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**Nuclear data analyses for improving the safety of
advanced lead-cooled reactors**

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Resumen

El Reactor Rápido refrigerado por Plomo (LFR) es una de las tres tecnologías seleccionadas por la Plataforma Tecnológica de Energía Nuclear Sostenible que pueden satisfacer las futuras necesidades energéticas europeas. Investigadores e industria están realizando importantes esfuerzos para superar los principales inconvenientes del despliegue industrial de los LFR, que son la falta de experiencia operacional y el impacto de las incertidumbres en el diseño del reactor, la operación y la evaluación de la seguridad.

En el diseño de reactores nucleares, las incertidumbres provienen principalmente de las propiedades de los materiales, las tolerancias de fabricación, las condiciones operativas, las herramientas de simulación y los datos nucleares. De hecho, la incertidumbre en los datos nucleares es una de las fuentes más importantes de incertidumbre en el diseño del reactor y en las simulaciones de la física del reactor y, en el pasado, se han obtenido sistemáticamente importantes diferencias entre las incertidumbres y las precisiones objetivo. Es necesario cumplir con la precisión objetivo no sólo para lograr el nivel de seguridad requerido para esta tecnología, sino también para minimizar el aumento de los costes debido a medidas de seguridad adicionales.

Con esos antecedentes, el objetivo principal de este trabajo ha sido analizar y mejorar los datos nucleares necesarios para el desarrollo, la evaluación de seguridad y el licenciamiento de los reactores LFR, reduciendo las incertidumbres en los parámetros de reactividad (para seguridad) debido a las incertidumbres en los datos nucleares, con el fin de alcanzar las precisiones objetivo definidas por investigadores, industria y reguladores.

Herramientas de sensibilidad e incertidumbre precisas y con alta fiabilidad son necesarias para estimar las incertidumbres en parámetros de seguridad clave del reactor (factor de multiplicación neutrónico, k_{eff} , fracción efectiva de neutrones diferidos, β_{eff} , tiempo efectivo de generación de neutrones, $\Lambda_{c\phi\phi}$, coeficientes de reactividad, ...) e identificar posibles debilidades

en los datos nucleares. Existen herramientas para calcular la incertidumbre de un parámetro del reactor debida a las incertidumbres en los datos nucleares. Sin embargo, estas herramientas poseen varias limitaciones, como carecer de capacidades de procesamiento en paralelo; necesidad de que el usuario seleccione los isótopos y canales de reacción a incluir en el análisis; uso de datos nucleares en estructura de multigrupos; uso de una librería de datos nucleares específica y/o una matriz de covarianza específica; y la limitación en la complejidad del sistema a analizar debido al número requerido de simulaciones.

Por lo tanto, en este trabajo, se ha desarrollado una Metodología de Sensibilidad e Incertidumbre para códigos de MONtecarlo (SUMMON). SUMMON es una herramienta concebida para realizar análisis automatizados completos de sensibilidad e incertidumbre de los parámetros de reactividad (para seguridad) más relevantes de diseños de reactores desde el punto de vista neutrónico, es decir, k_{eff} , β_{eff} , Λ_{eff} y los coeficientes de reactividad, utilizando librerías de datos nucleares y covarianzas de última generación. SUMMON se ha validado utilizando experimentos integrales del ICSBEP (*International Handbook of Evaluated Criticality Safety Benchmark Experiments*) y se ha verificado exhaustivamente con códigos consolidados como SCALE, SUS3D y SERPENT. Se ha encontrado un buen acuerdo entre los códigos.

Una vez SUMMON fue desarrollado, se llevaron a cabo análisis preliminares para el diseño de MYRRHA (*Multi-purpose hYbrid Research Reactor for High-tech Applications*), un reactor rápido refrigerado con plomo-bismuto. Primero, se utilizó la librería de datos nucleares ENDF/B-VII.0 para identificar los datos nucleares más importantes para las reacciones inducidas por neutrones en los cálculos de criticidad de los LFR. Posteriormente, la librería JEFF-3.3T1, versión beta en ese momento de la nueva versión de la librería de datos nucleares evaluada en Europa, se analizó utilizando los mejores conjuntos de datos experimentales dependientes de la energía disponibles. El bismuto y el plomo, identificados en los análisis anteriores como isótopos clave, fueron seleccionados como los principales objetos de estudio para la mejora de los datos nucleares, ya que son de vital importancia y no fueron cubiertos en el proyecto piloto CIELO. Se encontraron problemas en la región de resonancias resueltas en las evaluaciones del plomo y el bismuto en JEFF-3.3T1 y se dieron recomendaciones al proyecto JEFF, que se adoptaron en la versión final de dicha librería de datos nucleares.

A continuación, se realizaron análisis de sensibilidad e incertidumbre con las librerías de datos nucleares JEFF-3.3 y ENDF/B-VIII.0 mediante SUMMON para estimar las incertidumbres en los parámetros de criticidad de MYRRHA. Si bien se observó un buen acuerdo en las incertidumbres totales producidas por ambas librerías, las diferencias en las evaluaciones y la inexistencia de correlaciones y evaluaciones de covarianzas hicieron que los contribuyentes a la incertidumbre total difirieran. Además, las precisiones objetivo de diseño para algunos

parámetros de seguridad, como el factor de multiplicación neutrónica, se excedieron en más del doble para las evaluaciones de datos nucleares consideradas.

Con el fin de proporcionar datos nucleares ajustados, no sólo capaces de predecir las propiedades del reactor dentro de la precisión objetivo de diseño, sino también estadísticamente coherentes con los diversos experimentos diferenciales, se desarrolló el módulo de Asimilación de Datos Con summoN (DAWN). DAWN se basa en la combinación de datos de covarianza experimentales y experimentos integrales junto con técnicas avanzadas de ajuste estadístico (mínimos cuadrados generalizados). DAWN ha sido verificado utilizando el método TMC (*Total Monte Carlo*) para diferentes experimentos integrales.

Finalmente, DAWN se usó para realizar una asimilación de los principales contribuyentes a la incertidumbre mediante el uso de datos nucleares de JEFF-3.3 *a priori* y experimentos de masa crítica disponibles públicamente en el ICSBEP. La consistencia del ajuste se verificó con datos experimentales diferenciales y se encontró un buen acuerdo. Se obtuvo una reducción significativa en la incertidumbre utilizando los experimentos más representativos de MYRRHA, debido a la reducción en la incertidumbre de los contribuyentes principales y la presencia *a posteriori* de fuertes correlaciones cruzadas entre isótopos y reacciones que no existían *a priori*. Los resultados muestran que se puede lograr una reducción de casi 300 pcm realizando una asimilación con el experimento más sensible al mayor contribuyente a la incertidumbre. Esto demuestra que la combinación de datos de covarianza experimental y experimentos integrales junto con la técnica de mínimos cuadrados generalizados puede proporcionar datos nucleares ajustados capaces de predecir las propiedades del reactor con menor incertidumbre, coherentes con los datos diferenciales.

Abstract

The Lead-cooled Fast Reactor (LFR) is one of the three technologies selected by the Sustainable Nuclear Energy Technology Platform that can meet future European energy needs. Significant efforts are being made by researchers and industry to overcome the main drawbacks for the industrial deployment of LFR, which are the lack of operational experience and the impact of uncertainties in the reactor design, operation and safety assessment.

In nuclear reactor design the uncertainties mainly come from material properties, fabrication tolerances, operative conditions, simulation tools and nuclear data. Indeed, the uncertainty in nuclear data is one of the most important sources of uncertainty in reactor design and reactor physics simulations, and significant gaps between the uncertainties and the target accuracies have been systematically shown in the past. Meeting the target accuracy is required not only to achieve the requested level of safety for this technology, but also to minimize the increase in the costs due to additional security measures.

With that background, the main objective of this work has been to analyse and improve the nuclear data required for the development, safety assessment and licensing of LFR reactors, reducing the uncertainties in the criticality safety parameters due to the uncertainties in nuclear data, in order to reach the target accuracies defined by researchers, industry and regulators.

To estimate the uncertainties in reactor key parameters (effective neutron multiplication factor, k_{eff} , effective delayed neutron fraction, β_{eff} , effective neutron generation time, Λ_{eff} , safety coefficients, ...) and to identify possible nuclear data weaknesses, accurate and reliable tools for sensitivity analysis and uncertainty quantification are needed. Tools able to calculate the uncertainty of a response due to uncertainties in nuclear data are available. However they possess several limitations such as no parallel processing capabilities; user selection of isotope and reaction channels to be included in the analysis; use of multi-group nuclear data; use of specific

nuclear data library and/or specific covariance matrix; and limited complexity of the system under analysis due to the required number of simulations.

Hence, in the framework of this work, a Sensitivity and Uncertainty Methodology for MONte carlo codes (SUMMON) has been developed. SUMMON is a tool conceived to perform complete automated sensitivity and uncertainty analyses of the most relevant criticality safety parameters of detailed complex reactor designs from the neutronic point of view, i.e., k_{eff} , β_{eff} , Λ_{eff} and reactivity coefficients, using state-of-the-art nuclear data libraries and covariances. SUMMON has been validated using integral experiments from the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP) and extensively verified against consolidated codes such as SCALE, SUS3D and SERPENT. Good agreement between codes has been found.

Once SUMMON was developed, preliminary analyses were carried out for MYRRHA (Multi-purpose hYbrid Research Reactor for High-tech Applications) lead-bismuth cooled fast reactor design. First, the ENDF/B-VII.0 nuclear data library was used, in order to identify the most important nuclear data for neutron induced reactions for criticality safety calculations of LFRs. Then, the recently released JEFF-3.3T1 library, the beta proposal at the time for the next version of the European evaluated nuclear data library, was analysed using the best documented energy dependent experimental data sets available. Bismuth and lead, identified in the previous analyses as key isotopes, were chosen as the main objects of study for improvement of nuclear data since they are of vital importance and were not covered in the CIELO pilot project. Problems were found in the resolved resonance region of JEFF-3.3T1 bismuth and lead evaluations and recommendations were given to the JEFF project, which were adopted in the release version of the library.

Next, sensitivity and uncertainty analyses using the state-of-the-art JEFF-3.3 and ENDF/B-VIII.0 nuclear data libraries were performed with SUMMON to estimate the uncertainties in the criticality safety parameters of MYRRHA. While good agreement was observed in the total uncertainties yielded by both libraries, differences in evaluations, missing correlations and missing covariance evaluations, caused the contributors to the total uncertainty to differ. Furthermore, the design target accuracies for some criticality safety parameters, such as the effective neutron multiplication factor, still exceeded by more than a factor of two for the considered modern nuclear data evaluations.

In order to provide adjusted nuclear data, not only capable of predicting reactor properties within the target design accuracy, but also statistically consistent with the various differential measurements, the Data Assimilation With summoN (DAWN) module was developed. DAWN is based on the combination of experimental covariance data and integral experiments together

with advanced statistical adjustment techniques (Generalised Least Squares). DAWN has been verified against the Total Monte Carlo (TMC) method for several integral experiments.

Finally, DAWN was used to perform an assimilation on the main contributors to the uncertainty using JEFF-3.3 nuclear data as a prior and publicly available critical mass experiments from the ICSBEP. The consistency of the nuclear data adjustment was checked against differential experimental data and good agreement was found. A significant reduction in uncertainty was obtained using the experiments most representative of MYRRHA, due to the reduction in the uncertainty of the major contributors and to the presence *a posteriori* of strong cross-correlations between isotopes and reactions that did not exist *a priori*. Results show that a reduction of nearly 300 pcm can be achieved performing an assimilation with the most sensitive experiment to the major contributor to the uncertainty. It proves that the combination of experimental covariance data and integral experiments together with Generalised Least Squares technique, can provide adjusted nuclear data capable of predicting reactor properties with lower uncertainty and consistent with differential data.

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Abbreviations

1st PT	First order Perturbation Theory
ADS	Accelerator Driven Systems
ALFRED	Advanced Lead-cooled Fast Reactor European Demonstrator
ALLEGRO	Advanced European Gas-cooled Fast Reactor Demonstrator
ANL	Argonne National Laboratory
ASTRID	Advanced Sodium Technological Reactor for Industrial Demonstration
BMC	Bayesian Monte Carlo
BoC	Beginning of Cycle
BoL	Beginning of Life
CEA	Commissariat à l'Énergie Atomique et aux énergies alternatives
CIELO	Collaborative International Evaluated Library Organization
CLUTCH	Contribution-Linked eigenvalue sensitivity/Uncertainty estimation via Track length importance CHaracterization
CR	Control Rods
DA	Data Assimilation
DAWN	Data Assimilation With summoN
DICE	Database for the International handbook of evaluated Criticality safety benchmark Experiments
ENDF	Evaluated Nuclear Data File
EGPT	Equivalent Generalized Perturbation Theory
ESNII	European Sustainable Nuclear Industrial Initiative

EU	European Union
FALCON	Fostering ALfred CONstruction
FUDGE	For Updating Data and Generating Evaluations
GELINA	GEel LINear electron Accelerator
Gen-IV	Generation IV
GLS	Generalised Least Squares
GNDS	Generalised Nuclear Database Structure
GPT	Generalized Perturbation Theory
GRS	Gesellschaft für Anlagen- und Reaktorsicherheit
IAEA	International Atomic Energy Agency
ICSBEP	International Criticality Safety Benchmark Evaluation Project
IPPE	Institute of Physics and Power Engineering
IDAT	International reactor physics handbook Database and Analysis Tool
IFP	Iterated Fission Probability
INL	Idaho National Laboratory
IRPhE	International Reactor Physics Experiment Evaluation
IRSN	Institut de Radioprotection et de Sûreté Nucléaire
ISC	Integrated Sensitivity Coefficients
JAEA	Japanese Atomic Energy Agency
JEFF	Joint Evaluated Fission and Fusion
JSI	Jožef Stefan Institute
LANL	Los Alamos National Laboratory
LBE	Lead-Bismuth Eutectic
LFR	Lead-cooled Fast Reactor
LLNL	Lawrence Livermore National Laboratory
MC	Monte Carlo
MG	Multi-Group
MOX	Mixed Oxide Fuel
MYRRHA	Multi-purpose hYbrid Research Reactor for High-tech Applications
NEA	Nuclear Energy Agency
NRG	Nuclear Research and consultancy Group

OECD	Organization for Economic Cooperation and Development
ORELA	Oak Ridge Electron Linear Accelerator
ORNL	Oak Ridge National Laboratory
PIA	Progressive Incremental Adjustment
PSI	Paul Scherrer Institute
REWIND	Ranking Experiments by Weighting for Improved Nuclear Data
RRR	Resolved Resonance Region/Range
SCK•CEN	Studiecentrum voor Kernenergie • Centre d'Étude de l'énergie Nucléaire
SET Plan	Strategic Energy Technology Plan
SINBAD	Shielding Integral Benchmark Archive and Database
SNETP	Sustainable Nuclear Energy Technology Platform
SR	Safety Rods
S/U	Sensitivity and Uncertainty
SUMMON	Sensitivity and Uncertainty Methodology for MONte carlo codes
TMC	Total Monte Carlo
ToF	Time of Flight
UQ	Uncertainty Quantification
ULOF	Unprotected Loss Of Flow
URR	Unresolved Resonance Region/Range
UTOP	Unprotected Transient OverPower
VTT	Technical Research Centre of Finland
WNR	Weapons Neutron Research
WPEC	Working Party on International Nuclear Data Evaluation Co-operation
XGPT	eXtended Generalized Perturbation Theory

Part I

Introduction

Chapter 1

Introduction

1.1. Motivation

The estimated increase in world population to more than 9700 million people by 2050 [UN Department of Economic and Social Affairs, 2017], along with the need for a sustainable development to reduce CO₂ emissions and to combat climate change, the main environmental concern in the next 50 years [UN Framework Convention on Climate Change, 2002], make nuclear energy a part of the solution to meet future energy needs. The term sustainable, in the energy option context, involves the capability of producing energy for a long time without harming future generations, so that the environment is respected and the production is economically viable, safe and guaranteed regardless of location or geopolitical conflicts.

The European Union (EU) has set itself targets for reducing its greenhouse gas emissions progressively up to 2050 [European Commission, 2019a], in order to meet the objective committed in the Paris Agreement [European Commission, 2016] to limit global temperature increase under 2 °C, while striving to keep it to 1.5 °C. The EU has put in place legislations to reduce emissions by at least 40% (from 1990 levels) by 2030, as part of EU's 2030 climate and energy framework and contributing to the Paris Agreement, by increasing the share of renewable energies to at least 32% and improving 32.5% energy efficiency. Furthermore, on November 2018, the Commission presented its European strategic long-term vision for a prosperous, modern, competitive and climate neutral economy [European Commission, 2018], in which it is stated that: *“By 2050, more than 80% of electricity will be coming from renewable energy sources (increasingly located off-shore). Together with a nuclear power share of ca. 15%, this will be the backbone of a carbon-free European power system.”*

Therefore, renewable energies are the European main solution to address energy-demand and climate challenges; however, due to the high degree of volatility in very short time of their

availability factor [Pavel et al., 2017], they cannot operate without the help of other baseload carbon-free energy producing technologies capable also of load-following. This is where nuclear energy plays a key role.

Nuclear energy is a competitive and reliable emission-free power source that meets all the criteria mentioned above but also has drawbacks, such as the production of high activity radioactive waste, the potential production of nuclear weapons or the accident risk. However, fast reactors with closed fuel cycle can drastically reduce the volume of waste and the risk of producing weapon grade material (^{239}Pu and ^{235}U) [Brook et al., 2014], improving the economic competitiveness of fission reactors and having great availability factor and load-following capabilities [Wider et al., 2005]. One of the main challenges is showing that they are as safe as other existing reactors when they are to be built (2040 - 2050), being able to maintain the very low safety risk of the current responsibly managed nuclear power plants. Therefore, it is necessary to research and develop a new generation of advanced nuclear reactors, the so-called Generation IV (Gen-IV), to advance in sustainability, reliability, proliferation-resistance and safety.

Europe has defined a Strategic Energy Technology Plan (SET Plan), which aims to accelerate the development and deployment of low-carbon technologies [European Commission, 2019b], promoting research and innovation efforts by supporting the most impactful technologies in the EU's transformation to a low-carbon energy system. One of the Platforms created to support the implementation of the SET Plan is the Sustainable Nuclear Energy Technology Platform (SNETP) [Sustainable Nuclear Energy Technology Platform, 2019], whose objectives are: i) to preserve and strengthen the European technological leadership and nuclear industry through a strong and long-term research and development programme, involving fuel cycles and reactor systems of Generation II, III and IV types; ii) to enhance Europe's technological leadership in nuclear science and engineering; and iii) to contribute to the production of synthetic fuels and hydrogen.

Within SNETP, Europe has defined its strategy and set the necessary priorities for the development of Gen-IV fast reactors that can meet future European energy needs through the European Sustainable Nuclear Industrial Initiative (ESNII) [European Sustainable Nuclear Industrial Initiative, 2019]. To this end, it has selected the following technologies:

- The Sodium-cooled Fast Reactor (with the ASTRID reactor as the prototype) is the reference solution, with France strongly supporting this technology.
- As first alternative technology, the Lead-cooled Fast Reactor (ALFRED), with the construction of an experimental reactor to demonstrate the technology in Romania, and with the support of a lead-bismuth irradiation facility in Belgium (MYRRHA).

- As second technological alternative, the Gas-cooled Fast Reactor (ALLEGRO), which also requires the construction of a demonstrator in a European country.

In support of ESNII, the collaborative project “Preparing ESNII for Horizon 2020” (ESNII Plus) [European Commission, 2017a], co-funded by the European Commission within the 7th EURATOM Framework Programme, was launched in 2013. The aim of this project was to define strategic orientations and establish research priorities for the future Gen-IV reactor deployment in Europe.

The sodium-cooled fast reactor technology was the European reference choice; however, recent news [Thomson Reuters, 2018] seem to point out that France will halt research into the ASTRID project in 2019, with no plans to allocate a budget beyond 2020, and with the possibility of reducing ASTRID from a commercial-sized reactor demonstrator to a research reactor. On the other hand, on September 2018 the Belgian government approved 558 million euros in funding for MYRRHA and, in fact, MYRRHA’s project Phase 1 has already started with the construction of the 100 MeV particle accelerator and the pre-licensing of the reactor [SCK•CEN, 2019]. Additionally, on September 2017, stronger commitment was given by the organizations participating in the ALFRED project with the renewal of the consortium to achieve the construction of ALFRED [ALFRED, 2018]. Therefore, Lead-cooled Fast Reactors (LFR) have become a fundamental part of Europe’s long-term plan for nuclear energy.

However, significant drawbacks for the industrial deployment of LFR still exist, among which are the lack of operational experience and the little knowledge about the potential impact of uncertainties in the reactor design, operation and safety assessment.

Traditionally, expensive experimental facilities have been needed for the design of a new nuclear reactor in order to conduct dedicated experiments to cover a wide range of scenarios and aspects of the new system. Nowadays, considering the cost of such facilities, it would be desirable that the design of new systems could rely more on computer simulations. Accurate simulations can help to improve understanding and optimize the design and safety margins in any operational conditions. Hence, the capability to provide reliable predictions is recognized as a priority to support the development of LFR technologies.

The quantification of uncertainties associated with the computational outcomes is imperative to establish the credibility of the results and make robust decisions based on simulations. In nuclear reactor design, the uncertainties come from material properties, fabrication tolerances, operative conditions, simulation tools and nuclear data. The uncertainty in nuclear data is one of the most important sources of uncertainty in neutronic calculations and consequently in reactor design [Kodeli, 2007]. Accurate and reliable tools are therefore needed to propagate nuclear data uncertainties to reactor key parameters (neutron multiplication factor, safety coefficients, ...).

Significant gaps between the estimated uncertainties in reactor core parameters and the target accuracies (i.e., maximum acceptable uncertainties for a certain parameter) have been systematically shown in the past [Plompen and Harada, 2014], suggesting nuclear data weaknesses. Meeting the target accuracy is required not only to achieve the requested level of safety for this technology, but also to minimize the increase in the costs due to additional safety measures.

The European Commission within the 7th EURATOM Framework Programme launched in 2013 CHANDA project [European Commission, 2017b], whose acronym stands for “solving CHallenges in Nuclear DATA”. One of the objectives of the project was to address the challenges in the field of nuclear data for new reactors and nuclear fuel cycle facilities, preparing tools that solve the challenges of quantifying and certifying the accuracy of simulations based on available nuclear data uncertainties.

This Thesis work has been performed in the framework of CHANDA and ESNII+ projects, with the aim to respond to the specific nuclear data needs for LFR.

1.2. Objectives and original contributions

The main objective of this Thesis is to analyse and improve the nuclear data required for the development, safety assessment and licensing of LFR reactors, reducing the uncertainties in the criticality safety parameters due to the uncertainties in nuclear data, in order to reach the target accuracies defined by scientific community, industry and regulators. This is carried out by means of sensitivity and uncertainty analyses to quantify the impact of nuclear data uncertainties in reactor integral parameters, and data assimilation to constrain uncertainties. In addition, LFR coolant materials in JEFF-3.3 state-of-the-art nuclear data library are thoroughly analysed. LFR nuclear data needs are identified, improvements are proposed and recommendations are given.

The original contributions of this Thesis, with the references where they have been published, are:

- Development of a Sensitivity and Uncertainty Methodology for MONte carlo codes called SUMMON [Mills, 2018; Romojaro et al., 2019, 2018a, 2017a].
- Analysis, identification of errors and improvement of lead and bismuth files in JEFF-3.3 nuclear data library [Cabellos et al., 2017; Kodeli et al., 2018, 2016b; Romojaro et al., 2017c; Romojaro and Žerovnik, 2016; Žerovnik et al., 2017b, 2017a, 2016].
- Sensitivity and uncertainty quantification analyses and target accuracy assessments for ALFRED and MYRRHA reactors [García-Herranz et al., 2017; Grasso et al., 2018, 2017, Romojaro et al., 2018b, 2017b, 2017c, 2015].

- Development of a data assimilation module to utilize integral data to constrain uncertainties, called DAWN (Data Assimilation With summoN) [Romojaro et al., 2018b].
- Data assimilation studies to reduce uncertainties in LFR criticality safety parameters [Romojaro et al., 2018b].
- Identification of nuclear data weaknesses in JEFF-3.3 and recommendations for improvement to JEFF project [Žerovnik et al., 2017a, 2017b].

1.3. Structure

In Part I, the motivations that conducted to this Thesis are presented and the fundamental objectives and original contributions are established.

In Part II, a summary of Lead-cooled Fast Reactors is given in Chapter 2, while the state-of-the-art of nuclear data used throughout this Thesis and current methodologies for sensitivity and uncertainty analysis are presented in Chapter 3 and Chapter 4, respectively.

Part III is comprised of the developments performed during the Thesis and the applications of such developments. In Chapter 5, the theory used to develop Sensitivity and Uncertainty Methodology for MONte carlo (SUMMON) is presented and the implementation, validation and verification of SUMMON are detailed. Before nuclear data can be used for applications, exhaustive validation and verification studies must be carried out. Consequently, Chapter 6 focuses on the detailed analysis of lead and bismuth files in JEFF-3.3 nuclear data library, in order to be used as the reference library for the subsequent analyses performed in the following chapters. In Chapter 7, sensitivity and uncertainty analyses for MYRRHA criticality safety parameters are carried out and target accuracy assessments are performed. In Chapter 8, the theory in which Data Assimilation With summoN is based, is presented and the implementation and verification of this module are described. Furthermore, DAWN is applied to constrain the uncertainties in MYRRHA criticality safety parameters that do not meet target accuracies in Chapter 7.

Finally, in Part IV, the achievements of this Thesis are summarised, the main conclusions and recommendations are given and future lines of research are proposed.

Part II

State-of-the-art

Chapter 2

Lead-cooled Fast Reactors

Abstract – Europe has selected Lead-cooled Fast Reactors as one of the candidate reactor technologies that can meet future European energy needs. Nuclear systems cooled by lead, the Lead-cooled Fast Reactors and the Accelerator Driven Systems, are presented in this chapter. The first part of the chapter reviews the advantages and disadvantages, as well as the historical development of both lead-cooled systems. In the second part, MYRRHA and ALFRED reactors are described in more detail.

2.1. Lead-cooled reactors

Lead is used as coolant in fast reactors due to its very low neutron absorption and energy moderation properties, which allow maintaining a fast neutron flux (i.e., a neutron spectrum shifted to higher energies), and good thermodynamic properties. Two general types of fast reactors employ lead for cooling: critical Lead-cooled Fast Reactors and subcritical Accelerator Driven Systems (ADS). They will be described in the following.

2.1.1. LFR

Lead-cooled fast reactors (Figure 1) are fast spectrum reactors cooled by molten lead or lead-based alloys, among which the lead-bismuth eutectic (LBE) mixture is the most commonly considered. LFRs can operate at high temperature and at near atmospheric pressure because of the very high boiling point of the coolant (up to 1743 °C) and its low vapour pressure [Pioro, 2016]. Furthermore, lead is found abundantly in nature and can consequently be available in case of a large deployment of an LFR reactor fleet.

The LFR has excellent material management capabilities since it operates in the fast-neutron spectrum and uses a closed fuel cycle for efficient conversion of fertile uranium. It can also be

used as a burner to consume actinides from Light Water Reactor spent fuel and as a burner/breeder with thorium matrices [Gen-IV International Forum, 2019].

Figure 1. Lead-cooled Fast Reactor scheme [Gen-IV International Forum, 2019]

Furthermore, LFRs present enhanced safety due to the choice of lead as a coolant material, that is: i) no rapid chemical reactions with water or air (such as sodium); ii) the high boiling point eliminates the risk of core voiding due to coolant boiling; iii) lead provides a significant thermal inertia in case of loss of heat sink; iv) lead shields gamma radiation and retains fission products; v) lead low neutron moderation properties allow greater spacing between pins and reduced risk of flow blockage; and vi) thermodynamic properties of lead allow a high level of natural circulation cooling based on convection.

On the other hand, the LFR still has development needs and presents research challenges, such as inspection and monitoring of reactor in-core components as well as fuel handling due to the opacity of lead, the consideration of a structural design to prevent seismic impacts to the reactor system because of the high density and mass of lead and, the most significant challenge, lead corrosion at high temperature when in contact with structural steels.

2.2.2. ADS

Accelerator Driven Systems are advanced nuclear systems which are particularly suitable for transmutation objectives. An ADS consists of a high power proton accelerator, a heavy metal spallation target that produces neutrons when bombarded by the high power beam, and a subcritical core that is neutronically coupled to the spallation target [International Atomic Energy Agency, 2015]. Lead and LBE have been considered as coolants and as neutron spallation targets, due to their high-power density, for ADS.

Several objectives can be achieved with these systems: nuclear waste transmutation of selected isotopes, generation of electricity and/or heat, and production of fissile materials by irradiating fertile elements. Furthermore, they offer great flexibility on fuel composition since fuels not fissile with thermal neutrons, like thorium, can be used. However, the most important aspects of ADS are their enhanced safety features, due to the fact that the system cannot maintain criticality and shuts down once the accelerator is turned off.

Nevertheless, ADS are not exempted from design and operational disadvantages such as the stress, irradiation and corrosion that the beam window and targets are subjected to; the complexity of the installation; the reliability of the accelerator; and the reduction of electrical efficiency due to the accelerator consumption.

2.2. Development

The development of fast reactors with molten lead (or lead-based alloys) as a coolant was initially considered in West Europe in the 1950s, but discarded due to the anticipated problems with the corrosive nature of lead [Cacuci, 2010]. However, during the same timeframe, the Soviet Union initiated research on the use of lead-bismuth alloy at the Institute of Physics and Power Engineering (IPPE) in Obninsk, to pursue the technology for submarine propulsion. Eight submarines were built and operated along with two on-shore reactors, the 27/VT land prototype in 1959 at IPPE and the second land-based naval reactor prototype in 1978 at the Scientific Research Technological Institute in Sosnovy Bor. A total of 15 reactor cores were operated from the early 1960s until 1995, with the decommissioning of the final submarine.

Since 1990, Russia has shown a renewed interest on LFRs for civilian (i.e., electricity production) purposes. Two initiatives are currently being pursued: the lead-bismuth cooled SVBR-75/100 modular reactor [Zrodnikov et al., 2008] and the lead-cooled BREST-300 demonstrator reactor [Lemekhov et al., 2017].

In Europe, the European Lead-cooled System (ELSY) project was initiated in 2006 to demonstrate the possibility of designing a fast critical industrial-size LFR using simple engineered technical features, whilst fully complying with the Generation IV goals of sustainability [Cinotti et al., 2007]. This was followed in 2010 with the European Advanced Lead-cooled Demonstration (LEADER) project [De Bruyn et al., 2013], which continued the study of an industrial-sized reactor, and with the launch of the European Sustainable Nuclear Industrial Initiative (ESNII) [European Sustainable Nuclear Industrial Initiative, 2019] also in 2010. ESNII aimed at the construction of ALFRED [Alemberti et al., 2013], a reactor to act as demonstrator of the lead-cooled technology, in an European country willing to host the programme, supported by

MYRRHA [De Bruyn et al., 2014], a lead-bismuth irradiation facility project in Belgium that can operate as an LFR or ADS. As mentioned in Chapter 1, MYRRHA and ALFRED projects have been progressively gaining strong support in European countries, culminating with the start of the construction of the 100 MeV particle accelerator and the approval of funding for MYRRHA in 2018. Moreover, in Sweden, a collaboration between Chalmers University of Technology, the Royal Institute of Technology and Uppsala University has been initiated for the development of an education and training facility to test LFR technology and research on fast reactor dynamics, the European Lead-Cooled TRaining reactor (ELECTRA) project [Wallenius et al., 2012].

Additional LFR designs are being currently studied by other countries including USA, with the development of the Small Secure Transportable Autonomous Reactor (SSTAR) project [Smith et al., 2008], a small modular natural circulation reactor with lead as a coolant and a long-life (15-30 years) sealed core; South Korea, with the development of the Proliferation-resistant Environment-friendly Accident-tolerant Continuable-energy Economical lead-bismuth Reactor (PEACER) [Hwang et al., 2000] to transmute long-lived fission products in the spent nuclear fuel into short-lived low-intermediate-level waste, and the Battery-Optimized Reactor Integral System (BORIS) [Yu et al., 2006] multipurpose integral optimized lead-cooled fast reactor with an ultra-long-life core that aims at satisfying the needs of developing nations and especially remote communities; Japan, with the Pb-Bi cooled direct-contact boiling Water Fast Reactor (PBWFR) [Takahashi et al., 2005], the Steam Lift Pump-type LFR (SLPLFR) [Nakazima et al., 2006], and the Constant Axial Neutron During the Life of Energy (CANDLE) reactor [Sekimoto and Yan, 2008]; and China, with the China LEAd-based Reactor (CLEAR) project [Wu et al., 2013].

Regarding ADS, since the early 1990s the international scientific community began to consider the ADS as a concept suitable to be developed to properly demonstrate its potential to address the high-level waste issue. Several basic research programmes have been launched in Europe, Korea and Japan, leading to the definition of possible conceptual alternatives and to the related investigation of technological issues [International Atomic Energy Agency, 2015].

In Europe, the Energy Amplifier (EA) [Rubbia et al., 1995], one of the first ADS concepts, was conceived by C. Rubbia in 1993 at CERN. Starting from 1996, research activities were carried out by Italian, French and Spanish institutions due to the growing interest in the EA, that conducted to the LBE-cooled Reference Configuration of the ADS Experimental Facility (XADS) [Cinotti, 2001], which in turn evolved to the European PDS-XADS [Mueller, 2003]. In parallel, SCK•CEN began the ADONIS project in 1995 with the sole aim of producing ^{99}Mo , using a cyclotron coupled with a subcritical blanket [D'hondt et al., 1997]. However, it was decided in 1998 that ADONIS machine would become a material testing reactor to act as an ADS demonstrator of reasonable power scale; thus, the MYRRHA project was born. In 2005,

MYRRHA design, which consisted of a proton accelerator coupled to a subcritical 50 MW_{th} core, was integrated in the 6th Framework Programme EUROTRANS project [Abderrahim et al., 2009], which resulted in the XT-ADS design [De Bruyn et al., 2010b]. This design was taken in as reference in 7FP CDT project [De Bruyn et al., 2010a], in which the possibility of operating as a critical reactor was introduced in the new MYRRHA-FASTEF design [Sarotto et al., 2013]. Finally, the MYRRHA design was once again revised in 2014, evolving to MYRRHA rev. 1.6 [Malambu and Stankovskiy, 2014], which is the design employed in this Thesis.

ADS have been developed in Korea since 1997, with the HYbrid Power Extraction Reactor (HYPER) [Park et al., 2000] being designed for transmutation of long-lived nuclear wastes. HYPER uses LBE as both coolant and spallation target.

Moreover, in Japan, an ADS using LBE as a spallation target and coolant, with the thermal power of 800 MW has been designed, where 250 kg of minor actinides and some long-lived fission products can be transmuted annually [Cacuci, 2010].

As the European Gen-IV references for lead fast reactor technology, MYRRHA and ALFRED have been the main focus of this Thesis and will be briefly described in the following sections.

2.3. MYRRHA

The Multi-purpose hYbrid Research Reactor for High-tech Applications (MYRRHA) is a flexible experimental facility being designed at SCK•CEN, Mol, Belgium. It is conceived to operate both in sub-critical mode, as an Accelerator Driven System, and in critical mode, as a lead-bismuth cooled fast reactor.

MYRRHA will serve as an irradiation facility for material developments for fission and fusion reactors. Furthermore, it will help to demonstrate the ADS concept and allow the study of high-level waste transmutation. Moreover, MYRRHA will allow the production of radioisotopes for medical and industrial applications.

In order to take profit of the thermal inertia provided by a large coolant volume, a pool type configuration (Figure 2) has been selected, housing the components of the primary loop (i.e., pumps, heat exchangers, fuel handling tools, experimental rigs, etc.) inside the reactor vessel, which is located in an air controlled environment.

MYRRHA will have a high level requirement in terms of irradiation performances, with high flux levels ($\phi_{\text{tot}} > 5 \cdot 10^{15}$ n/cm²s) and high availability rate. Because of the desired high flux, the

high-power density lead-bismuth liquid metal has been chosen as coolant. Moreover, LBE allows operating at lower temperatures, due to its low melting point, limiting corrosion problems.

In ADS mode, the LBE target will produce 10^{17} neutrons per beam particle by means of spallation reactions with protons delivered by a 600 MeV, 4 mA beam produced by the linear proton accelerator. Consequently, LBE will have to evacuate the 1.43 MW heat produced by the beam. A windowless spallation target was selected for previous designs; however, the current design envisages a loopless window.

Figure 2. The MYRRHA reactor

Regarding the status of the project, the first phase of the programme was launched in early 2016 with the construction of the 100 MeV accelerator for research. In 2018 the Belgian government decided to support the construction and exploitation of the first phase and 558 million euros were allocated for MYRRHA's financing. The construction of the 600 MeV accelerator and the construction of the reactor, second and third phases of the project respectively, are planned to start in 2026. Start of operation of the reactor and full ADS are envisioned for 2033.

2.4. ALFRED

The Advanced Lead-cooled Fast Reactor European Demonstrator (ALFRED) is a 300 MW_{th} small-size pool type reactor cooled by lead, with the core, primary pumps and steam generators contained within the reactor vessel. Its primary system can be seen in Figure 3.

Figure 3. The ALFRED reactor [Alemberti et al., 2013]

ALFRED shall be connected to the electrical grid (125 MW_e). It will use already available technology, to speed up construction time, and corrosion-resistant structural materials compatible with lead (AISI 316LN and 15-15 Ti). Furthermore, coolant flow velocity will be limited to reduce lead erosive properties and natural circulation will be enhanced by low primary system pressure loops, to reach the expected high safety level. The design will allow removing components from the reactor vessel for inspection, maintenance and replacement; and shall be characterized by its robustness.

ALFRED core is composed by 171 hexagonal fuel assemblies divided in an inner and an outer zone, with different plutonium enrichments (higher enrichment in the outer region) to flatten the power distribution. Two rows of dummy elements will serve as reflector. Two different control systems will be employed, that is, control rods, for power regulation and reactivity swing compensation, and safety rods for shutdown purposes. A total of eight steam generators will be placed inside the vessel.

Regarding the current status of ALFRED, the actual realisation of the project continues progressing. Fostering ALfred CONstruction (FALCON) consortium agreement was established in 2013 to bring LFR technology to industrial maturity. It was then renewed in 2017, with the objective of a rapid deployment of ALFRED being shared by the new members. Romania, ALFRED's host country, has also demonstrated a firm commitment to ALFRED as a major project, as can be seen in Figure 4.

Figure 4. Romania's support to the ALFRED project [Alemberti, 2018]

Chapter 3

Nuclear data

Abstract – Nuclear data constitute the fundamental building of the nuclear physics research. This chapter introduces nuclear data and describes the cycle used by the nuclear data community to produce high quality data. Furthermore, existing state-of-the-art nuclear data evaluation projects and libraries are reviewed and the major formats used to store the data are briefly explained. Additionally, main processing codes used to produce application libraries for simulation tools are summarized.

3.1. Introduction

Reliable nuclear structure and reaction data constitute the fundamental building of nuclear physics research and are vital for many other applications. In nuclear physics simulations, two classes of data are required [Koning et al., 2011]: i) data describing neutron (and sometimes other particle) interaction with the nuclei conforming the system; and ii) data describing nuclear changes in system constituents, as a result of fission, activation or decay. All these data are considered nuclear data.

To produce high quality nuclear data, the life cycle presented in Figure 5 is followed. First, novel experimental nuclear reaction data are obtained with energy dependent measurements. Since it is not possible to measure everything, experimental data are usually completed by theoretical model calculations. Then, evaluators produce evaluated data sets through the process of selection, critical comparison, renormalization and averaging of the available data, to come up with a best judgement of the real values of the underlying nuclear reaction data. Evaluated data are exhaustively tested and verified before their release, in order to ensure that no errors have been made in the evaluation and that the format, in which the data are compiled, is respected. The compendium of such data, usually composed of data for several hundreds of nuclides, is known

as evaluated nuclear data libraries. The processing of nuclear data libraries with specialized computer codes (e.g., NJOY, PREPRO, AMPX or FUDGE), allows obtaining application libraries, which are the input data to computations for a wide variety of nuclear science and technology applications. Application libraries are validated using integral experimental data, by simulating the integral measurement (e.g., criticality simulation with a transport code such as PARTISN, MCNP, SERPENT, ...) and comparing the results from the calculation against the experimental data. Finally, application libraries are employed by users in specific applications (e.g., nuclear reactor simulations). The validation and use of application libraries allow identifying nuclear data needs and establishing nuclear data priorities to perform new measurements or re-evaluations and, thus, the cycle is once again repeated.

Figure 5. Life cycle of nuclear data

It is important to notice that nuclear data are not free of uncertainties. Experiments, by their nature, are imperfect. They are uncertain due to limitations of measurement procedures, as well as due to statistical fluctuations that are uncontrollable. Numerical values for physical parameters predicted by theoretical models are also uncertain [Smith and Otuka, 2012]. These uncertainties are analysed and evaluated, and then, provided within the nuclear data evaluations in the form of covariance matrices. However, uncertainty information is not always given and when it is, it may lack completeness or consistency.

3.2. Nuclear data libraries

As of the mid-1960s many nuclear data libraries existed. Each laboratory had its own data library, in its own format for its own computer codes, which was designed to get the “best” answers using the in-house laboratory computer codes, for the specific applications that each

laboratory was interested in. This often required nonphysical “fixes” or fits to force agreement between computer code and experimental results [Cacuci, 2010].

On the mid-1960s, an effort began to establish a nuclear data library, containing evaluated data based solely on the “best” available energy dependent measurements and nuclear model calculations. It was hoped that one common library of data could be universally adopted for use throughout the world [Cacuci, 2010]. Unfortunately, this goal has not been achieved yet and significant differences between the important evaluations in these various data libraries still exist.

The major nuclear data libraries used through this Thesis are:

- The Joint Evaluated Fission and Fusion (JEFF) nuclear data library, which is produced by a coordinated group of the Nuclear Energy Agency (NEA), that belongs to the Organisation for Economic Co-operation and Development (OECD). The latest version, JEFF-3.3 [Plompen, 2017], was officially released in November 2017. This library is the main focus of the Thesis.
- The ENDF/B nuclear data library, which is produced by the Cross Section Evaluation Working Group, which is a cooperative effort of the national laboratories, industry, and universities in the United States and Canada. The latest version, ENDF/B-VIII.0 [Brown et al., 2018], was released in February 2018.
- The Japanese Evaluated Nuclear Data Library (JENDL), which is produced by the Nuclear Data Centre at the Japan Atomic Energy Agency, with the aid of the Japanese Nuclear Data Committee. The latest complete version, JENDL-4.0 [Shibata et al., 2011], was released in May 2010. This release has been partially updated through JENDL-4.0u [Japan Atomic Energy Agency, 2016].
- The TALYS-based Evaluated nuclear data library (TENDL), which provides nuclear data based on the output of the TALYS [Koning and Rochman, 2012] nuclear model code system. Up to 2014, TENDL was produced by the Nuclear Research and consultancy Group (NRG) in Petten. Since 2015, TENDL is mainly developed by Paul Scherrer Institute (PSI) and the Nuclear Data Section of the International Atomic Energy Agency (IAEA). The latest version, TENDL-2017 [Rochman et al., 2017], was released in December 2017.

The two other major nuclear data libraries that, though not used in this Thesis, provide full coverage for nuclear calculations, are:

- The Chinese Evaluated Nuclear Data Library (CENDL), which is produced by the China Nuclear Data Center in cooperation with the China Nuclear Data Coordination Network. The latest version, CENDL-3.1 [Ge et al., 2011], was released in December 2009.
- The Russian evaluated neutron data library, which is produced by the Russian Nuclear Data Center. The latest version, BROND-3.1 [Blokhin et al., 2016], was released in 2016.

