_decay_matrix);

size(Actinides_capture_mat);



fission_sensitivities=xlsread('actinides_Inp_v33','sensitivity','C2:C82');

capture_sensitivities=xlsread('actinides_Inp_v33','sensitivity','D2:D82');

Yield_uncertainties=xlsread('actinides_Inp_v33','sensitivity','E2:E82');
```

---------- Fission yields----------

```
yeild_vector= xlsread('actinides_Inp_v33','yeilds_matrix','E3:E83');

yeild_matrix= xlsread('actinides_Inp_v33','yeilds_matrix','H3:CJ86');

test=yeild_matrix*yeild_vector;
```

----------Fission Products Input Data from the Excel file----------

```
[num1, fissionProHalfLives] = xlsread('fissionPro_Inp_v2','InputData','D9:D92');
```

```
LambdafissionPro = zeros(length(fissionProHalfLives),1);

for j = 1:length(fissionProHalfLives)

   LambdafissionPro(j)=log(2)/(eval(fissionProHalfLives{j}));

   if LambdafissionPro(j)< (7.32E-10*uSEC)

      LambdafissionPro(j)=0;

   end

end



Therm_cap_fissionPro=xlsread('fissionPro_Inp_v3','InputData','F9:F92')*uBARN;

Int_cap_fissionPro=xlsread('fissionPro_Inp_v3','InputData','G9:G92')*uBARN;

%fast_cap_fissionPro=xlsread('fissionPro_Inp_v2','actinide','K5:K85')*uBARN;



Ther_fac = ((pi/4)*(Temp1)/(Temp2))^(1/2);

Int_fac = 1/(log(0.821/0.000000625));

fast_fac = (1/0.755);



fissionPro_cap= (Ther_flux*Ther_fac*Therm_cap_fissionPro)+(Int_flux*Int_fac*Int_cap_fissionPro);
%+(Fast_flux*fast_fac*fast_cap_Actinide);



fissionPro_decay_matrix=xlsread('fissionPro_Inp_v3','decay_mat','C3:CH86');
```

----------The Simulink Model/ Run and Output Data----------

```
%%------------------ The Simulink model-----------------------------------

% All the data input in this input file and excel file are called to work

% space and used as an input in the SIMULINK model witch solve series of

% first order differential equations which basically calculate the number of

% different atoms of actinides or fission products in the fuel

% The output data after 2 years and 3 years of operations are recorded in:

% output_V1.xls excel file

sim('SCWR_V1')

tuse = [1/12 3/12 6/12 1 1.5 2 2.5 3]*uYR;

ppos = [];

Values = [];

for i = 1:length(tuse)

   [value,pos]=FINDNEAR(simout.time,tuse(i));

   ppos(i) = pos(1);

   Values(i,:) = simout.signals.values(ppos(i),:);

end

FuelCon = Values';
```

```
xlswrite('out.xls',FuelCon,'results_out','B2');

% time used for output the data (i.e. concentration of the isotopes is outputted as a function of time) the time can be set to any interval and units as required: Sec, Min, hours, days, months or years. Also it is not necessary to have equal intervals.

tuse1 = [1/12 3/12 6/12 1 1.5 2 2.5 3]*uYR;

ppos1 = [];

Values1 = [];

for i = 1:length(tuse1)

   [value1,pos1]=FINDNEAR(actinide.time,tuse1(i));

   ppos1(i) = pos(1);

   Values1(i,:) = actinide.signals.values(ppos1(i),:);

end

ActCon = Values1';

xlswrite('out.xls',ActCon,'results_out0','B2');

save rua.mat

run_is_completed= 1;