3.3. Nuclear data formats

Even though the international effort has not led to a common set of evaluated nuclear data, it has led to a common universally accepted format for the data [Cacuci, 2010]; i.e., the Evaluated Nuclear Data File format in its sixth version (ENDF-6) [Herman and Trkov, 2009] has been adopted by all the major evaluated nuclear data libraries. However, over the past six years, a new standard format for storing nuclear data is being designed, the Generalised Nuclear Database Structure (GNDS) [Descalle et al., 2018]. Despite ENDF-6 widespread acceptance, new applications in medical physics, space/radiation physics, homeland security, nuclear waste management and non-proliferation, drive this format far beyond its original design and intended uses [Mattoon et al., 2012] (i.e., ENDF-6 format offers limited support for correlated particle emission, limited numeric precision and general lack of extensibility). Both formats will coexist, but new evaluations will add data types not supported by ENDF-6 that will force the gradual transition of codes and users to GNDS format. In Figure 6, a comparison between ENDF-6 and GNDS formats can be seen.

0.000000+0	0.000000+0	0	0	0	09228 3	099999
9.223500+4	2.330248+2	0	0	0	09228 3	18 1
1.934054+8	1.934054+8	0	0	1	4359228 3	18 2
435	2				9228 3	18 3
1.000000-5	0.000000+0	2.250000+3	0.000000+0	2.250000+3	5.864859+09228 3	18 4
2.500000+3	5.385604+0	3.000000+3	5.084990+0	3.500000+3	4.784377+09228 3	18 5
4.000000+3	4.522516+0	4.500000+3	4.260654+0	5.000000+3	4.049612+09228 3	18 6
5.500000+3	3.838569+0	6.000000+3	3.564659+0	6.500000+3	3.290749+09228 3	18 7
7.000000+3	3.263572+0	7.500000+3	3.236395+0	8.000000+3	3.122824+09228 3	18 8
9.000000+3	3.064746+0	1.000000+4	3.063389+0	1.100000+4	2.949688+09228 3	18 9
1.200000+4	2.835987+0	1.300000+4	2.722286+0	1.400000+4	2.608585+09228 3	18 10
1.600000+4	2.463572+0	1.800000+4	2.400948+0	2.000000+4	2.338325+09228 3	18 11
2.100000+4	2.292500+0	2.200000+4	2.246675+0	2.300000+4	2.200851+09228 3	18 12
2.400000+4	2.155026+0	2.600000+4	2.128040+0	2.800000+4	2.101054+09228 3	18 13
3.000000+4	2.074069+0	3.100000+4	2.058953+0	3.200000+4	2.043838+09228 3	18 14

```

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      </piecewise>
    </resonancesWithBackground>
    <pointwise xData="XYs" length="268399" accuracy="0.01">
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        <axis index="1" label="crossSection" unit="b" frame="lab"/></axes>
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    </pointwise>
  </crossSection>

```

Figure 6. Comparison between nuclear data files in ENDF-6 format (top) and GNDS/XML [Mattoon et al., 2012] format (bottom)

3.3.1. ENDF-6

The ENDF-6 format uses 80-character records. The structure of an ENDF-6 format file is hierarchical, as can be seen in Figure 7. A single ENDF-6 file can contain several materials, which are identified by the MAT number. The data of each material is divided into different files containing data for a certain class of information, identified by the MF number, which in turn, are subdivided into sections, each one containing data for a particular reaction type, identified by the MT number. The sections themselves are structured in several records (MR).

Figure 7. Structure of an ENDF-6 file [Herman and Trkov, 2009]

The most relevant files for the applications studied during this Thesis are:

- File 1 (MF1), which provides a brief documentation of how the data were evaluated and a directory that summarizes the files and sections contained in the material. In the case of fissionable materials, it may contain up to five additional sections giving fission neutron and photon yields and energy release information.
- File 2 (MF2), which contains data for both resolved and unresolved resonance parameters.
- File 3 (MF3), in which reaction cross sections and auxiliary quantities are given as functions of E , where E is the incident particle energy in the laboratory system.
- Files 4-6 (MF4-6), which are used to describe the angular distribution of emitted particles; the energy distributions of secondary particles expressed as normalized probability distributions; and the distribution of reaction products (i.e., neutrons, photons, charged particles, and residual nuclei) in energy and angle, respectively.
- File 7 (MF7), containing neutron scattering data for the thermal neutron energy range ($E < 5$ eV) for moderating materials.
- File 31 (MF31), in which the covariances of the average number of neutrons per fission, given in File 1, are provided.

- File 32 (MF32), which contains the variances and covariances of the resonance parameters given in File 2.
- File 33 (MF33), providing covariances of neutron cross section information appearing in File 3.
- File 35 (MF35), in which covariance matrices for the energy distribution of secondary particles, provided in File 5, are given.

3.3.2. GNDS

GNDS is also a hierarchical file format, which can be stored in any format that supports nested data hierarchy such as XML, JSON and HDF5. GNDS format, among other properties: i) can store nuclear data in a hierarchy that reflects the understanding of nuclear reactions and decays, specifying all data; ii) supports any projectile/target combination and any combination of reaction products; iii) has backwards-compatibility with ENDF-6; and iv) is able to store both evaluated and processed data within the same hierarchy.

Within a GNDS file (Table 1), all data involving a given projectile and target for a given evaluation are organized inside a reactionSuite (also sometimes called a ‘PRO-TAR-E’ to indicate the combination of PROjectile, TARget and Evaluation) [Descalle et al., 2018]. Within the reactions node, a list of exclusive reaction nodes (sum of their cross sections is equal to the total cross section) is given, which contain a cross section and an output channel each. The output channel contains the reaction Q-value and a list of outgoing products. Multiplicity and probability distributions for outgoing product angle and/or energy are included in each product.

Table 1. Top-level nodes within reactionSuite used to organize data in GNDS files [Descalle et al., 2018]

Node	Description
documentation	Contains the top-level documentation.
styles	A list of all the types (e.g., evaluated, multi-group) of data stored in the file.
PoPs	Particle properties including masses, spins, etc.
resonances	Resonance parameter data.
reactions	A list of the exclusive reactions each stored as a ‘reaction’ node.
orphanProducts	List of products not associated with a particular reaction (e.g., like ENDF MT=3 gamma data).
sums	Sums of various data. For example, the total and/or inelastic cross sections.
productions	Cross-sections for production of unstable products
incompleteReactions	Reactions with incomplete data and thus not suitable for use in transport codes.
fissionComponents	Data about the various chance fissions (e.g., first or second chance fission).

Uncertainties and covariances may be stored alongside their central values, or they may be stored in a separate file called a ‘covarianceSuite’, and associated with their central values by links [OECD/NEA, 2016a]. More specifications can be found in Ref. [OECD/NEA, 2016a].

3.4. Processing codes

As mentioned in Section 3.2, processing codes are necessary to obtain application libraries, which are the input data to computations for a wide variety of nuclear science and technology applications, such as deterministic or stochastic neutron transport codes. The main processing codes used by the nuclear data community will be summarized in the following sections, giving a more detailed description of NJOY, which is the nuclear data processing code used in this Thesis.

3.4.1. NJOY

The NJOY nuclear data processing system [Muir et al., 2016] is a comprehensive computer code package, developed and maintained by Los Alamos National Laboratory, for producing pointwise and multigroup nuclear cross sections and related quantities from evaluated nuclear data in ENDF-6 format. Although, NJOY version 2016 has been used, a newer version exists (NJOY21), which is a ground-up rewrite of NJOY2016 with the objective of handling the new GNDS format.

NJOY consists of a set of main modules, each performing a well-defined processing task, which are linked by input and output files. The following NJOY modules and sequence have been used to process cross sections and covariance data (Figure 8):

Figure 8. NJOY sequences to process cross section (top) and covariance (bottom) data [Cabellos, 2014]

- MODER, to convert ENDF-6 files between ASCII and blocked binary modes;
- RECONR, to reconstruct pointwise (energy-dependent) cross sections from resonance parameters and interpolation schemes;
- BROADR, to perform Doppler-broadening and thinning pointwise cross sections;
- HEART, to generate pointwise heat and radiation damage production cross sections;
- GASPR, to generate pointwise gas production cross sections;
- THERMR, to produce cross sections and energy-to-energy matrices for free or bound scatterers in the thermal energy range;
- PURR, to generate unresolved-region probability tables for Monte Carlo codes;
- ACER, to generate libraries in ACE format for the MCNP code;
- GROUPE, to produce self-shielded multi-group cross sections;
- ERROR, to compute multi-group covariance data from pointwise data;
- and COVR, to process ERRORR output to BOXER format, which is a highly compressed, card-image format for storing covariance matrices.

3.4.2. *PREPRO*

The ENDF/B Pre-processing codes (PREPRO) [Cullen, 2018], originally written by D.E. Cullen and maintained nowadays by the International Atomic Energy Agency, is a collection of 18 computer codes, which are designed to convert ENDF formatted neutron and/or photon data from the form originally distributed by evaluations to a format in which the data can be used in applications. These codes also allow viewing the data, on-screen and/or hardcopy. PREPRO runs on virtually any computer and the code output is completely FORTRAN, C and C++ Compatible.

3.4.3. *AMPX*

AMPX [Rearden and Jessee, 2018] is a modular system developed and maintained by Oak Ridge National Laboratory, that generates continuous energy and multi-group AMPX format data libraries from ENDF-6 files. AMPX nuclear data libraries are used by SCALE code system. In addition to data processing modules, AMPX also includes a number of useful utility modules for checking, manipulating, and editing the libraries in SCALE.

3.4.4. *FUDGE*

For Updating Data and Generating Evaluations (FUDGE) [Beck, 2005] is a code developed by Lawrence Livermore National Laboratory for managing and processing nuclear data. FUDGE was originally written to handle LLNL's legacy nuclear data format but has been modified to support GNDS and handling ENDF-6. Currently, FUDGE is the main code for processing GNDS files.

Chapter 4

Sensitivity and Uncertainty analyses

Abstract – Sensitivity and uncertainty analyses are becoming increasingly widespread in many fields of engineering and sciences. Regarding reactor physics simulations, sensitivity analyses allow identifying the most important neutron-induced nuclear data and establishing a ranking of importance for the response of interest, while uncertainty analyses allow quantifying the uncertainty in the reactor response. In this chapter, the sensitivity and uncertainty analysis theory, employed by different codes/tools in the nuclear data analyses performed in this Thesis, is presented.

4.1. Introduction

Sensitivity and uncertainty analyses are becoming increasingly widespread in many fields of engineering and sciences, encompassing practically all of the experimental data processing activities as well as many computational modelling and process simulation activities [Cacuci et al., 2005].

Regarding nuclear data science and reactor physics simulations, sensitivity analyses study the variation of a reactor response when system parameters vary (i.e., how a reactor response such as the effective neutron multiplication factor changes when nuclear data change); and allow identifying the most important neutron-induced nuclear data and establishing a ranking of importance for the response studied. Uncertainty analyses allow quantifying the uncertainty in the reactor response due to uncertainties in nuclear data.

There are many methods, based either on deterministic or stochastic concepts, for performing sensitivity and uncertainty analysis. Deterministic methods are mostly based on local analysis, which aims at studying the behaviour of the system responses locally around a chosen point in

the combined phase space of parameters and state variables. Local sensitivities yield only the first order contributions to the total response variation and are valid only within sufficiently small neighbourhoods of the nominal values of the respective parameters [Cacuci, 2003]. Stochastic methods are usually used for global analysis, which aims at determining all of the system's critical points over the entire space of parameter variations, that is, they consider the whole variation range of input parameters [Saltelli et al., 2008].

Local sensitivity and uncertainty analyses are very efficient in computer time; however, they assume that the system response is linear. On the other hand, global analyses take into account high-order terms (non-linearity), but they require huge computational resources to analyse complex systems with a wide number of input parameters.

Reactors are very complex systems whose responses depend on thousands of input parameters (i.e., nuclides, reaction channels, energy, ...); moreover, reactor physics is in general concerned with integral quantities that can be considered linear with respect to the real and/or adjoint neutron fluxes, such as neutron multiplication factor, reactivity worths and neutron lifetimes [Gandini, 1967; Lewins, 1987]. Thus, linearity assumption is valid for calculating the sensitivity of reactor criticality safety parameters to cross sections, average number of emitted neutrons and average fission spectra. Therefore, the methodologies implemented in SUMMON, the sensitivity and uncertainty system developed in this Thesis, are based on local analysis.

The methods used by different codes/tools to perform sensitivity and uncertainty analyses during the course of this Thesis will be briefly described hereunder, while a detailed description of the methodologies implemented in SUMMON is provided in Chapter 5.

4.2. Sensitivity analyses

4.2.1. Deterministic methods

4.2.1.1. 1st order Perturbation Theory

First order Perturbation Theory [Cacuci, 2003] is a local expansion-based method. Let R be the response function of a system that satisfies $R = f(\alpha_1, \alpha_2, \dots, \alpha_k)$, where the true values of the parameters $(\alpha_1, \alpha_2, \dots, \alpha_k)$ are unknown, but their nominal values $(\alpha_1^0, \alpha_2^0, \dots, \alpha_k^0)$ are known together with their uncertainties $(\delta\alpha_1, \delta\alpha_2, \dots, \delta\alpha_k)$. The nominal parameters α_i^0 are usually taken to be the expected parameter values and their uncertainties $\delta\alpha_i$ given as standard deviation. Then, the true value of the parameters can be expressed as:

$$(\alpha_1, \alpha_2, \dots, \alpha_k) = (\alpha_1^0, \alpha_2^0, \dots, \alpha_k^0) + (\delta\alpha_1, \delta\alpha_2, \dots, \delta\alpha_k) = \alpha^0 + \delta\alpha \quad (4.1)$$

Writing the response R as a function of Eq. 4.1 and expanding using a Taylor series around the mean value α^0 , retaining the terms up to the n^{th} order in the variations $\delta\alpha_i$ around α_i^0 , yields:

$$\begin{aligned}
R(\alpha_1, \dots, \alpha_k) &\equiv R(\alpha_1^0 + \delta\alpha_1, \dots, \alpha_k^0 + \delta\alpha_k) \\
&= R(\alpha^0) + \sum_{i_1=1}^k \left(\frac{\partial R}{\partial \alpha_{i_1}} \right)_{\alpha_0} \delta\alpha_{i_1} + \frac{1}{2} \sum_{i_1, i_2=1}^k \left(\frac{\partial^2 R}{\partial \alpha_{i_1} \partial \alpha_{i_2}} \right)_{\alpha_0} \delta\alpha_{i_1} \delta\alpha_{i_2} \\
&+ \dots + \frac{1}{n!} \sum_{i_1, i_2, \dots, i_n=1}^k \left(\frac{\partial^n R}{\partial \alpha_{i_1} \partial \alpha_{i_2} \dots \partial \alpha_{i_n}} \right)_{\alpha_0} \delta\alpha_{i_1} \delta\alpha_{i_2} \dots \delta\alpha_{i_n}
\end{aligned} \tag{4.2}$$

Using Eq. 4.2, the various moments of the random variable $R(\alpha_1, \dots, \alpha_k)$, such as the mean value, the variance, etc., can be calculated. However, for large complex systems with many parameters, it is impractical to consider the non-linear terms (i.e., interactions between parameters). Thus, assuming linearity (truncating to the first order term of the expansion), the response function becomes:

$$R(\alpha_1, \dots, \alpha_k) = R(\alpha^0) + \sum_{i_1=1}^k \left(\frac{\partial R}{\partial \alpha_{i_1}} \right)_{\alpha_0} \delta\alpha_{i_1} = R^0 + \sum_{i_1=1}^k S_i \delta\alpha_{i_1} \tag{4.3}$$

where $R^0 \equiv R(\alpha^0)$ and $S_i \equiv (\partial R / \partial \alpha_i)$ is the sensitivity of the response to the parameter α_i .

This approach is valid for deriving sensitivities for a response whose dependence on α_i is only direct (e.g., effective neutron multiplication factor sensitivities).

4.2.1.2. Generalized Perturbation Theory

The effective neutron multiplication factor is not the only system response of interest in reactor sensitivity studies. In general [Cacuci, 2017], a perturbation $\delta\alpha_i$ would perturb a response $R(\alpha_1, \dots, \alpha_k, \varphi)$ such that the first order response perturbation $\delta R(\alpha_1, \dots, \alpha_k, \varphi)$, would take on the following expression:

$$\delta R = \frac{\partial R(\alpha_1, \dots, \alpha_k, \varphi)}{\partial \alpha_{i_1}} \delta\alpha_{i_1} + \frac{\partial R(\alpha_1, \dots, \alpha_k, \varphi)}{\partial \varphi} \delta\varphi \tag{4.4}$$

The first term of Eq. 4.4 can be computed using 1st order Perturbation Theory described in Section 4.2.1.1. However, the second term, the so-called indirect term, needs to satisfy a strict orthogonality condition [Cacuci, 2017]:

$$\left\langle \varphi, \frac{\partial R(\alpha_1, \dots, \alpha_k, \varphi)}{\partial \varphi} \right\rangle = 0 \tag{4.5}$$

Responses that satisfy Eq. 4.5 are called GPT-allowable responses and the linear perturbation methodology used to calculate the effects of perturbations $\delta\alpha_i$ on those responses is called

Generalized Perturbation Theory (GPT). With GPT, sensitivities of effective delayed neutron fraction, effective neutron generation time and reactivity worth can be derived. However, GPT requires generalized solutions that are more difficult to compute, due to the indirect term.

4.2.2. Stochastic methods

4.2.2.1. Sobol's method

According to Sobol's analysis of variance [Sobol', 2001], given a model expressed as a function $R = f(x)$, where $x = [x_1, x_2, \dots, x_n]$ is a vector of n uncorrelated random variables, the response function can be decomposed as:

$$f(x) = f_0 + \sum_i f_i(x_i) + \sum_{i < j} f_{ij}(x_i, x_j) + \dots + f_{1,2,\dots,n}(x_1, x_2, \dots, x_n) \quad (4.6)$$

where the terms in Eq. 4.6 meet the following condition:

$$\int_0^1 f_{i_1 \dots i_s}(x_{i_1}, \dots, x_{i_s}) dx_k = 0 \quad \text{for } k = i_1, \dots, i_s \quad (4.7)$$

which means that all terms in Eq. 4.6 are orthogonal and can be expressed as integrals of $f(x)$.

Assuming that $f(x)$ is square integrable, then Eq. 4.6 can be squared and integrated to get:

$$\int f^2(x) dx - f_0^2 = \sum_{s=1}^n \sum_{i_1 < \dots < i_s} \int f_{i_1 \dots i_s}^2 dx_{i_1} \dots dx_{i_s} \quad (4.8)$$

The left hand side of the Eq. 4.8 is equal to the variance of y and the right hand side represents the decomposed variance terms, which leads to:

$$V_R = \sum_{i=1}^n V_i + \sum_{i < j} V_{ij} + \dots + V_{1,2,\dots,n} \quad (4.9)$$

where V_i represents the response marginal variance, taken over all possible values of x_i , of the conditional mean $E[y|x_i]$, over all factors but x_i :

$$V_i = V_{x_i}(E[R|x_i]) \quad (4.10)$$

and the contribution of the interaction between x_i and x_j to the variance of the response is given by:

$$V_{ij} = V_{x_i, x_j}(E[R|x_i, x_j]) - V_{x_i}(E[R|x_i]) - V_{x_j}(E[R|x_j]) \quad (4.11)$$

The ratios:

$$S_{i,\dots,j} = \frac{V_{i,\dots,j}}{V_R} \quad (4.12)$$

are the global sensitivity indices [Sobol', 2001]. Finally, introducing these indices in Eq. 4.9:

$$\sum_{i=1}^n S_i + \sum_{i<j}^n S_{ij} + \dots + S_{1,2,\dots,n} = 1 \quad (4.13)$$

where $S_i = \frac{V_i}{V_R}$ is the individual sensitivity index of x_i (equivalent to the sensitivity derived using 1st order Perturbation Theory in Section 4.2.1.1). The total effect sensitivity index S_{T_i} , that provides the individual contribution plus all high order effects of x_i , is:

$$S_{T_i} = S_i + \sum_{i \neq j}^n S_{ij} + \dots + S_{1,\dots,i,\dots,n} \quad (4.14)$$

4.3. Uncertainty quantification

4.3.1. Deterministic methods

According to the ‘‘Propagation of Moments’’ method formulated in Ref. [Cacuci, 2003], the variance of the response function derived using 1st order Perturbation Theory (Eq. 4.3) can be obtained propagating the second order moment, μ_2 , as follows:

$$\begin{aligned} \mu_2(R) &= \text{var}(R) = E[(R - R^0)^2] = \int \left(\sum_{i=1}^k S_i \delta \alpha_i \right)^2 p(\alpha_1, \dots, \alpha_k) \delta \alpha_1 \delta \alpha_2 \dots \delta \alpha_k = \\ &= \sum_{i=1}^k S_i^2 \int_{S_\alpha} (\delta \alpha_i)^2 p(\alpha_1, \dots, \alpha_k) \delta \alpha_1 \delta \alpha_2 \dots \delta \alpha_k + 2 \sum_{i \neq j=1}^k S_i S_j \int_{S_\alpha} (\delta \alpha_i)(\delta \alpha_j) p(\alpha_1, \dots, \alpha_k) \delta \alpha_1 \delta \alpha_2 \dots \delta \alpha_k = \\ &= \sum_{i=1}^k S_i^2 \text{var}(\alpha_i) + 2 \sum_{i \neq j=1}^k S_i S_j \text{cov}(\alpha_i, \alpha_j) \end{aligned} \quad (4.15)$$

Eq. 4.15 can be written in matrix form as:

$$\text{var}(R) = S V_\alpha S^T \quad (4.16)$$

where V_α is the covariance matrix for the parameters $(\alpha_1, \dots, \alpha_k)$. Eq. 4.16 is commonly referred as the ‘‘Sandwich Rule’’.

4.3.2. Stochastic methods

Random sampling is a stochastic methodology where variables with uncertainties, considered as random variables, are sampled using mean values and covariance matrices with their associated probability distribution function. The random draws are fed into the mathematical model or code that derives the response functions studied. In this way, uncertainties are propagated to response functions due to the variation of system parameters [Díez, 2014]. This process is repeated a large number of times until statistical convergence of the response function is obtained (Figure 9). Then, the total uncertainty in the response function due to the variables' uncertainties can be quantified using statistical analysis.

This technique can also be used to study the individual effect of each system parameter and their contribution to the total uncertainty by sampling one-by-one the parameters or employing Sobol's method (see Section 4.2.2.1) with an extension of the theory to take into account correlated input parameters [Mara and Tarantola, 2012].

Figure 9. Random sampling scheme [Díez, 2014]

Part III

Developments & Applications

Chapter 5

Sensitivity and Uncertainty Methodology for MONte carlo codes

Abstract – Accurate and reliable tools for sensitivity analysis and uncertainty quantification are needed to estimate the uncertainties in key reactor parameters (k_{eff} , β_{eff} , Λ_{eff} , safety coefficients, ...) and to identify possible nuclear data weaknesses. Sensitivity and Uncertainty Methodology for MONte carlo codes (SUMMON) described in this chapter, has been developed to calculate the sensitivities of the criticality safety parameters to nuclear data as well as their uncertainties due to uncertainties in nuclear data, addressing limitations of existing tools. Furthermore, SUMMON has been validated using integral experiments from public databases and verified against well-consolidated codes.

This chapter shows, partially or completely, works already presented in the following references:

- International Conference Proceeding [Romojaro et al., 2017a]
- CHANDA Deliverable D9.5 [Mills, 2018]
- International Conference Proceeding [Romojaro et al., 2018a]
- International Journal Article [Grasso et al., 2018]
- International Journal Article [Romojaro et al., 2019]

5.1. Introduction

Numerous efforts are being made nowadays to address the increasing demand from nuclear research institutions, industry and regulators to support calculations of best-estimate predictions with their confidence bounds [Ivanov et al., 2013] and to address the nuclear data needs for the design and safety analysis of Advanced Fast Reactors and Advanced Fuel Cycle Scenarios. In nuclear reactor design the uncertainties mainly come from material properties, fabrication

tolerances, operative conditions, simulation tools and nuclear data. Furthermore, the uncertainty in nuclear data is one of the most important sources of uncertainty in reactor physics simulations [Kodeli, 2007]. Hence, accurate and reliable tools for sensitivity analysis and uncertainty quantification are needed to estimate the uncertainties in key reactor parameters (effective neutron multiplication factor, k_{eff} , effective delayed neutron fraction, β_{eff} , effective neutron generation time, Λ_{eff} , safety coefficients, ...) and to identify possible nuclear data weaknesses. Tools that can calculate the sensitivity of a response to nuclear data and/or the uncertainty of a response due to uncertainties in nuclear data are available, however they are affected by several limitations, as can be seen in Table 2 where a summary of existing state-of-the-art codes is presented.

Table 2. Summary of existing state-of-the-art tools for S/U analysis

Name	Institution	Sensitivity method	Uncertainty method	Limitation
SCALE [Rearden and Jessee, 2018]	ORNL (USA)	1 st PT, EGPT, GPT, IFP, CLUTCH	Sandwich, Sampling	Limited number of available nuclear data libraries processed to AMPX format
MCNP [Werner, 2017]	LANL (USA)	Differential operator, IFP	Sandwich	Sensitivity and uncertainty analysis of k_{eff} only
SERPENT [Leppänen et al., 2015]	VTT (Finland)	IFP, GPT, XGPT	-	User selection of isotope and reaction channels to be included in the analysis. No UQ capabilities
SUSD3D [Kodeli and Slavic, 2017]	JSI (Slovenia)	1 st PT	Sandwich	MG nuclear data
ERANOS [Rimpault, 2002]	CEA (France)	1 st PT, EGPT, GPT, IFP, CLUTCH	Sandwich	JEFF-3.1 MG nuclear data library only
SANDY [Fiorito et al., 2017]	SCK • CEN (Belgium)	Sobol	Sampling	Complexity of the system analysed due to required number of simulations
TMC [Koning and Rochman, 2008]	NRG (Netherlands)	-	Sampling	Complexity of the system analysed due to required number of simulations. No sensitivity capabilities
NUDUNA [Buss et al., 2011]	AREVA (Germany)	-	Sampling	Complexity of the system analysed due to required number of simulations. No sensitivity capabilities
XSUSA [Bostelmann et al., 2015]	GRS (Germany)	Multiple Squared Correlation Coefficient	Sampling	Complexity of the system analysed due to required number of simulations. MG nuclear data
NUSS-RF [Zhu et al., 2015]	PSI (Switzerland)	Sobol	Sampling	Complexity of the system analysed due to required number of simulations

Sensitivity and Uncertainty Methodology for MONte carlo codes (SUMMON) has been conceived as a tool to perform complete automated sensitivity and uncertainty analyses of the most relevant criticality safety parameters of detailed complex reactor designs from the neutronic point of view, i.e., k_{eff} , β_{eff} , Λ_{eff} and reactivity coefficients, using state-of-the-art nuclear data libraries and covariances.

SUMMON is based on the use of the KSEN card of the MCNP code [Werner, 2017], taking advantage of MCNP parallel computing implementation and allowing the use of any neutron induced nuclear data library, though any code that can calculate the energy dependent sensitivity of k_{eff} with respect to cross section changes can be used. Moreover, any covariance matrix can be used to propagate the uncertainties.

5.2. Theory

5.2.1. Sensitivity analysis

The methods implemented in the KSEN card of MCNP to calculate the sensitivity coefficients are based upon linear-perturbation theory using adjoint weighting. The adjoint weighting is performed in a forward calculation by means of the Iterated Fission Probability methodology [Kiedrowski et al., 2011; Kiedrowski and Brown, 2013; Nauchi and Kameyama, 2010], which is based on the interpretation of the adjoint flux as the neutron importance function, also called iterated fission probability, originally formulated by Hurwitz [Hurwitz, 1964]. The theory for the derivation of the sensitivity coefficients is presented below.

5.2.1.1. Eigenvalue sensitivity coefficients

Let the Boltzmann transport equation be written in the form:

$$[A - \lambda B]\phi = 0 \quad (5.1)$$

where ϕ is the neutron flux, λ represents the eigenvalues where the largest eigenvalue is $1/k_{eff}$, A is the operator that represents the scattering and total interactions terms and B is the operator that represents the fission term.

A perturbation in the transport operators and the eigenvalues can be defined as:

$$\begin{aligned} A' &= A + \partial A \\ B' &= B + \partial B \\ \lambda' &= \lambda + \partial \lambda \end{aligned} \quad (5.2)$$

where ∂A and ∂B represent small linear perturbations in the transport operators and $\partial \lambda$ represents the resulting change in the eigenvalues. The perturbed neutron transport equation can be written as:

$$[A' - \lambda' B']\phi' = 0 \quad (5.3)$$

The equation adjoint to Eq. 5.1 is:

$$[A^* - \lambda B^*]\phi^* = 0 \quad (5.4)$$

where ϕ^* is the adjoint flux and A^* and B^* are the adjoint operators.

Multiplying Eq. 5.3 by ϕ^* , integrating over all phase space and expanding in terms of Eq. 5.2 results in:

$$\langle \phi^*, (A - \lambda B + \partial A - \lambda \partial B - \partial \lambda B - \partial \lambda \partial B) \phi' \rangle = 0 \quad (5.5)$$

Using the adjoint properties and Eq. 5.4 yields:

$$\langle \phi^*, (\partial A - \lambda \partial B - \partial \lambda B - \partial \lambda \partial B) \phi' \rangle = 0 \quad (5.6)$$

Ignoring the second order perturbation term (i.e., $\partial \lambda \partial B$) and assuming that perturbations in the transport operator do not cause significant perturbations in the flux ($\phi' = \phi$), the eigenvalue perturbation becomes:

$$\frac{\partial \lambda}{\lambda} = \frac{\langle \phi^*, (\partial A - \lambda \partial B) \phi \rangle}{\langle \phi^*, (\lambda B) \phi \rangle} \quad (5.7)$$

The sensitivity of k to a change in some nuclear data α , which can be a cross section, the fission neutron multiplicity, ν , or the fission neutron spectrum, χ , is defined as:

$$S_{k,\alpha} = \frac{\alpha}{k} \frac{\partial k}{\partial \alpha} \quad (5.8)$$

Therefore, considering that $\lambda = 1/k$, where $k = k_{eff}$, and considering Eq. 5.7 and Eq. 5.8, the sensitivity coefficient can be expressed as:

$$S_{k_{eff},\alpha} = -\frac{\alpha}{\partial \alpha} \frac{\langle \phi^*, \left(\partial A - \frac{1}{k_{eff}} \partial B \right) \phi \rangle}{\langle \phi^*, \left(\frac{1}{k_{eff}} B \right) \phi \rangle} \quad (5.9)$$

As seen from Eq. 5.9, there are four adjoint weighting tallies (i.e., parameters to be scored in the Monte Carlo calculations), three involving scattering, total interactions and fission in the numerator and one for the fission in the denominator. The adjoint weighted tallies are computed using the IFP methodology, which interprets the adjoint function as the expected population of neutrons present in the system during some future generation that are descendants of the original event. In MCNP, the active generations are grouped into C contiguous blocks with index c of fixed size. In the first cycle within the block, original (non-adjoint-weighted) contributions, T_q , of tallies are evaluated and stored (the variables on the right side of $\langle \cdot, \cdot \rangle$), and the neutrons are tagged with index q (the total number of these indices within a block is Q). That way, it is known which neutron is associated with which contribution. The index q is distinct from the history index because whenever a neutron history branches, such as in an (n,2n) reaction or when an implicit capture event creates a fission neutron and the original neutron continues, a new index is needed.

These tags are inherited by subsequent progeny within the block of generations. In the final cycle within the block, fission neutron production estimates, R_q , are made and summed for all neutrons with the same tag and multiplied by the associated contributions T_q to obtain a score for the adjoint-weighted tally.

Once the asymptotic populations R_q are known from the forward simulation, the adjoint-weighted estimates of the numerator for block c , $N^{(c)}$, and the corresponding denominator, $D^{(c)}$, can be found by:

$$N^{(c)} = \frac{1}{Q} \sum_{q=1}^Q R_q T_q ; \quad D^{(c)} = \frac{1}{Q} \sum_{q=1}^Q R_q \quad (5.10)$$

Therefore, the sensitivity coefficient for block c is:

$$S_{k_{\text{eff}}, \alpha}^{(c)} = \frac{N^{(c)}}{D^{(c)}} \quad (5.11)$$

Finally, the sensitivity coefficient is calculated as an average over the C blocks, so:

$$S_{k_{\text{eff}}, \alpha} = \frac{1}{C} \sum_{c=1}^C S_{k_{\text{eff}}, \alpha}^{(c)} \quad (5.12)$$

The standard deviation of the sensitivity coefficients in MCNP is calculated using sample statistics as in any other tally.

5.2.1.2. Eigenvalue-difference response sensitivity coefficients

The methodology implemented in SUMMON's S/U calculation code, SUMMONR, to derive the sensitivity coefficients of a reactivity response is based on the eigenvalue definition of reactivity, which is equivalent to applying Equivalent Generalized Perturbation Theory (EGPT) [Gandini et al., 1986] in the case of reactivity responses. This methodology is also employed by the TSAR module of the SCALE system [Rearden and Jessee, 2018; Williams, 2007]. As discussed in Ref. [Gandini et al., 1986], an alternative formulation based on Generalized Perturbation Theory (GPT) exists [Greenspan, 1982], however, GPT requires generalized solutions that are more difficult to compute (see Section 4.2.1.2) and not available in all Monte Carlo codes. Therefore, the eigenvalue-difference approach is more convenient and has been selected for SUMMONR. This approach is derived in the lines below.

Let the system be initially in a defined state 1 with an eigenvalue λ_1 . The reactivity ρ for state 1 is:

$$\rho_1 = 1 - \lambda_1 \quad (5.13)$$

A perturbation in the system, such as a change in the fuel temperature, coolant density, a movement of the control rods, etc., transforms the original system in a new configuration designated as state 2 with an eigenvalue:

$$\lambda_2 = \lambda_1 + \Delta\lambda_{1 \rightarrow 2} \quad (5.14)$$

and a reactivity of:

$$\rho_2 = 1 - \lambda_2 \quad (5.15)$$

The change in reactivity (reactivity response $\rho_{1 \rightarrow 2}$) associated with the change in the state of the system can be defined as:

$$\rho_{1 \rightarrow 2} = \rho_2 - \rho_1 = \lambda_1 - \lambda_2 \quad (5.16)$$

with a statistical error due to Monte Carlo calculations equal to:

$$std_{\rho_{1 \rightarrow 2}}^2 \approx \left(\frac{\partial \rho_{1 \rightarrow 2}}{\partial \lambda_1} \right)^2 std_{\lambda_1}^2 + \left(\frac{\partial \rho_{1 \rightarrow 2}}{\partial \lambda_2} \right)^2 std_{\lambda_2}^2 = \left(\frac{1}{k_1} \right)^2 std_{k_1}^2 + \left(\frac{1}{k_2} \right)^2 std_{k_2}^2 \quad (5.17)$$

where std_{k_1} and std_{k_2} are statistical errors of the nominal and perturbed neutron multiplication factors respectively. It was assumed that their possible correlations, result of using the same models and methods in the corresponding Monte Carlo transport calculations, can be considered negligible. This assumption is reasonable as the covariance is limited according to the Schwartz inequality and reliable stochastic transport calculations are usually performed:

$$|cov_{k_1, k_2}| \leq std_{k_1} std_{k_2} \quad (5.18)$$

Then, the statistical error of $\rho_{1 \rightarrow 2}$ is bound as follows and can be controlled by the precision selected by the user:

$$\begin{aligned} std_{\rho_{1 \rightarrow 2}}^2 &\leq \left(\frac{\partial \rho_{1 \rightarrow 2}}{\partial k_1} \right)^2 std_{k_1}^2 + \left(\frac{\partial \rho_{1 \rightarrow 2}}{\partial k_2} \right)^2 std_{k_2}^2 + 2 \left(\frac{\partial \rho_{1 \rightarrow 2}}{\partial k_1} \right) \left(\frac{\partial \rho_{1 \rightarrow 2}}{\partial k_2} \right) std_{k_1} std_{k_2} \\ std_{\rho_{1 \rightarrow 2}}^2 &\leq \left[\left| \frac{\partial \rho_{1 \rightarrow 2}}{\partial k_1} \right| std_{k_1} + \left| \frac{\partial \rho_{1 \rightarrow 2}}{\partial k_2} \right| std_{k_2} \right]^2 \\ std_{\rho_{1 \rightarrow 2}} &\leq \left| \frac{\partial \rho_{1 \rightarrow 2}}{\partial k_1} \right| std_{k_1} + \left| \frac{\partial \rho_{1 \rightarrow 2}}{\partial k_2} \right| std_{k_2} = \frac{1}{k_1^2} std_{k_1} + \frac{1}{k_2^2} std_{k_2} \end{aligned} \quad (5.19)$$

Note that previous expression refers solely to the propagation of statistical uncertainties on the reactivity response. In the remainder of this Thesis, the symbol std will refer to the estimated standard deviation in a final response due to statistical errors in the parameters from which it was calculated, quantifying the impact of statistical fluctuations. It rules out any risk of confusion with the estimated variance in a final response due to the propagation of nuclear data uncertainties.

The relative sensitivity coefficient for the reactivity response is:

$$S_{\rho_{1 \rightarrow 2}, \alpha} = \frac{\alpha}{\rho_{1 \rightarrow 2}} \frac{\partial \rho_{1 \rightarrow 2}}{\partial \alpha} \quad (5.20)$$

Therefore, introducing Eq. 5.16 in Eq. 5.17, the relative sensitivity coefficient of the reactivity response $\rho_{1 \rightarrow 2}$ is:

$$S_{\rho_{1 \rightarrow 2}, \alpha} = \frac{\alpha}{\rho_{1 \rightarrow 2}} \left(\frac{\partial \lambda_1}{\partial \alpha} - \frac{\partial \lambda_2}{\partial \alpha} \right) = \frac{\lambda_1 S_{1, \alpha} - \lambda_2 S_{2, \alpha}}{\rho_{1 \rightarrow 2}} \quad (5.21)$$

and the standard deviation, std , can be derived from Eq. 5.19:

$$S_{\rho_{1 \rightarrow 2}, \alpha} = f(\lambda_1, \lambda_2, S_1, S_2) = f(k_1, k_2, S_1, S_2) \quad (5.22)$$

$$\begin{aligned} std_{S_{\rho_{1 \rightarrow 2}, \alpha}}^2 &= \left(\frac{\partial S_{\rho_{1 \rightarrow 2}, \alpha}}{\partial k_1} \right)^2 std_{k_1}^2 + \left(\frac{\partial S_{\rho_{1 \rightarrow 2}, \alpha}}{\partial k_2} \right)^2 std_{k_2}^2 + \left(\frac{\partial S_{\rho_{1 \rightarrow 2}, \alpha}}{\partial S_1} \right)^2 std_{S_1}^2 + \left(\frac{\partial S_{\rho_{1 \rightarrow 2}, \alpha}}{\partial S_2} \right)^2 std_{S_2}^2 \\ &+ 2 \left(\frac{\partial S_{\rho_{1 \rightarrow 2}, \alpha}}{\partial k_1} \right) \left(\frac{\partial S_{\rho_{1 \rightarrow 2}, \alpha}}{\partial k_2} \right) c_{k_1 k_2} std_{k_1} std_{k_2} + 2 \left(\frac{\partial S_{\rho_{1 \rightarrow 2}, \alpha}}{\partial S_1} \right) \left(\frac{\partial S_{\rho_{1 \rightarrow 2}, \alpha}}{\partial S_2} \right) c_{S_1 S_2} std_{S_1} std_{S_2} \\ &+ 2 \left(\frac{\partial S_{\rho_{1 \rightarrow 2}, \alpha}}{\partial k_1} \right) \left(\frac{\partial S_{\rho_{1 \rightarrow 2}, \alpha}}{\partial S_1} \right) c_{k_1 S_1} std_{k_1} std_{S_1} + 2 \left(\frac{\partial S_{\rho_{1 \rightarrow 2}, \alpha}}{\partial k_2} \right) \left(\frac{\partial S_{\rho_{1 \rightarrow 2}, \alpha}}{\partial S_2} \right) c_{k_2 S_2} std_{k_2} std_{S_2} \\ &+ 2 \left(\frac{\partial S_{\rho_{1 \rightarrow 2}, \alpha}}{\partial k_1} \right) \left(\frac{\partial S_{\rho_{1 \rightarrow 2}, \alpha}}{\partial S_2} \right) c_{k_1 S_2} std_{k_1} std_{S_2} + 2 \left(\frac{\partial S_{\rho_{1 \rightarrow 2}, \alpha}}{\partial k_2} \right) \left(\frac{\partial S_{\rho_{1 \rightarrow 2}, \alpha}}{\partial S_1} \right) c_{k_2 S_1} std_{k_2} std_{S_1} \end{aligned} \quad (5.23)$$

$$\begin{aligned} std_{S_{\rho_{1 \rightarrow 2}, \alpha}}^2 &= \left(\frac{k_2(S_1 - S_2)}{(k_2 - k_1)^2} \right)^2 std_{k_1}^2 + \left(\frac{k_1(S_2 - S_1)}{(k_2 - k_1)^2} \right)^2 std_{k_2}^2 + \left(\frac{k_2}{k_2 - k_1} \right)^2 std_{S_1}^2 \\ &+ \left(\frac{k_1}{k_1 - k_2} \right)^2 std_{S_2}^2 + 2 \frac{k_2^2(S_1 - S_2)}{(k_2 - k_1)^3} c_{k_1 S_1} std_{k_1} std_{S_1} \\ &+ 2 \frac{k_1^2(S_1 - S_2)}{(k_2 - k_1)^3} c_{k_2 S_2} std_{k_2} std_{S_2} \end{aligned} \quad (5.24)$$

Eq. 5.24 represents the standard deviation of the reactivity response sensitivity coefficient due to the propagation of the statistical uncertainties std in the parameters k_1 , k_2 , S_1 and S_2 . Correlations between both states of the system (i.e., $c_{k_1 k_2}$, $c_{S_1 S_2}$, $c_{k_1 S_2}$ and $c_{k_2 S_1}$) can be considered negligible due to the stochastic nature of Monte Carlo calculations. On the other hand, correlations between the eigenvalue and the sensitivities of a state, $c_{k_1 S_1}$ and $c_{k_2 S_2}$, cannot be neglected since they are calculated in a single calculation using the same particle histories. However, this correlation is not easily determined so, in order to be conservative, SUMMON assumes full positive or negative correlations depending on the case, therefore maximizing the standard deviation of the reactivity response sensitivity coefficient.

5.2.1.3. Effective delayed neutron fraction sensitivity coefficients

According to Keepin [Keepin, 1965], the effective delayed neutron fraction, β_{eff} , can be defined as the ratio between the adjoint weighted delayed ($P_{d,eff}$) and total (P_{eff}) neutron production:

$$\beta_{eff} = \frac{P_{d,eff}}{P_{eff}} \quad (5.25)$$

with:

$$P_{eff} = \int \phi^*(\vec{r}, E', \Omega') \chi(E') \nu(E) \Sigma_f(\vec{r}, E) \phi(\vec{r}, E, \Omega) \partial E \partial \Omega \partial E' \partial \Omega' \partial \vec{r} \quad (5.26)$$

$$P_{d,eff} = \int \phi^*(\vec{r}, E', \Omega') \chi_d(E') \nu_d(E) \Sigma_f(\vec{r}, E) \phi(\vec{r}, E, \Omega) \partial E \partial \Omega \partial E' \partial \Omega' \partial \vec{r} \quad (5.27)$$

where $\chi(E')$ is the energy spectrum of the generated fission neutrons, $\nu(E)$ is the average neutron multiplicity per fission ($\chi_d(E')$ and $\nu_d(E)$ are the same quantities defined before but for delayed neutrons) and $\Sigma_f(\vec{r}, E)$ is the macroscopic fission cross section of the material at position $\vec{r}$.

Eq. 5.25 can be rewritten as:

$$\beta_{eff} = \frac{P_{d,eff}}{P_{eff}} = 1 - \frac{P_{p,eff}}{P_{eff}} \cong 1 - \frac{k_p}{k_{eff}} \quad (5.28)$$

where $P_{p,eff}$ is the adjoint weighted prompt neutron production and k_p is the effective multiplication factor taking into account the prompt neutrons only. The formulation used to calculate β_{eff} in Eq. 5.28 is commonly known as the prompt method and is based on Bretscher's approximation [Bretscher, 1997; Meulekamp and Van der Marck, 2006], which assumes: i) the shape of χ is almost equal to that of χ_p ; and ii) ϕ and ϕ^* for a reactor with $\chi = \chi_p$ and $\nu = \nu_p$ have the same shapes as for the original system with χ and ν .

The statistical error of β_{eff} due to the statistical nature of the Monte Carlo transport calculations used to compute the effective and prompt neutron multiplication factors can be estimated from the propagation of error expressions, assuming that the correlation between the both factors is negligible (Eq. 5.17), as:

$$std_{\beta_{eff}}^2 \approx \left(\frac{\partial \beta_{eff}}{\partial k_{eff}} \right)^2 std_{k_{eff}}^2 + \left(\frac{\partial \beta_{eff}}{\partial k_p} \right)^2 std_{k_p}^2 = \left(\frac{k_p}{k_{eff}^2} \right)^2 std_{k_{eff}}^2 + \left(\frac{1}{k_{eff}} \right)^2 std_{k_p}^2 \quad (5.29)$$

The sensitivity of β_{eff} to changes in nuclear data α can be easily calculated following Eq. 5.28:

$$\begin{aligned}
S_{\beta_{eff},\alpha} &= \frac{\alpha}{\beta_{eff}} \frac{\partial \beta_{eff}}{\partial \alpha} = \frac{\alpha}{\beta_{eff}} \frac{\partial}{\partial \alpha} \left(1 - \frac{k_p}{k_{eff}} \right) = \frac{\alpha}{\beta_{eff}} \left(-\frac{1}{k_{eff}} \frac{\partial k_p}{\partial \alpha} + \frac{k_p}{k_{eff}^2} \frac{\partial k_{eff}}{\partial \alpha} \right) \\
&= \frac{k_p}{k_{eff} - k_p} \left(\frac{\alpha}{k_{eff}} \frac{\partial k_{eff}}{\partial \alpha} - \frac{\alpha}{k_p} \frac{\partial k_p}{\partial \alpha} \right) = \frac{k_p}{k_{eff} - k_p} (S_{k_{eff},\alpha} - S_{k_p,\alpha}) \quad (5.30)
\end{aligned}$$

where $S_{k_{eff},\alpha}$ and $S_{k_p,\alpha}$ correspond to the relative sensitivities to nuclear data of k_{eff} and k_p , which can be obtained using the KSEN card of MCNP and will consequently be affected by statistical errors. In MCNP, k_p and $S_{k_p,\alpha}$ are derived using the same methodology as in k_{eff} and $S_{k_{eff},\alpha}$ calculations, but deactivating the sampling of delayed fission neutrons with the TOTNU card [Werner, 2017]. This option is also available in other widely used MC neutron transport codes such as SERPENT and KENO-VI from the SCALE system.

The standard deviation of $S_{\beta_{eff},\alpha}$ due to the propagation of statistical uncertainties in the parameters k_{eff} , k_p , $S_{k_{eff},\alpha}$ and $S_{k_p,\alpha}$ can be derived from Eq. 5.30, taking into account that $S_{\beta_{eff},\alpha} = f(k_{eff}, k_p, S_{k_{eff},\alpha}, S_{k_p,\alpha})$. As in the case of $std_{S_{\rho_{1 \rightarrow 2},\alpha}}$ (Eq. 5.24), correlations between the multiplication factors of two states or between their sensitivity coefficients can be neglected due to the stochastic nature of Monte Carlo calculations, while correlations between the eigenvalue and the sensitivities of a state, $c_{k_{eff}S_{k_{eff},\alpha}}$ and $c_{k_pS_{k_p,\alpha}}$, cannot be neglected since they are calculated in a single calculation. Therefore, once again, SUMMON assumes full positive or negative correlations depending on the case:

$$\begin{aligned}
std_{S_{\beta_{eff},\alpha}}^2 &\approx \left(\frac{k_p (S_{k_p,\alpha} - S_{k_{eff},\alpha})}{(k_{eff} - k_p)^2} \right)^2 std_{k_{eff}}^2 + \left(\frac{k_{eff} (S_{k_{eff},\alpha} - S_{k_p,\alpha})}{(k_{eff} - k_p)^2} \right)^2 std_{k_p}^2 + \left(\frac{k_p}{k_{eff} - k_p} \right)^2 std_{S_{k_{eff},\alpha}}^2 \\
&+ \left(\frac{k_p}{k_p - k_{eff}} \right)^2 std_{S_{k_p,\alpha}}^2 + 2 \frac{k_p^2 (S_{k_p,\alpha} - S_{k_{eff},\alpha})}{(k_{eff} - k_p)^3} c_{k_{eff}S_{k_{eff},\alpha}} std_{k_{eff}} std_{S_{k_{eff},\alpha}} \\
&- 2 \frac{k_{eff} k_p (S_{k_{eff},\alpha} - S_{k_p,\alpha})}{(k_{eff} - k_p)^3} c_{k_pS_{k_p,\alpha}} std_{k_p} std_{S_{k_p,\alpha}} \quad (5.31)
\end{aligned}$$

where $std_{S_{k_{eff},\alpha}}$ and $std_{S_{k_p,\alpha}}$ are the statistical errors of $S_{k_{eff},\alpha}$ and $S_{k_p,\alpha}$. It can be seen that the standard deviation in the sensitivities of β_{eff} can be greater than the errors in k_{eff} , k_p , $S_{k_{eff},\alpha}$ or $S_{k_p,\alpha}$ if the difference in the multiplication factors is small, therefore a great number of histories is required to obtain accurate solutions. In order to reduce statistical uncertainties, a modification of the prompt method using a scaling factor has been proposed by Chiba [Chiba, 2009]. Let us consider the transport equation at a different fictitious state, where the adjoint weighted total neutron production from Eq. 5.24 is:

$$\overline{P_{eff}} = \int \phi^*(\vec{r}, E', \Omega') (\chi(E') \nu(E) + a \chi_d(E') \nu_d(E)) \Sigma_f(\vec{r}, E) \phi(\vec{r}, E, \Omega) \partial E \partial \Omega \partial E' \partial \Omega' \partial \vec{r} \quad (5.32)$$

in which a is a scaling factor for adjusting the perturbation from the reference state.

Then, following Keepin definition of β_{eff} from Eq. 5.25 and using similar formulation and approximations made by Bretscher:

$$\beta_{eff} = \frac{P_{d,eff}}{P_{eff}} = \frac{\frac{1}{a} (\overline{P_{eff}} - P_{eff})}{P_{eff}} \cong \frac{1}{a} \left(\frac{\overline{k_{eff}}}{k_{eff}} - 1 \right) \quad (5.33)$$

and:

$$\begin{aligned} std_{\beta_{eff}}^2 &\approx \left(\frac{\partial \beta_{eff}}{\partial k_{eff}} \right)^2 std_{k_{eff}}^2 + \left(\frac{\partial \beta_{eff}}{\partial \overline{k_{eff}}} \right)^2 std_{\overline{k_{eff}}}^2 \\ &= \frac{1}{a^2} \left[\left(\frac{\overline{k_{eff}}}{k_{eff}^2} \right)^2 std_{k_{eff}}^2 + \left(\frac{1}{k_{eff}} \right)^2 std_{\overline{k_{eff}}}^2 \right] \end{aligned} \quad (5.34)$$

Using Chiba's approximation of β_{eff} , $S_{\beta_{eff}, \alpha}$ can be derived as in Eq. 5.30:

$$S_{\beta_{eff}, \alpha} = \frac{\alpha}{\beta_{eff}} \frac{\partial \beta_{eff}}{\partial \alpha} = \frac{\overline{k_{eff}}}{k_{eff} - \overline{k_{eff}}} (S_{k_{eff}, \alpha} - S_{\overline{k_{eff}}, \alpha}) \quad (5.35)$$

and the standard deviation of $S_{\beta_{eff}, \alpha}$ due to the propagation of statistical uncertainties can be obtained making analogous assumptions as in Eqs. 5.24 and 5.31:

$$\begin{aligned} std_{S_{\beta_{eff}, \alpha}}^2 &\approx \left(\frac{\overline{k_{eff}} (S_{\overline{k_{eff}, \alpha}} - S_{k_{eff}, \alpha})}{(k_{eff} - \overline{k_{eff}})^2} \right)^2 std_{k_{eff}}^2 + \left(\frac{k_{eff} (S_{k_{eff}, \alpha} - S_{\overline{k_{eff}, \alpha}})}{(k_{eff} - \overline{k_{eff}})^2} \right)^2 std_{\overline{k_{eff}}}^2 + \left(\frac{\overline{k_{eff}}}{k_{eff} - \overline{k_{eff}}} \right)^2 std_{S_{k_{eff}, \alpha}}^2 \\ &\quad + \left(\frac{\overline{k_{eff}}}{k_{eff} - \overline{k_{eff}}} \right)^2 std_{S_{\overline{k_{eff}, \alpha}}}^2 + 2 \frac{\overline{k_{eff}}^2 (S_{\overline{k_{eff}, \alpha}} - S_{k_{eff}, \alpha})}{(k_{eff} - \overline{k_{eff}})^3} c_{k_{eff} S_{k_{eff}, \alpha}} std_{k_{eff}} std_{S_{k_{eff}, \alpha}} \\ &\quad - 2 \frac{k_{eff} \overline{k_{eff}} (S_{k_{eff}, \alpha} - S_{\overline{k_{eff}, \alpha}})}{(k_{eff} - \overline{k_{eff}})^3} c_{\overline{k_{eff}} S_{\overline{k_{eff}, \alpha}}} std_{\overline{k_{eff}}} std_{S_{\overline{k_{eff}, \alpha}}} \end{aligned} \quad (5.36)$$

Chiba's modified method is superior to the prompt method in terms of reducing the statistical uncertainty of β_{eff} and its sensitivities [Iwamoto et al., 2018], as can be seen from Eqs. 5.29 and 5.34 where, if the statistical uncertainties in k_{eff} , k_p and $\overline{k_{eff}}$ are similar, $std_{\beta_{eff}}$ is smaller by a factor $|a|$ using the modified method.

However, Chiba's modified method requires in practice the use of modified nuclear data files in the calculations, where ν_d evaluated values are multiplied by $(a + 1)$ and ν_T values are adjusted accordingly (Figure 10), something which is not feasible in some Monte Carlo codes,

such as the KENO-VI MC code. Consequently, while both methods are available in SUMMON, Chiba's method will only be able to be used in conjunction with Monte Carlo codes that can employ the modified libraries in the calculations.

Figure 10. Comparison between ENDF/B-VII.0 original $^{235}\text{U } \nu_d$ and modified $^{235}\text{U } \nu_d$ for a perturbation $a = 20$

5.2.1.4. Effective neutron generation time sensitivity coefficients

The effective neutron generation time, Λ_{eff} , is defined by:

$$\Lambda_{eff} = \frac{\langle \phi^*, \frac{1}{v} \phi \rangle}{\langle \phi^*, B \phi \rangle} \quad (5.37)$$

where v is the neutron speed. Λ_{eff} can be interpreted as the reciprocal of the average neutron production probability or the average time before one neutron produces another [Lewins, 1965; Verboomen et al., 2006].

Three methods are available [Louis, 2014] for calculating Λ_{eff} :

1. the adjoint weighted method, which requires the calculation of the adjoint flux;
2. the perturbation method, which requires the calculation of a variation of reactivity due to a perturbation of the original system;
3. and the iterated fission probability method.

The approach used by SUMMON to compute the sensitivity of Λ_{eff} to changes in nuclear data α is based on the perturbation method and the IFP method, the latter of which is used by MCNP to calculate the effective neutron generation time. The first methodology has once again been discarded because it requires the use of GPT.

The perturbation method is based on Miller and Lewis first-order perturbation formula for reactivity increments [Miller and Lewis, 1993], which in the case of a $1/v$ perturbation, yields:

$$\Delta\rho = \rho_c - \rho_0 = -\frac{\langle\phi^*, \frac{c}{v}\phi\rangle}{\langle\phi^*, B\phi\rangle} \quad (5.38)$$

where ρ_c is the reactivity of the system exposed to a uniform c/v perturbation, ρ_0 is the nominal state of the system and c is the amplitude of the perturbation.

Consequently, the first order perturbation formula for the effective neutron generation time can be obtained using Eqs. 5.37 and 5.38:

$$\Lambda_{eff} = -\frac{\Delta\rho}{c} \quad (5.39)$$

To perform the perturbation, the $1/v$ insertion method [Templin, 1963] is used, in which the entire reactor is perturbed by a dilute and uniform distribution of a purely $1/v$ neutron absorber, so that [Verboomen et al., 2006]:

$$\Sigma_p(c) = \frac{c}{v} = N(c)\sigma_p = N(c)\frac{A}{v} \quad (5.40)$$

where $\Sigma_p(c)$ is the macroscopic capture cross section of the neutron absorber material, $N(c)$ is the atom density, σ_p is the microscopic cross section and A is a constant used to normalize σ_p .

Figure 11. Comparison between JEFF-3.2 ^{10}B [OECD/NEA Data Bank, 2014] and SUMMON artificial material cross sections

In other works [Bretscher, 1997; Louis, 2014], ^{10}B has been used as an absorber material to perform the perturbation, which serves as a good approximation for a purely $1/v$ absorber.

However, although this is true for thermal systems, the use of ^{10}B for fast systems has been found to yield incorrect results due to the low ^{10}B cross section in the fast energy range. Therefore, an artificial $1/v$ absorber has been created for use in SUMMON. The artificial file contains only the (n,γ) cross section normalized to ~ 5000 barn at 0.0253 eV. A comparison between the capture cross section of ^{10}B and the artificial material is shown in Figure 11.

Therefore, according to Eqs. 5.39 and 5.40, Λ_{eff} can be defined as:

$$\Lambda_{eff} = \frac{1}{A} \frac{(\rho_0 - \rho_c)}{N(c)} \quad (5.41)$$

The standard deviation due to the propagation of statistical errors in the multiplication factors can be estimated as follows:

$$\begin{aligned} std_{\Lambda_{eff}}^2 &\approx \left(\frac{\partial \Lambda_{eff}}{\partial k_0} \right)^2 std_{k_0}^2 + \left(\frac{\partial \Lambda_{eff}}{\partial k_c} \right)^2 std_{k_c}^2 \\ &= \frac{1}{(A N(c))^2} \left[\left(\frac{1}{k_0^2} \right)^2 std_{k_0}^2 + \left(\frac{1}{k_c^2} \right)^2 std_{k_c}^2 \right] \end{aligned} \quad (5.42)$$

The methodology implemented in SUMMON uses both the perturbation method and the Iterated Fission Probability method to calculate Λ_{eff} and the corresponding size of the perturbation, c , that yields the IFP Λ_{eff} estimated value. Once the size of the perturbation has been obtained, first, the sensitivity coefficients of the effective neutron multiplication factor of the perturbed system, $S_{k_c, \alpha}$, are calculated, and then the sensitivity of Λ_{eff} to changes in some nuclear data α , $S_{\Lambda_{eff}, \alpha}$, is estimated as follows:

$$\begin{aligned} S_{\Lambda_{eff}, \alpha} &= \frac{\alpha}{\Lambda_{eff}} \frac{\partial \Lambda_{eff}}{\partial \alpha} = \frac{\alpha}{\Lambda_{eff}} \frac{\partial}{\partial \alpha} \left(\frac{1}{A} \frac{(\rho_0 - \rho_c)}{N(c)} \right) = \frac{\alpha}{\Lambda_{eff} A N(c)} \frac{\partial}{\partial \alpha} \left(\frac{1}{k_c} - \frac{1}{k_0} \right) \\ &= \frac{\alpha}{\Lambda_{eff} A N(c)} \left(-\frac{1}{k_c^2} \frac{\partial k_c}{\partial \alpha} + \frac{1}{k_0^2} \frac{\partial k_0}{\partial \alpha} \right) = \frac{1}{\Lambda_{eff} A N(c)} \left(\frac{S_{k_0, \alpha}}{k_0} - \frac{S_{k_c, \alpha}}{k_c} \right) \end{aligned} \quad (5.43)$$

The standard deviation of $S_{\Lambda_{eff}, \alpha}$ due to the propagation of statistical uncertainties can be obtained using the same formulation and approximations that have been used in Eqs. 5.22, 5.31 and 5.36:

$$\begin{aligned} std_{S_{\Lambda_{eff}, \alpha}}^2 &\approx \frac{1}{(\Lambda_{eff} A N(c))^2} \left[\frac{1}{\Lambda_{eff}^2} \left(\frac{S_{k_c, \alpha}}{k_c} - \frac{S_{k_0, \alpha}}{k_0} \right)^2 std_{\Lambda_{eff}}^2 + \left(\frac{S_{k_0, \alpha}}{k_0^2} \right)^2 std_{k_0}^2 \right. \\ &\quad + \left(\frac{S_{k_c, \alpha}}{k_c^2} \right)^2 std_{k_c}^2 + \left(\frac{1}{k_0} \right)^2 std_{S_{k_0, \alpha}}^2 + \left(\frac{1}{k_c} \right)^2 std_{S_{k_c, \alpha}}^2 - 2 \frac{S_{k_0, \alpha}}{k_0^3} c_{k_0 S_{k_0, \alpha}} std_{k_0} std_{S_{k_0, \alpha}} \\ &\quad \left. + 2 \frac{1}{\Lambda_{eff}} \frac{S_{k_0, \alpha}}{k_0^2} \left(\frac{S_{k_0, \alpha}}{k_0} - \frac{S_{k_c, \alpha}}{k_c} \right) c_{k_0 \Lambda_{eff}} std_{k_0} std_{\Lambda_{eff}} \right] \end{aligned}$$

$$\begin{aligned}
& + 2 \frac{1}{\Lambda_{eff}} \frac{1}{k_0} \left(\frac{S_{k_c, \alpha}}{k_c} - \frac{S_{k_0, \alpha}}{k_0} \right) c_{S_{k_0, \alpha} \Lambda_{eff}} std_{S_{k_0, \alpha}} std_{\Lambda_{eff}} - 2 \frac{S_{k_c, \alpha}}{k_c^3} c_{k_c S_{k_c, \alpha}} std_{k_c} std_{S_{k_c, \alpha}} \\
& + 2 \frac{1}{\Lambda_{eff}} \frac{S_{k_c, \alpha}}{k_c^2} \left(\frac{S_{k_c, \alpha}}{k_c} - \frac{S_{k_0, \alpha}}{k_0} \right) c_{k_c \Lambda_{eff}} std_{k_c} std_{\Lambda_{eff}} \\
& + 2 \frac{1}{\Lambda_{eff}} \frac{1}{k_c} \left(\frac{S_{k_0, \alpha}}{k_0} - \frac{S_{k_c, \alpha}}{k_c} \right) c_{S_{k_c, \alpha} \Lambda_{eff}} std_{S_{k_c, \alpha}} std_{\Lambda_{eff}} \Big] \quad (5.44)
\end{aligned}$$

It is important to notice that in order to accurately employ this method, especially for fast systems, the use of the artificial material file is recommended. However, if the MC code utilized with SUMMON cannot use this file, ^{10}B would serve as a good approximation in Λ_{eff} and $S_{\Lambda_{eff}, \alpha}$ calculations for thermal systems.

5.2.2. Uncertainty quantification

Once the sensitivity coefficients to nuclear data have been obtained, it is possible to propagate the nuclear data uncertainties to the final responses. The relative variance of a response R (i.e., k_{eff} , β_{eff} , Λ_{eff} and reactivity coefficients) can be calculated using the “Sandwich Rule” of the “Propagation of Moments” method formulated in Section 4.3.1:

$$\sigma_R^2 = S_{R, \alpha} C_{\alpha\alpha} S_{R, \alpha}^T \quad (5.45)$$

where $C_{\alpha\alpha}$ denotes the covariance matrix for the nuclear data $(\alpha_1, \dots, \alpha_k)$ and $S_{R, \alpha}$ are the sensitivity coefficients collapsed to the same energy group structure as the covariance matrix.

Since sensitivities are affected by statistical errors due to the statistical nature of the Monte Carlo transport calculations used to compute them, it is possible to propagate the statistical errors to the estimated variance of the response due to nuclear data uncertainties. The standard deviation of the variance of a response R due to the statistical uncertainties in the sensitivities can be derived from the “Sandwich Rule” (Eq. 5.45):

$$std_{\sigma_R}^2 = std_{S_R}^2 (C_{\alpha\alpha} S_R^T)^2 + (S_R C_{\alpha\alpha})^2 std_{S_R}^2 \quad (5.46)$$

In summary, when a final response is calculated from parameters computed from Monte Carlo transport calculations (and consequently affected by the statistical nature of the stochastic method), they will be affected by two different kinds of uncertainties:

- A statistical uncertainty or error in the final response, due to the propagation of the statistical errors in the parameters from which the response is calculated. It quantifies the impact of the statistical fluctuations on the response and can be controlled by the user increasing the number of histories.

- A nuclear data propagated uncertainty in the final response, due to the propagation of the uncertainties in nuclear data (assuming nuclear data as the dominant source of input data uncertainties). Since the sensitivity coefficients used for uncertainty quantification will be also affected by statistical errors, the uncertainty in the final response due to nuclear data will be also accompanied by a statistical deviation.

When final responses are obtained from reliable stochastic transport calculations, it can be seen that the influence of the statistical errors is negligible compared to the effect of the nuclear data uncertainties. Consequently, for example in order to assess the impact of uncertainties in reactivity effects on transients driven by them, uncertainties due to nuclear data will have to be used to establish a possible range of confidence for the reactivity effects [Grasso et al., 2017].

5.3. Implementation

The SUMMON system has been written in FORTRAN 90 programming language [Adams et al., 1992] and is composed of more than 3000 lines of code divided in 17 subroutines:

- **summonr.f90** is the main program interface.
- **KSEN2sdf.f90** converts the output of the KSEN card of MCNP to sensitivity data file format.
- **reg_int.f90** calculates the energy integrated sensitivity coefficients.
- **gettida.f90** introduces time and date in the form: hh:mm:ss mm/dd/yy.
- **getexearg.f90** introduces in character string buffer the contents of the execution line message (input file name) excluding the command name.
- **allocat.f90** reads the sensitivity and covariance files in BOXER format to get the values for the allocation of matrices.
- **sdf_reader.f90** reads the sensitivity coefficients in the sensitivity data file.
- **cov_allocat.f90** allocates space in memory for the covariance matrix.
- **cov_reader.f90** reads the contents of the covariance matrix.
- **collaps.f90** collapses the sensitivity coefficients to the covariance matrix energy group structure.
- **response.f90** calculates $S_{\rho_{1 \rightarrow 2}, \alpha}$.
- **bettaeff.f90** calculates $S_{\beta_{eff}, \alpha}$ with the prompt method.

- **bettaeff2.f90** calculates $S_{\beta_{eff},\alpha}$ with Chiba's method.
- **lambda.f90** calculates $S_{\Lambda_{eff},\alpha}$.
- **srule.f90** calculates the uncertainties using the sandwich rule.
- **sdfoutline.f90** writes the results of the sensitivity analysis in an output file.
- **output.f90** writes the results of the uncertainty quantification in an output file.

Figure 12. General flow diagram of SUMMON's S/U module

In Figure 12, the general flow diagram of SUMMON is presented. First, the evaluated data files are processed with the NJOY code [Muir et al., 2016] to obtain MCNP-compatible ACE files. Any evaluated nuclear library in ENDF-6 format [Herman and Trkov, 2009] can be used. Additionally, modified nuclear data files for $S_{\beta_{eff},\alpha}$ calculations and an artificial material file for $S_{\Lambda_{eff},\alpha}$ calculations have been created (see Sections 5.2.1.3 and 5.2.1.4) and are provided to SUMMON. Then, if the parameter to be studied is the effective neutron multiplication factor, one single MCNP calculation with the KSEN card is run to obtain the sensitivity coefficients. On the other hand, two different MCNP/KSEN calculations are run, one for the nominal state and other for the perturbed state, if the sensitivity analysis of the following quantities of interest is to be performed: i) a reactivity response, corresponding to the difference in critical eigenvalues for two distinct states of a system (temperature effects, void worth, control rod worth, expansion effects, ...); ii) the effective delayed neutron fraction, corresponding to the difference in critical eigenvalues for the nominal state of the system and the system taking into account only prompt neutrons; and iii) the effective neutron generation time, corresponding to the reactivity difference

between the nominal state of the system and a perturbed state in which an artificial $1/\nu$ absorber material has been introduced in the whole system. Once the energy dependent sensitivity coefficients have been obtained the KSEN2sdf code translates the MCNP/KSEN output to sensitivity data file (.sdf) format [Rearden and Jessee, 2018]. Finally, the SUMMONR code is called to perform the sensitivity analysis of the required quantities of interest (k_{eff} , reactivity response, β_{eff} or Λ_{eff}) using the data previously produced and performs the uncertainty quantification.

State-of-the-art covariance libraries are employed by the SUMMONR code to propagate the uncertainties in k_{eff} and in the criticality safety parameters due to uncertainties in nuclear data. COMMARA-2.0 [Herman et al., 2011], SCALE6.1 [*Scale: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design*, 2011], SCALE6.2 [Rearden and Jessee, 2018] and covariance matrices from the evaluated nuclear data libraries JEFF-3.3 [Plompen, 2017], ENDF/B-VIII.0 [Brown et al., 2018] and JENDL-4.0 [Shibata et al., 2011] can be used for the uncertainty assessment. These matrices have been processed to BOXER format [Muir et al., 2016] which allows large data compression factors significantly reducing the size of the covariance files, except COMMARA-2.0 which is directly used by SUMMONR without any previous processing. Additionally, any new nuclear data library which contains covariance data can be easily processed with the NJOY code to BOXER format, thus giving SUMMONR the capability of always using state-of-the-art covariance libraries.

Another important feature of the SUMMONR code is its capability of calculating energy-dependent uncertainties. This allows identifying the specific energy regions of a nuclide and reaction channel where nuclear data uncertainties must be improved in order to reach the target accuracy for a specific application.

Although the SUMMON methodology is based on the use of MCNP to calculate the sensitivities, other codes can be used to perform this task such as KENO-VI, SERPENT, etc. The only requirement is that the group structure of the energy dependent sensitivity coefficients share some of the 308 standard groups used by SUMMONR, which have been defined to be compatible with the energy binning of COMMARA-2.0 and SCALE covariance matrices and can be found in Annex A.

5.4. Verification

In order to verify the SUMMON system and to check the quality of the written code and internal routines, as well as the applicability of the proposed methodologies, several calculations have been performed.

For the verification of the eigenvalue and eigenvalue-difference response sensitivity estimation and uncertainty quantification capabilities, SUMMON has been applied to calculate the sensitivities and uncertainties in k_{eff} and two reactivity responses, corresponding to an increase of the fuel temperature from 1200 K to 1500 K and a 20% increase of the coolant density, of the ALFRED lead-cooled fast reactor (see Chapter 2). The innovative reactor concept has been modelled at Beginning of Cycle (BoC) and nominal conditions with MCNP code and SCALE system. A detailed description of the core specifications and the model developed can be found at Refs [Grasso et al., 2018, 2017; Grasso and Mansani, 2014]. The ENDF/B-VII.0 nuclear data library [Chadwick et al., 2006] and SCALE6.1-44g ENDF/VII.0 based covariance matrix have been used with SUMMONR and the consolidated and well-validated TSUNAMI-3D MG and TSAR modules [Rearden and Jessee, 2018] of SCALE and the results obtained by both systems have been compared.

For the verification of the sensitivities estimation of the effective delayed neutron fraction and effective neutron generation time, experiments from the International Criticality Safety Benchmark Exaluation Project (ICSBEP) Handbook [OECD/NEA, 2016b] and the International Reactor Physics Experiment Evaluation (IRPhE) [OECD/NEA, 2017a] Project databases have been used to perform the S/U analyses with the ENDF/B-VII.0 library. The results obtained with SUMMONR have been compared against SUD3D, SERPENT and XSUSA codes.

However, as discussed in bibliography [Aufiero et al., 2015], one of the most severe limitations of EGPT applied to Monte Carlo simulations are statistical uncertainties. The methods implemented in SUMMONR to derive the sensitivity coefficients of the reactivity response, effective delayed neutron fraction using Bretscher's approximation and effective neutron generation time (Eqs. 5.19, 5.30 and 5.43) are equivalent to applying EGPT and are consequently affected by the same limitations. Therefore first, several calculations with MCNP/KSEN were performed in order to study the impact of statistics in the sensitivity coefficient calculations. In Figure 13 and Figure 14, the sensitivity profiles of k_{eff} to ^{239}Pu ν and $^{238}\text{U}(n,n)$ using different statistics are shown. The standard deviation of the neutron multiplication factor of the initial calculation, given in pcm (1 pcm = 10^{-5}), has been reduced from 8 pcm to 1 pcm using a higher amount of neutron histories, therefore, improving the statistics of the successive calculations.

Figure 13. k_{eff} sensitivity to $^{239}\text{Pu } \nu$ using different number of neutron histories

Small differences can be observed in the calculated sensitivity profiles of $^{239}\text{Pu } \nu$ (Figure 13), however, the impact of statistics in the ^{238}U elastic scattering cross section is very high (Figure 14). This is reflected in the $^{238}\text{U}(n,n)$ energy-integrated sensitivity coefficients presented in Table 3, where differences between the TSUNAMI-3D MG value, taken as a reference, and the MCNP/KSEN sensitivity coefficient values reduce considerably when the statistics are improved. Additionally, the statistical uncertainty of the calculated sensitivity coefficients reduces by 86% when the statistical uncertainty in k_{eff} is reduced from 8 pcm to 1 pcm.

Figure 14. k_{eff} sensitivity to $^{238}\text{U}(n,n)$ using different number of neutron histories

Table 3. Energy-integrated sensitivity coefficients of k_{eff} to $^{238}\text{U}(\text{n},\text{n})$ obtained with MCNP/KSEN

$$^{238}\text{U}(\text{n},\text{n}) - \text{STSUMANI-3D MG} = 1.3515 \cdot 10^{-2} \pm 8.1 \cdot 10^{-5}$$

k_{eff} std.	Sensitivity	Diff. (%)
8 pcm	$1.6741 \cdot 10^{-2} \pm 7.8 \cdot 10^{-5}$	23.87
4 pcm	$1.5564 \cdot 10^{-2} \pm 4.5 \cdot 10^{-5}$	15.16
2 pcm	$1.1200 \cdot 10^{-2} \pm 2.3 \cdot 10^{-5}$	17.13
1 pcm	$1.2370 \cdot 10^{-2} \pm 1.1 \cdot 10^{-5}$	8.48

The same behaviour can be observed in the sensitivity coefficients of k_{eff} to elastic and inelastic scattering cross section sensitivity profiles and statistical uncertainties of other key elements. Hence, when using the KSEN card of MCNP, it is highly recommended to perform calculations with a sufficient number of neutron histories so that the statistical uncertainty in k_{eff} is not greater than 2 pcm, in order to have a low statistical uncertainty in the sensitivity coefficients. On the other hand, achieving such statistical uncertainties might be too computationally costly depending on the application, so the user must evaluate the accuracy of the calculations when less statistics are employed. For ALFRED sensitivity calculations, CPU times on a ~2000 core cluster are presented in Table 4.

Table 4. CPU times for SCALE and MCNP sensitivity calculations

Code	Number of processors	Number of neutrons	k_{eff} std.	t (minutes)
SCALE6.1/TSUNAMI-3D MG	1*	$1.20 \cdot 10^8$	9 pcm	6120
		$6.00 \cdot 10^7$	8 pcm	330
MCNP/KSEN	64	$1.60 \cdot 10^8$	4 pcm	878
		$5.60 \cdot 10^8$	2 pcm	2793
		$2.28 \cdot 10^9$	1 pcm	13514

*Note: SCALE6.1 does not have parallel capabilities

From this point forward, all MCNP/KSEN calculations shown in this Thesis have been performed with enough particles so that a statistical error of 1 pcm in the neutron multiplication factor has been reached.

5.4.1. Eigenvalue, eigenvalue-difference sensitivities and uncertainty quantification

To ensure the consistency of the calculations, the results have been compared against sensitivity coefficients obtained by the direct perturbation method [Radulescu et al., 2008], which uses variations of nuclide density that result in small k_{eff} variations consistent with the linear perturbation approximation and allows determining the total sensitivity coefficients.

Table 5 shows the total sensitivity to the eight most relevant nuclides for ALFRED reactor (i.e., the nuclides for which k_{eff} has the highest sensitivity) obtained with both MCNP/KSEN and

SCALE/TSUNAMI-3D MG (238 energy groups) and their comparison with direct perturbation calculations. It can be seen that the MCNP and SCALE total sensitivity coefficients for the fuel materials are consistent with the direct perturbation calculations, with differences smaller than 4%, except for ^{242}Pu calculated with MCNP (6.6%).

Table 5. Total sensitivity (%/%) of the most relevant isotopes compared with direct perturbations for ALFRED

Isotope	Direct Perturbation	MCNP/KSEN		SCALE/TSUNAMI-3D MG	
		Total Sensitivity	Diff. (%)	Total Sensitivity	Diff. (%)
^{239}Pu	$4.4988 \cdot 10^{-1}$	$4.5724 \cdot 10^{-1}$	1.64	$4.4520 \cdot 10^{-1}$	1.05
^{238}U	$-1.2187 \cdot 10^{-1}$	$-1.2073 \cdot 10^{-1}$	0.94	$-1.2134 \cdot 10^{-1}$	0.44
^{241}Pu	$6.3706 \cdot 10^{-2}$	$6.4335 \cdot 10^{-2}$	0.99	$6.3264 \cdot 10^{-2}$	0.70
^{240}Pu	$3.0313 \cdot 10^{-2}$	$3.0941 \cdot 10^{-2}$	2.07	$2.9943 \cdot 10^{-2}$	1.24
^{16}O	$-3.1652 \cdot 10^{-2}$	$-3.0412 \cdot 10^{-2}$	3.92	$-3.1648 \cdot 10^{-2}$	0.01
^{56}Fe	$-2.0278 \cdot 10^{-2}$	$-2.1564 \cdot 10^{-2}$	6.34	$-1.7899 \cdot 10^{-2}$	13.29
^{242}Pu	$4.2390 \cdot 10^{-3}$	$4.5176 \cdot 10^{-3}$	6.57	$4.2049 \cdot 10^{-3}$	0.81
^{208}Pb	$7.9280 \cdot 10^{-3}$	$8.8876 \cdot 10^{-3}$	12.10	$6.8858 \cdot 10^{-3}$	15.14

Table 6. Uncertainty quantification ($\Delta k_{eff}/k_{eff}$ %) in k_{eff} for ALFRED

Quantity	SCALE	SUMMON		
		Sensitivities taken from SCALE		Sensitivities taken from MCNP
		44 groups	44 groups	44 groups 56 groups
$^{239}\text{Pu } \nu$	$0.703 \pm 5 \cdot 10^{-6}$	$0.703 \pm 6 \cdot 10^{-6}$	$0.713 \pm 2 \cdot 10^{-6}$	$0.056 \pm 2 \cdot 10^{-8}$
$^{238}\text{U } (n,n')$	$0.534 \pm 4 \cdot 10^{-4}$	$0.533 \pm 4 \cdot 10^{-4}$	$0.534 \pm 1 \cdot 10^{-5}$	$0.544 \pm 2 \cdot 10^{-5}$
$^{239}\text{Pu } (n,\gamma)$	$0.266 \pm 2 \cdot 10^{-5}$	$0.266 \pm 1 \cdot 10^{-5}$	$0.262 \pm 2 \cdot 10^{-7}$	$0.252 \pm 4 \cdot 10^{-7}$
$^{240}\text{Pu } \nu$	$0.243 \pm 5 \cdot 10^{-7}$	$0.243 \pm 7 \cdot 10^{-7}$	$0.245 \pm 3 \cdot 10^{-7}$	$0.061 \pm 2 \cdot 10^{-8}$
$^{239}\text{Pu } \chi$	$0.214 \pm 3 \cdot 10^{-6}$	$0.213 \pm 4 \cdot 10^{-6}$	$0.166 \pm 1 \cdot 10^{-6}$	$0.127 \pm 5 \cdot 10^{-7}$
$^{238}\text{U } (n,\gamma)$	$0.201 \pm 1 \cdot 10^{-5}$	$0.200 \pm 8 \cdot 10^{-6}$	$0.198 \pm 2 \cdot 10^{-7}$	$0.174 \pm 2 \cdot 10^{-7}$
$^{239}\text{Pu } (n,f)$	$0.198 \pm 3 \cdot 10^{-6}$	$0.198 \pm 3 \cdot 10^{-6}$	$0.202 \pm 2 \cdot 10^{-7}$	$0.196 \pm 2 \cdot 10^{-7}$
$^{238}\text{Pu } (n,f)$	$0.149 \pm 1 \cdot 10^{-6}$	$0.149 \pm 1 \cdot 10^{-6}$	$0.029 \pm 5 \cdot 10^{-8}$	$0.001 \pm 1 \cdot 10^{-10}$
$^{238}\text{U } (n,n) - ^{238}\text{U } (n,n')$	$0.131 \pm 4 \cdot 10^{-5}$	$0.131 \pm 3 \cdot 10^{-5}$	$0.156 \pm 9 \cdot 10^{-6}$	$0.154 \pm 1 \cdot 10^{-5}$
$^{238}\text{U } \nu$	$0.101 \pm 2 \cdot 10^{-7}$	$0.101 \pm 2 \cdot 10^{-7}$	$0.102 \pm 6 \cdot 10^{-8}$	$0.103 \pm 1 \cdot 10^{-7}$
TOTAL	$1.073 \pm 5 \cdot 10^{-4}$	$1.066 \pm 4 \cdot 10^{-4}$	$1.048 \pm 2 \cdot 10^{-5}$	$0.917 \pm 2 \cdot 10^{-5}$

Uncertainty quantification analyses have been performed with both SCALE and SUMMON. In a first step, the SUMMONR code has been executed with the sensitivity profiles obtained by SCALE and with SCALE6.1 covariance matrix (i.e., using exactly the same inputs for the uncertainty quantification with both codes), to verify that the uncertainty propagation methodology has been correctly implemented. The results are included in the second and third columns of Table 6, showing that both methodologies provide differences lower than 1% for the total uncertainty (taking into account all contributors) and for the uncertainties in the 10 most

relevant quantities (i.e., 10 most relevant nuclides and reactions). These differences, as well as the slight discrepancies in the standard deviation of the uncertainties, can be attributed to rounding errors due to differences in the programming implementation of the variables in both systems and due to the use of covariance matrices in binary format by SCALE and in ASCII format by SUMMON.

Furthermore, once the verification has been carried out, in a second step, uncertainty quantification analyses in k_{eff} due to the uncertainty in nuclear data ($\Delta k_{eff}/k_{eff}$), have been performed with SUMMON using MCNP/KSEN sensitivities and SCALE6.1-44g and SCALE6.2-56g covariance matrices (based on ENDF/B-VII.0 and ENDF/B-VII.1 nuclear data libraries, respectively). The results are shown in the fourth and fifth columns of Table 6, where a good agreement between the uncertainties propagated from the same covariance matrix (SCALE6.1-44g) using SCALE and KSEN sensitivities is observed, except for ^{238}Pu (n,f) uncertainty which is five times lower when using KSEN sensitivities due to differences in the energy-dependent sensitivities obtained by SCALE/TSUNAMI-3D MG and MCNP/KSEN for this particular quantity (i.e., nuclide and reaction) (Figure 15). However, differences arise between the uncertainties derived using KSEN sensitivities and SCALE6.1-44g and SCALE6.2-56g covariance matrices, which are caused by differences in SCALE's covariance matrix libraries. In particular, the uncertainties in the average number of neutrons emitted per fission ν , the average fission spectrum χ and the fission cross section reaction have been reduced for a number of nuclides, mainly Pu, in SCALE6.2 covariance library, something which is clearly observed in Table 6, when the uncertainty is propagated using this covariance matrix.

Figure 15. Comparison between SCALE/TSUNAMI-3D MG and MCNP/KSEN for energy-dependent sensitivity coefficients of k_{eff} to ^{238}Pu (n,f) cross section for ALFRED model

The implementation of the methodology for the calculation of the eigenvalue-difference response sensitivity coefficients, described in Section 5.2, has been verified comparing SUMMONR and TSAR results when the same inputs are used for a reactivity response case, as can be seen in the second and third columns of Table 7. The values of the absolute sensitivity coefficients obtained by TSAR and SUMMONR are exactly the same, while the errors predicted by SUMMONR are higher as a result of taking into account the correlations between the eigenvalue and the sensitivities of a state of the system, something which is neglected by SCALE due to the use of a different method to derive the sensitivity coefficients.

Table 7. List of highest absolute integrated sensitivity coefficients (pcm) for a 20% increment in coolant density for ALFRED

Quantity	SCALE/TSAR	SUMMONR/SUMMONR	
		Sensitivities taken from SCALE	Sensitivities taken from MCNP
$^{239}\text{Pu } \nu$	7.293 ± 0.032	7.293 ± 0.893	4.860 ± 0.049
$^{239}\text{Pu } (n,f)$	5.810 ± 0.116	5.810 ± 0.677	3.383 ± 0.038
$^{238}\text{U } \nu$	-5.657 ± 0.009	-5.657 ± 0.615	-3.574 ± 0.031
$^{238}\text{U } (n,\gamma)$	-5.290 ± 0.092	-5.290 ± 0.358	-3.656 ± 0.019
$^{238}\text{U } (n,f)$	-3.456 ± 0.034	-3.456 ± 0.372	-2.003 ± 0.018
$^{16}\text{O } (n,n)$	-2.592 ± 2.499	-2.592 ± 2655	-6.626 ± 0.075
$^{206}\text{Pb } (n,n')$	-2.561 ± 0.085	-2.561 ± 0.298	-1.983 ± 0.018
$^{240}\text{Pu } \nu$	-1.884 ± 0.005	-1.884 ± 0.212	-1.161 ± 0.011
$^{207}\text{Pb } (n,n')$	-1.864 ± 0.070	-1.864 ± 0.171	-1.365 ± 0.010
$^{241}\text{Pu } \nu$	1.659 ± 0.005	1.659 ± 0.141	1.132 ± 0.008

In the fourth column of Table 7, the absolute sensitivities derived by SUMMONR using MCNP/KSEN sensitivities for the nominal and perturbed state of the system are shown and significant differences between the eigenvalue-difference sensitivities, calculated using SCALE and MCNP eigenvalue sensitivities, can be appreciated. These differences are caused by differences in the eigenvalue sensitivities $S_{k,\alpha}$ calculated by SCALE/TSUNAMI-3D MG and MCNP/KSEN, which are magnified when using EGPT to calculate $S_{\rho_{1 \rightarrow 2}, \alpha}$. These differences using EGPT have also been reported by the SCALE team when using TSAR to compute sensitivities in reactivity coefficients [ORNL, 2013].