Check_the_output_V1_excelfile_for_result=1
```

Appendix F:
UNCERTAINTIES IN THORIUM CROSS SECTIONAL DATA

Th-232 absorption cross section uncertainties were used as an example to demonstrate how FICST is used to perform sensitivity analysis. The following data were gathered from reference [36]to support the values that have been used in this example.

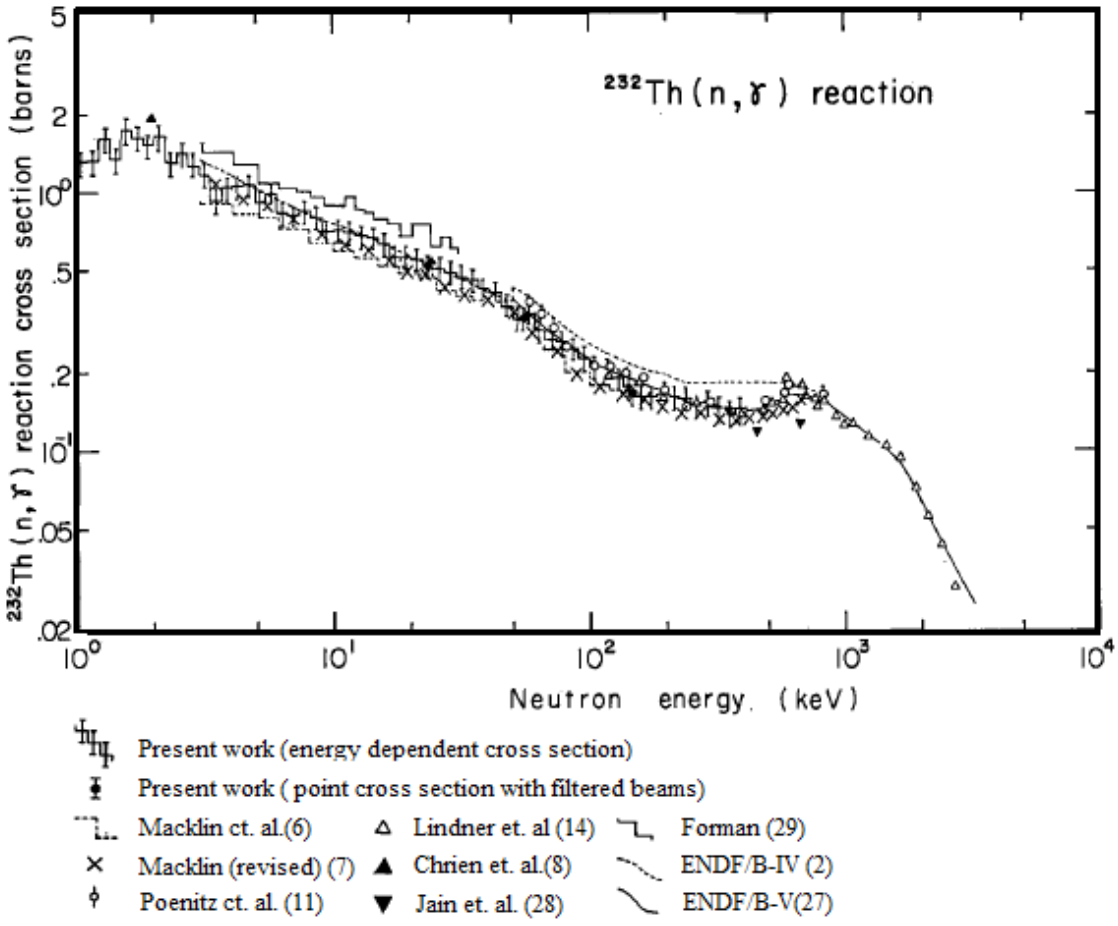


Figure F-1: Cross Section for Th-232 (n, γ) Reaction and Its Uncertainties [36]

Table F-1: Th-232 Neutron Capture Cross Section Uncertainties [36]

Neutron energy (keV)		Cross Sections	Error	Neutron energy (keV)		Cross Sections	Error
E_{max}	E_{min}	(mb)	(mb)	E_{max}	E_{min}	(mb)	(mb)
408	369	145	±15.9	20.2	18.3	566	± 56.3
369	334	138	±14.7	18.3	16.6	57 1	± 56.7
334	302	144	±15.1	16.6	15	636	±63.9
302	273	152	±15.8	15	13.6	67 1	± 67.5
273	247	149	±15.2	13.6	12.3	683	± 68.2
247	224	159	±16.0	12.3	11	702	±70.3
224	202	161	±16.0	11	10	712	±71.3
202	183	164	±16.3	10	9.07	707	±70.1