After the verification of the implementation of the eigenvalue-difference response sensitivity calculation method was carried out, the uncertainty in the reactivity change for both scenarios was calculated with SCALE and SUMMON, using sensitivities derived by SCALE/TSUNAMI-3D MG and MCNP/KSEN together with SCALE6.1-44g covariance matrix (Table 8 and Table 9). As in the case of the uncertainty quantification in k_{eff} (Table 6), differences lower than 1% for the total uncertainty and for the uncertainties in the most relevant quantities are observed between

SCALE and SUMMON when the same sensitivities from SCALE are used to propagate the uncertainty.

Table 8. Uncertainty quantification of $\Delta\rho/\rho$ (%) for a 20% increment in coolant density for ALFRED

$$SCALE/TSAR: \rho_{+20\%} = -47 \pm 14 \text{ pcm}$$

$$SUMMON/MCNP: \rho_{+20\%} = -64 \pm 1 \text{ pcm}$$

Quantity	SCALE	SUMMON	
		Sensitivities taken from SCALE	Sensitivities taken from KSEN
$^{238}\text{U} (n,n')$	$37.6 \pm 1 \cdot 10^{+0}$	$37.6 \pm 2 \cdot 10^{+0}$	$13.8 \pm 6 \cdot 10^{-2}$
$^{206}\text{Pb} (n,n')$	$18.2 \pm 1 \cdot 10^{-1}$	$18.2 \pm 1 \cdot 10^{-1}$	$14.4 \pm 2 \cdot 10^{-2}$
$^{207}\text{Pb} (n,n')$	$18.0 \pm 1 \cdot 10^{-1}$	$18.0 \pm 1 \cdot 10^{-1}$	$11.5 \pm 1 \cdot 10^{-2}$
$^{238}\text{U} (n,n) - (n,n')$	$13.5 \pm 1 \cdot 10^{-1}$	$13.5 \pm 1 \cdot 10^{-1}$	$17.0 \pm 1 \cdot 10^{-1}$
$^{239}\text{Pu } \nu$	$13.3 \pm 4 \cdot 10^{-3}$	$13.3 \pm 5 \cdot 10^{-3}$	$8.8 \pm 8 \cdot 10^{-3}$
$^{239}\text{Pu } \chi$	$10.5 \pm 1 \cdot 10^{-2}$	$10.5 \pm 3 \cdot 10^{-2}$	$10.0 \pm 2 \cdot 10^{-2}$
<i>Most relevant contributors according to SUMMON if not yet included</i>			
$^{204}\text{Pb} (n,n)$	$1.2 \pm 2 \cdot 10^{-3}$	$1.2 \pm 7 \cdot 10^{-3}$	$24.3 \pm 1 \cdot 10^{-1}$
$^{238}\text{U} (n,n)$	$3.0 \pm 1 \cdot 10^{-2}$	$2.9 \pm 2 \cdot 10^{-2}$	$13.8 \pm 6 \cdot 10^{-2}$
$^{16}\text{O} (n,n)$	$5.6 \pm 4 \cdot 10^{-1}$	$5.6 \pm 6 \cdot 10^{-1}$	$11.3 \pm 3 \cdot 10^{-2}$
$^{207}\text{Pb} (n,n)$	$0.8 \pm 1 \cdot 10^{-2}$	$0.8 \pm 7 \cdot 10^{-3}$	$10.1 \pm 4 \cdot 10^{-2}$
TOTAL	$56.3 \pm 1 \cdot 10^{+0}$	$55.5 \pm 1 \cdot 10^{+0}$	$51.4 \pm 3 \cdot 10^{-1}$

However, when the uncertainty is propagated by SUMMONR code using KSEN sensitivities, significant differences with SCALE-derived uncertainties are observed in the contribution of most quantities in both cases, as well as in the total uncertainty in the +300 K temperature scenario (Table 9). These differences are caused by differences in the reactivity response sensitivities, which are in turn caused by differences in the eigenvalue sensitivities, as explained before for the results included in Table 7. An example is given in Figure 16, where the energy-dependent sensitivities of $^{238}\text{U} (n,n')$ for the +20% increase in coolant density scenario obtained with SUMMON using SCALE/TSUNAMI-3D MG and MCNP/KSEN eigenvalue sensitivities are presented. While the energy integrated sensitivity (ISC) is very similar due to compensations, as shown also in the direct perturbation calculations included in Table 5, there are differences of nearly one order of magnitude in some energy bins. Furthermore, the statistical uncertainty of the sensitivities derived from SCALE is 20 times higher than the one derived from MCNP, as a consequence of the higher number of particles used in the MCNP simulations. These differences between energy-dependent sensitivities have a significant impact when the uncertainty is propagated, resulting in different predictions of the impact of some quantities in the uncertainty of the reactivity responses, particularly for the scattering reactions of coolant and fuel materials (Table 8 and Table 9).

Table 9. Uncertainty quantification of $\Delta\rho/\rho$ (%) for a $\Delta T=+300$ K in fuel temperature for ALFRED

$$SCALE/TSAR: \rho_{+300K} = -112 \pm 14 \text{ pcm}$$

$$SUMMON/MCNP: \rho_{+300K} = -122 \pm 2 \text{ pcm}$$

Quantity	SCALE	SUMMON	
		Sensitivity from SCALE	Sensitivity from KSEN
^{238}U (n,n')	$8.5 \pm 1 \cdot 10^{+0}$	$8.5 \pm 1 \cdot 10^{+0}$	$10.4 \pm 1 \cdot 10^{-1}$
^{239}Pu (n,n')	$1.5 \pm 1 \cdot 10^{-1}$	$1.5 \pm 1 \cdot 10^{-1}$	$11.9 \pm 1 \cdot 10^{-1}$
^{207}Pb (n,n')	$1.2 \pm 2 \cdot 10^{-2}$	$1.2 \pm 2 \cdot 10^{-2}$	$0.8 \pm 1 \cdot 10^{-3}$
^{239}Pu v	$1.1 \pm 1 \cdot 10^{-3}$	$1.1 \pm 4 \cdot 10^{-3}$	$1.8 \pm 1 \cdot 10^{-3}$
^{238}U (n, γ)	$1.1 \pm 5 \cdot 10^{-3}$	$1.1 \pm 7 \cdot 10^{-3}$	$0.6 \pm 7 \cdot 10^{-5}$
^{206}Pb (n,n')	$1.1 \pm 1 \cdot 10^{-2}$	$1.1 \pm 1 \cdot 10^{-2}$	$2.2 \pm 3 \cdot 10^{-3}$
<i>Most relevant contributors according to SUMMON if not yet included</i>			
^{62}Ni (n,n)	$0.07 \pm 2 \cdot 10^{-3}$	$0.07 \pm 2 \cdot 10^{-3}$	$8.4 \pm 1 \cdot 10^{-1}$
^{144}Nd (n,n)	$0.02 \pm 1 \cdot 10^{-5}$	$0.02 \pm 2 \cdot 10^{-5}$	$8.3 \pm 3 \cdot 10^{-2}$
^{204}Pb (n,n)	$0.06 \pm 6 \cdot 10^{-4}$	$0.06 \pm 8 \cdot 10^{-4}$	$7.6 \pm 8 \cdot 10^{-2}$
^{238}U (n,n) - (n,n')	$-0.79 \pm 8 \cdot 10^{-2}$	$-0.80 \pm 7 \cdot 10^{-2}$	$6.0 \pm 6 \cdot 10^{-2}$
TOTAL	$9.2 \pm 1 \cdot 10^{+0}$	$9.2 \pm 1 \cdot 10^{+0}$	$33.0 \pm 3 \cdot 10^{-1}$

Figure 16. Comparison between SCALE/TSUNAMI-3D MG and MCNP/KSEN energy-dependent sensitivity coefficients to ^{238}U (n,n') for a 20% increment in coolant density for ALFRED

Additionally, it can be seen that the statistical uncertainties in the reactivity responses using SCALE are significant and comparable to the total uncertainties due to nuclear data. This shows that the calculations performed with SCALE are not accurate enough for estimating these

reactivity responses and should be repeated, increasing the number of histories to reduce statistical uncertainties. On the other hand, statistical uncertainties calculated with SUMMON are well below nuclear data uncertainties.

5.4.2. Effective delayed neutron fraction sensitivities

Table 10 shows the integral benchmark experiments selected for the β_{eff} verification process from the ICSBEP, as well as the experimental and the calculated β_{eff} values obtained with adjoint-weighting (SUSD3D) [Kodeli, 2013], the IFP methodology (MCNP) and the prompt and modified methods (SUMMONR), using the ENDF/B-VII.0 nuclear data library. For each benchmark, the β_{eff} values calculated with the different methodologies are within 2σ of the experimental value.

Table 10. Experimental and calculated values of β_{eff} in pcm

Benchmark	Experiment	SUSD3D	MCNP	SUMMONR (Bretscher)	SUMMONR (Chiba)
PU-MET-FAST-001 [OECD/NEA, 2015a]	194 ± 10	185	182 ± 2	184 ± 1	185 ± 0.1
PU-MET-FAST-006 [OECD/NEA, 2015b]	276 ± 7	277	278 ± 2	276 ± 1	274 ± 0.1
HEU-MET-FAST-028 [OECD/NEA, 2015c]	665 ± 13	688	693 ± 3	689 ± 1	687 ± 0.1
U233-MET-FAST-006 [OECD/NEA, 2015d]	360 ± 9	374	372 ± 2	374 ± 1	369 ± 0.1
IEU-MET-FAST-007 [OECD/NEA, 2015e]	720 ± 7	720	726 ± 4	722 ± 1	703 ± 0.1
SNEAK-LMFR-EXP-001-A [OECD/NEA, 2017b]	395 ± 20	373	370 ± 3	366 ± 2	357 ± 0.1
SNEAK-LMFR-EXP-001-B [OECD/NEA, 2017b]	413 ± 25	419	410 ± 2	416 ± 1	400 ± 0.1

For the verification of the methodologies implemented in SUMMON to calculate $S_{\beta_{eff}, \alpha}$, the results reported by Kodeli [Kodeli, 2013] were used. First, the $S_{\beta_{eff}, \alpha}$ values obtained with SUMMONR module using the prompt method were compared against values calculated with the deterministic code SUSD3D. The energy-integrated sensitivity coefficients of β_{eff} for the U233-MET-FAST-006 benchmark obtained with SUMMONR are given in Table 11, while the sensitivity coefficients calculated with SUSD3D are presented in Table 12.

Table 11. Relative β_{eff} sensitivities in %/% for U233-MET-FAST-006 with SUMMONR using the prompt method

	(n,n)	(n,n')	(n,f)	(n, γ)	ν_d	ν_p	ν_t
^{233}U	$-0.131 \pm 1.3 \cdot 10^{-3}$	$-0.012 \pm 6.6 \cdot 10^{-4}$	$-0.266 \pm 1.6 \cdot 10^{-3}$	$-0.019 \pm 5.2 \cdot 10^{-5}$	$0.695 \pm 4.5 \cdot 10^{-4}$	$-0.902 \pm 1.9 \cdot 10^{-3}$	$-0.207 \pm 1.7 \cdot 10^{-3}$
^{234}U	$0.022 \pm 1.7 \cdot 10^{-4}$	$0.012 \pm 8.2 \cdot 10^{-5}$	$-0.001 \pm 1.1 \cdot 10^{-5}$	$-2.4 \cdot 10^{-4} \pm 8.1 \cdot 10^{-7}$	$0.007 \pm 6.3 \cdot 10^{-6}$	$-0.009 \pm 1.5 \cdot 10^{-5}$	$-0.002 \pm 1.1 \cdot 10^{-5}$
^{235}U	$-0.020 \pm 1.9 \cdot 10^{-4}$	$-0.011 \pm 7.5 \cdot 10^{-5}$	$0.016 \pm 1.2 \cdot 10^{-4}$	$-4.2 \cdot 10^{-4} \pm 1.8 \cdot 10^{-6}$	$0.015 \pm 9.7 \cdot 10^{-6}$	$0.003 \pm 1.2 \cdot 10^{-4}$	$0.017 \pm 1.2 \cdot 10^{-4}$
^{238}U	$0.133 \pm 2.2 \cdot 10^{-3}$	$-0.149 \pm 9.8 \cdot 10^{-4}$	$0.174 \pm 5.0 \cdot 10^{-4}$	$-0.026 \pm 1.2 \cdot 10^{-4}$	$0.274 \pm 3.3 \cdot 10^{-4}$	$-0.082 \pm 3.9 \cdot 10^{-4}$	$0.191 \pm 5.0 \cdot 10^{-4}$

Good agreement between SUMMONR and SUS3D is observed for the U233-MET-FAST-006 β_{eff} sensitivities for the (n,f) and (n, γ) reactions and the average delayed, prompt and total neutron fission multiplicities (ν_d , ν_p and ν_t), whereas large differences are found in the (n,n) and (n,n') β_{eff} sensitivities. As explained in Section 5.4.1, these differences can be attributed to the different $S_{k,\alpha}$ values predicted by MCNP and SUS3D codes, i.e., if the sensitivity of k to nuclear data for a particular reaction does not have perfect agreement between codes, the differences in $S_{k,\alpha}$ values are magnified when using EGPT to calculate $S_{\beta_{eff},\alpha}$. Furthermore, elastic scattering has a high statistical uncertainty in Monte Carlo calculations due to high cancelation of gain and loss terms, so differences for this reaction are expected [Kodeli et al., 2016a].

Table 12. Relative β_{eff} sensitivities in %/% for U233-MET-FAST-006 with SUS3D [Kodeli, 2013]

	(n,n)	(n,n')	(n,f)	(n, γ)	ν_d	ν_p	ν_t
^{233}U	-0.005	-0.034	-0.231	-0.016	0.700	-0.885	-0.185
^{234}U	$2 \cdot 10^{-5}$	-0.001	-0.001	$-2 \cdot 10^{-4}$	0.007	-0.009	-0.002
^{235}U	0.001	-0.001	0.015	-0.001	0.015	0.002	0.017
^{238}U	0.075	-0.129	0.167	-0.033	0.274	-0.104	0.170

β_{eff} sensitivities for the SNEAK-LMFR-EXP-001-B integral experiment calculated with SUMMONR and SUS3D are presented in Table 13 and Table 14, respectively. Furthermore, energy-dependent sensitivities of β_{eff} calculated with SUMMONR for ^{239}Pu prompt and delay neutron yields, as well as inelastic scattering and capture reactions, are shown in Figure 17. Additionally, β_{eff} sensitivities obtained with the GPT based SERPENT code [Aufiero et al., 2015; Kodeli et al., 2016a] and with the sampling based XSUSA code [Kodeli et al., 2016a; Kodeli and Zwermann, 2014] are shown in Table 15 and Table 16, respectively.

Figure 17. Energy-dependent β_{eff} sensitivities to ^{239}Pu for SNEAK-LMFR-EXP-001-B

Table 13. Relative β_{eff} sensitivities in %/% for SNEAK-LMFR-EXP-001-B with SUMMONR using the prompt method

	(n,n)	(n,n')	(n,f)	(n,g)	v_d	v_p	v_t
^{235}U	$0.030 \pm$	$-0.005 \pm$	$0.034 \pm$	$-0.003 \pm$	$0.104 \pm$	$-0.066 \pm$	$0.038 \pm$
	$3.8 \cdot 10^{-4}$	$1.3 \cdot 10^{-4}$	$2.5 \cdot 10^{-4}$	$9.8 \cdot 10^{-6}$	$5.4 \cdot 10^{-5}$	$2.6 \cdot 10^{-4}$	$2.5 \cdot 10^{-4}$
^{238}U	$0.484 \pm$	$-0.116 \pm$	$0.235 \pm$	$-0.059 \pm$	$0.558 \pm$	$-0.356 \pm$	$0.201 \pm$
	$3.7 \cdot 10^{-3}$	$1.4 \cdot 10^{-3}$	$5.9 \cdot 10^{-4}$	$2.1 \cdot 10^{-4}$	$6.2 \cdot 10^{-4}$	$6.5 \cdot 10^{-4}$	$5.4 \cdot 10^{-4}$
^{239}Pu	$0.146 \pm$	$-0.063 \pm$	$-0.204 \pm$	$-0.008 \pm$	$0.305 \pm$	$-0.536 \pm$	$-0.230 \pm$
	$1.1 \cdot 10^{-3}$	$3.7 \cdot 10^{-4}$	$9.7 \cdot 10^{-4}$	$5.6 \cdot 10^{-5}$	$1.5 \cdot 10^{-4}$	$1.0 \cdot 10^{-3}$	$9.7 \cdot 10^{-4}$
^{240}Pu	$-0.003 \pm$	$0.002 \pm$	$-0.010 \pm$	$-8.3 \cdot 10^{-5} \pm$	$0.010 \pm$	$-0.022 \pm$	$-0.013 \pm$
	$3.5 \cdot 10^{-4}$	$1.0 \cdot 10^{-4}$	$3.4 \cdot 10^{-5}$	$6.5 \cdot 10^{-6}$	$5.9 \cdot 10^{-6}$	$3.7 \cdot 10^{-5}$	$3.4 \cdot 10^{-5}$
^{241}Pu	$0.014 \pm$	$0.002 \pm$	$0.004 \pm$	$-3.7 \cdot 10^{-5} \pm$	$0.008 \pm$	$-0.005 \pm$	$0.003 \pm$
	$9.6 \cdot 10^{-5}$	$3.4 \cdot 10^{-5}$	$1.2 \cdot 10^{-5}$	$3.4 \cdot 10^{-7}$	$4.3 \cdot 10^{-6}$	$1.2 \cdot 10^{-5}$	$1.2 \cdot 10^{-5}$

Table 14. Relative β_{eff} sensitivities in %/% for SNEAK-LMFR-EXP-001-B with SUSD3D [Kodali, 2013]

	(n,n)	(n,n')	(n,f)	(n,g)	v_d	v_p	v_t
^{235}U	$-2 \cdot 10^{-4}$	-0.002	0.061	-0.001	0.114	-0.052	0.061
^{238}U	-0.019	-0.164	0.267	0.011	0.564	-0.334	0.230
^{239}Pu	-0.001	-0.008	-0.233	-0.001	0.300	-0.579	-0.280
^{240}Pu	$-1 \cdot 10^{-4}$	-0.001	-0.010	$5 \cdot 10^{-5}$	0.009	-0.022	-0.013
^{241}Pu	$-7 \cdot 10^{-6}$	$-7 \cdot 10^{-5}$	0.003	$1 \cdot 10^{-5}$	0.008	-0.005	0.003

Again, in the SNEAK-LMFR-EXP-001-B there is a relatively good agreement between codes for the averaged neutron multiplicities and the (n,f) and (n, γ) reactions, except for $^{238}\text{U}(n,\gamma)$, and $^{239}\text{Pu}(n,f)$ and $^{238}\text{U } \nu_p$ in SERPENT, while differences arise in elastic and inelastic scattering sensitivities. The same phenomenology is found in the PU-MET-FAST-001 (Table 17 and Table 18), PU-MET-FAST-006 (Table 19 and Table 20), HEU-MET-FAST-028 (Table 21 and Table 22), IEU-MET-FAST-007 (Table 23 and Table 24) and SNEAK-LMFR-EXP-001-A (

Table 25 and Table 26) integral benchmark experiments.

Table 15. Relative β_{eff} sensitivities in %/% with relative statistical uncertainties for SNEAK-LMFR-EXP-001-B with SERPENT [Kodeli et al., 2016a]

	(n,n)	(n,n')	(n,f)	(n, γ)	ν_d	ν_p	ν_t
^{235}U	$-0.001 \pm 99\%$	$-0.001 \pm 21\%$	$0.061 \pm 0.9\%$	$-0.002 \pm 8.3\%$	$0.111 \pm 0.2\%$	$-0.048 \pm 0.9\%$	-
^{238}U	$0.013 \pm 53\%$	$-0.124 \pm 1.9\%$	$0.259 \pm 0.3\%$	$-0.016 \pm 6\%$	$0.560 \pm 0.1\%$	$0.349 \pm 0.2\%$	-
^{239}Pu	$0.003 \pm 60\%$	$-0.006 \pm 11.5\%$	$0.227 \pm 0.4\%$	$-0.008 \pm 4.6\%$	$0.304 \pm 0.1\%$	$-0.565 \pm 0.1\%$	-

Table 16. Relative β_{eff} sensitivities in %/% for SNEAK-LMFR-EXP-001-B with XSUSA [Kodeli et al., 2016a]

	(n,n)	(n,n')	(n,f)	(n, γ)	ν_d	ν_p	ν_t
^{235}U	-	-	-	-	0.124	-	-
^{238}U	-	-0.170	0.347	-	0.624	-0.288	-
^{239}Pu	-	-	-0.306	-	0.334	-0.700	-

Table 17. Relative β_{eff} sensitivities in %/% for PU-MET-FAST-001 with SUMMONR using the prompt method

	(n,n)	(n,n')	(n,f)	(n, γ)	ν_d	ν_p	ν_t
^{239}Pu	$-0.524 \pm$	$-0.004 \pm$	$0.058 \pm$	$-0.023 \pm$	$0.947 \pm$	$-0.946 \pm$	$0.001 \pm$
	$3.6 \cdot 10^{-3}$	$1.6 \cdot 10^{-4}$	$4.3 \cdot 10^{-3}$	$9.7 \cdot 10^{-5}$	$1.5 \cdot 10^{-3}$	$4.9 \cdot 10^{-3}$	$4.3 \cdot 10^{-3}$
^{240}Pu	$-0.069 \pm$	$0.026 \pm$	$0.003 \pm$	$-0.001 \pm$	$0.043 \pm$	$-0.048 \pm$	$-0.005 \pm$
	$8.9 \cdot 10^{-4}$	$4.2 \cdot 10^{-4}$	$1.5 \cdot 10^{-4}$	$6.3 \cdot 10^{-6}$	$7.9 \cdot 10^{-5}$	$1.8 \cdot 10^{-4}$	$1.4 \cdot 10^{-4}$
^{241}Pu	$0.028 \pm$	$0.008 \pm$	$0.005 \pm$	$-6.3 \cdot 10^{-5} \pm$	$0.007 \pm$	$-0.002 \pm$	$0.005 \pm$
	$1.9 \cdot 10^{-4}$	$1.3 \cdot 10^{-4}$	$1.5 \cdot 10^{-5}$	$3.8 \cdot 10^{-7}$	$1.0 \cdot 10^{-5}$	$1.4 \cdot 10^{-5}$	$1.5 \cdot 10^{-5}$

Table 18. Relative β_{eff} sensitivities in %/% for PU-MET-FAST-001 with SUSD3D [Kodeli, 2013]

	(n,n)	(n,n')	(n,f)	(n, γ)	ν_d	ν_p	ν_t
^{239}Pu	0.079	0.009	-0.014	-0.022	0.948	-0.947	0.002
^{240}Pu	0.005	$3.0 \cdot 10^{-4}$	-0.002	-0.001	0.043	-0.049	-0.007
^{241}Pu	$2.0 \cdot 10^{-4}$	$7.0 \cdot 10^{-5}$	0.005	$-7.0 \cdot 10^{-5}$	0.007	-0.002	0.005

Table 19. Relative β_{eff} sensitivities in %/% for PU-MET-FAST-006 with SUMMONR using the prompt method

	(n,n)	(n,n')	(n,f)	(n, γ)	v_d	v_p	v_t
^{235}U	$0.017 \pm 2.7 \cdot 10^{-4}$	$0.002 \pm 1.2 \cdot 10^{-4}$	$0.012 \pm 2.0 \cdot 10^{-4}$	$-2.9 \cdot 10^{-4} \pm 2.9 \cdot 10^{-6}$	$0.020 \pm 1.8 \cdot 10^{-5}$	$-0.006 \pm 2.0 \cdot 10^{-4}$	$0.014 \pm 2.0 \cdot 10^{-4}$
^{238}U	$0.388 \pm 3.3 \cdot 10^{-3}$	$-0.147 \pm 1.5 \cdot 10^{-3}$	$0.152 \pm 7.4 \cdot 10^{-4}$	$-0.015 \pm 2.0 \cdot 10^{-4}$	$0.360 \pm 5.9 \cdot 10^{-4}$	$-0.186 \pm 7.1 \cdot 10^{-4}$	$0.175 \pm 7.7 \cdot 10^{-4}$
^{239}Pu	$0.069 \pm 2.0 \cdot 10^{-3}$	$0.001 \pm 9.7 \cdot 10^{-4}$	$-0.203 \pm 2.3 \cdot 10^{-3}$	$-0.013 \pm 6.6 \cdot 10^{-5}$	$0.587 \pm 5.4 \cdot 10^{-4}$	$-0.763 \pm 2.5 \cdot 10^{-3}$	$-0.176 \pm 2.3 \cdot 10^{-3}$
^{240}Pu	$-0.047 \pm 4.7 \cdot 10^{-4}$	$-0.004 \pm 2.3 \cdot 10^{-4}$	$-0.012 \pm 7.7 \cdot 10^{-5}$	$-9.7 \cdot 10^{-4} \pm 4.6 \cdot 10^{-6}$	$0.024 \pm 2.9 \cdot 10^{-5}$	$-0.039 \pm 9.3 \cdot 10^{-5}$	$-0.014 \pm 7.5 \cdot 10^{-5}$
^{241}Pu	$-3.7 \cdot 10^{-4} \pm 1.1 \cdot 10^{-4}$	$-0.002 \pm 5.8 \cdot 10^{-5}$	$0.003 \pm 7.7 \cdot 10^{-6}$	$-5.1 \cdot 10^{-5} \pm 2.5 \cdot 10^{-7}$	$0.005 \pm 4.0 \cdot 10^{-6}$	$-0.002 \pm 7.6 \cdot 10^{-2}$	$0.003 \pm 7.5 \cdot 10^{-6}$

Table 20. Relative β_{eff} sensitivities in %/% for PU-MET-FAST-006 with SUSD3D [Kodeli, 2013]

	(n,n)	(n,n')	(n,f)	(n, γ)	v_d	v_p	v_t
^{235}U	0.001	-0.001	0.027	-0.001	0.020	0.010	0.030
^{238}U	0.103	-0.170	0.261	-0.050	0.361	-0.083	0.278
^{239}Pu	-0.010	-0.042	-0.305	-0.017	0.588	-0.879	-0.292
^{240}Pu	$-3.0 \cdot 10^{-4}$	-0.002	-0.015	-0.001	0.024	-0.043	-0.019
^{241}Pu	$-4.0 \cdot 10^{-5}$	$-1.0 \cdot 10^{-4}$	0.002	$-5.0 \cdot 10^{-5}$	0.005	-0.002	0.002

Table 21. Relative β_{eff} sensitivities in %/% for HEU-MET-FAST-028 with SUMMONR using the prompt method

	(n,n)	(n,n')	(n,f)	(n, γ)	v_d	v_p	v_t
^{234}U	$0.023 \pm 1.0 \cdot 10^{-4}$	$-0.003 \pm 4.9 \cdot 10^{-5}$	$-0.004 \pm 8.2 \cdot 10^{-6}$	$-2.8 \cdot 10^{-4} \pm 5.8 \cdot 10^{-7}$	$0.005 \pm 2.0 \cdot 10^{-6}$	$-0.010 \pm 9.7 \cdot 10^{-6}$	$-0.005 \pm 8.2 \cdot 10^{-6}$
^{235}U	$-0.083 \pm 9.5 \cdot 10^{-4}$	$0.002 \pm 5.0 \cdot 10^{-4}$	$-0.045 \pm 8.5 \cdot 10^{-4}$	$-0.035 \pm 6.3 \cdot 10^{-5}$	$0.834 \pm 2.9 \cdot 10^{-4}$	$-0.809 \pm 9.3 \cdot 10^{-4}$	$0.025 \pm 8.4 \cdot 10^{-4}$
^{238}U	$0.275 \pm 1.3 \cdot 10^{-3}$	$0.006 \pm 5.6 \cdot 10^{-4}$	$-0.006 \pm 2.0 \cdot 10^{-4}$	$-0.007 \pm 6.9 \cdot 10^{-5}$	$0.152 \pm 1.0 \cdot 10^{-4}$	$-0.173 \pm 2.5 \cdot 10^{-4}$	$-0.020 \pm 2.0 \cdot 10^{-4}$

Table 22. Relative β_{eff} sensitivities in %/% for HEU-MET-FAST-028 with SUSD3D [Kodeli, 2013]

	(n,n)	(n,n')	(n,f)	(n, γ)	v_d	v_p	v_t
^{234}U	$2.0 \cdot 10^{-4}$	$-2.0 \cdot 10^{-4}$	-0.004	$-3.0 \cdot 10^{-4}$	0.004	-0.010	-0.005
^{235}U	0.016	-0.014	-0.059	-0.033	0.836	-0.843	-0.007
^{238}U	0.047	-0.051	0.028	-0.013	0.153	-0.140	0.013

Table 23. Relative β_{eff} sensitivities in %/% for IEU-MET-FAST-007 with SUMMONR using the prompt method

	(n,n)	(n,n')	(n,f)	(n, γ)	ν_d	ν_p	ν_t
^{234}U	$-8.5 \cdot 10^{-4} \pm$	$-0.008 \pm$	$-0.002 \pm$	$-2.6 \cdot 10^{-4} \pm$	$0.001 \pm$	$-0.003 \pm$	$-0.002 \pm$
	$1.1 \cdot 10^{-4}$	$3.8 \cdot 10^{-5}$	$3.3 \cdot 10^{-6}$	$3.8 \cdot 10^{-7}$	$4.1 \cdot 10^{-7}$	$3.6 \cdot 10^{-6}$	$3.3 \cdot 10^{-6}$
^{235}U	$-0.083 \pm$	$-0.010 \pm$	$-0.092 \pm$	$-0.035 \pm$	$0.543 \pm$	$-0.531 \pm$	$0.013 \pm$
	$1.1 \cdot 10^{-3}$	$4.3 \cdot 10^{-4}$	$8.4 \cdot 10^{-4}$	$4.9 \cdot 10^{-5}$	$1.9 \cdot 10^{-4}$	$8.5 \cdot 10^{-4}$	$8.3 \cdot 10^{-4}$
^{238}U	$0.275 \pm$	$-0.059 \pm$	$0.062 \pm$	$-0.173 \pm$	$0.445 \pm$	$-0.457 \pm$	$-0.011 \pm$
	$3.6 \cdot 10^{-3}$	$1.5 \cdot 10^{-3}$	$4.7 \cdot 10^{-4}$	$2.4 \cdot 10^{-4}$	$2.8 \cdot 10^{-4}$	$5.9 \cdot 10^{-4}$	$4.4 \cdot 10^{-4}$

Table 24. Relative β_{eff} sensitivities in %/% for IEU-MET-FAST-007 with SUSD3D [Kodeli, 2013]

	(n,n)	(n,n')	(n,f)	(n, γ)	ν_d	ν_p	ν_t
^{234}U	$1.0 \cdot 10^{-5}$	$-3.0 \cdot 10^{-5}$	-0.001	$-8.0 \cdot 10^{-5}$	0.001	-0.003	-0.002
^{235}U	0.001	-0.005	0.016	-0.012	0.548	-0.516	0.032
^{238}U	0.009	-0.061	0.046	-0.041	0.443	-0.473	-0.030

Table 25. Relative β_{eff} sensitivities in %/% for SNEAK-LMFR-EXP-001-A with SUMMONR using the prompt method

	(n,n)	(n,n')	(n,f)	(n, γ)	ν_d	ν_p	ν_t
^{235}U	$-0.044 \pm$	$0.037 \pm$	$0.079 \pm$	$0.001 \pm$	$0.060 \pm$	$0.018 \pm$	$0.078 \pm$
	$9.4 \cdot 10^{-4}$	$3.1 \cdot 10^{-4}$	$6.4 \cdot 10^{-4}$	$2.8 \cdot 10^{-5}$	$5.1 \cdot 10^{-5}$	$6.3 \cdot 10^{-4}$	$6.4 \cdot 10^{-4}$
^{238}U	$-0.722 \pm$	$-0.478 \pm$	$0.250 \pm$	$-0.155 \pm$	$0.495 \pm$	$-0.251 \pm$	$0.243 \pm$
	$1.1 \cdot 10^{-2}$	$4.2 \cdot 10^{-3}$	$1.4 \cdot 10^{-4}$	$6.7 \cdot 10^{-4}$	$1.0 \cdot 10^{-3}$	$1.3 \cdot 10^{-3}$	$1.3 \cdot 10^{-3}$
^{239}Pu	$0.651 \pm$	$0.052 \pm$	$-0.406 \pm$	$-0.090 \pm$	$0.414 \pm$	$-0.726 \pm$	$-0.311 \pm$
	$4.5 \cdot 10^{-3}$	$1.3 \cdot 10^{-3}$	$3.7 \cdot 10^{-3}$	$3.3 \cdot 10^{-4}$	$3.5 \cdot 10^{-4}$	$3.7 \cdot 10^{-3}$	$3.7 \cdot 10^{-3}$
^{240}Pu	$0.046 \pm$	$0.016 \pm$	$-0.008 \pm$	$-0.008 \pm$	$0.014 \pm$	$-0.027 \pm$	$-0.013 \pm$
	$1.3 \cdot 10^{-3}$	$3.9 \cdot 10^{-4}$	$1.3 \cdot 10^{-4}$	$4.3 \cdot 10^{-5}$	$1.7 \cdot 10^{-5}$	$1.4 \cdot 10^{-4}$	$1.3 \cdot 10^{-4}$
^{241}Pu	$-0.018 \pm$	$0.002 \pm$	$2.3 \cdot 10^{-4} \pm$	$-5.7 \cdot 10^{-4} \pm$	$0.012 \pm$	$-0.010 \pm$	$0.002 \pm$
	$3.7 \cdot 10^{-4}$	$1.3 \cdot 10^{-4}$	$4.8 \cdot 10^{-5}$	$2.0 \cdot 10^{-6}$	$9.7 \cdot 10^{-6}$	$4.8 \cdot 10^{-5}$	$4.8 \cdot 10^{-5}$

Table 26. Relative β_{eff} sensitivities in %/% for SNEAK-LMFR-EXP-001-A with SUSD3D [Kodeli, 2013]

	(n,n)	(n,n')	(n,f)	(n, γ)	ν_d	ν_p	ν_t
^{235}U	$-2.0 \cdot 10^{-4}$	-0.001	0.052	-0.001	0.080	-0.025	0.055
^{238}U	-0.011	-0.151	0.276	-0.017	0.488	-0.233	0.255
^{239}Pu	-0.002	-0.012	-0.252	-0.006	0.402	-0.700	-0.298
^{240}Pu	$-3.0 \cdot 10^{-4}$	-0.001	-0.012	$-4.0 \cdot 10^{-4}$	0.014	-0.030	-0.016
^{241}Pu	$-2.0 \cdot 10^{-5}$	$-1.0 \cdot 10^{-4}$	0.005	$-2.0 \cdot 10^{-5}$	0.011	-0.007	0.005

Once the verification of the prompt method was carried out, Chiba's modified method was also verified using the same integral benchmark experiments (Table 27 - Table 33). The size of the scaling factor was chosen according to Iwamoto et al. [Iwamoto et al., 2018], who concluded that a factor $a = 20$ appears to yield sufficiently small statistical uncertainties. It can be seen that in all integral experiments and for all nuclides and reactions, Chiba's method yields superior results than the prompt method, as in the case of $^{233}\text{U}(n,n')$ in U233-MET-FAST-006 (Table 27).

Table 27. Relative β_{eff} sensitivities in %/% for U233-MET-FAST-006 with SUMMONR using Chiba's method

	(n,n)	(n,n')	(n,f)	(n, γ)	ν_d	ν_p	ν_t
^{233}U	$0.002 \pm 2.7 \cdot 10^{-4}$	$-0.030 \pm 6.7 \cdot 10^{-5}$	$-0.207 \pm 2.6 \cdot 10^{-4}$	$-0.017 \pm 2.2 \cdot 10^{-6}$	$0.698 \pm 1.4 \cdot 10^{-4}$	$-0.854 \pm 1.5 \cdot 10^{-4}$	$-0.155 \pm 2.5 \cdot 10^{-4}$
	$-9.4 \cdot 10^{-4} \pm 2.5 \cdot 10^{-5}$	$-0.001 \pm 9.3 \cdot 10^{-6}$	$-0.001 \pm 1.1 \cdot 10^{-6}$	$-2.2 \cdot 10^{-4} \pm 5.2 \cdot 10^{-8}$	$0.007 \pm 1.3 \cdot 10^{-6}$	$-0.009 \pm 3.0 \cdot 10^{-8}$	$-0.002 \pm 7.6 \cdot 10^{-7}$
^{235}U	$1.5 \cdot 10^{-4} \pm 3.2 \cdot 10^{-5}$	$-0.001 \pm 8.6 \cdot 10^{-6}$	$0.015 \pm 3.9 \cdot 10^{-5}$	$-4.7 \cdot 10^{-4} \pm 4.0 \cdot 10^{-8}$	$0.015 \pm 6.2 \cdot 10^{-6}$	$0.001 \pm 2.7 \cdot 10^{-5}$	$0.016 \pm 3.9 \cdot 10^{-5}$
	$0.072 \pm 5.2 \cdot 10^{-4}$	$-0.108 \pm 1.4 \cdot 10^{-4}$	$0.142 \pm 8.2 \cdot 10^{-5}$	$-0.030 \pm 4.0 \cdot 10^{-6}$	$0.255 \pm 5.3 \cdot 10^{-5}$	$-0.114 \pm 7.7 \cdot 10^{-7}$	$0.141 \pm 8.1 \cdot 10^{-5}$

Table 28. Relative β_{eff} sensitivities in %/% for SNEAK-LMFR-EXP-001-B with SUMMONR using Chiba's method

	(n,n)	(n,n')	(n,f)	(n, γ)	ν_d	ν_p	ν_t
^{235}U	$2.7 \cdot 10^{-4} \pm 6.9 \cdot 10^{-5}$	$-4.5 \cdot 10^{-4} \pm 1.9 \cdot 10^{-5}$	$0.062 \pm 9.5 \cdot 10^{-5}$	$-0.001 \pm 5.0 \cdot 10^{-7}$	$0.109 \pm 2.4 \cdot 10^{-5}$	$-0.045 \pm 3.7 \cdot 10^{-6}$	$0.063 \pm 9.2 \cdot 10^{-5}$
	$0.006 \pm 7.6 \cdot 10^{-4}$	$-0.114 \pm 1.6 \cdot 10^{-4}$	$0.240 \pm 9.5 \cdot 10^{-5}$	$-0.017 \pm 1.3 \cdot 10^{-5}$	$0.522 \pm 9.5 \cdot 10^{-5}$	$-0.330 \pm 3.9 \cdot 10^{-7}$	$0.192 \pm 8.1 \cdot 10^{-5}$
^{239}Pu	$-0.005 \pm 1.8 \cdot 10^{-4}$	$-0.004 \pm 5.7 \cdot 10^{-5}$	$-0.212 \pm 1.2 \cdot 10^{-4}$	$-0.008 \pm 1.5 \cdot 10^{-6}$	$0.312 \pm 5.9 \cdot 10^{-5}$	$-0.556 \pm 3.6 \cdot 10^{-6}$	$-0.244 \pm 1.7 \cdot 10^{-4}$
	$-5.9 \cdot 10^{-4} \pm 6.1 \cdot 10^{-5}$	$-0.001 \pm 1.4 \cdot 10^{-5}$	$-0.011 \pm 1.5 \cdot 10^{-6}$	$-6.4 \cdot 10^{-4} \pm 2.2 \cdot 10^{-7}$	$0.009 \pm 1.8 \cdot 10^{-6}$	$-0.023 \pm 3.2 \cdot 10^{-7}$	$-0.014 \pm 1.6 \cdot 10^{-6}$
^{241}Pu	$-5.8 \cdot 10^{-4} \pm 1.7 \cdot 10^{-5}$	$-1.6 \cdot 10^{-4} \pm 4.8 \cdot 10^{-6}$	$0.003 \pm 4.2 \cdot 10^{-6}$	$-2.2 \cdot 10^{-5} \pm 1.8 \cdot 10^{-8}$	$0.009 \pm 1.7 \cdot 10^{-6}$	$-0.005 \pm 1.1 \cdot 10^{-7}$	$0.003 \pm 4.1 \cdot 10^{-6}$

Table 29. Relative β_{eff} sensitivities in %/% for PU-MET-FAST-001 with SUMMONR using Chiba's method

	(n,n)	(n,n')	(n,f)	(n, γ)	ν_d	ν_p	ν_t
^{239}Pu	$0.098 \pm 6.7 \cdot 10^{-4}$	$0.009 \pm 2.3 \cdot 10^{-4}$	$-0.015 \pm 5.5 \cdot 10^{-4}$	$-0.021 \pm 1.6 \cdot 10^{-6}$	$0.947 \pm 3.7 \cdot 10^{-4}$	$-0.944 \pm 3.7 \cdot 10^{-4}$	$0.002 \pm 5.6 \cdot 10^{-4}$
	$0.011 \pm 1.5 \cdot 10^{-4}$	$1.7 \cdot 10^{-4} \pm 5.5 \cdot 10^{-5}$	$-0.003 \pm 1.1 \cdot 10^{-5}$	$-0.001 \pm 3.6 \cdot 10^{-7}$	$0.042 \pm 1.6 \cdot 10^{-5}$	$-0.049 \pm 2.2 \cdot 10^{-6}$	$-0.007 \pm 9.8 \cdot 10^{-6}$
^{241}Pu	$-0.001 \pm 1.8 \cdot 10^{-5}$	$-5.1 \cdot 10^{-4} \pm 1.2 \cdot 10^{-5}$	$0.005 \pm 3.8 \cdot 10^{-6}$	$-6.5 \cdot 10^{-5} \pm 2.2 \cdot 10^{-8}$	$0.007 \pm 2.7 \cdot 10^{-6}$	$-0.002 \pm 1.5 \cdot 10^{-6}$	$0.005 \pm 3.7 \cdot 10^{-6}$

Table 30. Relative β_{eff} sensitivities in %/% for PU-MET-FAST-006 with SUMMONR using Chiba's method

	(n,n)	(n,n')	(n,f)	(n, γ)	ν_d	ν_p	ν_t
^{235}U	$-0.002 \pm 3.7 \cdot 10^{-5}$	$-0.001 \pm 1.5 \cdot 10^{-5}$	$0.027 \pm 5.8 \cdot 10^{-5}$	$-0.001 \pm 3.6 \cdot 10^{-8}$	$0.021 \pm 9.6 \cdot 10^{-6}$	$0.009 \pm 4.6 \cdot 10^{-5}$	$0.030 \pm 5.8 \cdot 10^{-5}$
^{238}U	$0.086 \pm 7.3 \cdot 10^{-4}$	$-0.152 \pm 1.7 \cdot 10^{-4}$	$0.238 \pm 1.3 \cdot 10^{-4}$	$-0.052 \pm 2.9 \cdot 10^{-6}$	$0.343 \pm 9.4 \cdot 10^{-5}$	$-0.097 \pm 3.7 \cdot 10^{-6}$	$0.246 \pm 1.3 \cdot 10^{-4}$
^{239}Pu	$3.7 \cdot 10^{-4} \pm 3.0 \cdot 10^{-4}$	$-0.041 \pm 8.7 \cdot 10^{-5}$	$-0.273 \pm 3.2 \cdot 10^{-4}$	$-0.018 \pm 1.1 \cdot 10^{-6}$	$0.586 \pm 1.6 \cdot 10^{-4}$	$-0.846 \pm 2.2 \cdot 10^{-4}$	$-0.260 \pm 3.2 \cdot 10^{-4}$
^{240}Pu	$-0.001 \pm 7.7 \cdot 10^{-5}$	$-0.003 \pm 2.7 \cdot 10^{-5}$	$-0.015 \pm 3.7 \cdot 10^{-6}$	$-0.001 \pm 2.1 \cdot 10^{-7}$	$0.023 \pm 6.2 \cdot 10^{-6}$	$-0.042 \pm 8.5 \cdot 10^{-7}$	$-0.019 \pm 3.6 \cdot 10^{-6}$
^{241}Pu	$2.3 \cdot 10^{-4} \pm 1.6 \cdot 10^{-5}$	$-7.6 \cdot 10^{-5} \pm 8.3 \cdot 10^{-6}$	$0.002 \pm 2.0 \cdot 10^{-6}$	$-5.6 \cdot 10^{-5} \pm 1.7 \cdot 10^{-8}$	$0.005 \pm 1.2 \cdot 10^{-6}$	$-0.002 \pm 1.0 \cdot 10^{-6}$	$0.003 \pm 1.9 \cdot 10^{-6}$

In quantities where significant differences were observed between the prompt and deterministic methods, e.g., $^{239}\text{Pu}(n,n')$ and $^{240}\text{Pu}(n,f)$ in SNEAK-LMFR-EXP-001-A (Table 25 and Table 26), negligible differences are obtained with Chiba's method (Table 33). Elastic scattering sensitivities still differ from SUS3D sensitivities, however, closer results to the reference values are obtained with the modified method, as can be seen for $^{239,240}\text{Pu}$ in PU-MET-FAST-001 (Table 29) and for ^{238}U in IEU-MET-FAST-007 (Table 32). Quantities with low sensitivity, such as $^{240}\text{Pu}(n,\gamma)$ and $^{241}\text{Pu}(n,\gamma)$ in SNEAK-LMFR-EXP-001-B (Table 28), still differ from SUS3D values.

Table 31. Relative β_{eff} sensitivities in %/% for HEU-MET-FAST-028 with SUMMONR using Chiba's method

	(n,n)	(n,n')	(n,f)	(n, γ)	ν_d	ν_p	ν_t
^{234}U	$-3.7 \cdot 10^{-4} \pm 1.8 \cdot 10^{-5}$	$-8.4 \cdot 10^{-6} \pm 8.3 \cdot 10^{-6}$	$-0.004 \pm 2.0 \cdot 10^{-7}$	$-2.7 \cdot 10^{-4} \pm 4.0 \cdot 10^{-8}$	$0.004 \pm 4.8 \cdot 10^{-7}$	$-0.010 \pm 5.3 \cdot 10^{-9}$	$-0.005 \pm 2.3 \cdot 10^{-7}$
^{235}U	$0.022 \pm 2.3 \cdot 10^{-4}$	$-0.011 \pm 7.3 \cdot 10^{-5}$	$-0.045 \pm 1.8 \cdot 10^{-4}$	$-0.035 \pm 2.6 \cdot 10^{-6}$	$0.847 \pm 9.8 \cdot 10^{-5}$	$-0.837 \pm 5.6 \cdot 10^{-5}$	$0.010 \pm 1.7 \cdot 10^{-4}$
^{238}U	$0.040 \pm 3.3 \cdot 10^{-4}$	$-0.041 \pm 8.8 \cdot 10^{-5}$	$0.014 \pm 3.0 \cdot 10^{-5}$	$-0.013 \pm 4.4 \cdot 10^{-6}$	$0.133 \pm 1.8 \cdot 10^{-5}$	$-0.137 \pm 4.1 \cdot 10^{-8}$	$-0.005 \pm 2.5 \cdot 10^{-5}$

Table 32. Relative β_{eff} sensitivities in %/% for IEU-MET-FAST-007 with SUMMONR using Chiba's method

	(n,n)	(n,n')	(n,f)	(n, γ)	ν_d	ν_p	ν_t
^{234}U	$-3.2 \cdot 10^{-5} \pm 2.2 \cdot 10^{-5}$	$9.7 \cdot 10^{-5} \pm 6.4 \cdot 10^{-6}$	$-0.001 \pm 2.0 \cdot 10^{-8}$	$-7.1 \cdot 10^{-5} \pm 2.5 \cdot 10^{-8}$	$0.001 \pm 1.4 \cdot 10^{-7}$	$-0.002 \pm 2.9 \cdot 10^{-9}$	$-0.001 \pm 3.2 \cdot 10^{-8}$
^{235}U	$0.003 \pm 2.3 \cdot 10^{-4}$	$-0.003 \pm 6.7 \cdot 10^{-5}$	$0.046 \pm 2.4 \cdot 10^{-4}$	$-0.013 \pm 1.9 \cdot 10^{-6}$	$0.569 \pm 7.1 \cdot 10^{-5}$	$-0.502 \pm 2.4 \cdot 10^{-5}$	$0.067 \pm 2.2 \cdot 10^{-4}$
^{238}U	$-0.004 \pm 7.1 \cdot 10^{-4}$	$-0.019 \pm 2.6 \cdot 10^{-4}$	$0.021 \pm 6.5 \cdot 10^{-5}$	$-0.048 \pm 1.5 \cdot 10^{-5}$	$0.393 \pm 4.6 \cdot 10^{-5}$	$-0.459 \pm 9.5 \cdot 10^{-8}$	$-0.065 \pm 2.5 \cdot 10^{-5}$

Table 33. Relative β_{eff} sensitivities in %/% for SNEAK-LMFR-EXP-001-A with SUMMONR using Chiba's method

	(n,n)	(n,n')	(n,f)	(n, γ)	ν_d	ν_p	ν_t
^{235}U	$-0.006 \pm 1.7 \cdot 10^{-4}$	$-0.001 \pm 3.1 \cdot 10^{-5}$	$0.036 \pm 1.7 \cdot 10^{-4}$	$-0.001 \pm 1.1 \cdot 10^{-6}$	$0.061 \pm 3.6 \cdot 10^{-5}$	$-0.023 \pm 3.2 \cdot 10^{-5}$	$0.038 \pm 1.6 \cdot 10^{-4}$
^{238}U	$0.013 \pm 1.4 \cdot 10^{-3}$	$-0.097 \pm 3.7 \cdot 10^{-4}$	$0.284 \pm 2.0 \cdot 10^{-4}$	$-0.031 \pm 3.3 \cdot 10^{-5}$	$0.461 \pm 1.6 \cdot 10^{-4}$	$-0.241 \pm 6.5 \cdot 10^{-7}$	$0.219 \pm 1.9 \cdot 10^{-4}$
^{239}Pu	$0.005 \pm 6.3 \cdot 10^{-4}$	$-0.009 \pm 1.7 \cdot 10^{-4}$	$-0.216 \pm 5.0 \cdot 10^{-4}$	$-0.017 \pm 9.5 \cdot 10^{-6}$	$0.417 \pm 1.5 \cdot 10^{-4}$	$-0.663 \pm 4.2 \cdot 10^{-5}$	$-0.245 \pm 6.0 \cdot 10^{-4}$
^{240}Pu	$-0.009 \pm 1.6 \cdot 10^{-4}$	$-0.003 \pm 3.8 \cdot 10^{-5}$	$-0.013 \pm 5.3 \cdot 10^{-6}$	$-0.001 \pm 2.1 \cdot 10^{-6}$	$0.014 \pm 5.1 \cdot 10^{-6}$	$-0.031 \pm 1.9 \cdot 10^{-6}$	$-0.017 \pm 4.4 \cdot 10^{-6}$
^{241}Pu	$4.0 \cdot 10^{-5} \pm 5.5 \cdot 10^{-5}$	$3.5 \cdot 10^{-4} \pm 1.7 \cdot 10^{-5}$	$0.005 \pm 1.4 \cdot 10^{-5}$	$-6.2 \cdot 10^{-5} \pm 1.3 \cdot 10^{-7}$	$0.012 \pm 4.6 \cdot 10^{-6}$	$-0.006 \pm 1.4 \cdot 10^{-6}$	$0.005 \pm 1.3 \cdot 10^{-5}$

Differences in elastic sensitivities and in quantities with low sensitivities can be attributed to the subtraction of nearly equal sensitivity profiles when using Eqs. 5.30 and 5.35. An example is given in Figure 18 where the energy-dependent sensitivities of k_{eff} to $^{241}\text{Pu}(n,\gamma)$ calculated for the nominal case, S_k , and for the perturbed cases using only prompt neutrons (prompt method), $S_{kprompt}$, and the perturbed libraries (modified method), S_{kchiba} , are shown. It can be seen that the differences between the sensitivity profiles calculated for the nominal and perturbed cases are nearly negligible, which turns the subtraction to be very sensitive to the statistical uncertainties of the energy-dependent sensitivity coefficients. This problem is not observed in quantities with high sensitivities (Figure 19), where differences between sensitivity profiles are significant when using both methods. In fact, elastic reactions with high sensitivity, as in the case of $^{238}\text{U}(n,n)$ in PU-MET-FAST-006 (Table 30) and HEU-MET-FAST-028 (Table 31) integral experiments, are very close to the reference deterministic values when using Chiba's method.

Figure 18. Energy-dependent β_{eff} sensitivities to $^{241}\text{Pu}(n,\gamma)$ for SNEAK-LMFR-EXP-001-B

Figure 19. Energy-dependent β_{eff} sensitivities to $^{239}\text{Pu}(n,n')$ for SNEAK-LMFR-EXP-001-A

5.4.3. Effective neutron generation time sensitivities

First, the implementation of the I / ν insertion method in SUMMON for thermal and fast systems was validated using the LEU-COMP-THERM-077-003 [OECD/NEA, 2015f] and HEU-COMP-FAST-100-002 [OECD/NEA, 2015g] integral experiments from the ICSBEP Handbook, the ENDF/B-VII.0 nuclear data library and the artificial material shown in Figure 11. These two experiments are the only ones available in public available in databases ICSBEP and IRPhE with referenced experimental Λ_{eff} values. The calculated Λ_{eff} for these experiments with both the IFP methodology (MCNP) and the I / ν method (SUMMON) using different perturbation sizes are shown in Table 34 and Table 35. Relative differences between SUMMON and the experimental value are included in the last column of these tables.

Table 34. Λ_{eff} values calculated by IFP and I / ν for LEU-COMP-THERM-077-003

$$\Lambda_{eff\,exp} = 31.96 \pm 0.35 \mu s$$

MCNP (IFP)	SUMMON (I / ν method)					
$\Lambda_{eff}(\mu s)$	N(c) (a/b·cm)	c (s ⁻¹)	k _c	Δp (pcm)	$\Lambda_{eff}(\mu s)$	Rel. diff. (%)
27.32 ± 0.005	$1 \cdot 10^{-9}$	$1 \cdot 10^0$	1.00356	1.99	19.86 ± 140.42	-37.87
	$1 \cdot 10^{-8}$	$1 \cdot 10^1$	1.00330	27.81	27.81 ± 14.05	-12.99
	$1 \cdot 10^{-7}$	$1 \cdot 10^2$	1.00084	272.79	27.28 ± 1.41	-14.65
	$1 \cdot 10^{-6}$	$1 \cdot 10^3$	0.97690	2721.35	27.21 ± 0.14	-14.85
	$1 \cdot 10^{-5}$	$1 \cdot 10^4$	0.79295	26468.08	26.47 ± 0.02	-17.18

For the thermal system (Table 34), there is a difference of nearly 15% between the experimental Λ_{eff} and the calculated Λ_{eff} with both methodologies, however, the best estimate Λ_{eff} values predicted by the IFP and the $1/v$ methods differ by less than 1% when using a 300 pcm perturbation. The difference between the experimental and calculated values can be attributed to the nuclear data library employed in the calculation. This agrees with the results contained within the IRPhE database [OECD/NEA, 2017a], with an estimated value for Λ_{eff} using MCNP-4C code [Briesmeister, 2000] of 26.67 μ s with ENDF/B-VI.8, 29.67 μ s with JEFF-3.1 and 29.47 μ s with JENDL-3.3 nuclear data libraries.

In Table 35, Λ_{eff} values predicted by both methods are in agreement with the experimental result within 1σ of uncertainty. It can clearly be seen that the optimum size of the perturbation using the $1/v$ method, to have a good agreement with the IFP Λ_{eff} (less than 5% difference with experimental value), is higher than for the thermal system (between 500 - 5000 pcm instead of 30 - 300 pcm). Indeed, Verboomen et al. [Verboomen et al., 2006] reported that though a perturbation of 300 pcm is in the range of applicability of the first-order perturbation formula for reactivity increments (Eq. 5.41) for thermal systems, the corresponding value of c is much larger for fast systems. However, in light of the results shown in Table 34, it seems that perturbations two orders of magnitude higher than 300 pcm are still within the range of applicability for thermal systems. That is not the case in fast systems, where linearity starts to be lost around perturbations of 5000 pcm due to the high absorber material concentration needed to further perturb the system. Nevertheless, for the HEU-COMP-FAST-100-002 integral experiment the IFP and $1/v$ perturbation Λ_{eff} calculated values differ less than 1% for a perturbation of nearly 600 pcm.

Table 35. Λ_{eff} values calculated by IFP and $1/v$ for HEU-COMP-FAST-100-002

$$\Lambda_{eff\ exp} = 5.94 \pm 0.59\ ns$$

MCNP (IFP)	SUMMON ($1/v$ method)					
Λ_{eff} (ns)	N(c) (a/b·cm)	c (s ⁻¹)	k _c	$\Delta\rho$ (pcm)	Λ_{eff} (ns)	Rel. diff. (%)
5.724 ± 0.002	1·10 ⁻⁶	1·10 ³	0.99820	1.00	10.04 ± 14.19	68.96
	1·10 ⁻⁵	1·10 ⁴	0.99816	5.02	5.02 ± 1.42	-15.52
	1·10 ⁻⁴	1·10 ⁵	0.99765	56.23	5.62 ± 0.14	-5.33
	1·10 ⁻³	1·10 ⁶	0.99258	568.23	5.68 ± 0.01	-4.34
	1·10 ⁻²	1·10 ⁷	0.94626	5499.88	5.50 ± 0.002	-7.41
	1·10 ⁻¹	1·10 ⁸	0.68355	46115.76	4.61 ± 0.0002	-22.36

An additional validation was carried out using ¹⁰B instead of the artificial material for cases where the MC code cannot use the modified libraries provided with SUMMON (Table 36). It can be seen that for the thermal system ¹⁰B provides nearly the same Λ_{eff} calculated value than the

artificial material, confirming that, as stated in Section 5.2.1.4, ^{10}B serves as a good approximation in Λ_{eff} and $S_{\Lambda_{eff},\alpha}$ calculations for thermal systems. On the other hand, the use of ^{10}B in the calculation with the fast system causes a significant deviation from the artificial material and experimental Λ_{eff} values. Therefore, the use of the methodology implemented in SUMMON without employing the artificial material library is not recommended for fast systems.

Table 36. Λ_{eff} values calculated by IFP and $1/\nu$ for HEU-COMP-FAST-100-002

System	SUMMON ($1/\nu$ method)					
	N(c) (a/b·cm)	c (s ⁻¹)	k _c	$\Delta\rho$ (pcm)	Λ_{eff}	Rel. diff. (%)
LCT-077-003	$1 \cdot 10^{-7}$	$1 \cdot 10^2$	1.00126	230.88	$27.31 \pm 1.41 \mu\text{s}$	-14.55
HCF-100-002	$1 \cdot 10^{-3}$	$1 \cdot 10^6$	0.99596	226.32	$2.68 \pm 0.01 \text{ ns}$	-54.94

The methodology proposed to calculate Λ_{eff} sensitivity to a change in some nuclear data α was verified comparing SUMMON results for the PU-MET-FAST-001 integral experiment with the effective prompt lifetime sensitivities, $S_{l_{eff},\alpha}$, SERPENT calculations performed by Aufiero et al. [Aufiero et al., 2015] using the ENDF/B-VII.0 evaluation, as no other reference to this type of calculations could be found in bibliography. The effective prompt lifetime sensitivities were derived from the relation between the effective neutron generation time and the effective prompt lifetime; that is:

$$\Lambda_{eff} = \frac{l_{eff}}{k_{eff}} \Rightarrow \frac{\alpha}{\Lambda_{eff}} \frac{\partial \Lambda_{eff}}{\partial \alpha} = \frac{\alpha}{\partial \alpha} \left(\frac{\partial l_{eff}}{l_{eff}} - \frac{\partial k_{eff}}{k_{eff}} \right) \Rightarrow S_{\Lambda_{eff},\alpha} = S_{l_{eff},\alpha} - S_{k_{eff},\alpha} \quad (5.47)$$

A calculation was performed with MCNP to determine Λ_{eff} . Then, according to the results obtained for HEU-COMP-FAST-100-002, perturbations between 500 pcm and 5000 pcm with the $1/\nu$ insertion method were carried out to determine the optimum value of c . Differences of less than 3% were obtained between the IFP Λ_{eff} value and the $1/\nu$ insertion Λ_{eff} values for perturbations smaller than 3000 pcm, while the last perturbation results in an inaccurate Λ_{eff} due to the loss of linearity, as can be seen in Table 37.

Table 37. Calculated Λ_{eff} for different perturbations of the parameter c using the $1/\nu$ insertion method for PU-MET-FAST-001

MCNP (IFP)	SUMMON ($1/\nu$ method)					
	N(c) (a/b·cm)	c (s ⁻¹)	k _c	$\Delta\rho$ (pcm)	Λ_{eff} (ns)	Rel. diff. (%)
2.87 ± 0.002	$5 \cdot 10^{-3}$	$5 \cdot 10^6$	0.98593	1414.08	2.83 ± 0.003	-1.53
	$1 \cdot 10^{-2}$	$1 \cdot 10^7$	0.97264	2799.96	2.80 ± 0.001	-2.51
	$5 \cdot 10^{-2}$	$5 \cdot 10^7$	0.88386	13127.09	2.63 ± 0.0003	-8.59

Finally, for each perturbation, Λ_{eff} and l_{eff} sensitivities were calculated with the SUMMONR module and compared against SERPENT values (Table 38). For the smallest perturbation (~ 1500 pcm), SUMMONR $S_{l_{eff},\alpha}$ values yield differences of less than 6%, except for the elastic and inelastic reactions which can be attributed to the same problem identified in Section 5.4.2. The ~ 3000 pcm perturbation also gives values close to SERPENT, although the relative difference between SUMMONR and SERPENT values is increased. The biggest perturbation produces the highest differences between both codes.

Therefore, for calculating $S_{\Lambda_{eff},\alpha}$ in fast systems, perturbations around 500 pcm to 3000 pcm are recommended so that linearity is preserved. The perturbation with the smallest difference between the best estimate MCNP Λ_{eff} value and the one calculated with the Eq. 5.41 should be chosen to estimate $S_{\Lambda_{eff},\alpha}$.

Table 38. Comparison between l_{eff} sensitivities calculated with SUMMONR for different perturbation sizes for PU-MET-FAST-001. Statistical uncertainties of $S_{l_{eff},\alpha}$ are neglected and all sensitivities are given in %/% units

		SERPENT $S_{l_{eff},\alpha}$	SUMMONR								
			$c = 5 \times 10^6 \text{ s}^{-1},$ $\Delta\rho \sim 1500 \text{ pcm}$			$c = 1 \times 10^7 \text{ s}^{-1},$ $\Delta\rho \sim 3000 \text{ pcm}$			$c = 5 \times 10^7 \text{ s}^{-1},$ $\Delta\rho \sim 13000 \text{ pcm}$		
			$S_{\Lambda_{eff},\alpha}$	$S_{l_{eff},\alpha}$	Diff. (%)	$S_{\Lambda_{eff},\alpha}$	$S_{l_{eff},\alpha}$	Diff. (%)	$S_{\Lambda_{eff},\alpha}$	$S_{l_{eff},\alpha}$	Diff. (%)
^{239}Pu	(n,f)	-0.247	$-0.978 \pm 8.0 \cdot 10^{-4}$	-0.250	-1.31	$-0.967 \pm 4.1 \cdot 10^{-4}$	-0.239	3.26	$-0.946 \pm 9.4 \cdot 10^{-5}$	-0.217	12.03
	(n,n)	0.227	$0.174 \pm 3.7 \cdot 10^{-4}$	0.237	-3.18	$0.142 \pm 1.8 \cdot 10^{-4}$	0.205	10.81	$0.106 \pm 3.6 \cdot 10^{-5}$	0.169	26.52
	(n,n')	0.202	$0.142 \pm 2.2 \cdot 10^{-4}$	0.181	10.18	$0.148 \pm 1.1 \cdot 10^{-4}$	0.188	7.09	$0.137 \pm 2.4 \cdot 10^{-5}$	0.176	12.90
	(n, γ)	-0.037	$-0.027 \pm 1.5 \cdot 10^{-5}$	-0.034	5.90	$-0.024 \pm 7.1 \cdot 10^{-6}$	-0.032	12.85	$-0.016 \pm 1.3 \cdot 10^{-6}$	-0.024	35.74
	ν	0.010	$-0.956 \pm 8.8 \cdot 10^{-4}$	0.009	2.26	$-0.957 \pm 4.5 \cdot 10^{-4}$	0.009	3.78	$-0.957 \pm 1.0 \cdot 10^{-4}$	0.009	10.56
^{240}Pu	(n,f)	-0.013	$-0.036 \pm 3.0 \cdot 10^{-5}$	-0.013	-0.01	$-0.036 \pm 1.5 \cdot 10^{-5}$	-0.013	2.16	$-0.036 \pm 3.6 \cdot 10^{-6}$	-0.012	3.53
	(n,n)	0.013	$-1.8 \cdot 10^{-4} \pm 7.9 \cdot 10^{-5}$	0.003	76.40	$0.007 \pm 3.9 \cdot 10^{-5}$	0.010	21.63	$0.006 \pm 7.8 \cdot 10^{-6}$	0.010	27.81
	(n,n')	0.008	$0.010 \pm 4.5 \cdot 10^{-5}$	0.012	-36.09	$0.003 \pm 2.2 \cdot 10^{-5}$	0.005	43.21	$0.006 \pm 4.6 \cdot 10^{-6}$	0.008	5.27
	(n, γ)	-0.002	$-0.002 \pm 9.4 \cdot 10^{-7}$	-0.002	4.77	$-0.001 \pm 4.5 \cdot 10^{-7}$	-0.002	11.78	$-0.001 \pm 8.2 \cdot 10^{-8}$	-0.002	34.02
	ν	-0.010	$-0.041 \pm 3.3 \cdot 10^{-5}$	-0.010	4.46	$-0.041 \pm 1.7 \cdot 10^{-5}$	-0.010	5.77	$-0.041 \pm 3.9 \cdot 10^{-6}$	-0.009	10.77

5.5. Application to MYRRHA

Sensitivity and uncertainty analyses of the effective neutron multiplication factor and of two reactivity changes in ALFRED lead-cooled fast reactor were performed in Section 5.4.1, which allowed not only verifying the SUMMON system, but also identifying the most important nuclear data for neutron induced reactions for criticality safety calculations of ALFRED. To confirm that the quantities obtained in the previous S/U analyses are the most important from the neutronic point of view of an LFR and to make an additional verification, SUMMON was applied, together with the ENDF/B-VII.0 nuclear data library, to perform a complete S/U analysis of k_{eff} in MYRRHA lead-bismuth cooled fast reactor. A description of the model can be found in Chapter 7, Section 7.2. Results obtained from the analysis were compared against results from the SCALE system and SUD3D code, obtained within the CHANDA project [Romojaro et al., 2015].

5.5.1. Sensitivity analysis

The Integrated Sensitivity Coefficients (ISC), obtained by SCALE and MCNP, using the ENDF/B-VII.0 library, and by SUD3D, using the ENDF/B-VII.1 library [Chadwick et al., 2011], for the 10 major contributors to the uncertainty in k_{eff} for the MYRRHA critical core are shown in Table 39.

Table 39. ISC of the major contributors to the k_{eff} uncertainty for the critical core obtained by different codes

Quantity	Integrated Sensitivity Coefficients (%/%)		
	MCNP/KSEN ENDF/B-VII.0	SCALE ENDF/B-VII.0	SUD3D ENDF/B-VII.1 [Romojaro et al., 2015]
$^{239}\text{Pu } \nu$	$7.06 \cdot 10^{-1} \pm 3 \cdot 10^{-6}$	$6.98 \cdot 10^{-1} \pm 2 \cdot 10^{-5}$	$6.99 \cdot 10^{-1}$
$^{239}\text{Pu}(n,f)$	$4.93 \cdot 10^{-1} \pm 4 \cdot 10^{-6}$	$4.83 \cdot 10^{-1} \pm 2 \cdot 10^{-4}$	$4.88 \cdot 10^{-1}$
$^{238}\text{U}(n,\gamma)$	$-1.17 \cdot 10^{-1} \pm 2 \cdot 10^{-6}$	$-1.19 \cdot 10^{-1} \pm 6 \cdot 10^{-5}$	$-1.20 \cdot 10^{-1}$
$^{240}\text{Pu } \nu$	$8.02 \cdot 10^{-2} \pm 2 \cdot 10^{-6}$	$7.91 \cdot 10^{-2} \pm 3 \cdot 10^{-5}$	$7.83 \cdot 10^{-2}$
$^{239}\text{Pu}(n,\gamma)$	$-5.59 \cdot 10^{-2} \pm 2 \cdot 10^{-7}$	$-5.80 \cdot 10^{-2} \pm 3 \cdot 10^{-4}$	$-5.71 \cdot 10^{-2}$
$^{238}\text{U}(n,n')$	$-1.90 \cdot 10^{-2} \pm 2 \cdot 10^{-5}$	$-1.84 \cdot 10^{-2} \pm 4 \cdot 10^{-4}$	$-1.87 \cdot 10^{-2}$
$^{56}\text{Fe}(n,\gamma)$ - whole core	-	$-1.81 \cdot 10^{-2} \pm 9 \cdot 10^{-6}$	$-1.45 \cdot 10^{-2}$
$^{238}\text{U}(n,n)$	$1.54 \cdot 10^{-2} \pm 3 \cdot 10^{-5}$	$1.67 \cdot 10^{-2} \pm 2 \cdot 10^{-4}$	$8.09 \cdot 10^{-3}$
$^{238}\text{Pu}(n,f)$	$2.22 \cdot 10^{-3} \pm 6 \cdot 10^{-7}$	$1.30 \cdot 10^{-2} \pm 3 \cdot 10^{-6}$	$1.26 \cdot 10^{-2}$
$^{56}\text{Fe}(n,\gamma)$ - active zone	$-7.57 \cdot 10^{-3} \pm 4 \cdot 10^{-7}$	$-8.50 \cdot 10^{-3} \pm 5 \cdot 10^{-6}$	$-8.65 \cdot 10^{-3}$
$^{239}\text{Pu } \chi$	$0.00 \pm 5 \cdot 10^{-6}$	$0.00 \pm 3 \cdot 10^{-5}$	0.00

It can be highlighted that:

- $^{238}\text{Pu}(n,f)$ MCNP sensitivity has an 83% difference regarding the SCALE result due to differences in ^{238}Pu nuclear data files, which agrees with the results obtained in Section 5.4.1 (Figure 15);
- $^{238}\text{U}(n,n)$ (Figure 20), obtained by SUS3D, has a difference of 51% to the value provided by SCALE, which can be mainly attributed to omitting the implicit sensitivity contribution (not taking into account the effects associated with changes in resonance-shielded MG data) in SUS3D. An assessment with the SCALE code revealed that the contribution of the implicit term to the total sensitivity for this quantity is 30%. The rest of the difference can be attributed to differences in the group structure and in the model;
- $^{56}\text{Fe}(n,\gamma)$ (Figure 21) has a difference of 11% (active zone only) between MCNP and SCALE and 20% (whole core) between SUS3D and SCALE. The differences obtained for this quantity between SUS3D and SCALE are mostly due to different models used in SUS3D (2D cylindrical) and SCALE (3D). Note that in the active zone SUS3D and SCALE results differ by less than 2%;
- other ISC values are very close between codes, most of them with a difference smaller than 4%. Sensitivity profiles of the most relevant quantities are given in Figure 22 - Figure 24.

Figure 20. Sensitivity coefficients of MYRRHA k_{eff} to $^{238}\text{U}(n,n)$ provided by the different codes for the critical core and whole energy interval

Figure 21. Sensitivity coefficients of MYRRHA k_{eff} to $^{56}\text{Fe}(n,\gamma)$ provided by the different codes for the active zone of the critical core and whole energy interval

Figure 22. Sensitivity coefficients of MYRRHA k_{eff} to $^{239}\text{Pu } \nu$ provided by the different codes for the critical core and whole energy interval

Figure 23. Sensitivity coefficients of MYRRHA k_{eff} to $^{238}\text{U}(n,n')$ provided by the different codes for the critical core

Figure 24. Sensitivity coefficients of MYRRHA k_{eff} to $^{238}\text{U}(n,\gamma)$ provided by the different codes for the critical core and whole energy interval

5.5.2. Uncertainty quantification

The uncertainty quantification analysis for MYRRHA is shown in Table 40. SCALE6.1-44g covariance library has been used by all the codes to propagate the uncertainty in nuclear data. It can be ascertained, by the similarity of the major contributors, that the most relevant quantities are nearly identical for ALFRED (Table 6) and MYRRHA reactors for what concerns k_{eff} uncertainty quantification. The total uncertainty in k_{eff} due to uncertainties in nuclear data for both reactors, according to SCALE's ENDF/B-VII.0-based nuclear data library, is around 1%.

Table 40. Main contributors to the k_{eff} uncertainty for MYRRHA. Statistical uncertainties have been omitted

Quantity	$\Delta k_{eff}/k_{eff}$ (%)		
	SUMMON	SCALE	SUSD3D [Romojaro et al., 2015]
$^{239}\text{Pu } \nu$	0.716	0.705	0.701
$^{238}\text{U}(n,n')$	0.320	0.319	0.324
$^{239}\text{Pu}(n,\gamma)$	0.263	0.270	0.265
$^{240}\text{Pu } \nu$	0.238	0.235	0.227
$^{239}\text{Pu}(n,f)$	0.188	0.188	0.188
$^{239}\text{Pu } \chi$	0.130	0.182	0.183
$^{238}\text{Pu}(n,f)$	0.030	0.161	0.160
$^{238}\text{U}(n,\gamma)$	0.151	0.156	0.152
$^{238}\text{U}(n,n) - (n,n')$	0.123	0.122	0.085
$^{238}\text{U } \nu$	0.083	0.094	0.083
$^{56}\text{Fe}(n,\gamma)$	0.055	0.216	0.073
TOTAL	0.959	0.957	0.945

5.6. Conclusions

Due to the limitations of existing tools, Sensitivity and Uncertainty Methodology for MONte carlo codes (SUMMON), a general methodology to calculate the sensitivities and uncertainties of the criticality safety parameters, has been developed. SUMMON has been conceived as a tool to perform complete automated sensitivity and uncertainty analyses of the most relevant criticality safety parameters of detailed complex reactor designs from the neutronic point of view, i.e., k_{eff} , β_{eff} , Λ_{eff} and reactivity coefficients, using nuclear data and corresponding covariance matrices from state-of-the-art nuclear data libraries.

The methodology is based on the use of the KSEN card of MCNP code to perform the eigenvalue sensitivity calculations, although any code that can provide sensitivity coefficients can be used. The sensitivity coefficients of a reactivity response are calculated using the eigenvalue definition of reactivity, which is equivalent to applying the Equivalent Generalized Perturbation

Theory. Moreover, the effective delayed neutron fraction sensitivity coefficients are derived from Bretscher's approximation or employing Chiba's modified method, whereas the sensitivity coefficients of the effective neutron generation time are obtained using the $1/\nu$ insertion method and the Equivalent Generalized Perturbation Theory. Uncertainties are propagated using the "Sandwich Rule" of the "Propagation of Moments" method employing covariance data from state-of-the-art covariance libraries.

The model of the GEN-IV Lead-cooled Fast Reactor ALFRED has been used to verify the implementation of the eigenvalue and eigenvalue-difference response sensitivity estimation and uncertainty quantification capabilities. Additionally, the effect of Monte Carlo statistical uncertainties in the methodology has been studied. Good agreement between KSEN and TSUNAMI-3D MG has been found in the sensitivity analyses when using a sufficient number of neutrons in the calculations so that in the studied cases the statistical uncertainty in k_{eff} does not exceed 2 pcm. Good agreement has also been found between TSUNAMI-3D MG and the SUMMONR code in the uncertainty quantification.

SUMMON's implementations to derive the sensitivity of the effective delayed neutron fraction method have been verified using integral benchmark experiments from the International Handbook of Evaluated Criticality Safety Benchmark Experiments and comparing SUMMON with the deterministic code SUS3D. For each benchmark, the β_{eff} values calculated with the prompt methodology are within 2σ of the experimental values. For the prompt method, good agreement has been found in (n,f) and (n, γ) reactions and the average delayed, prompt and total neutron fission multiplicities, whereas differences are found in the (n,n) and (n,n') β_{eff} sensitivities due to differences in the k_{eff} sensitivity to nuclear data predicted by both codes for those particular reactions. Chiba's method has been also verified using the same integral benchmarks and improved results have been obtained, except for the (n,n) reaction due to the inherent difficulty of accurately estimating the sensitivity to elastic scattering.

The implementation in of the $1/\nu$ method for the estimation of Λ_{eff} has been validated using a thermal and a fast integral experiment. Furthermore, the limits of the applicability of the first-order perturbation formula for reactivity increments have been studied. For both systems, the difference between the IFP and perturbed method is less than 1%. A method to calculate Λ_{eff} sensitivities using the $1/\nu$ insertion method and Equivalent Generalized Perturbation Theory has also been proposed. This method has been tested deriving l_{eff} sensitivities from Λ_{eff} sensitivities and comparing the results against the SERPENT code for the PU-MET-FAST-001 benchmark. Likewise, good agreement was found for all reactions except (n,n) and (n,n').

Finally, SUMMON has been applied to the model of the MYRRHA lead-bismuth cooled fast reactor to confirm that the quantities obtained in the ALFRED S/U analyses are the most important from the neutronic point of view of an LFR and to make an additional verification.

From the sensitivity and uncertainty analyses performed in this chapter and published in Ref. [Romojaro et al., 2015], it can be concluded that the following list of quantities are relevant from the criticality safety point of view of LFR reactors:

- ^{239}Pu v fast, $^{239}\text{Pu}(n,\gamma)$ both resonance and fast, $^{239}\text{Pu}(n,f)$ fast, ^{239}Pu fission spectrum;
- $^{238}\text{U}(n,n')$ fast, $^{238}\text{U}(n,\gamma)$ resonance and fast, ^{238}U elastic scattering in resonance and fast energy regions;
- ^{240}Pu v fast;
- $^{238}\text{Pu}(n,f)$ both resonance and fast;
- $^{56}\text{Fe}(n,\gamma)$ both resonance and fast, ^{56}Fe elastic and inelastic;
- and $^{204,206,207,208}\text{Pb}$ elastic and inelastic scattering in resonance and fast regions.

Additionally, due to the flexibility of MYRRHA facility in providing various irradiation environments, it is expedient to consider also $^{209}\text{Bi}(n,\gamma)$ and (n,n') in resonance and fast energy regions [Romojaro et al., 2015].

Chapter 6

Contributions to the JEFF-3.3 Nuclear Data Library

Abstract – Before nuclear data can be used for practical applications, a thorough verification/validation must be performed in order to ensure that the data is consistent with energy dependent and integral experimental measurements. In this chapter, validation and benchmarking studies performed for JEFF-3.3 evaluations of LFR coolant materials (i.e., lead and bismuth) are shown. First, the origins of the evaluations are established and then, the nuclear data evaluations are validated against energy dependent and integral experimental data. A final verification and benchmarking are carried out for ALFRED and MYRRHA reactors, in order to analyse the impact of the differences between the previous lead and bismuth evaluations and the new ones on the criticality and neutronics of both reactors.

This chapter shows, partially or completely, works already presented in the following references:

- CHANDA Deliverable D10.3 [Romojaro and Žerovnik, 2016]
- CHANDA Milestone MS10.1 [Kodeli et al., 2016b]
- JRC Technical Report [Žerovnik et al., 2016]
- International Conference Proceeding [Romojaro et al., 2017c]
- International Conference Proceeding [Cabellos et al., 2017]
- CHANDA Deliverable D10.5 [Žerovnik et al., 2017b]
- JRC Technical Report [Žerovnik et al., 2017a]
- CHANDA Deliverable D10.4 [Kodeli et al., 2018]

6.1. Introduction

The Joint Evaluated Fission and Fusion (JEFF) project involves evaluation efforts that cover the main nuclear data needs in the fields of fission and fusion applications. Although JEFF is an OECD/NEA coordinated project, the OECD member states USA and Japan continue to develop their own nuclear data libraries, and therefore the JEFF project involves essentially scientists from European countries. While existing reactors and fuel cycles remain the areas of essential application for JEFF, innovative reactor concepts (Generation IV systems), transmutation of radioactive waste, fusion, medical applications, and various non-energy related industrial applications also make use of the JEFF data files. The European Fusion File (EFF) project contributes to this initiative through specific tasks on nuclear data evaluations, library production, verification of data, development of computer programs and validation of nuclear data through integral experiments [Koning, 2007].

The latest version of the JEFF library, JEFF-3.3, was released in November 2017. Several beta versions were released previously: JEEF-3.3T1 in March 2016, JEFF-3.3T2 in July 2016, JEFF-3.3T3 in March 2017 and JEFF-3.3T4 in August 2017. JEFF-3.3 contains a neutron-induced reaction data library with data for 562 nuclides or elements, thermal scattering law data for 20 materials and thousands of files containing special purpose spontaneous and neutron induced fission yield data, decay data, alpha particle induced data, deuteron induced data, displacement data, gamma induced data, ^3He induced data and proton induced data.

Before nuclear data can be used for practical applications, a thorough verification/validation must be performed in order to ensure that the data is consistent with energy dependent and integral experimental measurements [Trkov, 2005]. Consequently, before the final version of the library was released, thorough validation, verification and benchmarking was performed within the JEFF collaboration in order to ensure the quality and accuracy of the data.

In this chapter the validation, verification and benchmarking of key nuclear data for LFRs will be shown. In particular, from the list of the key quantities for a lead-cooled fast reactor established in Chapter 5, the coolant materials, lead and bismuth, were chosen as the main objects of study since they are of vital importance for the neutronic performance and criticality safety and were not covered in the CIELO pilot project [Chadwick et al., 2018], a collaborative international effort which brought together nuclear data experimentalists and evaluators towards the production of new generation neutron data files for the most important nuclides for reactor applications, including ^{56}Fe , $^{235,238}\text{U}$ and ^{239}Pu .

6.2. Origin of the JEFF-3.3 lead and bismuth evaluations

6.2.1. ^{204}Pb

The JEFF-3.3 file is taken from the JEFF-3.2 evaluation [OECD/NEA Data Bank, 2014], which is an NRG evaluation [Rochman and Koning, 2008], based on the JEFF-3.1 file [Koning et al., 2006]. Resonance parameters were updated based on the Atlas of neutron resonances [Mughabghab, 2006]. The Resolved Resonance Region (RRR) was extended up to 900 keV, however only the part up to 100 keV is used in the RRR. The original JEFF-3.1 evaluation is based on a theoretical analysis with the nuclear model code TALYS [Koning and Rochman, 2012]. The resonance parameters below 50 keV were adopted from JENDL-3.3. Also, above the RRR, the evaluation was tested against experimental data for natural lead, in particular to data of Finlay [Finlay et al., 1993]. Finally, for evaluation of inelastic scattering, (n,p) and neutron multiplicity reactions, data of Plompen et al. [Plompen et al., 2002] were taken into account.

6.2.2. ^{206}Pb

The JEFF-3.3 file is based on JENDL-4.0 evaluation [Shibata et al., 2011] with modifications in the elastic scattering, total inelastic scattering and level inelastic scattering cross sections and with covariance data included. JENDL-4.0 resonance parameters are based on the Atlas of neutron resonances and the experimental data of Domingo-Pardo [Domingo-Pardo et al., 2007] and Borella [Borella et al., 2007]. The total cross section is based on experimental data from Horen [Horen et al., 1979] and Foster Jr. [Foster Jr and Glasgow, 1971] and calculations with the CCONE code [Iwamoto, 2007]. Cross sections of all relevant reactions were calculated by CCONE, except the (n, α) cross section below 820 keV which was calculated from resonance parameters, by assuming a mean alpha width of $9.0 \cdot 10^{-8}$ eV for s-wave resonances and $1.5 \cdot 10^{-7}$ eV for p- and d-wave resonances. The total inelastic and level inelastic scattering cross sections were modified to include renormalized experimental data by Mihailescu et al. [Negret et al., 2015] up to 3.1 MeV. Above this energy the original JENDL-4.0 evaluation was scaled by a linearly energy dependent factor that achieves continuity at 3.1 MeV and equals 1 at 20 MeV. The total inelastic cross section is the sum of all the level inelastic cross sections. The elastic scattering cross section was obtained by subtraction of the non-elastic cross sections from the total cross section. Covariances for the elastic scattering and capture cross sections in the RRR were obtained by the kernel approximation [Obložinský, 2010] while covariances for the total cross section from 820 keV to 5.5 MeV were obtained based on the average cross section of the experimental data [Foster Jr and Glasgow, 1971; Horen et al., 1979]. The rest of the covariance data were evaluated with CCONE and KALMAN [Kawano, 1997] codes.

6.2.3. ^{207}Pb

The JEFF-3.3 evaluation is based on JENDL-4.0 evaluation with modifications in the elastic scattering, total inelastic scattering and level inelastic scattering cross sections and with covariance data included. The resonance parameters are based on the Atlas of neutron resonances and the experimental data of Domingo-Pardo [Domingo-Pardo et al., 2006a]. The total cross section is based on experimental data from Horen [Horen et al., 1978] and calculations with the CCONE code. Cross sections of all relevant reactions were calculated by CCONE. Exception is the (n, α) cross section, which was below 680 keV calculated from resonance parameters, by assuming a mean alpha width of $1.0 \cdot 10^{-5}$ eV (below 550 keV) and $5.0 \cdot 10^{-7}$ eV (above 550 keV) for s-wave resonances and $5.0 \cdot 10^{-7}$ eV for p- and d-wave resonances. The total inelastic scattering and level inelastic scattering cross sections were modified to include renormalized experimental data by Mihailescu et al. [Mihailescu, 2006] up to 3.2 MeV. Above this energy the original evaluation was scaled by a linearly energy dependent factor that achieves continuity at 3.2 MeV and equals 1 at 20 MeV. Consequently, the elastic scattering cross section, which was obtained by subtracting the non-elastic cross sections from the total cross section, and the energy grid of the total cross section was modified. Covariances for the elastic scattering and capture cross sections in the RRR were obtained by the kernel approximation while covariances for the total cross section from 680 keV to 6 MeV were obtained based on the average cross section of the experimental data [Horen et al., 1978]. The rest of the covariance data were evaluated with CCONE and KALMAN codes.

6.2.4. ^{208}Pb

The JEFF-3.3 file is based on JENDL-4.0 evaluation with modifications in the elastic scattering, total inelastic scattering and level inelastic scattering cross sections and with covariance data included. The resonance parameters are based on the compilation of Mughabghab [Mughabghab, 2006]. The total cross section is based on the experimental data by Carlton [Carlton, 1991], Harvey [Harvey, 1999] and calculations with the CCONE code. Cross sections of all relevant reactions were calculated by CCONE. The total inelastic scattering and level inelastic scattering cross sections were modified to include renormalized experimental data by Mihailescu [Mihailescu et al., 2008a] up to 4.1 MeV. Above this energy the original JENDL-4.0 evaluation was scaled by a linearly energy dependent factor that achieves continuity at 4.1 MeV and equals 1 at 20 MeV. The elastic cross section was obtained by subtraction of the non-elastic cross sections from the total cross section. The total cross section is unchanged from JENDL-4.0 but the energy binning has been modified. Covariances for the elastic scattering and capture cross sections in the RRR were obtained by the kernel approximation. Covariances for the total cross section from 1 MeV to 7 MeV were obtained based on the average cross section of the

experimental data [Carlton, 1991; Harvey, 1999]. The rest of the covariance data were evaluated with CCONE and KALMAN codes.