183	166	161	±15.8	9.07	8.21	799	±79.9
166	150	162	±15.9	8.21	7.43	844	± 84.5
150	136	177	±17.3	7.43	6.72	820	± 81.9
136	123	189	±18.5	6.72	6.08	832	± 82.8
123	110	209	±21.3	6.08	5.5	1,002	±101.8
110	100	211	±21.4	5.5	4.98	921	±92.0
100	90.7	229	±23.3	4.98	4.5	1,084	±109.7
90.7	82.1	248	±25.2	4.5	4.08	1,057	±106.9
82.1	74.3	263	±25.9	4.08	3.69	1,049	±110.9
74.3	67.2	269	±26.3	3.69	3.34	935	±98.9
67.2	60.8	294	±29.0	3.34	3.02	1,194	±123.0
60.8	55	337	±33.6	3.02	2.73	1,294	±144.0
55	49.8	322	±31.7	2.73	2.47	1,423	±155.2
49.8	45	369	±36.9	2.47	2.24	1,316	±134.3
45	40.8	417	±41.9	2.24	2.02	1,655	±171.7
40.8	36.9	425	±42.8	2.02	1.83	1,515	±155.1
36.9	33.4	462	±46.2	1.83	1.66	1,632	±168.7
33.4	30.2	474	±47.2	1.66	1.5	1,739	±192.2
30.2	27.3	492	±49.1	1.5	1.36	1,345	±144.6
27.3	24.7	511	±51.2	1.36	1.23	1,614	±176.9
24.7	22.4	520	±52.0	1.23	1.1	1,328	±142.2
22.1	20.2	554	±55.7	1.1	1	1,304	±138.4

Appendix G:
FISSION YIELDS DATA FOR THE MAIN ACTINIDES