6.2.5. ^{209}Bi

^{209}Bi in the JEFF-3.3 file is also based on the JENDL-4.0 file with modifications in the elastic scattering, total inelastic scattering and level inelastic scattering cross sections. The JENDL-4.0 evaluation was adopted from the previous versions of the same library (original evaluation in the version 3.0) with some modifications. The resolved resonance parameters (up to 200 keV) were mainly adopted from Mughabghab [Mughabghab, 1984], updated for the version 4.0 taking into account the Domingo-Pardo et al. data [Domingo-Pardo et al., 2006b], measured at the n_TOF facility. A bound state was introduced to reproduce the capture cross section at the thermal energy recommended by Mughabghab [Mughabghab, 2006]. Up to 200 keV, a background cross section is added to the contribution from resonances. Above 200 keV the cross section is mainly based on measurements dating back to 1960s, except the capture cross section, which was normalized at 500 keV to the measurements by Saito et al. [Saito et al., 2004] with the Time of Flight (ToF) method at the Pelletron accelerator at the Tokyo Institute of Technology. Covariances of statistical model calculations were estimated with the KALMAN code. Covariances of optical model parameters were obtained by assuming 5% standard deviations of calculated total cross sections. Standard deviations of the target level density and the deformation parameters for distorted-wave Born approximation were assumed to be 2% and 10%, respectively. Renormalized Mihailescu experimental data [Mihailescu et al., 2008b] for the total inelastic and level inelastic cross sections up to 4 MeV were added to the JEFF-3.3 evaluation. Above that energy, TENDL-2015 [Koning et al., 2015] excitation functions were scaled to achieve continuity. The 12th level and continuum inelastic cross sections were modified to reflect the remaining TENDL-2015 discrete levels and continuum inelastic cross sections. JENDL-4.0 total cross section was not changed. The elastic scattering, non-elastic and total inelastic scattering cross sections were changed to respect the sum rules.

6.3. Validation with energy dependent experimental data

Once the detailed origin of each nuclear data file involved in the study has been established, a comparison against energy dependent experimental data has been performed in order to validate the JEFF-3.3 lead and bismuth evaluations. The EXFOR database [Otuka et al., 2014] has been used to search for experimental transmission ToF data, particularly focusing on experiments in the RRR, in the Unresolved Resonance energy Region (URR) and in the fast energy region, which are the relevant energy regions of operation for a lead-cooled fast reactor. The results available in

EXFOR were derived from experimental data using the SAMMY code [Larson, 2008], so resolution broadening was taken into account.

Transmission data are required to determine accurate neutron scattering data in the resonance region (i.e., scattering radii and neutron widths of individual resonances). Furthermore, the total cross section can be derived from transmission data using the following equation:

$$T = e^{-n_A \sigma_{tot}} \Rightarrow \sigma_{tot} = -\frac{\ln T}{n_A} \quad (6.1)$$

where T is the transmission coefficient, n_A is the areal density of the sample in at/b and σ_{tot} is the total cross section.

For the validation, the total cross section of each isotope contained in the libraries has been converted to transmission to reproduce the experiments using Eq. 6.1. Comparisons have been made using the first beta version of the library, JEFF-3.3T1, the final version, JEFF-3.3, and the JENDL-4.0 nuclear data library, which contained high-quality evaluations for these elements before the production version of JEFF-3.3 was released.

6.3.1. ^{204}Pb

Only few experiments have been performed with enriched ^{204}Pb samples due to the low natural abundance of this isotope (around 1.4%). Two cylindrical samples with aerial density of 0.1378 at/b and enriched to 71.41% ^{204}Pb were used to measure the total cross section in a transmission experiment at the Oak Ridge Electron Linear Accelerator (ORELA) facility by Carlton et al. [Carlton, 2003]. The facility is well characterized, including the resolution function. A 200 m flight path and Ne-110 plastic scintillator detectors were employed in the measurement. Results of the experiment have been corrected for the contribution of the other lead isotopes.

Figure 25. ^{204}Pb transmission comparison with experimental data from 35 to 90 keV

The RRR in JEFF-3.3T1 and JEFF-3.3 reaches up to 100 keV, while in the JENDL-4.0 evaluation the RRR ends at 75 keV but there are resonances added in the background cross section until 1.8 MeV. Consequently, in Figure 25 JENDL-4.0 is in perfect agreement with the experimental data, while JEFF-3.3T1 and JEFF-3.3 underestimate the total cross section (overestimate the transmission) by $\sim 12\%$. In the URR (Figure 26), JENDL-4.0 is in agreement with the experimental data whereas JEFF-3.3T1 and JEFF-3.3 give an average as a background cross section. In the fast energy region, Carlton's data is overestimated by JENDL-4.0, JEFF-3.3T1 and JEFF-3.3 from 3 MeV to 9 MeV (Figure 27), while there is a good agreement between the experimental data and the three evaluations from 9 MeV up to 20 MeV.

Figure 26. ^{204}Pb transmission comparison with experimental data in the URR

Figure 27. ^{204}Pb transmission comparison with experimental data in the fast energy range

6.3.2. ^{206}Pb

Horen et al. [Horen et al., 1979] and Borella et al. [Borella et al., 2007] transmission measurements are the most complete experimental data set available in the MYRRHA-relevant energy region (0.1 keV – 4 MeV), while the transmission experiment performed by Foster Jr. et al. [Foster Jr and Glasgow, 1971] is the one with better resolution in the fast energy range. Horen's measurement was performed at the ORELA facility using a 200 m flight path, a 99.5% ^{206}Pb

enriched sample with an areal density of 0.0989 at/b and Ne-100 plastic scintillator detectors. The measurement performed by Borella was done at the LINear Electron Accelerator facility in Geel (GELINA) using a 9.1 m flight path, two metallic samples with an enrichment of 99.82% in ^{206}Pb with an areal density of 0.03 at/b and Li-glass scintillator detectors. Foster's measurement was carried out on the Van de Graaff generator of the Pacific Northwest Laboratories using a 6.14 m flight path, a 92.4% ^{206}Pb enriched sample and a Ne-213 liquid scintillator detector.

Figure 28. ^{206}Pb transmission comparison with experimental data below 70 keV. The transmission coefficient has been calculated with respect to Horen's sample areal density for comparison purposes

A disagreement can be observed between Borella's and Horen's data in the region where they overlap. An analysis of the bibliography reveals that, in the energy region below 70 keV, Horen uses an uncompensated sample of ^{206}Pb , so the $^{207,208}\text{Pb}$ content in the sample is not taken into account. This may cause the overestimation of the total cross section (underestimation of transmission) due to $^{207,208}\text{Pb}$ having a larger cross section, as shown in Figure 28. Additionally, Borella's measurement has better resolution. It can also be observed that JENDL-4.0 and JEFF-3.3 evaluations follow Horen's dataset while JEFF-3.3T1 evaluation is in agreement with Borella's dataset. Consequently, JEFF-3.3T1 seems to overestimate the transmission, according to Horen's experimental data, in the rest of the RRR (Figure 29). In the URR, JEFF-3.3T1 seems to have an unphysical behaviour from 820 keV to 900 keV, missing resonances in this energy region.

Figure 29. ^{206}Pb transmission comparison with experimental data in the upper limits of the RRR. The transmission coefficient has been calculated with respect to Horen's sample areal density for comparison purposes

In the fast energy range (Figure 30), there is also a disagreement between the two datasets (Horen's and Foster's) in the region where they overlap, Horen's measurement pointing to a lower ^{206}Pb total cross section. Nevertheless, all evaluations agree with Foster's data in the fast region.

Figure 30. ^{206}Pb transmission comparison with experimental data in the fast energy region. The transmission coefficient has been calculated with respect to Horen's sample areal density for comparison purposes

6.3.3. ^{207}Pb

Horen et al. [Horen et al., 1978] ToF transmission measurements with 80 m and 200 m flight paths and a ^{207}Pb sample enriched to 92.4% with an effective thickness of 0.1503 at/b, produced the most consistent experimental data set in the RRR, URR and fast energy regions for this nuclide. The results from both flight paths were averaged into a single data set by the National Nuclear Data Center.

JENDL-4.0 and JEFF-3.3 have a good agreement with Horen et al. transmission data in the RRR and URR, as can be seen in Figure 31. On the contrary, JEFF-3.3T1 evaluation overestimates the total cross section. In the fast energy region (Figure 32), good agreement is found between all evaluations and the experimental data. There has been a significant improvement from JEFF-3.3T1 to JEFF-3.3.

Figure 31. ^{207}Pb transmission comparison with experimental data in the RRR

Figure 32. ^{207}Pb transmission comparison with experimental data in the fast energy range

6.3.4. ^{208}Pb

Two transmission measurements were carried out by Carlton et al. [Carlton, 1991] and Harvey et al. [Harvey, 1999] at the ORELA facility with a 200 m flight path, using a ^{208}Pb sample with an areal density of 0.18594 at/b and ^6Li glass detectors and a ^{208}Pb sample with an areal density of 0.16882 at/b and Ne-110 plastic scintillators detectors, respectively. Carlton's experimental dataset has been used for nuclear data validation due to having better experimental resolution in the MYRRHA-relevant energy region.

For the fast energy region, an additional measurement carried out by Finlay et al. [Finlay et al., 1993] was found in bibliography. The experiment was performed at the Weapons Neutron Research facility (WNR) in LANL with a 38.14 m flight path, using two samples (i.e., ^{206}Pb enriched sample and a sample enriched in ^{208}Pb and mixed with natural lead) and a BC-404 plastic scintillator detector.

Figure 33. ^{208}Pb transmission comparison with experimental data in the RRR and URR

In Figure 33, perfect agreement with experimental data is found until the upper limit of the RRR (1 MeV) for all ^{208}Pb evaluations. In the URR, JENDL-4.0 and JEFF-3.3 perfectly match Carlton's data while JEFF-3.3T1 evaluation also follows the experimental data but is interpolated within a coarser energy grid. In the fast energy region (Figure 34), good agreement between Carlton's and Finlay's measurements, as well as between the experimental data sets and the three evaluations, is observed.

Figure 34. ^{208}Pb transmission comparison with experimental data in the fast energy range. The transmission coefficient has been calculated with respect to Carlton's sample areal density for comparison purposes

6.3.5. ^{209}Bi

Harvey et al. [Harvey, 1975] transmission data is the best documented data set available in the RRR and URR. The ToF experiment was done at the ORELA facility in a 200 m flight path using a Bi sample with an areal density of 0.5651 at/b and Ne-110 plastic scintillator detectors. For the fast energy region, the measurements performed by Das et al. [Das and Finlay, 1990] and Finlay et al. [Finlay et al., 1993] are available. The experiment carried out by Das was also performed at the ORELA facility with a 201.52 m flight path, using a sample with a 0.14406 at/b areal density and Ne-110 plastic scintillators, while Finlay's experiment was performed at the Weapons Neutron Research facility with a 38.14 m flight path, using a 0.3153 at/b areal density sample and a BC-404 plastic scintillator detector.

Figure 35. ^{209}Bi transmission comparison with experimental data in the RRR and URR

JENDL-4.0 and JEFF-3.3 libraries have a good agreement with experimental data in the RRR (10 μeV - 200 keV). In the URR JENDL-4.0 and JEFF-3.3 total cross sections are fitted. Figure 35 shows that JEFF-3.3T1 overestimates the total cross section (underestimates the transmission) in the RRR (up to 100 keV) and has a clearly unphysical cross section shape from 100 to 250 keV, missing resonances at the upper end of the RRR (from 100 to 200 keV) and providing only the background. In the fast energy region (Figure 36), JENDL-4.0 and JEFF-3.3 evaluations agree with the experimental data produced by Das et al. and by Finlay et al. up to 20 MeV. On the other hand, JEFF-3.3T1 only agrees with the experimental data until 15 MeV where the cross section is underestimated up to 25 MeV. There has been a significant improvement from JEFF-3.3T1 to JEFF-3.3.

Figure 36. ^{209}Bi transmission comparison with experimental data in the fast energy range. The transmission coefficient has been calculated with respect to Harvey's sample areal density for comparison purposes

6.4. Validation with integral experiments

Integral benchmarks provide extensively peer-reviewed data that can be used by the international nuclear data community for testing and improvement of nuclear data files and by the international reactor physics, criticality safety, and math & computation communities for validation of analytical methodologies used for reactor physics, fuel cycle, nuclear facility safety analysis and design, and advanced modeling and simulation efforts [Briggs et al., 2014].

Three databases have been used:

- Database for the International Handbook of Evaluated Criticality Safety Benchmark Experiments (DICE) of the ICSBEP;
- International Reactor Physics Handbook Database and Analysis Tool (IDAT) of the IRPhE project;
- and the Shielding Integral Benchmark Archive and Database (SINBAD).

DICE is the database for the ICSBEP [OECD/NEA, 2016b], which is an official activity of the Organization for Economic Cooperation and Development of the Nuclear Energy Agency (OECD/NEA). It provides 567 evaluations with benchmark specifications, that have been derived from experiments performed at various nuclear critical facilities around the world, for 4.874 critical, near critical or subcritical configurations, 31 criticality alarm placement/shielding

configurations with multiple dose points for each, and 207 configurations that have been categorized as fundamental physics measurements that are relevant to criticality safety applications. Reactor physics benchmark specifications for 143 different experimental series that were performed at 50 different nuclear facilities can be found at IDAT, the database for the IRPhE project [OECD/NEA, 2017a], which has been created following the pattern of ICSBEP. Furthermore, SINBAD [Kodeli et al., 2006] contains an internationally established set of radiation shielding and dosimetry data from experiments relevant for reactor shielding, fusion blanket neutronics and accelerator shielding.

6.4.1. Lead

A significant number of experiments have been performed with lead due to its use in nuclear engineering as a shielding and coolant material. The databases contain numerous benchmarks with high sensitivity to lead cross section changes; three benchmarks from DICE with the highest sensitivity to cross sections of lead nuclides in the LFR-relevant energy region, one benchmark from IDAT and one benchmark from SINBAD have been selected. One additional benchmark, the Lawrence Livermore National Laboratory (LLNL) lead pulsed sphere experiment, has been found in an extra bibliographic search [Wong et al., 1972].

The DICE and IDAT benchmarks are sensitive to lead data in the resolved and unresolved energy regions. A comparison between the sensitivity coefficients of k_{eff} to cross sections of lead nuclides in MYRRHA lead-bismuth cooled fast reactor and the selected DICE benchmarks can be found in Table 41. The sensitivity in the benchmarks is at least one order of magnitude higher than in MYRRHA, which denotes that differences in lead cross sections evaluations will have a significant impact in these benchmarks.

Table 41. Sensitivity coefficients of k_{eff} to cross sections of lead nuclides in the selected DICE benchmarks and the MYRRHA model

Integral experiment	ISC (%/%)			
	$^{204}\text{Pb}(n,tot)$	$^{206}\text{Pb}(n,tot)$	$^{207}\text{Pb}(n,tot)$	$^{208}\text{Pb}(n,tot)$
MYRRHA - Fuel Assembly	-0.00040	-0.00033	0.00122	0.00637
HEU-MET-FAST-064-002 [OECD/NEA, 2015h]	0.00394	0.06106	0.06162	0.13038
HEU-MET-FAST-057-005 [OECD/NEA, 2015i]	-	0.05399	0.05325	0.11183
LEU-COMP-THERM-010-001 [OECD/NEA, 2015j]	0.00033	0.01697	0.00549	0.03708

The k_{eff} values computed by MCNP using JENDL-4.0, JEFF-3.3T1 and JEFF-3.3 nuclear data libraries, as well as the differences between the calculated and experimental k_{eff} in pcm, for the DICE and IDAT benchmarks are presented in Table 42. Very accurate MCNP simulations

(i.e., statistical uncertainty in k_{eff} lower than 5 pcm) have been performed, therefore the statistical uncertainty in MCNP results has been omitted.

Table 42. Results of MCNP criticality calculations for selected DICE and IDAT benchmarks using different nuclear data libraries

Integral experiment	U_{exp} (pcm)	JENDL-4.0		JEFF-3.3T1		JEFF-3.3	
		k_{eff}	$\Delta k_{eff,exp}$ (pcm)	k_{eff}	$\Delta k_{eff,exp}$ (pcm)	k_{eff}	$\Delta k_{eff,exp}$ (pcm)
HEU-MET-FAST-064-002	100	0.99982	22	0.99668	-292	1.00315	355
HEU-MET-FAST-057-005	190	1.02575	2575	1.02287	2287	1.02847	2847
LEU-COMP-THERM-010-001	370	1.00801	801	1.00492	492	1.00847	847
ZPR-FUND-EXP-018 [OECD/NEA, 2015k]	250	0.98099	869	0.96454	-776	0.97364	134

Significant differences between the experimental and calculated k_{eff} values can be seen in Table 42 for all evaluations. JENDL-4.0 and JEFF-3.3 estimate k_{eff} within the experimental uncertainty for HEU-MET-FAST-064-002 and ZPR-FUND-EXP-018, respectively, while the evaluations give underestimated results for the rest of the integral experiments. On the other hand, JEFF-3.3T1 evaluation disagrees with all the benchmarks.

However, even if these benchmarks are highly sensitive to changes in lead cross sections, the presence of other materials in the experiment makes impossible to attribute variations in the integral parameter (i.e., k_{eff}) to a single nuclide or reaction channel. Therefore, in order to study the contribution of cross sections of lead nuclides to the discrepancies between computed and experimental data and assess JEFF-3.3T1 and JEFF-3.3 evaluations, the particular impact of each nuclide has been computed by MCNP after substituting the JENDL-4.0 lead evaluation by nuclear data from JEFF-3.3T1 and JEFF-3.3 (Table 43). That is, JENDL-4.0 has been always used as reference library.

Table 43. Contribution of JEFF-3.3T1 and JEFF-3.3 cross sections of lead nuclides to k_{eff} calculated by MCNP models of the selected DICE and IDAT benchmarks taking JENDL-4.0 as the reference library. Differences in k_{eff} are expressed in units of pcm

Integral experiment	JEFF-3.3T1					JEFF-3.3				
	All	²⁰⁴ Pb	²⁰⁶ Pb	²⁰⁷ Pb	²⁰⁸ Pb	All	²⁰⁴ Pb	²⁰⁶ Pb	²⁰⁷ Pb	²⁰⁸ Pb
HEU-MET-FAST-064-002	-665	28	-296	435	-833	-15	30	8	-56	-5
HEU-MET-FAST-057-005	-614	-	-248	426	-785	-54	-	2	-47	-7
LEU-COMP-THERM-010-001	-294	8	-52	-22	-192	-11	5	2	-7	-6
ZPR-FUND-EXP-018	-612	63	-427	101	-385	-31	66	-15	-78	-9

Table 43 shows that JEFF-3.3T1 lead evaluations produce a decrease in reactivity with respect to JENDL-4.0 evaluations, which brings the calculated k_{eff} closer to the experimental

value. On the other hand, the impact of replacing JENDL-4.0 lead evaluations with JEFF-3.3 evaluations can be considered negligible.

The decrease in reactivity due to JEFF-3.3T1 substitution is produced by ^{206}Pb and ^{208}Pb which is partially compensated with an increase by ^{204}Pb and ^{207}Pb . JEFF-3.3T1 and JEFF-3.3 ^{204}Pb evaluations are taken from JEFF-3.2, therefore they produce identical results when ^{204}Pb JENDL-4.0 file is substituted (i.e., a slight increase in reactivity contrary to the experimental k_{eff}). The reactivity decrease produced by ^{206}Pb can be explained by the lower total cross section due to the use of Borella's data in the evaluation, which means that there is an increase in the leakage and a slight decrease in the amount of fissions due to a hardening of the neutron spectrum. The differences in reactivity due to ^{208}Pb can be attributed to the interpolation scheme in the fast energy region.

Regarding JEFF-3.3, differences obtained with ^{206}Pb and ^{208}Pb are within the statistical uncertainty of MCNP calculations, while the slight decrease in reactivity produced by ^{207}Pb can be attributed to differences in the inelastic cross section introduced by the consideration of Mihailescu experimental data in JEFF-3.3 evaluation.

For the fast energy region, the high energy neutron spectra generated by 590 MeV protons on a thick lead target [Cierjacks et al., 1981] from SINBAD and LLNL pulsed sphere [Wong et al., 1972] experiments have been used for the validation of lead nuclear data.

Figure 37. High energy neutron spectra generated by 590-MeV protons on a thick Pb target

In Figure 37, a comparison between the experimental neutron spectrum generated by 590 MeV protons and the calculated spectrum using JENDL-4.0, JEFF-3.3T1 and JEFF-3.3 evaluations can be seen. At the three libraries overestimate the experimental spectrum up to the

upper energy limit of the evaluations (20 MeV). However, above 20 MeV MCNP internal model is used and there is a good agreement between the experiment and calculations.

LLNL Pb pulsed sphere neutron spectrum calculated with the different evaluations is presented in Figure 38. Once again, differences can be observed at lower energies (up to 40%), while from 5 MeV up to higher energies a good agreement between the calculated and experimental spectrum is found, except for JEFF-3.3T1 evaluation from 8 to 11 MeV where a significant underestimation of the number of counts measured by the detector is obtained.

Figure 38. Neutron spectrum for LLNL experiment with the Pb pulsed sphere

6.4.2. Bismuth

An extensive search has been conducted in the databases mentioned above. However, there is a lack of integral benchmarks with enough sensitivity to ^{209}Bi in DICE and IDAT in the relevant energy region (300 eV – 10 MeV). In Table 44, it can be observed that the highest sensitivity to this quantity in a benchmark in these two databases is two orders of magnitude less than in MYRRHA. Kochetkov et al. [Kochetkov et al., 2006] describe a series of benchmark experiments for lead and bismuth neutron data testing that are candidates for IRPhEP, but they are not available yet and hence cannot be used within the framework of this Thesis.

Nevertheless, the SINBAD database contains one benchmark that can be used for ^{209}Bi data validation: the IPPE neutron transmission benchmark experiment with ^{252}Cf fission neutrons through a bismuth shell [Simakov et al., 1999]. In Figure 39, a comparison of the simulated neutron leakage spectrum against the experimental spectrum from 0.06 MeV to 15 MeV is presented. The spectrum is well predicted by all evaluations in the fast energy region.

Table 44. List of DICE and IDAT benchmarks most sensitive to the $^{209}\text{Bi}(n,\text{tot})$ cross section

MYRRHA $^{209}\text{Bi}(n,\text{tot})$ Integrated Sensitivity Coefficient = $4.3955 \cdot 10^{-2} \text{ \%/\%}$

Benchmark	$^{209}\text{Bi}(n,\text{tot})$ ISC (%/%)
HEU-MET-FAST-059-001 [OECD/NEA, 2015l]	$-3.0633 \cdot 10^{-4}$
HEU-MET-FAST-059-002 [OECD/NEA, 2015l]	$4.0288 \cdot 10^{-5}$
HEU-MET-FAST-051-016 [OECD/NEA, 2015m]	$2.2906 \cdot 10^{-5}$
HEU-MET-FAST-076-001 [OECD/NEA, 2015n]	$2.1494 \cdot 10^{-5}$
HEU-MET-FAST-071-016 [OECD/NEA, 2015o]	$1.4574 \cdot 10^{-5}$

Figure 39. Experimental and simulated neutron leakage spectra from IPPE Bi shell over the whole energy region

A more detailed analysis reveals that at upper limit of the RRR (200 keV), JENDL-4.0 and JEFF-3.3 are consistent with the experimental data (Figure 40). On the contrary, the shape of the neutron leakage spectra obtained with JEFF-3.3T1 from 100 to 200 keV is not compatible to the experimental spectra's shape. This is a consequence of JEFF-3.3T1 ^{209}Bi unphysical evaluation from 100 to 250 keV, as stated in Section 6.2.5.

Figure 40. Experimental and simulated neutron leakage spectra from IPPE Bi shell from 0.06 to 0.5 MeV

6.5. Verification & Benchmarking

Data validation involves not only the identification and selection of experimental data sets and the modelling of integral measurements, it also includes the processing of nuclear data files into application libraries and the benchmarking of nuclear applications.

Focusing on LFRs, ALFRED and MYRRHA reactor concept designs have been used to test the JEFF-3.3T1 and JEFF-3.3 evaluations, using the previous production version of the JEFF library, JEFF-3.2 [OECD/NEA Data Bank, 2014], as the reference library, in order to analyse the impact of the differences between the previous lead and bismuth evaluations and the new ones on the criticality and neutronics of both reactors.

The neutron multiplication factors, average number of neutrons produced per fission and fission and capture probabilities (i.e., number of fissions and captures per source particle, which can be interpreted as reaction rates considering that no time dependence exists in MCNP transport calculations) are presented in Table 45 and Table 46 for ALFRED and MYRRHA, respectively.

Table 45. k_{eff} , ν , fission and capture probabilities for ALFRED model. Statistical uncertainty in k_{eff} lower than 10 pcm for all calculations

	JEFF-3.2	JEFF-3.3T1	Difference	JEFF-3.3	Difference
k_{eff}	0.99220	0.99124	-96 pcm	0.99937	717 pcm
ν	2.94	2.91	-0.78%	2.91	-0.78%
Total fission probability	$3.38 \cdot 10^{-1}$	$3.40 \cdot 10^{-1}$	0.69%	$3.43 \cdot 10^{-1}$	1.52%
Total capture probability	$6.35 \cdot 10^{-1}$	$6.36 \cdot 10^{-1}$	0.19%	$6.32 \cdot 10^{-1}$	-0.37%
^{204}Pb capture probability	$8.64 \cdot 10^{-3}$	$8.48 \cdot 10^{-3}$	-1.91%	$8.62 \cdot 10^{-3}$	-0.25%
^{206}Pb capture probability	$1.16 \cdot 10^{-2}$	$1.26 \cdot 10^{-2}$	8.09%	$1.27 \cdot 10^{-2}$	9.10%
^{207}Pb capture probability	$1.17 \cdot 10^{-2}$	$2.37 \cdot 10^{-2}$	103.10%	$1.25 \cdot 10^{-2}$	6.68%
^{208}Pb capture probability	$1.16 \cdot 10^{-3}$	$1.48 \cdot 10^{-3}$	28.12%	$1.03 \cdot 10^{-3}$	-10.44%

In the case of ALFRED, the neutron multiplication factor slightly decreases with JEFF-3.3T1, but significantly increases with JEFF-3.3 due to an increase of 1.52% in the fission probability and a decrease of 0.37% in the capture probability, which are partially compensated by a decrease of 0.78% in the average number of neutrons per fission. On the other hand, similar differences (around 250 pcm) are obtained for MYRRHA with JEFF-3.3T1 and JEFF-3.3 nuclear data libraries. Nevertheless, it can be seen that the differences and inconsistencies in the lead and bismuth evaluations found and described in previous sections have a direct impact in the criticality and neutronics of both reactors, being especially significant in the case of JEFF-3.3T1 evaluations. The overestimation of the total cross section by ^{207}Pb JEFF-3.3T1 evaluation (Section 6.3.3) or the ^{209}Bi unphysical evaluation as a result of the missing resonances at the upper end of the RRR (Section 6.3.5), produce a significant increase on the number of neutrons captured by these coolant materials.

Table 46. k_{eff} , ν , fission and capture probabilities for MYRRHA model. Statistical uncertainty in k_{eff} lower than 10 pcm for all calculations

	JEFF-3.2	JEFF-3.3T1	Difference	JEFF-3.3	Difference
k_{eff}	1.00479	1.00737	258 pcm	1.00722	247 pcm
ν	2.93	2.91	-0.72%	2.91	-0.75%
Total fission probability	$3.43 \cdot 10^{-1}$	$3.46 \cdot 10^{-1}$	1.01%	$3.46 \cdot 10^{-1}$	0.99%
Total capture probability	$6.64 \cdot 10^{-1}$	$6.60 \cdot 10^{-1}$	-0.53%	$6.60 \cdot 10^{-1}$	-0.54%
^{204}Pb capture probability	$3.62 \cdot 10^{-3}$	$3.41 \cdot 10^{-3}$	-5.99%	$3.62 \cdot 10^{-3}$	-0.08%
^{206}Pb capture probability	$4.47 \cdot 10^{-3}$	$4.77 \cdot 10^{-3}$	6.79%	$4.83 \cdot 10^{-3}$	8.15%
^{207}Pb capture probability	$9.24 \cdot 10^{-3}$	$1.30 \cdot 10^{-2}$	41.10%	$9.55 \cdot 10^{-3}$	3.30%
^{208}Pb capture probability	$4.58 \cdot 10^{-4}$	$5.74 \cdot 10^{-4}$	25.22%	$3.84 \cdot 10^{-4}$	-16.18%
^{209}Bi capture probability	$1.07 \cdot 10^{-2}$	$1.66 \cdot 10^{-2}$	54.08%	$1.07 \cdot 10^{-2}$	-0.71%

6.6. Conclusions

The coolant materials of advanced LFR's (i.e., lead and bismuth) present in the latest version of the JEFF nuclear data library, JEFF-3.3, have been thoroughly studied. First, the origin of each evaluation has been analysed; then, JENDL-4.0, JEFF-3.3T1 and JEFF-3.3 lead and bismuth files have been validated using time of flight transmission and integral experiments; and finally, benchmarking has been carried out using ALFRED and MYRRHA advanced reactor designs in order to analyse the impact of the differences between the previous lead and bismuth evaluations and the new ones on the criticality and neutronics of both reactor concepts.

Several problems were found in the RRR of JEFF-3.3T1 lead and bismuth. These problems, as well as the recommendation to employ the RRR from JENDL-4.0 for these nuclides in the final version of JEFF-3.3, were communicated to the JEFF collaboration [Plompen, 2016; Romojaro and Alvarez-Velarde, 2016; Romojaro and Žerovnik, 2016; Žerovnik et al., 2017b, 2016] and, as can be seen in Section 6.2, the recommendations were adopted in the production version of JEFF-3.3 nuclear data library, except for ^{204}Pb which is still based on the JEFF-3.2 evaluation.

While numerous integral benchmarks sensitive to cross sections of lead nuclides have been found in the criticality and reactor databases, a lack of integral benchmarks with enough sensitivity to bismuth cross sections has been observed and only one benchmark is currently available for bismuth data validation. JEFF-3.3T1 lead evaluation disagrees with all lead integral benchmarks in the RRR and URR energy ranges, whereas bismuth evaluation is not compatible with the transmission benchmark experimental data from 100 to 250 keV due to ^{209}Bi unphysical evaluation. Better agreement is observed for JENDL-4.0 and JEFF-3.3 lead and bismuth evaluations with integral experiments.

The neutron multiplication factors of ALFRED and MYRRHA increase with respect to JEFF-3.2 using JEFF-3.3 evaluation, due to an increase in the fission probability and a decrease in the capture probability, which are partially compensated by a decrease in the average number of neutrons. The differences and inconsistencies found in lead and bismuth evaluations have a direct impact in the criticality and neutronics of both reactors.

JEFF-3.3 lead and bismuth evaluations have better agreement with energy dependent and integral experimental data than JEFF-3.3T1; therefore, they can be considered a significant improvement over the first beta evaluations for these materials in JEFF-3.3T1.

From this point forward, the state-of-the-art JEFF-3.3 nuclear data library will be used as the reference library to perform the S/U analyses and data adjustment, since extensive validation, verification and benchmarking of this library has been performed within his Thesis and within the JEFF project.

Chapter 7

Target Accuracy Assessment of MYRRHA

Abstract – Target accuracy assessments allow identifying nuclear data needs and requirements. Employing the SUMMON system, described in Chapter 5, and using the JEFF-3.3 nuclear data library, for which LFR coolant materials were thoroughly analysed in Chapter 6, a complete target accuracy assessment of MYRRHA lead-cooled fast reactor is performed in this chapter. MYRRHA model, developed by SCK•CEN, is first described and then sensitivity and uncertainty analyses of MYRRHA criticality safety parameters are carried out. Quantified uncertainties in reactor parameters are compared against target accuracies defined by NEA WPEC Subgroup 26 and a list nuclear data needs is given.

This chapter shows, partially or completely, works already presented in the following references:

- CHANDA Deliverable D10.1 [Romojaro et al., 2015]
- International Journal Article [Romojaro et al., 2017b]
- ESNII + Deliverable D6.1.6-1 [Grasso et al., 2017]
- International Conference Proceeding [García-Herranz et al., 2017]
- International Conference Proceeding [Romojaro et al., 2017c]
- International Journal Article [Grasso et al., 2018]
- International Conference Proceeding [Romojaro et al., 2018b]

7.1. Introduction

Target accuracy assessments allow identifying nuclear data needs and requirements (by nuclide, nuclear reaction and energy channel), in order to reduce margins, achieving the requested level of safety and minimizing the increase in the costs due to additional security measures, in the

preliminary conceptual design and in later design phases of selected reactor and fuel cycle concepts.

In 2008, the NEA Working Party on International Nuclear Data Evaluation Co-operation (WPEC) Subgroup 26 performed an uncertainty assessment for innovative systems using covariance data evaluations available at the time [Salvatores and Jacqmin, 2008]. Even though the uncertainty in nuclear data is one of the most important sources of uncertainty in reactor design and reactor physics simulations, significant gaps between the uncertainties and the target accuracies (i.e., maximum acceptable uncertainties for a certain reactor parameter) were systematically shown [Plompen and Harada, 2014] for reactor core parameters. In Table 47, target accuracies established by researchers and industry for fast reactors at Beginning of Life (BoL) are presented.

Table 47. Fast reactor target accuracies. No target accuracy for Λ_{eff} has been found in bibliography

Multiplication Factor [Salvatores and Jacqmin, 2008]	300 pcm
Delayed neutron fraction [D’Angelo and Rowlands, 2002; Rudstan et al., 2002]	3%
Reactivity coefficients (coolant void and Doppler) [Salvatores and Jacqmin, 2008]	7%

Since the accuracy and priorities strongly depend on the assumed initial uncertainty data [Plompen and Harada, 2014] and since numerous nuclear data libraries with updated uncertainty evaluations have been released in the past ten years (i.e., ENDF/B-VIII.0, JEFF-3.3, TENDL-2017 [Rochman et al., 2017], JENDL-4.0u [Japan Atomic Energy Agency, 2016] and BROND-3.1 [Blokhin et al., 2016], among others), it is necessary to repeat the analyses in order to study the impact of the new nuclear data evaluations on advanced reactor design parameters.

In this chapter, the SUMMON system will be used to perform a complete target accuracy assessment of an advanced LFR-representative, employing the state-of-the-art JEFF-3.3 nuclear data library. MYRRHA has been chosen as the main object of study, due to the key role it will play in the development of the Pb-alloy technology needed for the LFR GEN-IV concept [Van den Eynde et al., 2015] as an LFR pilot plant. Furthermore, strong support has been given by the Belgian government and numerous countries and, in fact, MYRRHA’s project Phase 1 has already started with the construction of the 100 MeV particle accelerator and with the pre-licensing of the reactor.

7.2. MYRRHA model

MYRRHA’s updated core design is described in detail in Ref. [Van den Eynde et al., 2015]. For the sensitivity and uncertainty analyses, a simplified model developed and provided by

SCK•CEN [Stankovski and Van den Eynde, 2014], homogenised on fuel assembly level, of the critical core configuration in nominal conditions at BoL has been used. The layout of the core is shown in Figure 41.

Figure 41. Critical MYRRHA core layout [Stankovski and Van den Eynde, 2014]

The hexagonal fuel assemblies consist of 127 fuel pins containing Mixed Oxide Fuel (MOX) with an enrichment of 30% Pu+Am in heavy metals. They have been divided into five axial parts comprising fuel pin active part, top and bottom reflectors (YZrO) and parts of the assembly above and below. Principal materials such as MOX fuel, fuel pin clad (15-15Ti stainless-steel), lead-bismuth eutectic coolant, assembly wrapper and gas plenum have been mixed resulting in homogenized material compositions.

Besides the 78 fuel assemblies, the core contains 4 in-pile sections for material testing, 4 irradiation rigs for medical isotope production (Mo-99), 3 sub-assemblies containing gravity driven safety rods (SR), 6 sub-assemblies containing buoyancy driven control rods (CR), 32 dummy assemblies filled with LBE and 84 reflector assemblies containing BeO-loaded rods.

The core is enforced with a stainless-steel jacket and is enclosed in 3 cm thick core barrel with 179.2 cm external diameter. The structure is enclosed in a vessel with 874 cm diameter and 860 cm height. The space outside the core barrel is filled with LBE. The model is limited to LBE free surface above the core (353 cm above core mid-plane). The shrinking of the model in radial direction or below the core has not been done since there is no physical boundary which can be used as separator (such as LBE free surface on top) [Stankovski and Van den Eynde, 2014]. The model vertical layout is given in Figure 42.

Figure 42. Vertical layout of the MYRRHA model (dimensions given in cm) [Stankovskiy and Van den Eynde, 2014]

Material compositions and their main characteristics (temperatures, densities) used to create the homogenised core are provided in Ref. [Stankovskiy and Van den Eynde, 2014].

Even though the original heterogeneous core was not available for the analyses, the models with homogenization on assembly level adequately reproduce the physics of reference heterogeneous models (Figure 43) and can be safely used for a wide range of neutronic calculations [Stankovskiy and Van den Eynde, 2014].

Figure 43. Neutron spectra in MYRRHA critical core averaged over the inner ring of fuel assemblies and whole core [Stankovskiy and Van den Eynde, 2014]

7.3. k_{eff}

From the designer's point of view, the determination of the k_{eff} target accuracy is a rather complex issue due to the number of factors to take into account, such as reactor criticality, rods' safety margins, safety parameters, etc. The estimated reactivity worth of the safety rods in MYRRHA's critical configuration is ~ 5000 pcm. Regarding the safety aspect, the combined uncertainty from all sources, nuclear data among them, should not exceed this value. On the other hand, a possible underestimation of k_{eff} will require loading of additional fuel assemblies in the core periphery to reach the criticality. Given that MYRRHA has a certain rotational symmetry, 3 or 6 fuel assemblies would have to be added. Taking into account that the reactivity worth of a peripheral fuel assembly is ~ 50 pcm [Malambu and Stankovskiy, 2014], a k_{eff} target accuracy of 300 pcm is deemed by MYRRHA designers to be satisfactory in order to minimize the increase in the costs of additional fuel assemblies, which agrees with the k_{eff} target accuracy established by the NEA WPEC Subgroup 26 for fast reactors [Salvatores and Jacqmin, 2008].

Table 48. k_{eff} and k_{eff} ISC to the 10 most important neutron induced nuclear data for MYRRHA with JEFF-3.3 library

$$k_{eff} = 1.000719 \pm 0.00001$$

MYRRHA – k_{eff} ISC (%/%)		
Quantity		JEFF-3.3
^{239}Pu	ν	$0.696 \pm 2.9 \cdot 10^{-6}$
^{239}Pu	(n,f)	$0.482 \pm 2.9 \cdot 10^{-6}$
^{238}U	(n, γ)	$-0.112 \pm 3.7 \cdot 10^{-7}$
^{241}Pu	ν	$0.091 \pm 4.5 \cdot 10^{-7}$
^{240}Pu	ν	$0.081 \pm 4.5 \cdot 10^{-7}$
^{238}U	ν	$0.070 \pm 6.1 \cdot 10^{-7}$
^{241}Pu	(n,f)	$0.064 \pm 4.6 \cdot 10^{-7}$
^{240}Pu	(n,f)	$0.055 \pm 4.6 \cdot 10^{-7}$
^{239}Pu	(n, γ)	$-0.053 \pm 3.1 \cdot 10^{-7}$
^{209}Bi	(n,n)	$0.052 \pm 1.1 \cdot 10^{-5}$

In Table 48, k_{eff} and the energy and region integrated sensitivity coefficients to the ten most important nuclides and reactions (quantities) for MYRRHA's effective multiplication factor are presented. Very similar values to the ones obtained with ENDF/B-VII.0 library for the preliminary analysis (Table 39) can be observed. On the other hand, in Table 49 the major contributors and the total uncertainty in k_{eff} due to these contributors derived with JEFF-3.3 strongly differ from the results obtained in the preliminary analysis (Table 40). This shows the strong reliance of UQ analyses on the assumed initial uncertainty data and the importance of choosing a comprehensive set of nuclear data (i.e., nuclear data library) that has been extensively verified and validated and that possesses a complete and realistic set of covariance evaluations, in order to obtain accurate results in the analyses. An additional UQ analysis with the state-of-the-art ENDF/B-VIII.0

covariance library using the sensitivities derived with JEFF-3.3 library is also provided in Table 49 to illustrate this point.

While a good agreement can be observed in the total k_{eff} uncertainty derived by JEFF-3.3 and ENDF/B-VIII.0 due to compensations, the contributors to this uncertainty significantly vary. This can be attributed to differences in the uncertainty evaluations, such as the case of $^{208}\text{Pb}(n,n')$ (Figure 44); to missing correlations, such as $^{240}\text{Pu}(n,f)$ - $^{240}\text{Pu}(n,\gamma)$ in the fast energy range for ENDF/B-VIII.0 (Figure 45); and to missing covariance evaluations, such as $^{209}\text{Bi}(n,n)$ in JEFF-3.3, which, as shown in Table 48, is one of the most important neutron induced reactions for MYRRHA's multiplication factor and the third major contributor to the total uncertainty when using ENDF/B-VIII.0 covariance library. This causes JEFF-3.3 to underestimate the total uncertainty in any system parameter with a strong sensitivity to $^{209}\text{Bi}(n,n)$, such as k_{eff} for MYRRHA.

Table 49. k_{eff} nuclear data uncertainty quantification for MYRRHA with JEFF-3.3 and ENDF/B-VIII.0 libraries

MYRRHA					
JEFF-3.3				ENDF/B-VIII.0	
Quantity		$\Delta k_{eff}/k_{eff}(\%)$	Quantity		$\Delta k_{eff}/k_{eff}(\%)$
^{240}Pu (n,f)	^{240}Pu (n,f)	$0.543 \pm 7.3 \cdot 10^{-7}$	^{239}Pu (n,f)	^{239}Pu (n,f)	$0.550 \pm 5.4 \cdot 10^{-7}$
^{240}Pu (n,f)	^{240}Pu (n, γ)	$-0.420 \pm 1.4 \cdot 10^{-7}$	^{239}Pu (n, γ)	^{239}Pu (n, γ)	$0.227 \pm 1.2 \cdot 10^{-7}$
^{239}Pu ν_p	^{239}Pu ν_p	$0.321 \pm 1.1 \cdot 10^{-7}$	^{209}Bi (n,n)	^{209}Bi (n,n)	$0.222 \pm 3.3 \cdot 10^{-6}$
^{239}Pu (n,f)	^{239}Pu (n,f)	$0.295 \pm 2.6 \cdot 10^{-7}$	^{239}Pu ν_p	^{239}Pu ν_p	$0.187 \pm 4.0 \cdot 10^{-8}$
^{239}Pu χ	^{239}Pu χ	$0.261 \pm 2.0 \cdot 10^{-6}$	^{238}U (n, γ)	^{238}U (n, γ)	$0.139 \pm 2.7 \cdot 10^{-8}$
^{240}Pu (n, γ)	^{240}Pu (n, γ)	$0.197 \pm 2.3 \cdot 10^{-8}$	^{239}Pu χ	^{239}Pu χ	$0.128 \pm 3.5 \cdot 10^{-7}$
^{239}Pu (n,f)	^{239}Pu (n, γ)	$0.174 \pm 4.3 \cdot 10^{-8}$	^{238}U (n,n')	^{238}U (n,f)	$-0.095 \pm 2.6 \cdot 10^{-7}$
^{238}U (n, γ)	^{238}U (n, γ)	$0.167 \pm 3.6 \cdot 10^{-8}$	^{240}Pu (n, γ)	^{240}Pu (n, γ)	$0.091 \pm 6.2 \cdot 10^{-9}$
^{239}Pu (n, γ)	^{239}Pu (n, γ)	$0.151 \pm 6.7 \cdot 10^{-8}$	^{238}U ν_p	^{238}U ν_p	$0.087 \pm 4.3 \cdot 10^{-8}$
^{238}U (n,n')	^{238}U (n,f)	$-0.138 \pm 5.6 \cdot 10^{-7}$	^{238}U (n,n')	^{238}U (n, γ)	$0.081 \pm 1.5 \cdot 10^{-7}$
Total uncertainty in k_{eff}		$0.772 \pm 3.7 \cdot 10^{-6}$	Total uncertainty in k_{eff}		$0.771 \pm 3.9 \cdot 10^{-6}$

Nevertheless, regarding the target accuracy assessment, a target accuracy of 300 pcm in the effective neutron multiplication factor was specified for fast reactors at BoL. However, nearly 800 pcm of uncertainty in k_{eff} have been obtained in the UQ using the state-of-the-art JEFF-3.3 and ENDF/B-VIII.0 libraries; therefore, the design target accuracy is still exceeded by more than a factor of two for the considered modern nuclear data evaluations.

Figure 44. JEFF-3.3 (left) and ENDF/B-VIII.0 (right) covariance matrices for $^{208}\text{Pb}(n,n')$

Figure 45. JEFF-3.3 (left) and ENDF/B-VIII.0 (right) cross-covariance matrices for $^{240}\text{Pu}(n,f)$ - $^{240}\text{Pu}(n,\gamma)$

7.4. β_{eff}

Kinetic parameters such as β_{eff} and Λ_{eff} play a key role in the control and safety of nuclear reactors. Furthermore, besides their importance in reactor safety analysis and interpretation of measurements, β_{eff} can be also valuable for nuclear data validation [Kodeli, 2018]. β_{eff} can provide complementary information to k_{eff} for other quantities, such as v_d [Kodeli, 2013]. Moreover, in Ref. [Stankovski and Van den Eynde, 2014] it is concluded that “*precise knowledge of the β_{eff} uncertainty will be particularly important for the future reactor systems using a wider range of actinide isotopes with lower values of β_{eff} (Pu isotopes), making the reactor control of MOX fueled cores more challenging*”.

In Table 50, β_{eff} and the energy and region integrated sensitivity coefficients to the ten most important nuclides and reactions (quantities) for MYRRHA’s effective delayed neutron fraction, obtained with Chiba’s method, are presented.

Table 50. β_{eff} and β_{eff} ISC to the 10 most important neutron induced nuclear data for MYRRHA with JEFF-3.3 library

$$\beta_{eff} = 328 \pm 1 \text{ pcm}$$

MYRRHA – β_{eff} ISC (%/%)		
Quantity		JEFF-3.3
^{239}Pu	v_p	$-0.594 \pm 9.8 \cdot 10^{-6}$
^{239}Pu	v_d	$0.413 \pm 9.9 \cdot 10^{-6}$
^{238}U	v_d	$0.297 \pm 6.7 \cdot 10^{-5}$
^{238}U	(n,f)	$0.192 \pm 7.5 \cdot 10^{-5}$
^{239}Pu	(n,f)	$-0.167 \pm 3.0 \cdot 10^{-4}$
^{241}Pu	v_d	$0.131 \pm 3.3 \cdot 10^{-5}$
^{238}U	v_p	$-0.126 \pm 9.2 \cdot 10^{-8}$
^{240}Pu	v_p	$-0.116 \pm 6.0 \cdot 10^{-7}$
^{241}Pu	v_p	$-0.068 \pm 5.4 \cdot 10^{-6}$
^{240}Pu	v_d	$0.063 \pm 1.4 \cdot 10^{-5}$

Indeed, it can be seen that the most important quantities from the effective delayed neutron fraction point of view are v_d and v_p for U and Pu nuclides in the MOX fuel. These values are very similar to the ones obtained by Kodeli [Kodeli, 2018] in a MYRRHA S/U analysis using the deterministic SUS3D code and ENDF/B-VII.1 nuclear data library.

Table 51. β_{eff} nuclear data uncertainty quantification for MYRRHA with JEFF-3.3 and JENDL-4.0u2 libraries

MYRRHA					
JEFF-3.3				JENDL-4.0u2	
Quantity		$\Delta\beta_{eff}/\beta_{eff}(\%)$		Quantity	
^{241}Pu	v_d	^{241}Pu	v_d	$0.653 \pm 2.2 \cdot 10^{-6}$	
^{239}Pu	χ	^{239}Pu	χ	$0.500 \pm 4.2 \cdot 10^{-5}$	
^{238}U	(n,f)	^{238}U	(n,f)	$0.440 \pm 1.1 \cdot 10^{-5}$	
^{238}U	(n,n')	^{238}U	(n,f)	$-0.321 \pm 1.8 \cdot 10^{-5}$	
^{241}Pu	χ	^{241}Pu	χ	$0.283 \pm 9.9 \cdot 10^{-6}$	
^{240}Pu	(n,f)	^{240}Pu	(n,f)	$0.277 \pm 5.8 \cdot 10^{-6}$	
^{239}Pu	v_p	^{239}Pu	v_p	$0.270 \pm 4.6 \cdot 10^{-8}$	
^{238}U	(n,n')	^{238}U	(n,n')	$0.197 \pm 2.2 \cdot 10^{-5}$	
^{238}U	χ	^{238}U	χ	$0.144 \pm 3.7 \cdot 10^{-6}$	
^{10}B	(n,n')	^{10}B	(n,n')	$0.139 \pm 2.5 \cdot 10^{-5}$	
Total uncertainty in β_{eff}		$1.100 \pm 1.2 \cdot 10^{-4}$		Total uncertainty in β_{eff}	
				$2.300 \pm 6.0 \cdot 10^{-5}$	

JEFF-3.3 nuclear data library does not contain uncertainty evaluations for the average number of prompt, v_p , and delayed, v_d , neutrons per fission for ^{240}Pu and of v_d for ^{235}U , ^{238}U , ^{239}Pu and ^{242}Pu , as can be inferred from Table 51, where β_{eff} uncertainty quantification analysis for MYRRHA with JEFF-3.3 nuclear data library is shown. Missing these evaluations causes JEFF-3.3 to severely underestimate the uncertainty in β_{eff} . Consequently, an additional UQ analysis with the state-of-the-art JENDL-4.0u2 covariance library using the sensitivities from JEFF-3.3 has been performed, in order to obtain a realistic estimation of β_{eff} uncertainty. Once again, results for the total β_{eff} uncertainty and major contributors are very similar to the ones obtained by Kodeli [Kodeli, 2018] using JENDL-4.0 covariance library. The average number of delayed neutrons per fission and the neutron fission spectra, χ , of Pu nuclides and ^{238}U are the major contributors to β_{eff} uncertainty. The total uncertainty in β_{eff} was found to be around 2.3% using the most complete covariance library for this parameter (i.e., JENDL-4.0), which is lower than the target accuracy requested by experts [D'Angelo and Rowlands, 2002; Rudstan et al., 2002].

7.5. Λ_{eff}

As mentioned in Section 7.4, Λ_{eff} plays a key role in reactor dynamics and safety analysis. However, neither the target accuracy for Λ_{eff} nor the UQ analysis for this parameter in any reactor concept have been found in bibliography.

In Table 52, Λ_{eff} values derived with MCNP and SUMMON, as well as the energy and region integrated sensitivity coefficients to the ten most important nuclides and reactions (quantities) for MYRRHA's effective neutron generation time, are shown.

Table 52. Λ_{eff} and Λ_{eff} ISC to the 10 most important neutron induced nuclear data for MYRRHA with JEFF-3.3 library

$$MCNP: \Lambda_{eff} = 1.798 \pm 0.006 \mu s$$

$$SUMMON: \Lambda_{eff} = 1.756 \pm 0.028 \mu s$$

MYRRHA – Λ_{eff} ISC (%/%)		
Quantity		JEFF-3.3
⁵⁶ Fe	(n,n)	$-1.712 \pm 3.6 \cdot 10^{-2}$
¹⁶ O	(n,n)	$1.567 \pm 3.8 \cdot 10^{-2}$
²⁰⁹ Bi	(n,n)	$-1.086 \pm 4.4 \cdot 10^{-2}$
²³⁸ U	(n,n)	$-0.772 \pm 3.3 \cdot 10^{-2}$
²³⁹ Pu	(n,f)	$-0.721 \pm 1.3 \cdot 10^{-2}$
⁵⁷ Fe	(n,n)	$0.719 \pm 9.8 \cdot 10^{-3}$
²⁰⁶ Pb	(n,n)	$0.679 \pm 1.9 \cdot 10^{-2}$
⁵² Cr	(n,n)	$-0.659 \pm 1.3 \cdot 10^{-2}$
²³⁹ Pu	v	$-0.655 \pm 1.4 \cdot 10^{-2}$
²³⁸ U	(n,n')	$-0.444 \pm 1.1 \cdot 10^{-2}$

A total uncertainty in Λ_{eff} around 20% is obtained in the UQ analysis for MYRRHA with JEFF-3.3 nuclear data library, as shown in Table 53. Once again, ²⁰⁹Bi elastic scattering is one of the most important neutron-induced reactions (Table 48 and Table 52); therefore, the total uncertainty in Λ_{eff} with JEFF-3.3 nuclear data library is underestimated since no uncertainty evaluation exists for this quantity. An additional UQ analysis has been performed using ENDF/B-VIII.0 library and an uncertainty of 6.8% due to ²⁰⁹Bi(n,n) has been obtained, which would rise the total uncertainty predicted by JEFF-3.3 to 22%.

In Table 53, the uncertainty in ¹⁰B(n,n') can also be highlighted given that it is not one of the quantities with highest Λ_{eff} sensitivity, which denotes a high uncertainty for this cross section in the fast energy range. In Figure 46, JEFF-3.3, ENDF/B-VIII.0 and BROND-3.1 uncertainty evaluations for ¹⁰B(n,n') are shown. A relative uncertainty of 500000% can be observed in the threshold of the reaction for JEFF-3.3, while from 0.82 to 4 MeV the uncertainty highly exceeds 100%. The impact of this uncertainty is such that ¹⁰B(n,n') turns to be the major contributor to the uncertainty in Λ_{eff} . The same behaviour is observed in ENDF/B-VIII.0 evaluation. While JEFF-3.3 and ENDF/B-VIII.0 ¹⁰B covariances for the most important reactions, like (n,α), are based on international standard analyses [Carlson et al., 2009] and can be therefore considered of high quality, no information about the origin of ¹⁰B(n,n') uncertainty evaluations is provided in the

ENDF-6 files. On the other hand, BROND-3.1 nuclear data library provides an uncertainty of less than 8% in the threshold of the inelastic reaction based on model calculations.

Table 53. Λ_{eff} nuclear data uncertainty quantification for MYRRHA with JEFF-3.3

MYRRHA				
JEFF-3.3				
Quantity				$\Delta\Lambda_{eff}/\Lambda_{eff}(\%)$
^{10}B	(n,n')	^{10}B	(n,n')	$9.769 \pm 1.7 \cdot 10^{-1}$
^{57}Fe	(n,n)	^{57}Fe	(n,n)	$7.649 \pm 3.1 \cdot 10^{-2}$
^{56}Fe	(n,n)	^{56}Fe	(n,n)	$7.551 \pm 5.5 \cdot 10^{-2}$
^{54}Fe	(n,n)	^{54}Fe	(n,n)	$6.081 \pm 4.5 \cdot 10^{-2}$
^{240}Pu	(n,n')	^{240}Pu	(n,n')	$5.078 \pm 9 \cdot 2 \cdot 10^{-3}$
^{240}Pu	(n,n)	^{240}Pu	(n,n)	$4.183 \pm 5.0 \cdot 10^{-3}$
^{239}Pu	χ	^{239}Pu	χ	$3.792 \pm 2.6 \cdot 10^{-2}$
^{238}U	(n,n')	^{238}U	(n,n')	$3.587 \pm 1.6 \cdot 10^{-2}$
^{16}O	(n,n)	^{16}O	(n,n)	$3.478 \pm 1.4 \cdot 10^{-2}$
^{208}Pb	(n,n)	^{208}Pb	(n,n)	$3.427 \pm 3.6 \cdot 10^{-2}$
Total uncertainty in Λ_{eff}				$20.754 \pm 2.0 \cdot 10^{-1}$

Figure 46. $^{10}\text{B}(\text{n},\text{n}')$ relative standard deviation in JEFF-3.3, ENDF/B-VIII.0 and BROND-3.1 evaluations

Even though there is no existing target accuracy, neutron noise measurements in VENUS-F CC10 core during the MYRTE project [Bécares and Villamarín, 2018] can give an approximation of the value of Λ_{eff} and, consequently, of the validity of the uncertainty in Λ_{eff} predicted by JEFF-3.3, comparing the Λ_{eff} value and its uncertainty due to nuclear data calculated with SUMMON against the measured Λ_{eff} . VENUS-F CC10 core configuration serves as a mock-up of MYRRHA

reactor and the neutron noise experiments allow for the determination of the kinetic parameters (i.e., β_{eff} and Λ_{eff}) in the critical state. The values of the kinetic parameters have been experimentally evaluated to be $\Lambda_{eff} = 2.31 \pm 0.11 \mu s$ and $\beta_{eff} = 659 \pm 22 pcm$. While MYRRHA's β_{eff} would highly differ from VENUS-F CC10 configuration due to the latter one having 30% enriched metallic U fuel [Bécares and Villamarín, 2018] and not possessing Pu (β_{eff} is mainly governed by ν_d and ν_p for Pu isotopes in the MOX fuel), a relatively similar Λ_{eff} to the one determined experimentally in VENUS-F can be expected in MYRRHA since Λ_{eff} dynamics are highly sensitive to materials that serve as a moderator, that is, to the elastic scattering reactions with coolant and structural materials (Table 52). This means that the true Λ_{eff} value would be underpredicted by around 20% by JEFF-3.3 with the IFP and 1/v insertion methods, which also agrees with the deviations between the experimental and calculated Λ_{eff} for LEU-COMP-THERM-077-003 (Table 34). However, if we considered the uncertainty in Λ_{eff} due to nuclear data derived with JEFF-3.3 nuclear data library (around 20%), there would be an agreement between the experimental determined and calculated values. Consequently, the uncertainty obtained with JEFF-3.3 can be accepted due to the spread that exists between experimental and calculated Λ_{eff} values for MYRRHA and VENUS-F mock-up core, even considering the anomalous behaviour of $^{10}B(n,n')$ uncertainty. Nevertheless, a more rigorous and exhaustive evaluation should be performed to confirm this target accuracy (20%).

Figure 47. Energy dependent $S_{\Lambda_{eff}}$ to the three most important quantities for Λ_{eff} in MYRRHA

Additionally, SUMMON is capable of obtaining energy dependent sensitivities and uncertainties. These values, for the most important quantities for Λ_{eff} , are given in Figure 47 and

Figure 48, respectively. It can be confirmed that the energy region of interest is the fast spectrum, as expected.

Figure 48. Energy dependent uncertainty contribution from the two most important quantities for $\Delta\Lambda_{eff}$ in MYRRHA

7.6. Reactivity coefficients

Reactivity coefficients indicate the change in core reactivity produced by an external perturbation and provide the information needed to perform the analysis of operational and accidental transients. They are therefore necessary to make a full safety assessment of the core design.

It is important to note that the use of a homogenized model to simulate the reactivity change scenarios can introduce a bias in the calculations since the change in core conditions cannot be accurately modelled in MCNP.

7.6.1. Doppler coefficient

The Doppler effect, when acting as a reduction in the self-shielding by the widening of the absorption resonances, is one of the key factors in the dynamic behaviour of the reactor [Cacuci, 2010]. Its effect on the reactivity is practically logarithmic with respect to temperature.

In Table 54, the reactivity response of a scenario corresponding to an increase of 400 K from the reference 800 K in fuel temperature (i.e., increase to 1200 K), ρ_T , as well as the energy and region integrated sensitivity coefficients of the ten most important nuclides and reactions (quantities) for MYRRHA for this reactivity effect, are shown. An increase of fuel temperature

of 400 K introduces a ~200 pcm decrease in reactivity. A high sensitivity to fuel primary materials and reactions (i.e., ^{239}Pu fission and ν and ^{238}U capture), as well as to the elastic scattering of coolant and structural materials is observed.

Table 54. ρ_T and ρ_T ISC to the 10 most important neutron induced nuclear data for MYRRHA with JEFF-3.3 library for a fuel temperature increase of 400 K

$$\rho_T = -192 \pm 1 \text{ pcm}$$

MYRRHA – ρ_T ISC (%/%)		
Quantity		JEFF-3.3
^{239}Pu	(n,f)	$0.924 \pm 2.8 \cdot 10^{-3}$
^{239}Pu	ν	$0.612 \pm 2.9 \cdot 10^{-3}$
^{16}O	(n,n)	$-0.582 \pm 8.3 \cdot 10^{-3}$
^{207}Pb	(n,n)	$-0.532 \pm 4.5 \cdot 10^{-3}$
^{238}U	(n, γ)	$-0.422 \pm 6.4 \cdot 10^{-4}$
^{206}Pb	(n,n)	$0.370 \pm 4.5 \cdot 10^{-3}$
^{208}Pb	(n,n)	$-0.330 \pm 7.4 \cdot 10^{-3}$
^{52}Cr	(n,n)	$-0.305 \pm 6.5 \cdot 10^{-3}$
^{27}Al	(n,n)	$0.303 \pm 3.1 \cdot 10^{-3}$
^{54}Fe	(n,n)	$-0.220 \pm 3.0 \cdot 10^{-3}$

ρ_T uncertainty quantification analysis for MYRRHA with JEFF-3.3 nuclear data library is shown in Table 55. Once again, $^{10}\text{B}(\text{n},\text{n}')$ is a major contributor to ρ_T uncertainty even if the sensitivity of the reactivity response to a change of 400 K in fuel temperature to $^{10}\text{B}(\text{n},\text{n}')$ is not one of the top 10. However, the elastic scattering of iron nuclides is once more a major contributor to the uncertainty of a parameter that is mainly driven by the physics of the fuel materials (Table 52 and Table 54). While $^{54}\text{Fe}(\text{n},\text{n})$ and $^{56}\text{Fe}(\text{n},\text{n})$ can be mostly explained by the convolution of their high ISC (10th and 15th, respectively) with their uncertainty in JEFF-3.3, $^{57}\text{Fe}(\text{n},\text{n})$ contribution denotes a high uncertainty in JEFF-3.3 evaluation, which is based on JEFF-3.2. In Figure 49, a maximum uncertainty of 8% in the fast energy region for ^{56}Fe , unrealistically high relative uncertainties, except above the threshold for the inelastic scattering (~15%) where resonances are missing, of up to 500% for ^{54}Fe and up to 1000% for ^{57}Fe can be observed in the MYRRHA relevant energy range (0.1 keV – 4 MeV).

Figure 49. Relative standard deviation of elastic scattering for iron nuclides in JEFF-3.3 evaluations

Table 55. ρ_p uncertainty quantification for MYRRHA with JEFF-3.3

MYRRHA				
JEFF-3.3				
Quantity				$\Delta\rho_T/\rho_T(\%)$
^{10}B	(n,n')	^{10}B	(n,n')	$4.925 \pm 1.1 \cdot 10^{-7}$
^{57}Fe	(n,n)	^{57}Fe	(n,n)	$3.385 \pm 1.2 \cdot 10^{-8}$
^{56}Fe	(n,n)	^{56}Fe	(n,n)	$3.304 \pm 6.9 \cdot 10^{-8}$
^{54}Fe	(n,n)	^{54}Fe	(n,n)	$2.438 \pm 1.4 \cdot 10^{-8}$
^{55}Mn	(n,n)	^{55}Mn	(n,n)	$1.918 \pm 6.9 \cdot 10^{-9}$
^{58}Ni	(n,n)	^{58}Ni	(n,n)	$1.864 \pm 4.5 \cdot 10^{-9}$
^{208}Pb	(n,n)	^{208}Pb	(n,n)	$1.793 \pm 5.6 \cdot 10^{-8}$
^{240}Pu	(n,n)	^{240}Pu	(n,n')	$-1.514 \pm 2.8 \cdot 10^{-9}$
^{240}Pu	(n,n')	^{240}Pu	(n,n')	$1.441 \pm 1.1 \cdot 10^{-8}$
^{240}Pu	(n,f)	^{240}Pu	(n,f)	$1.422 \pm 6.3 \cdot 10^{-8}$
Total uncertainty in ρ_T				$9.051 \pm 3.1 \cdot 10^{-7}$

With regard to the target accuracy, the total uncertainty in ρ_T due to uncertainty in nuclear data is around 9%, which makes the target accuracy for this criticality parameter to be slightly exceeded. Without the anomalous contributions of $^{10}\text{B}(\text{n},\text{n}')$ and elastic scattering of Fe nuclides, the target accuracy would not be exceeded.

7.6.2. Coolant expansion coefficient

Unlike in sodium reactors, in LFR the lead voiding scenario can be assumed as unreal (the evaporation temperature of lead is 1749 °C and of lead-bismuth eutectic is 1670 °C, much higher temperatures than the coolant nominal temperature). Therefore, the lead voiding scenario simulation (decreasing lead density) is performed to maintain consistency with SFR analysis and

not because it is a real accidental scenario; even if large losses of coolant (mitigated by the pool-type reactor configuration) or a large steam injection, due to a massive rupture of the steam generators tubes [Cacuci, 2010], are assumed.

To evaluate the coolant expansion effect, a decrease of 5% in coolant density in the fuel active region, which corresponds to a temperature increase of 400 K in the fuel (scenario in Section 7.6.1), was assumed. In Table 56, the reactivity response of the 5% decrease in coolant density scenario, ρ_ρ , as well as the energy and region integrated sensitivity coefficients of the ten most important nuclides and reactions (quantities) for MYRRHA for this reactivity effect, are shown.

A decrease in coolant density implies a reduction of interactions between neutrons and coolant nuclides. Therefore:

- i. the spectrum, due to a decrease in the interactions with the coolant, becomes harder and reactivity increases;
- ii. in leakage, because of a reduction in the interactions with lead, there are more neutrons with higher energy available. Although the probability of interaction or absorption depends on each nuclide, it usually decreases with the energy; so the leakage increases in the core and the reactivity decreases.
- iii. Although it is a relatively low effect, the reactivity increases due to fewer captures.

Consequently, reactivity changes will depend on the sum of these three effects. A reactivity decrease as a result of a decrease in coolant density or coolant voiding is required from the safety point of view.

Table 56. ρ_ρ and ρ_ρ ISC to the 10 most important neutron induced nuclear data for MYRRHA with JEFF-3.3 library for a coolant density decrease of 5%

$$\rho_\rho = -97 \pm 1 \text{ pcm}$$

MYRRHA – ρ_ρ ISC (%/%)		
Quantity		JEFF-3.3
¹⁶ O	(n,n)	$-2.286 \pm 2.8 \cdot 10^{-2}$
⁵⁸ Ni	(n,n)	$-1.291 \pm 1.2 \cdot 10^{-2}$
²⁰⁹ Bi	(n,n)	$-1.288 \pm 2.8 \cdot 10^{-2}$
⁵⁶ Fe	(n,n)	$1.064 \pm 2.3 \cdot 10^{-2}$
²⁰⁷ Pb	(n,n)	$-0.740 \pm 1.3 \cdot 10^{-2}$
²⁰⁸ Pb	(n,n)	$-0.718 \pm 2.0 \cdot 10^{-2}$
²³⁸ U	v	$0.672 \pm 3.2 \cdot 10^{-3}$
⁶² Ni	(n,n)	$0.552 \pm 3.5 \cdot 10^{-3}$
⁵³ Cr	(n,n)	$0.541 \pm 6.3 \cdot 10^{-3}$
²³⁹ Pu	(n,f)	$-0.523 \pm 9.7 \cdot 10^{-3}$

For MYRRHA, the increase in leakage overcomes the positive effect on the neutron spectra and captures decrease in the active part, so a negative reactivity effect of ~ 100 pcm is introduced (Table 56). Elastic scattering of fuel, structural and coolant materials (i.e., ^{16}O , ^{58}Ni , ^{209}Bi , ^{56}Fe and ^{207}Pb) are the most important reactions for this reactivity response.

ρ_p uncertainty quantification analysis for MYRRHA with JEFF-3.3 nuclear data library is shown in Table 57. As in Δ_{eff} and ρ_T , $^{10}\text{B}(n,n')$ and $^{54,56,57}\text{Fe}(n,n)$ are the major contributors to the uncertainty; though, in this reactivity effect, $^{238}\text{U}(n,n')$ and its correlation with elastic scattering are also key contributors. The sum of the uncertainties of all contributors involved in this effect yields a total ρ_p uncertainty of 20%, which is once again underestimated due to JEFF-3.3 missing $^{209}\text{Bi}(n,n)$ covariance evaluation but still exceeds by more than a factor of 2 the target accuracy. In this case, even if the anomalous uncertainties of $^{10}\text{B}(n,n')$ and Fe nuclides would be corrected, the target accuracy would still be exceeded.

Table 57. ρ_p nuclear data uncertainty quantification for MYRRHA with JEFF-3.3

MYRRHA				
JEFF-3.3				
Quantity				$\Delta\rho_p/\rho_p(\%)$
^{10}B	(n,n')	^{10}B	(n,n')	$10.400 \pm 4.9 \cdot 10^{-8}$
^{57}Fe	(n,n)	^{57}Fe	(n,n)	$8.069 \pm 5.4 \cdot 10^{-9}$
^{56}Fe	(n,n)	^{56}Fe	(n,n)	$7.415 \pm 3.1 \cdot 10^{-8}$
^{54}Fe	(n,n)	^{54}Fe	(n,n)	$5.318 \pm 6.1 \cdot 10^{-9}$
^{240}Pu	(n,n')	^{240}Pu	(n,n')	$4.745 \pm 5.1 \cdot 10^{-9}$
^{16}O	(n,n)	^{16}O	(n,n)	$4.514 \pm 6.6 \cdot 10^{-9}$
^{208}Pb	(n,n)	^{208}Pb	(n,n)	$3.591 \pm 2.5 \cdot 10^{-8}$
^{238}U	(n,n')	^{238}U	(n,n')	$3.394 \pm 5.6 \cdot 10^{-8}$
^{238}U	(n,n)	^{238}U	(n,n)	$3.393 \pm 3.7 \cdot 10^{-8}$
^{58}Ni	(n,n)	^{58}Ni	(n,n)	$3.157 \pm 2.0 \cdot 10^{-9}$
Total uncertainty in ρ_p				$20.311 \pm 1.4 \cdot 10^{-7}$

7.6.3. Control rod worth

The safety and control rod systems are key components for the safe and reliable operation of any nuclear reactor. In normal operation, reactivity is controlled by CRs while SRs are fully extracted. SRs, together with CRs, are only inserted during an emergency reactor shutdown which takes less than one second in MYRRHA design [Proffir et al., 2015]. Control rod reactivity worth is derived by assessing the reactivity decrease due to a small CR insertion ($\sim 10\%$) in successive steps until the CRs are fully inserted. This allows nuclear reactor designers to obtain a clear picture of control rod dynamics. However, in the homogeneous model control rod insertion is simulated by changing the material composition of the CR assemblies and only two options are available,

CR fully extracted or CR fully inserted. Consequently, to evaluate the reactivity response due to control rod movement, full CR insertion was simulated. In Table 58, the reactivity response due to a full CR insertion, ρ_{CR} , as well as the energy and region integrated sensitivity coefficients of the ten most important nuclides and reactions (quantities) for MYRRHA for this reactivity effect, are shown.

The buoyancy-driven control rods in MYRRHA employ 90% ^{10}B -enriched boron carbide, B_4C , as an absorbing material. Besides the availability of boron and the ease of its fabrication, therefore, the low costs related to the adoption to B_4C -based control systems, the neutronic properties of the ^{10}B isotope are excellent even in the fast spectrum because of its (n,α) reaction cross section [Cacuci, 2010]. Thus, $^{10}\text{B}(n,\alpha)$ is expected to be a key quantity in this reactivity change scenario, together with reactions produced in the fuel material due to the shift in the neutron spectrum caused by the insertion of CRs.

Table 58. ρ_{CR} and ρ_{CR} ISC to the 10 most important neutron induced nuclear data for MYRRHA with JEFF-3.3 library for a full CR insertion

$$\rho_p = -10177 \pm 2 \text{ pcm}$$

MYRRHA – ρ_{CR} ISC (%/%)		
Quantity		JEFF-3.3
^{239}Pu	(n,f)	$0.653 \pm 4.7 \cdot 10^{-5}$
^{239}Pu	v	$0.575 \pm 4.7 \cdot 10^{-5}$
^{10}B	(n, α)	$-0.359 \pm 2.8 \cdot 10^{-5}$
^{240}Pu	v	$0.166 \pm 7.7 \cdot 10^{-6}$
^{238}U	v	$0.154 \pm 1.1 \cdot 10^{-5}$
^{240}Pu	(n,f)	$0.143 \pm 7.7 \cdot 10^{-6}$
^{238}U	(n,f)	$0.122 \pm 1.1 \cdot 10^{-5}$
^{238}U	(n, γ)	$0.115 \pm 7.3 \cdot 10^{-6}$
^{239}Pu	(n, γ)	$0.105 \pm 5.2 \cdot 10^{-6}$
^{209}Bi	(n,n)	$0.082 \pm 1.6 \cdot 10^{-4}$

ρ_{CR} uncertainty quantification analysis for MYRRHA with JEFF-3.3 nuclear data library is shown in Table 59; **Error! La autoreferencia al marcador no es válida.** $^{240}\text{Pu}(n,f)$ is the major contributor to the uncertainty, as in the case of k_{eff} (Section 7.3), because of the significant relative standard deviation (around 35%) of this evaluation in the MYRRHA-relevant energy region (Figure 50). On the other hand, even if the uncertainty of $^{239}\text{Pu}(n,f)$ cross section is less than 5% (Figure 50), $^{239}\text{Pu}(n,f)$ is the second major contributor to the uncertainty as a consequence of its high sensitivity coefficient. $^{238}\text{U}(n,n')$, which was a major source of uncertainty in all criticality safety coefficients due its uncertainty in older evaluations [Grasso et al., 2018; Romojaro et al., 2017b] is still a major contributor, but its uncertainty has been significantly reduced in JEFF-3.3 and ENDF/B-VIII.0 state-of-the-art nuclear data libraries (Figure 51). JEFF-3.3 ^{10}B covariance

data were taken from the standards analysis [Carlson et al., 2009], therefore the covariances should be considered to be of high quality. Uncertainties for the standard (n,α) reaction are near 1% and, subsequently, the contribution of this reaction to the total uncertainty is lower than for nuclides present in fuel, in spite of its large ISC.

Table 59. ρ_{CR} nuclear data uncertainty quantification for MYRRHA with JEFF-3.3

MYRRHA				
JEFF-3.3				
Quantity				$\Delta\rho_{CR}/\rho_{CR}(\%)$
²⁴⁰ Pu	(n,f)	²⁴⁰ Pu	(n,f)	$1.284 \pm 3.1 \cdot 10^{-7}$
²³⁹ Pu	(n,f)	²³⁹ Pu	(n,f)	$0.689 \pm 1.1 \cdot 10^{-7}$
²³⁹ Pu	χ	²³⁹ Pu	χ	$0.535 \pm 8.6 \cdot 10^{-7}$
²³⁹ Pu	(n,γ)	²³⁹ Pu	(n,γ)	$0.468 \pm 3.0 \cdot 10^{-8}$
²³⁸ U	(n,n')	²³⁸ U	(n,f)	$-0.407 \pm 2.4 \cdot 10^{-7}$
²³⁸ U	(n,n')	²³⁸ U	(n,n')	$0.382 \pm 6.3 \cdot 10^{-7}$
²³⁸ U	(n,n)	²³⁸ U	(n,n')	$-0.327 \pm 4.1 \cdot 10^{-7}$
²³⁸ U	(n,f)	²³⁸ U	(n,f)	$0.307 \pm 4.9 \cdot 10^{-8}$
²³⁸ U	(n,n)	²³⁸ U	(n,f)	$0.289 \pm 3.1 \cdot 10^{-7}$
²³⁹ Pu	(n,f)	²³⁹ Pu	(n,γ)	$-0.286 \pm 1.8 \cdot 10^{-8}$
Total uncertainty in ρ_{CR}				$1.802 \pm 1.6 \cdot 10^{-6}$

Figure 50. Relative standard deviation of ²³⁹Pu and ²⁴⁰Pu fission cross section in JEFF-3.3

The total uncertainty in the reactivity response due to the uncertainty in nuclear data corresponding to a full CR insertion is 1.8% (183 pcm). No target accuracy for this effect has been established by expert groups or industry, nevertheless, if we assume the same target accuracy requested for Doppler and void reactivity coefficients (Table 47), target accuracy is met.

Figure 51. Relative standard deviation of ^{238}U inelastic scattering in ENDF/B-VII.1, ENDF/B-VIII.0 and JEFF-3.3

7.7. Conclusions

A target accuracy assessment of the latest MYRRHA design has been performed with the SUMMON system and JEFF-3.3 nuclear data library. Integrated sensitivity coefficients, total uncertainties and main contributors to the uncertainty in the criticality safety coefficients (i.e., k_{eff} , β_{eff} , Λ_{eff} , change in fuel temperature, change in coolant density and control rod worth) have been obtained. Significant differences and inconsistencies for some nuclides and reactions in JEFF-3.3, ENDF/B-VIII.0 and JENDL4.0u2 covariance evaluations have been found. ^{238}U , $^{239,240}\text{Pu}$, $^{10}\text{B}(n,n')$, $^{54,56,57}\text{Fe}(n,n)$ and $^{208}\text{Pb}(n,n)$ have been identified as major contributors to the uncertainty in the criticality safety parameters.

The target accuracy assessment has allowed identifying the following nuclear data needs and requirements in JEFF-3.3 nuclear data library:

- No covariance evaluation for ^{209}Bi elastic scattering cross section exists. This causes an underestimation of the total uncertainty in k_{eff} , Λ_{eff} and change in coolant density scenario.
- No covariance evaluations exist for the average number of prompt and delayed neutrons emitted per fission in ^{240}Pu and for the number of delayed neutrons emitted per fission in ^{235}U , ^{238}U , ^{239}Pu and ^{242}Pu . This produces a significant underestimation of the total uncertainty in β_{eff} .
- $^{240}\text{Pu}(n,f)$ uncertainty is a major contributor to the total uncertainty in k_{eff} , fuel temperature increase scenario and control rod worth. Reduction of the uncertainty in this quantity, which reaches up to 30% in the MYRRHA-relevant energy range (0.1 keV – 4 MeV), is needed to meet target accuracies.

- $^{10}\text{B}(\text{n},\text{n}')$ has an unphysical relative uncertainty of 500000% in the near threshold region of the reaction, while from 0.82 to 4 MeV the uncertainty highly exceeds 100%. The impact of this uncertainty is such that $^{10}\text{B}(\text{n},\text{n}')$ turns to be the major contributor to the uncertainty in Λ_{eff} and fuel and coolant density change scenarios, even if the sensitivity coefficient of this quantity is not one of the highest. Significant reduction of the total uncertainty in the criticality coefficients would be achieved if the uncertainty for this quantity was reduced.
- Large uncertainties are found in ^{54}Fe and ^{57}Fe elastic scattering JEFF-3.3 evaluation (up to 500% and 1000% respectively) in the MYRRHA-relevant energy range, which introduce significant uncertainties in Λ_{eff} , which is highly sensitive to reflector materials, and fuel and coolant density change scenarios. A reduction of the uncertainty in these quantities is recommended to meet target accuracies. A new evaluation of the $^{57}\text{Fe}(\text{n},\text{n}')$ cross section is also needed.
- Even if the uncertainty in $^{208}\text{Pb}(\text{n},\text{n})$ cross section is less than 7% in the energy range of interest for MYRRHA, ^{208}Pb elastic scattering is also a major contributor in Λ_{eff} and fuel and coolant density change scenarios. The uncertainty of this quantity in the MYRRHA relevant energy region should be reduced.
- Uncertainty in $^{238}\text{U}(\text{n},\text{n}')$ cross section has been significantly reduced in modern evaluations but is still one of the main contributors to the uncertainty and, consequently, there is still need for improvement.

Furthermore, target accuracies defined by industry and experts are exceeded for k_{eff} , change in fuel temperature and change in coolant density scenarios. No established target accuracy has been found for Λ_{eff} and control rod worth, however, comparison with experimental results from VENUS-F CC 10 core configuration, which serves as a mock-up of MYRRHA critical core, indicate that the uncertainty in Λ_{eff} due to nuclear data obtained with JEFF-3.3 may be acceptable and explains the spread between the existing experimental and calculated results. Target accuracy in control rod worth is met, assuming the same target accuracies requested for Doppler and void reactivity change scenarios.

To achieve the goal of reducing nuclear data uncertainties in LFR safety coefficients, the reduction of nuclear data uncertainties in JEFF-3.3 in the quantities identified in the S/U analyses is needed. Thus, three options are available at this point, adopt other state-of-the-art-evaluations incorporating new uncertainty evaluations (e.g., BROND-3.1 $^{10}\text{B}(\text{n},\text{n}')$ or ENDF/B-VIII.0 CIELO-based $^{54}\text{Fe}(\text{n},\text{n})$ and ^{57}Fe evaluations), perform new high-quality experiments to obtain new cross section data with reduced uncertainties or use integral benchmark data together with

advanced statistical adjustment techniques to incorporate already available experimental data to the uncertainty evaluations.

Chapter 8

Data Assimilation With summoN

Abstract – Target accuracies defined by industry and experts for k_{eff} , change in fuel temperature and change in coolant density scenarios were exceeded for the MYRRHA case study in Chapter 7. Data Assimilation With summoN (DAWN) module is developed to perform data assimilation using integral experiments from public databases, with the aim of providing adjusted nuclear data, not only capable of predicting reactor properties within the target design accuracy, but also statistically consistent with the various energy dependent measurements. In this chapter, the DAWN module is described. Furthermore, in order to verify DAWN a data assimilation with JEFF-3.3 is performed and results are compared against adjustments with Bayesian Monte Carlo methodology using TALYS-generated nuclear data. Finally, DAWN is used to perform data assimilation with JEFF-3.3 nuclear data library on the nuclides identified in Chapter 7 as major contributors to MYRRHA’s uncertainty in k_{eff} , Doppler effect and change in coolant density, aiming to produce a new covariance data set capable of predicting the criticality safety coefficients with uncertainties lower than the established target accuracies.

This chapter shows, partially or completely, works already presented in the following reference:

- International Conference Proceeding [Romojaro et al., 2018b]

8.1. Introduction

Uncertainties in nuclear data are one of the most important sources of uncertainty in reactor physics simulations. Therefore, target accuracies required for innovative reactor concepts such as MYRRHA or ALFRED can only be met if accurate nuclear data are available. Neutron cross sections and neutron spectra can be obtained either by measurements of cross sections versus neutron energy, or as the measurement of a critical size or a criticality factor of a well-defined

system. The former measurements are called energy dependent experiments, the latter integral experiments [Tellier, 1981].

The level of accuracy needed in nuclear data cannot be obtained using only energy dependent experiments [Brown et al., 2018; Kuroi and Mitani, 1975; Salvatores et al., 2014], even if “innovative” or “novel” experiments designed to reduce counting and systematic uncertainties (resolution function, detector efficiency and instrumentation among others) of a conventional experiment are used. Furthermore, correlations between measurements are hard to quantify. The sources of uncertainties in integral experiments are different from those of energy dependent measurements, so they provide a complementary point of view on nuclear data. The use of integral experiments has proven crucial to support the design of new reactor concepts. Moreover, they have been extensively used for nuclear data validation and the development of new simulation tools.

The combination of experimental covariance data and integral experiments together with advanced statistical adjustment techniques, such as Generalised Least Squares (GLS) [Smith, 1991], can provide adjusted nuclear data, not only capable of predicting reactor properties within the target design accuracy, but also statistically consistent with the various energy dependent measurements [Kuroi and Mitani, 1975].

Table 60. Summary of state-of-the-art tools for data adjustment

Name	Institution	Adjustment method*	Comments
GMADJ [Poenitz, n.d.]	ANL (USA)	GLS	Not public
CONRAD [Archier et al., 2014]	CEA (France)	Bayes' theorem method	Not public
AMARA [Gandini and Petilli, 1973]	INL (USA)	Lagrange multiplier's method	Maximum number of integral data is 60. Maximum number of nuclear data is 200
INDECS [Manturov, 1984]	IPPE (Russia)	Maximum likelihood method	Not public
In-house development [Dragt et al., 1977]	JAEA (Japan)	Bayesian parameter-estimation method	Not public
ZOTT-VL [Muir, 1989]	IAEA (Austria)	Partitioned least-square method	Integrated in the GANDR system
BERING [Ivanova et al., 2017]	IRSN (France)	GLS	Not public
BMC [Rochman et al., 2018]	NRG (Netherlands)	BMC	Complexity of the system due to number of simulations
SCALE [Rearden and Jessee, 2018]	ORNL (USA)	GLS	Use of SCALE covariance libraries for adjustment

* ANL, CEA, INL, IPPE, JAEA, IAEA and IRSN apply mathematically identical equations. ORNL equations use an additional factor [De Saint Jean et al., 2011].

Tools/codes that can perform consistent nuclear data adjustment exist, however some of them are not available to the public while others have limitations, as can be seen in Table 60 where a summary of state-of-the-art codes is presented.

Despite its recognized potential, data adjustment requires tracking and solving a series of issues [Palmiotti et al., 2015; Salvatores et al., 2014]: i) physical meaning of the individual adjustments; ii) possible compensation effects; iii) use of the *a posteriori* covariance matrix; and iv) definition of the application domain of the adjusted data sets.

In this chapter, the methodology implemented in SUMMON system to perform consistent nuclear data adjustment, also known as data assimilation (DA), is summarized. Furthermore, the methodology is verified against existing nuclear data adjustments performed using the Bayesian Monte Carlo (BMC) methodology and integral benchmark experiments from ICSBEP database.

8.2. Theory

The Working Party on International Nuclear Data Evaluation Co-operation of the OECD/NEA Nuclear Science Committee established a subgroup (called “Subgroup 33”) on “Methods and issues for the combined use of integral experiments and covariance data”. Its main objective was to study methods and issues of the combined use of integral experiments and covariance data with the objective of recommending a set of best and consistent practices in order to improve evaluated nuclear data files. A detailed description of the methodology implemented in SUMMON can be found in the subgroup intermediate [De Saint Jean et al., 2011] and final [Salvatores et al., 2013] reports.

8.2.1. Data adjustment

The current methodology is based on the GLS technique [De Saint Jean et al., 2011; Smith, 1991]. Let it be N_E integral parameters and N_σ neutron multi-group cross sections. Let $\sigma_j (j = 1, N_\sigma)$ and M_σ define the *a priori* expectation and covariance matrix of the cross sections. Then, the following quantities can be defined:

- $E_i (i = 1, \dots, N_E)$: experimental value of measured integral parameter i ;
- $C_i (i = 1, \dots, N_E)$: *a priori* calculated value of integral parameter i ;
- $\sigma'_j (j = 1, \dots, N_\sigma)$: *a posteriori* cross sections;
- S_{ij} : sensitivity coefficients for integral parameter i and cross section j ;
- M_E : relative integral parameter $i \times i$ covariance matrix due to measurement covariance;
- M_C : relative integral parameter $i \times i$ covariance matrix due to calculation covariance;
- $M_{EC} = (M_E + M_C)$: relative integral parameter $i \times i$ covariance matrix;

- M'_σ : *a posteriori* cross section $j \times j$ covariance matrix.