The following graphs demonstrate the fission yield data for the main actinides in the fresh fuel. These graphs were developed using the Nuclear Data Center, Japan Atomic Energy Agency. JENDL FP Fission Yields Data File 2011 **[41]**

A comparison between the cumulative and independent fission yields data of different actinide was performed using the JAEA nuclear data graphical tool. As shown in Figure G- 1 to Figure G-4, the fission yield of the plutonium isotopes are relatively similar, whereas a significant difference can be observed with Th-232. It seems that thorium's two humps are more toward the isotopes with lower atomic number compared to the plutonium humps.

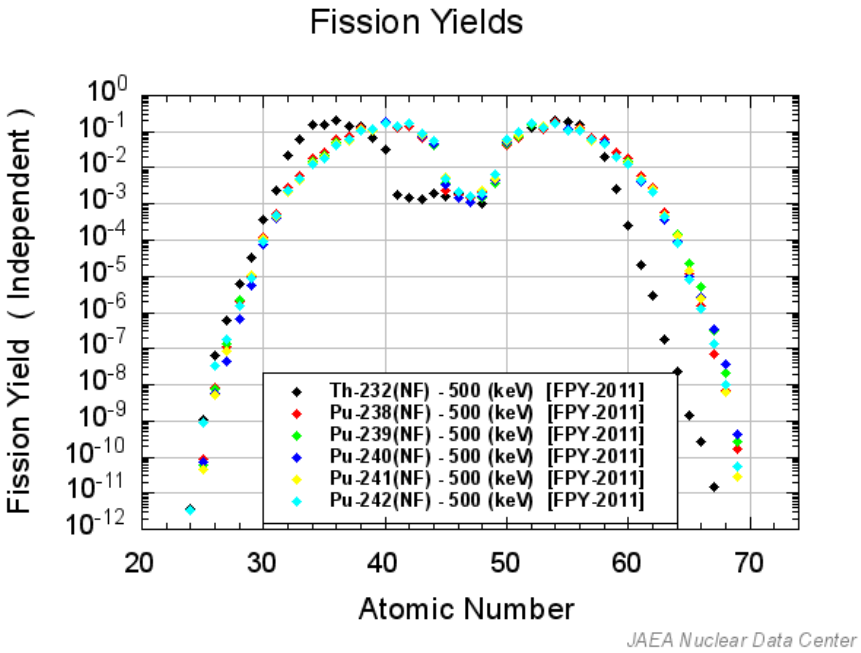


Figure G- 1: Comparison between the Independent Fission Yields of the Main Actinides (Log Scale)

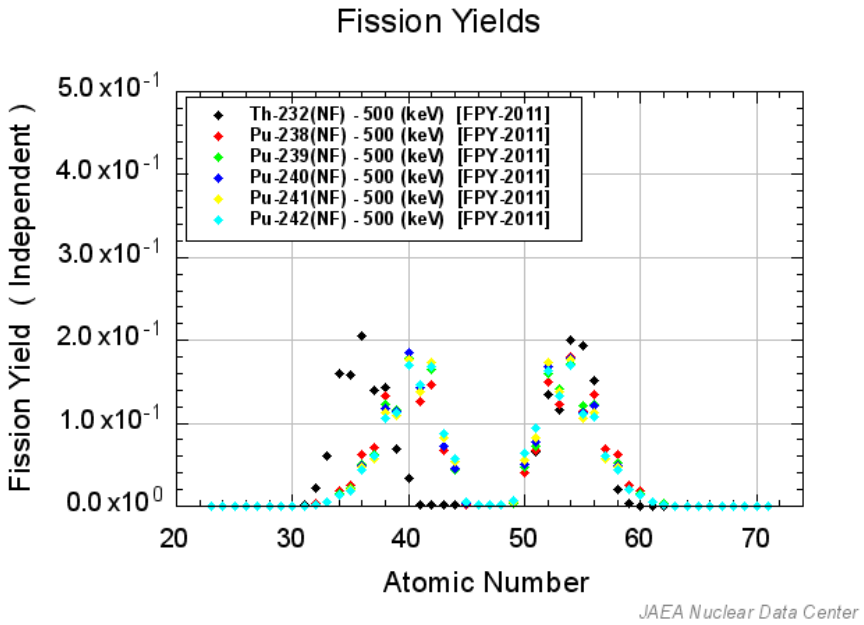


Figure G- 2: Comparison between the Independent Fission Yields of the Main Actinides (Linear Scale)

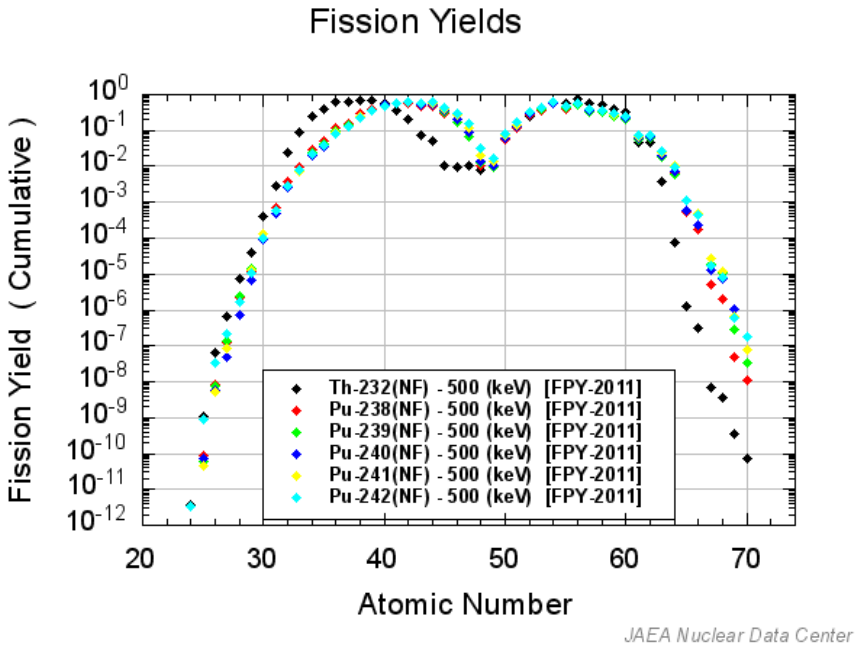


Figure G- 3: Comparison between the Independent Fission Yields of the Main Actinides (Log Scale)

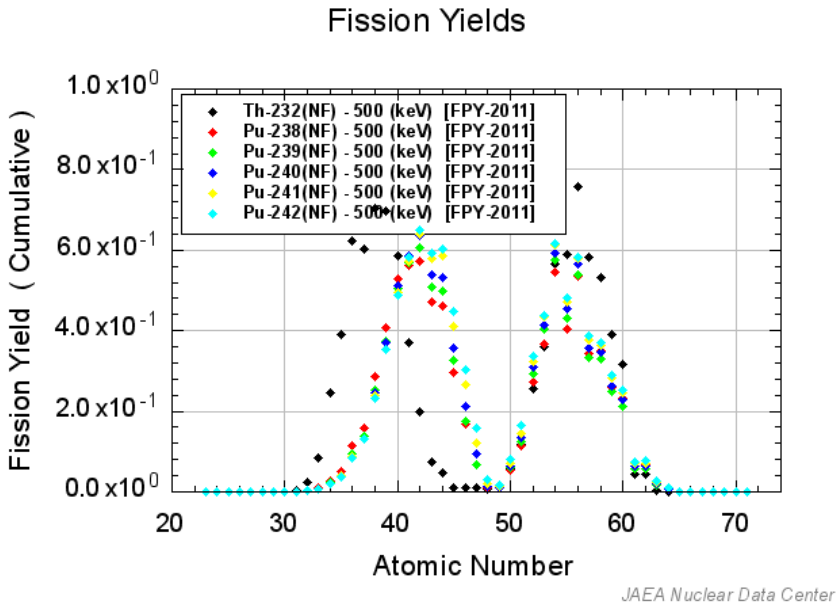


Figure G- 4: Comparison between the Independent Fission Yields of the Main Actinides (Linear Scale)

Different codes tend to use different libraries, not considering that even different revision of the same code sometime uses different library data. The library data are being updated

and more information becomes available. Figure G- 5 and Figure G- 6 demonstrate the differences between fission yields of Pu-242 and Th-232 in J40-2010 and FPY-2011.

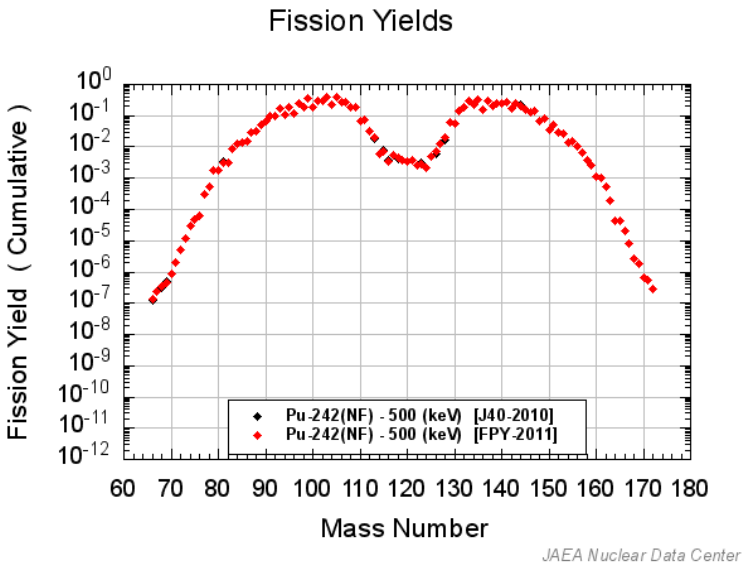


Figure G- 5: Comparison between the Cumulative Fission Yields of Pu-242 obtained from the Two Different Library Data (J40-2010 and FPY-2011)

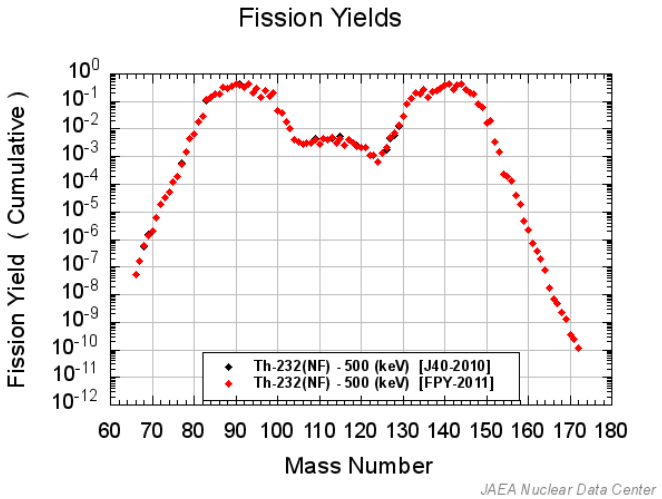


Figure G- 6: Comparison between the Cumulative Fission Yields of Th-232 obtained from the Two Different Library Data (J40-2010 and FPY-2011)