Let the following assumptions be made [Cabellos and Fiorito, 2018]:

- Experimental and nuclear data are normally distributed;
- All observables can be approximated linearly;
- Model and experimental data are uncorrelated.

Then, the evaluation of posterior expectation and covariances is done by finding the minimum of the following cost function (a generalised least-squares), which has been derived using Bayesian inference and assuming that prior and posterior probabilities are normally distributed [De Saint Jean et al., 2017]:

$$\chi^2 = \left(\frac{\sigma' - \sigma}{\sigma} \right)^T M_\sigma^{-1} \left(\frac{\sigma' - \sigma}{\sigma} \right) + \left(\frac{E - C}{C} \right)^T M_{EC}^{-1} \left(\frac{E - C}{C} \right) \quad (8.1)$$

The cross sections modifications that minimize the χ^2 thanks to the adjustment are:

$$\left(\frac{\sigma' - \sigma}{\sigma} \right) = M_\sigma S^T G^{-1} \left(\frac{E - C}{C} \right) \quad (8.2)$$

$G = (M_{EC} + S M_\sigma S^T)$ being the relative total integral $i \times i$ covariance matrix.

The associated *a posteriori* cross section covariance matrix is:

$$M'_\sigma = M_\sigma - M_\sigma S^T G^{-1} S M_\sigma = M_\sigma (I - S^T G^{-1} S M_\sigma) \quad (8.3)$$

Finally, the χ^2 after adjustment can be computed as:

$$\chi'^2 = \left(\frac{E - C}{C} \right)^T G^{-1} \left(\frac{E - C}{C} \right) \quad (8.4)$$

It should be noted that to ensure a valid cross section adjustment, the following premises are required: i) no missing and/or underestimation of uncertainty; ii) reliable nuclear data M_σ , experiment M_E and calculation M_C covariances; and iii) consistency of C/E values and covariance matrices.

Missing nuclides and reactions in nuclear data covariance can cause unreliable variations of other cross sections due to compensations or missing correlations, while underestimation of uncertainty could give again unreliable results.

If more than a single experiment is used at the same time in the adjustment (i.e., complete adjustment), some considerations must be taken regarding the experimental covariance matrix M_E . Experimental uncertainties of an integral parameter are usually given by the experimenters in the form of components. However, correlations between integral parameters are scarcely found

in the experiment reports [Salvatores et al., 2014]. Correlation coefficient data of uncertainties in criticality cases, derived from IPPE and from ANL for the ZPR/ZPPR values and publicly available in DICE [“DICE: User’s Manual,” 2016], together with the final experimental uncertainty reported for each experiment in the ICSBEP Handbook [OECD/NEA, 2016b], have been used to generate M_E . In consequence, the adjustment methodology implemented in SUMMON in the framework of this Thesis is limited to the use of these 93 critical mass experiments (i.e., k_{eff} experiments) for data assimilation.

The calculation covariance matrix M_C is derived from the statistical error of the MC code used to simulate the experiment. Ueki et al. [Ueki et al., 1997] and Shim et al. [Shim and Kim, 2009] have pointed out that MC codes cannot depend on the effect of correlation among the fission source over successive MC cycles to evaluate the statistical error; therefore, according to [Salvatores et al., 2013], the statistical error evaluated with the MC code should be multiplied by a factor of 2 in order to not underestimate the real statistical error. Furthermore, due to the random nature of the MC method, the correlations between calculations are basically 0, except if the integral measurements correspond to two reaction rate ratios that have the same denominator, in which case the correlation is 0.5.

Lastly, the consistency of C/E values and covariance matrices can be assured if the following condition is satisfied:

$$\frac{\chi'^2}{N_E} \approx 1 \quad (8.5)$$

8.2.1.1. M_σ^{-1}

As discussed in Ref. [Geraldo and Smith, 1988]: “*It is essential to realize that covariance matrices are introduced when statistical methods are employed in the modeling of physical phenomena - namely, in the area of uncertainty. For this reason it is important to insure that the mathematical models which are developed conform to physical reality. It is intuitively evident that all sets of information with which one deals in practical situations involve at least some random uncertainty, and, very likely, sources of systematic uncertainty as well. Realistic covariance matrices should reflect this fact. Covariance matrices must, therefore, be positive definite in order to represent uncertainties which are positive, not vanishing or imaginary. In fact, it is evident that investigators in this field have not always satisfied this important physical requirement in their work with covariance matrices*”. Indeed, when trying to invert nuclear data covariance matrices, problems arise with state-of-the-art evaluations due to the presence of zero and/or negative eigenvalues (not positive definite covariances), mostly because of rounding or truncations which can distort the eigenvalues of a symmetric matrix.

In order to produce invertible matrices, several steps have been taken:

- Instead of using SUMMON's 308 groups, covariance matrices with the same energy group structure that is given by evaluators in the nuclear data files have been produced with NJOY for each nuclide and reaction (e.g., 33g for ^{239}Pu or 44g for ^{240}Pu). This way, rounding errors due to interpolation inside covariance matrices and numerical stability problems due to the closeness of some energy bin limits are avoided.
- To include in the covariance matrices all the significant digits that appear in the nuclear data files, NJOY has been modified setting the *nfv* variable, which controls the number of significant digits written to BOXER format, to 13 in the covr.f90 module. If this is not done, the resulting matrices are not invertible due to rounding errors.
- If the whole energy range is taken into consideration for threshold reactions, such as (n,n') or (n,2n), a block of 0s in the variances and covariances appear up to the reaction threshold in the matrices, which makes them non-invertible. Therefore, to avoid that problem, SUMMON only employs the non-0 part, that is, a smaller block/matrix.

8.2.2. Experiment selection

Before nuclear data can be adjusted, the first step is to select a comprehensive set of complimentary experiments, representative of the target application, that provide information on “elementary” phenomena, on separated individual physics effects related to specific isotopes or on specific energy ranges [Palmiotti et al., 2017]. In practice, this means calculating correlations among the reactor concept and experiments to determine how representative is the latter of the former.

The representativity factor, f_{RE} , is defined as:

$$f_{RE} = \frac{S_R^T M_\sigma S_E}{\sqrt{(S_R^T M_\sigma S_R)(S_E^T M_\sigma S_E)}} \quad (8.6)$$

where S_R is the sensitivity vector for the targeted reactor and S_E is the sensitivity vector for the experiment. The closer f_{RE} is to one, the more similarity exists between the reactor and the experiment. General guidance is that f_{RE} values greater than 0.9 demonstrate similarity between two experiments or models, and f_{RE} values between 0.8 and 0.9 demonstrate moderate similarity. Values closer to zero indicate systems that are totally dissimilar [Parry et al., 2009].

The complementarity between an experiment E and another experiment E' can be established by the correlation factor, $f_{EE'}$:

$$f_{EE'} = \frac{S_E^T M_\sigma S_{E'}}{\sqrt{(S_E^T M_\sigma S_E)(S_{E'}^T M_\sigma S_{E'})}} \quad (8.7)$$

Opposite to the representativity factor, $f_{EE'} \ll 1$ indicates that a strong complementarity between experiments exist and that both are useful for the adjustment.

Once the representative experiments have been selected, several parameters have been defined to analyse if each individual experiment will be useful for the adjustment [Palmiotti et al., 2015]. Three parameters have been implemented in SUMMON to determine if an experiment should be kept or discarded before the adjustment.

The first parameter is the adjustment margin, AM :

$$AM_i = U_{\sigma}^i + U_{EC}^i - \left| \left(\frac{E^i - C^i}{C^i} \right) \right| \quad (8.8)$$

where U_{σ}^i is the uncertainty in the experiment parameter i due to nuclear data uncertainties and U_{EC}^i is the combined uncertainty of the measurement and the calculation for parameter i . Negative values of AM indicate inconsistencies in the covariance matrix due to low nuclear data uncertainties, underestimation of experimental or calculation errors, missing experimental correlations and/or the presence of an undetected systematic error in the experiment.

The parameter proposed by ORNL [De Saint Jean et al., 2011] to quantify the individual contribution of an integral experiment i to χ^2 , taking into account the correlations among integral experiments and cross sections to some extent, is $\chi_{diag}^{i^2}$:

$$\chi_{diag}^{i^2} = \left(\frac{E^i - C^i}{C^i} \right)^2 G_{ii}^{-1}(i, i) \quad (8.9)$$

$\chi_{diag}^{i^2}$ uses only the diagonal values of the inverse total integral covariance matrix, $G_{ii}^{-1}(i, i)$. If $\chi_{diag}^{i^2} \gg 1$, the same inconsistencies identified for AM may exist. A value of less than three is recommended [Palmiotti et al., 2015] in order to keep the experiment i in the adjustment.

The last parameter used by SUMMON to determine if an integral experiment i will be useful for the adjustment is the Ishikawa factor, IS_i , which allows estimating the expected reduced uncertainty gain before adjustment and can also point out inconsistencies between the nuclear data M_{σ} , experiment M_E and calculation M_C covariance matrices. It is defined as:

$$IS_i = S_i M_{\sigma} S_i^T (M_{EC})_{ii}^{-1} \quad (8.10)$$

If $IS_i \gg 1$, the experiment i is very useful and the nuclear data covariance matrix after adjustment M'_{σ} will be reduced to the same level as the integral parameter covariance M_{EC} . On the contrary, if $IS_i \ll 1$, the experiment i is not useful and the cross section remain unchanged

after adjustment. Finally, if $IS_i \approx 1$, then the experiment i is useful and the nuclear data covariance matrix after adjustment M'_σ will be reduced approximately by half.

8.2.2.1. Compensation effects

Unreliable results may be produced by the adjustment if compensation effects exist, e.g., different nuclide cross section variations that have opposite/compensating effects ($^{240}\text{Pu}(n,f)$ increase associated to $^{239}\text{Pu}(n,\gamma)$ increase in fast reactors).

Two new strategies have been recently proposed by Palmiotti et al. [Palmiotti and Salvatores, 2017] in order to limit the effect of compensations, based on giving priority to elemental type experiments (those sensitive to a specific cross section) in the adjustment: the Progressive Incremental Adjustment (PIA) methodology and the Ranking Experiments by Weighting for Improved Nuclear Data (REWIND) methodology. REWIND provides a scientifically based way (i.e., mathematical formulation) for ranking experiments while PIA relies on user judgment. Both strategies have been adopted by SUMMON.

PIA gives priority to the utilization of experiments of elemental type, following a definite hierarchy on which type of experiment to use [Palmiotti and Salvatores, 2017]. Once an adjustment step is performed, both the new adjusted data and the new covariance matrix are kept. This limits the range of variability of the adjusted cross sections. In the final steps integral experiments that are sensitive to a large variety of cross sections are added. However, even if elemental experiments are used, experiments can still be correlated, therefore correlations between experiments must be taken into account to avoid biasing or compensations.

REWIND is based on a technique that has been developed for optimizing portfolios of investment assets [Palmiotti and Palmiotti, 2015] by calculating the optimal weights that maximize the portfolio “Sharpe Ratio” [Sharpe, 1966]; that is, by maximizing the average return earned in excess of the risk-free rate per unit of volatility or total risk. Applied to nuclear data adjustment, the return of each asset is the potential gain an experiment can produce by reducing the uncertainty.

First, let the covariance of the set of integral experiments, M_P , be defined as:

$$M_P^{ii'} = U_\sigma^i fr_{ii'} U_\sigma^{i'} \quad (8.11)$$

where $fr_{ii'}$ corresponds to the correlation factor between experiment i and experiment i' (Eq. 8.7).

Then, the standard deviation of the set of integral experiments, SD_P , is:

$$SD_P = w_i M_P^{ii} w_i^T \quad (8.12)$$

while the internal correlation of the set of experiments, C_P , is defined as:

$$C_P = \frac{SD_P - SD_P^{cu}}{SD_P^{cc}} \quad (8.13)$$

where w_i is the weight for each experiment i ($\sum w_i = 1$), whereas SD_P^{cu} and SD_P^{cc} are the standard deviations of the complete uncorrelated and complete correlated set of integral experiments respectively, expressed as:

$$SD_P^{cu} = \sqrt{\sum_{i=1}^{N_E} (w_i U_\sigma^i)^2} \quad (8.14)$$

$$SD_P^{cc} = \sum_{i=1}^{N_E} w_i U_\sigma^i \quad (8.15)$$

A C_P value close to 0 is desired, which means that experiments are orthogonal (i.e., uncorrelated) and they provide diversified information.

Finally, the Sharpe Ratio to find the optimal experiment weights is:

$$SR_P = \frac{\sum_{i=1}^{N_E} w_i (U_\sigma^i - U_{EC}^i)}{SD_P} \quad (8.16)$$

An optimization algorithm has been implemented in SUMMON in order to find the optimal weights w_i (i.e., maximum Sharpe Ratio) and, therefore, the ranking of experiments. The set of experiments with an internal correlation C_P very close to zero (almost uncorrelated) and the experiments with non-zero weights (useful for the adjustment) will be finally chosen for the data adjustment.

Once the ranking of experiments has been obtained, a progressive adjustment can be made starting from the top-ranked experiment, then recalculating new C/E with the new adjusted cross sections and related covariance matrices and proceeding to do the same with the next experiment, and so on; which is in fact the principle of the PIA methodology but relying on expert judgement to rank the experiments.

However, complete adjustments (described in Section 8.2.1) with non-zero weight experiments predicted by REWIND are recommended when SUMMON is used in conjunction with MCNP, because progressive adjustments are biased due to MCNP not computing the effect of the cross section self-shielding on the sensitivity coefficients in multi group calculations [Pelowitz, 2014; Werner, 2017]. In consequence, while the cross section relative modifications due to the adjustment are obtained in the data assimilation process and could be implemented in

308 group cross sections in ACE format, they cannot be used for calculating the new sensitivity coefficients after the adjustment since the implicit effect would not be considered, which will lead to incorrect results, as observed in Romojaro et al. [Romojaro et al., 2017b] for $^{238}\text{U}(\text{n},\text{n})$ sensitivity. Nevertheless, progressive and complete adjustments yield quite similar results when using k_{eff} experiments for data assimilation [Palmiotti and Salvatores, 2017] and, as described in Section 8.2.1, only k_{eff} experiments are used by SUMMON because of limited available correlation coefficient data in state-of-the-art databases, so correct results are expected even with such constraints.

Nonetheless, the complete methodology has been implemented in SUMMON so that the full potential of the data assimilation methodology can be reached when other code, with no limitations in the sensitivity coefficient calculation using multi group cross sections, is used, or more data on correlations of uncertainties in integral experiments are available.

8.2.3. Assessment after adjustment

After the adjustment is performed, several assessments must be made in order to determine if the changes obtained in the cross sections and nuclear data covariance matrix can be adopted and to analyse if the adjustment is consistent and valid.

8.2.3.1. Acceptance of adjusted central values

In order to avoid unreliable and/or unphysical cross section changes, SUMMON checks for:

- cross section changes larger than 1σ of the *a priori* standard deviation;
- negative *a posteriori* cross section values;
- large cross section variations in energy regions, nuclides or reactions that are not the main target of the adjustment;
- large cross section variations with a small *a posteriori* standard deviation.

Furthermore, to ensure the consistency of the adjustment, comparison of the *a posteriori* results with reliable energy dependent measurements and/or validated nuclear data files are carried out for the main adjustment targets.

8.2.3.2. Chi-filtering

After adjustment, if $\chi'^2 > 1$, then experiments can be removed based on their chi-square contribution, χ'^2_{con} :

$$\chi'^2_{\text{con}} = \frac{(E_i - C_i)G_{ii}^{-1}(E_i - C_i)}{N_E} \quad (8.11)$$

An experiment i should be removed from the adjustment if its $\chi_{con}^{i^2}$ has a large positive value due to possible unreliable changes in the cross sections. On the other hand, a negative value of $\chi_{con}^{i^2}$ means that the experiment is very effective in the adjustment.

8.2.3.3. *A posteriori* covariance matrix and application domain of the adjusted data sets

A consequence of the adjustment is that the *a posteriori* covariance matrix M'_σ is full because the experiment sensitivity coefficients detect and establish new correlations among missing quantities [Palmiotti et al., 2015]. Hence, M'_σ is fully correlated not only with the *a posteriori* cross sections, but also with the *a priori* and *a posteriori* integral parameters.

Therefore, due to such strong correlations, it is recommended to only use the adjusted nuclear data (*a posteriori* cross sections and covariances) for the reactor concept which have been adjusted, or for a system with a representativity factor f_{RE} close to one with the targeted reactor or experiments used in the adjustment. It is fundamental to keep in mind that, from a general-purpose library, we have generated with the adjustment procedure a specific-application library.

8.3. Implementation

The data assimilation methodology described in Section 8.2 has been implemented in the DAWN (Data Assimilation With summoN) module. DAWN has been developed to perform data assimilation using integral experiments from public databases, with the aim of providing adjusted nuclear data capable of predicting properties within the target design accuracy of advanced reactor designs. The DAWN module has been written in FORTRAN 90 programming language and is composed of 2890 lines of code. The main work has been divided in 4 specific subroutines:

- **dawn.f90** is the module interface.
- **similar.f90** calculates the correlation between two systems due to nuclear data.
- **adjust.f90** performs the adjustment.
- **newcov.f90** produces the new file in BOXER format with adjusted cross sections, uncertainties and covariances.

In Figure 52, the general flow diagram of DAWN is presented. First, the sensitivities of the reactor parameter of interest (i.e., k_{eff} , β_{eff} , Λ_{eff} and reactivity coefficients) are calculated with SUMMONR. Then, a search is conducted in ICSBEP and IRPhE databases to find integral experiments in which experimental data for the same integral parameter are provided. Sensitivities of the integral experiment are calculated with SUMMONR. Once the sensitivities have been obtained, the correlations among the reactor concept and experiment due to nuclear data, f_{RE} , are

derived. If f_{RE} is lower than 0.7, the experiment is discarded and another experiment is selected from the databases, repeating the previously described process. However, if the representativity factor is equal or greater than 0.7, data adjustment is performed with the *adjust* subroutine using the integral experiment and user selected covariance data and new cross section and covariance data in BOXER format is obtained with *newcov* subroutine.

Covariances from JEFF-3.3, ENDF/B-VIII.0 and JENDL-4.0 nuclear data libraries have been processed to BOXER format with the NJOY modification, following the guidelines given in Section 8.2.1.1, and can be used in the adjustment. Furthermore, any new nuclear data library which contains covariance data can be easily processed, thus conferring DAWN the same capability as SUMMONR of always using state-of-the-art covariance libraries.

Figure 52. General flow diagram of SUMMON's DAWN module

8.4. Verification

In order to verify the data assimilation module, ^{235}U , ^{238}U and ^{239}Pu data assimilation performed by Cabellos and Fiorito [Cabellos and Fiorito, 2019] and by Rochman [Rochman et al., 2018], using BMC methodology with TALYS-generated nuclear data and critical mass experiments from ICSBEP database, has been carried out with DAWN using JEFF-3.3 nuclear data library. Each experiment has been considered individually (i.e., single adjustment), therefore no progressive or complete adjustment has been performed.

In Table 61, a summary of the results obtained with the different codes and methodologies is presented. It can be seen that the prior uncertainty due to nuclear data predicted by BMC and SUMMON is higher than the experimental uncertainty, U_E , by a factor 3 at least. This indicates that there is a good potential for nuclear data adjustment. Indeed, the posterior uncertainties (i.e., total uncertainties due to nuclear data derived using adjusted covariance matrices), have been constrained to the same level as the experimental uncertainty. Furthermore, very good agreement between SUMMON and BMC can be observed, even if there are significant differences, up to 1000 pcm, between prior uncertainties in systems with intermediate uranium enrichment (IMF integral experiments).

Table 61. Summary of ^{235}U , ^{238}U and ^{239}Pu assimilation with DAWN and BMC

Integral Experiment		Prior				Posterior		Ref.
		SUMMON		BMC	SUMMON	BMC		
		E	U _E (pcm)	Unc. (pcm)	Unc. (pcm)	Unc. (pcm)	Unc. (pcm)	
HMF1	[OECD/NEA, 2015p]	1.00000	100	1358	1119	100	100	[Cabellos and Fiorito, 2019]
PMF1		1.00000	200	663	780	192	195	
PMF2	[OECD/NEA, 2015q]	1.00000	200	611	670	190	192	
PMF8	[OECD/NEA, 2015r]	1.00000	60	641	734	60	59	
PMF22	[OECD/NEA, 2015s]	1.00000	210	664	796	200	200	
IMF1-1	[OECD/NEA, 2015t]	0.99890	90	1440	910	90	90	[Rochman et al., 2018]
IMF2	[OECD/NEA, 2015u]	1.00000	300	1774	835	295	284	
IMF7		1.00450	70	1842	850	70	70	
MMF1	[OECD/NEA, 2015v]	1.00000	160	644	670	155	160	
MMF3	[OECD/NEA, 2015w]	0.99930	160	613	640	155	155	

Table 62. Prior and posterior UQ for HEU-MET-FAST-001 with SUMMON

A PRIORI					A POSTERIORI				
Quantity		$\Delta k_{eff}/k_{eff}(\%)$			Quantity		$\Delta k_{eff}/k_{eff}(\%)$		
^{235}U	(n,n')	^{235}U	(n,n')	$0.699 \pm 3.3 \cdot 10^{-6}$	^{235}U	(n,n')	^{235}U	(n,n')	$0.536 \pm 2.6 \cdot 10^{-5}$
^{235}U	(n,n')	^{235}U	(n,f)	$0.697 \pm 3.1 \cdot 10^{-6}$	^{235}U	(n,n')	^{235}U	(n, γ)	$-0.526 \pm 8.7 \cdot 10^{-6}$
^{235}U	(n,f)	^{235}U	(n,f)	$0.657 \pm 1.4 \cdot 10^{-6}$	^{235}U	v_p	^{235}U	v_p	$0.471 \pm 2.2 \cdot 10^{-6}$
^{235}U	v_p	^{235}U	v_p	$0.508 \pm 1.9 \cdot 10^{-7}$	^{235}U	v_p	^{235}U	(n,f)	$-0.446 \pm 2.3 \cdot 10^{-6}$
^{235}U	(n,n')	^{235}U	(n, γ)	$-0.424 \pm 4.4 \cdot 10^{-7}$	^{235}U	v_p	^{235}U	(n,n')	$-0.412 \pm 5.1 \cdot 10^{-6}$
^{235}U	(n, γ)	^{235}U	(n, γ)	$0.400 \pm 1.9 \cdot 10^{-7}$	^{235}U	(n,f)	^{235}U	(n,f)	$0.396 \pm 9.2 \cdot 10^{-6}$
^{235}U	χ	^{235}U	χ	$0.374 \pm 5.2 \cdot 10^{-6}$	^{235}U	(n, γ)	^{235}U	(n, γ)	$0.385 \pm 2.4 \cdot 10^{-6}$
^{235}U	(n,f)	^{235}U	(n, γ)	$0.350 \pm 1.8 \cdot 10^{-7}$	^{235}U	χ	^{235}U	χ	$0.360 \pm 6.6 \cdot 10^{-5}$
^{235}U	(n,n)	^{235}U	(n,n')	$-0.293 \pm 9.6 \cdot 10^{-7}$	^{235}U	χ	^{235}U	(n,f)	$-0.329 \pm 1.1 \cdot 10^{-5}$
^{235}U	(n,n)	^{235}U	(n,f)	$-0.241 \pm 1.2 \cdot 10^{-6}$	^{235}U	χ	^{235}U	(n,n')	$-0.303 \pm 1.0 \cdot 10^{-5}$
Total uncertainty in k_{eff}		$1.357 \pm 7.2 \cdot 10^{-6}$			Total uncertainty in k_{eff}		$0.100 \pm 7.8 \cdot 10^{-5}$		

To better understand the significant differences after the data assimilation, prior and posterior major contributors to the total uncertainty in HEU-MET-FAST-001 are shown in

Table 62 and Figure 53 to Figure 55 are provided. The strong reduction in the k_{eff} uncertainty can be attributed to a significant reduction in the uncertainty of important contributors, such as $^{235}\text{U}(n,f)$ or $^{235}\text{U}(n,\gamma)$ (Figure 53). Moreover, new strong negative cross-correlations between reactions that have large sensitivities appear after the adjustment due to the physical constraints introduced by the experiment, such as $^{235}\text{U} v - ^{235}\text{U}(n,f)$ (Figure 54). When the sensitivity of the nuclear data is zero or in energy regions where sensitivity is zero, such as thermal energy region

for $^{235}\text{U}(n,f)$, no correlation is generated (Figure 54). On the other hand, modifications in the cross section central values are nearly negligible using this integral experiment, ensuring that no unphysical cross sections are present after adjustment (Figure 55).

Figure 53. Prior (JEFF-3.3) and posterior nuclear data uncertainties in $^{235}\text{U}(n,n')$ and $^{235}\text{U}(n,f)$ using HEU-MET-FAST-001 for DA

Figure 54. Posterior cross-correlations between ν (MT 456) and (n,f) (MT 18) after adjustment with HEU-MET-FAST-001

Figure 55. Ratio between posterior and prior (JEFF-3.3) for different ^{235}U MG nuclear data using HEU-MET-FAST-001 for DA

8.5. Application to MYRRHA

In Chapter 7, sensitivity and uncertainty analyses were performed for MYRRHA lead-cooled fast reactor concept. Target accuracies defined by industry and experts were exceeded in k_{eff} , Doppler and change in coolant density criticality safety coefficients. In Chapter 8, SUMMON's data assimilation module (DAWN), developed to produce adjusted nuclear data in order to constrain uncertainties and predict reactor parameters within target accuracies, was presented.

In this section, DAWN will be used to perform data assimilation with JEFF-3.3 nuclear data library on the nuclides identified in Chapter 7 as major contributors to the uncertainty (i.e., ^{238}U , $^{239,240}\text{Pu}$, $^{10}\text{B}(n,n')$, $^{54,56,57}\text{Fe}(n,n)$ and $^{208}\text{Pb}(n,n)$), aiming to produce a new covariance data set capable of predicting the above-mentioned criticality coefficients with uncertainties lower than the established target accuracies. ^{209}Bi has not been targeted in the adjustment since no covariance information exists for the elastic scattering reaction channel in JEFF-3.3 and no critical mass experiment with enough sensitivity is available in the databases (Chapter 6).

Individual critical mass experiments from ICSBEP that provide information on separated individual physics effects related to the nuclides with highest sensitivity were chosen to perform data assimilation. No progressive or complete adjustments will be made (i.e., PIA or REWIND methodologies will not be employed) due to the limitations of SUMMON's current implementation with MCNP (see Chapter 8). A single nuclide or element will be adjusted with each integral experiment in order to avoid compensations since no information about correlations between selected experiments are available in ICSBEP database. Following this procedure, while cross-correlations between nuclides will not be produced *a posteriori*, possible compensations

due to the use of correlated integral experiments with unknown correlations between experimental uncertainties will be avoided.

To re-assess the posterior uncertainty in reactor criticality safety parameters, sensitivities calculated *a priori* (sensitivities derived in the target accuracy calculations in Chapter 7) will be used to propagate the uncertainties of the adjusted nuclear data, as in Chapter 8, which serves as a good approximation when the central values of the cross sections undergo very small adjustments *a posteriori*.

8.5.1. Data Assimilation

Publicly available critical mass experiments from the ICSBEP database with high sensitivity to ^{238}U , $^{239,240}\text{Pu}$, ^{10}B , Fe and Pb were assessed and a set of six experiments was obtained (Table 63).

Table 63. Integral experiments selected for DA

Integral experiment	Acronym	Targeted isotope
HEU-MET-FAST-010 [OECD/NEA, 2015x]	HMF010	^{10}B
PU-MET-FAST-028 [OECD/NEA, 2015y]	PMF028	$^{54,56,57,58}\text{Fe}$
HEU-MET-FAST-064	HMF064	$^{204,206,207,208}\text{Pb}$
PU-MET-FAST-006	PMF006	^{238}U
PU-MET-FAST-001	PMF001	^{239}Pu
PU-MET-FAST-002	PMF002	^{240}Pu

In Table 64, the representativity factors between MYRRHA and the six experiments are shown. No complementarity between experiments due to nuclear data will exist in the adjustment ($f_{EE'} = 0$), because in each experiment a different single material has been targeted (i.e., sensitivities have only been calculated for the material that will be adjusted with the experiment). ALFRED's representativity factor has also been included in order to evaluate the similarity between MYRRHA and ALFRED regarding nuclear data.

Table 64. Representativity factor of ALFRED and the selected integral experiments

f_{RE}	MYRRHA
ALFRED	0.97
HMF010	0.39
PMF028	0.42
HMF064	0.56
PMF006	0.81
PMF001	0.82
PMF002	0.94

If the sensitivity coefficients are similar and the cross section uncertainties are high, f_{RE} between two systems is significant. As indicated in Section 8.2.2, values greater than 0.9 demonstrate similarity between two experiments and values between 0.8 and 0.9 demonstrate moderate similarity. ALFRED and MYRRHA have a correlation factor of nearly one, therefore, from the point of view of nuclear data, they can be treated as the same system and, consequently, the adjustment will be valid for both reactors. In fact, any other LFR design that uses MOX fuel should have a similar representativity factor.

To study how much room for k_{eff} is present in order to accommodate in the adjustment the discrepancy between the measured and calculated values [Palmiotti et al., 2015], the adjustment margin of each experiment has been quantified (Table 65). The uncertainty due to nuclear data of each experiment, U_{σ} , has been calculated considering only the uncertainties of the nuclide targeted in the adjustment. The highest adjustment margins are produced in experiments with significant nuclear data uncertainties, that is, in the ones used for adjusting nuclides present in fuel. Consequently, fuel related integral experiments have also a significant similarity factor while lead, iron and boron experiments have low similarity with MYRRHA. However, the latter experiments will be kept in the adjustment because they will serve to moderately constrain nuclear data uncertainties.

Table 65. Adjustment margin of the integral experiments

Integral experiment	E	U_E (%)	C	U_c (%)	U_{EC} (%)	U_{σ} (%)	AM (%)
HMF010	1.00000	0.10	0.99728	0.001	0.10	0.01	-0.17
PMF028	1.00000	0.24	0.99906	0.001	0.24	0.41	0.56
HMF064	0.99960	0.10	1.00318	0.001	0.10	0.33	0.08
PMF006	1.00000	0.30	1.00334	0.001	0.30	0.75	0.72
PMF001	1.00000	0.11	1.00019	0.001	0.11	0.66	0.75
PMF002	1.00000	0.20	1.00128	0.001	0.20	0.84	0.91

The HMF010 experiment has a negative adjustment margin. Negative values of AM indicate possible inconsistencies in the covariance matrix due to low nuclear data uncertainties, underestimation of experimental or calculation errors, missing experimental correlations and/or the presence of an undetected systematic error in the experiment. If the experiment is kept in the adjustment, unphysical changes in the cross sections may be produced [Palmiotti et al., 2015], therefore, HMF010 has been discarded.

After the adjustment was performed, the posterior uncertainties obtained using the adjusted covariance matrix were re-assessed in a first step for the integral experiments (Table 66). For each experiment, the uncertainty in k_{eff} due to uncertainties in nuclear data has been reduced by at least 50%, meeting all experiments the target accuracy established for k_{eff} . The significant reductions in uncertainty are mainly caused by the appearance of strong negative correlations between reaction channels that were not present *a priori* in the covariance matrix, such as $^{239}\text{Pu } \chi - ^{239}\text{Pu } v_p$ or $^{239}\text{Pu } v_p - ^{239}\text{Pu}(n,f)$, as can be seen in Table 67 where the *a priori* and *a posteriori* UQ for PMF001 is shown. Nevertheless, the uncertainties in the major contributors a priori, such as $^{239}\text{Pu } v$, have also been constrained (Figure 56), contributing to the uncertainty reduction.

Table 66. Prior and posterior uncertainties due to nuclear data in the experiments used for DA

Integral experiment	U_σ (%)	U_σ' (%)
PMF028	0.41	0.21
HMF064	0.33	0.10
PMF006	0.75	0.28
PMF001	0.66	0.11
PMF002	0.84	0.19

Table 67. Prior and posterior UQ for PU-MET-FAST-001 with SUMMON. Statistical uncertainties can be considered negligible

A PRIORI					A POSTERIORI				
Quantity		$\Delta k_{eff}/k_{eff}$ (%)			Quantity		$\Delta k_{eff}/k_{eff}$ (%)		
$^{239}\text{Pu } \chi$	$^{239}\text{Pu } \chi$			0.470	$^{239}\text{Pu } \chi$	$^{239}\text{Pu } v_p$			-0.407
$^{239}\text{Pu } v_p$	$^{239}\text{Pu } v_p$			0.412	$^{239}\text{Pu } \chi$	$^{239}\text{Pu } \chi$			0.336
$^{239}\text{Pu } (n,n)$	$^{239}\text{Pu } (n,n)$			0.101	$^{239}\text{Pu } v_p$	$^{239}\text{Pu } v_p$			0.325
$^{239}\text{Pu } (n,n)$	$^{239}\text{Pu } (n,n')$			0.162	$^{239}\text{Pu } (n,f)$	$^{239}\text{Pu } (n,f)$			0.294
$^{239}\text{Pu } (n,n)$	$^{239}\text{Pu } (n,2n)$			0.030	$^{239}\text{Pu } (n,n')$	$^{239}\text{Pu } (n,f)$			-0.238
$^{239}\text{Pu } (n,n)$	$^{239}\text{Pu } (n,f)$			-0.200	$^{239}\text{Pu } \chi$	$^{239}\text{Pu } (n,f)$			-0.217
$^{239}\text{Pu } (n,n)$	$^{239}\text{Pu } (n,\gamma)$			-0.075	$^{239}\text{Pu } (n,n)$	$^{239}\text{Pu } (n,f)$			-0.201
$^{239}\text{Pu } (n,n')$	$^{239}\text{Pu } (n,n')$			0.132	$^{239}\text{Pu } v_p$	$^{239}\text{Pu } (n,f)$			-0.190
$^{239}\text{Pu } (n,n')$	$^{239}\text{Pu } (n,2n)$			0.035	$^{239}\text{Pu } (n,n)$	$^{239}\text{Pu } (n,n')$			0.162
$^{239}\text{Pu } (n,n')$	$^{239}\text{Pu } (n,f)$			-0.239	$^{239}\text{Pu } (n,n')$	$^{239}\text{Pu } (n,n')$			0.132
Total uncertainty in k_{eff}		0.663			Total uncertainty in k_{eff}		0.109

Figure 56. Prior (JEFF-3.3) and posterior nuclear data uncertainties in ^{239}Pu ν_p

The consistency of the assimilation was assessed against experimental data. An example of the consistency checks is given in Figure 57, where the prior and posterior $^{240}\text{Pu}(n,f)$ cross sections after the assimilation with PMF002 integral experiment are represented. It can be seen that the central value of the cross section has been modified in the fast energy region and is compatible with the various experimental energy dependent data.

Figure 57. $^{240}\text{Pu}(n,f)$ prior (JEFF-3.3) and posterior cross sections compared with experimental data

8.5.2. Target accuracy assessment with the adjusted covariances

Once the assimilation was carried out, the total uncertainty in k_{eff} , Doppler coefficient ρ_T and change in coolant density ρ_p criticality safety coefficients was re-assessed using the new adjusted covariances. In Table 68, Table 69 and Table 70 comparisons between the *a priori* and *a posteriori* UQ analyses for k_{eff} , ρ_T and ρ_p , respectively, are presented. Statistical uncertainties are negligible; hence they are not shown in the tables for simplicity purposes.

Table 68. Prior and posterior k_{eff} uncertainty quantification for MYRRHA

A PRIORI				A POSTERIORI			
Quantity		$\Delta k_{eff}/k_{eff}(\%)$		Quantity		$\Delta k_{eff}/k_{eff}(\%)$	
²⁴⁰ Pu (n,f)	²⁴⁰ Pu (n,f)	0.543		²³⁹ Pu (n,f)	²³⁹ Pu (n,f)	0.291	
²⁴⁰ Pu (n,f)	²⁴⁰ Pu (n, γ)	-0.420		²³⁹ Pu χ	²³⁹ Pu ν_p	-0.268	
²³⁹ Pu ν_p	²³⁹ Pu ν_p	0.321		²³⁹ Pu ν_p	²³⁹ Pu ν_p	0.254	
²³⁹ Pu (n,f)	²³⁹ Pu (n,f)	0.295		²³⁹ Pu χ	²³⁹ Pu χ	0.187	
²³⁹ Pu χ	²³⁹ Pu χ	0.261		²³⁹ Pu (n,f)	²³⁹ Pu (n, γ)	0.173	
²⁴⁰ Pu (n, γ)	²⁴⁰ Pu (n, γ)	0.197		²³⁸ U (n, γ)	²³⁸ U (n, γ)	0.167	
²³⁹ Pu (n,f)	²³⁹ Pu (n, γ)	0.174		²³⁹ Pu (n, γ)	²³⁹ Pu (n, γ)	0.151	
²³⁸ U (n, γ)	²³⁸ U (n, γ)	0.167		²³⁹ Pu ν_p	²³⁹ Pu (n,f)	-0.137	
²³⁹ Pu (n, γ)	²³⁹ Pu (n, γ)	0.151		²⁴⁰ Pu (n,f)	²⁴⁰ Pu (n,f)	0.135	
²³⁸ U (n,n')	²³⁸ U (n,f)	-0.138		²³⁹ Pu χ	²³⁹ Pu (n,f)	-0.132	
Total uncertainty in k_{eff}		0.772		Total uncertainty in k_{eff}		0.529	

Table 69. Prior and posterior ρ_T uncertainty quantification for MYRRHA

A PRIORI				A POSTERIORI			
Quantity		$\Delta \rho_T/\rho_T(\%)$		Quantity		$\Delta \rho_T/\rho_T(\%)$	
¹⁰ B (n,n')	¹⁰ B (n,n')	4.925		¹⁰ B (n,n')	¹⁰ B (n,n')	4.925	
⁵⁷ Fe (n,n)	⁵⁷ Fe (n,n)	3.385		⁵⁷ Fe (n,n)	⁵⁷ Fe (n,n)	3.379	
⁵⁶ Fe (n,n)	⁵⁶ Fe (n,n)	3.304		⁵⁶ Fe (n,n)	⁵⁶ Fe (n,n)	3.221	
⁵⁴ Fe (n,n)	⁵⁴ Fe (n,n)	2.438		⁵⁴ Fe (n,n)	⁵⁴ Fe (n,n)	2.435	
⁵⁵ Mn (n,n)	⁵⁵ Mn (n,n)	1.918		⁵⁵ Mn (n,n)	⁵⁵ Mn (n,n)	1.918	
⁵⁸ Ni (n,n)	⁵⁸ Ni (n,n)	1.864		⁵⁸ Ni (n,n)	⁵⁸ Ni (n,n)	1.864	
²⁰⁸ Pb (n,n)	²⁰⁸ Pb (n,n)	1.793		²⁴⁰ Pu (n,n)	²⁴⁰ Pu (n,n')	-1.425	
²⁴⁰ Pu (n,n)	²⁴⁰ Pu (n,n')	-1.514		²⁰⁸ Pb (n,n)	²⁰⁸ Pb (n,n)	1.408	
²⁴⁰ Pu (n,n')	²⁴⁰ Pu (n,n')	1.441		¹⁶ O (n,n)	¹⁶ O (n,n)	1.318	
²⁴⁰ Pu (n,f)	²⁴⁰ Pu (n,f)	1.422		¹³ Al (n,n)	¹³ Al (n,n)	1.315	
Total uncertainty in ρ_T		9.051		Total uncertainty in ρ_T		8.725	

The total uncertainty in the reactor criticality safety parameters has been reduced but target accuracies are still not met. Since the most significant adjustments and anticorrelations were generated for ²⁴⁰Pu and ²³⁹Pu, the strongest decrease in uncertainty using the adjusted covariance data has been experimented by k_{eff} (nearly ~250 pcm). On the other hand, the reduction in the reactivity coefficients uncertainty due to the adjustment of iron and lead cross sections can be considered negligible (

Table 69 and Table 70).

Table 70. Prior and posterior ρ_p uncertainty quantification for MYRRHA

A PRIORI					A POSTERIORI				
Quantity		$\Delta\rho_p/\rho_p(\%)$			Quantity		$\Delta\rho_p/\rho_p(\%)$		
¹⁰ B	(n,n')	¹⁰ B	(n,n')	10.400	¹⁰ B	(n,n')	¹⁰ B	(n,n')	10.400
⁵⁷ Fe	(n,n)	⁵⁷ Fe	(n,n)	8.069	⁵⁷ Fe	(n,n)	⁵⁷ Fe	(n,n)	8.053
⁵⁶ Fe	(n,n)	⁵⁶ Fe	(n,n)	7.415	⁵⁶ Fe	(n,n)	⁵⁶ Fe	(n,n)	7.329
⁵⁴ Fe	(n,n)	⁵⁴ Fe	(n,n)	5.318	⁵⁴ Fe	(n,n)	⁵⁴ Fe	(n,n)	5.309
²⁴⁰ Pu	(n,n')	²⁴⁰ Pu	(n,n')	4.745	¹⁶ O	(n,n)	¹⁶ O	(n,n)	4.514
¹⁶ O	(n,n)	¹⁶ O	(n,n)	4.514	²⁴⁰ Pu	(n,n')	²⁴⁰ Pu	(n,n')	4.023
²⁰⁸ Pb	(n,n)	²⁰⁸ Pb	(n,n)	3.591	²⁰⁸ Pb	(n,n)	²⁰⁸ Pb	(n,n)	3.512
²³⁸ U	(n,n')	²³⁸ U	(n,n')	3.394	⁵⁸ Ni	(n,n)	⁵⁸ Ni	(n,n)	3.157
²³⁸ U	(n,n)	²³⁸ U	(n,n')	3.393	⁶⁰ Ni	(n,n)	⁶⁰ Ni	(n,n)	2.539
⁵⁸ Ni	(n,n)	⁵⁸ Ni	(n,n)	3.157	²³⁸ U	(n,n)	²³⁸ U	(n,n')	2.514
Total uncertainty in ρ_p		20.311			Total uncertainty in ρ_p		19.459		

The strong reduction in uncertainty after assimilation in the selected integral experiments sensible to lead and iron (Table 66) can be nearly exclusively attributed to the new cross-correlations and not to cross section uncertainties being constrained (e.g., ⁵⁴Fe(n,n) in Figure 58). However, the total uncertainty introduced by those cross-correlations can be either positive or negative depending on the behaviour of the sensitivity coefficients, which can significantly vary between criticality safety coefficients due to the physics involved in the reactivity effect studied, as can be seen in Figure 59, where sensitivities of k_{eff} and ρ_p to elastic scattering of ⁵⁴Fe and ⁵⁶Fe are compared. This is the reason why the strong reduction in k_{eff} uncertainty experimented by PMF028 *a posteriori* is not observed in ρ_T and ρ_p for MYRRHA.

Figure 58. Prior (JEFF-3.3) and posterior nuclear data uncertainties in ⁵⁴Fe(n,n)

Figure 59. k_{eff} (left) and $\rho\rho$ (right) sensitivities to ^{54}Fe and ^{56}Fe elastic scattering

8.6. Conclusions

Data Assimilation With summonN (DAWN) module has been developed to perform data assimilation using integral experiments from public databases, with the aim of providing adjusted nuclear data, not only capable of predicting reactor properties within the target design accuracy, but also statistically consistent with the various energy dependent measurements.

The implemented methodology is based on the GLS technique and the use of integral experiments from ICSBEP and IRPhE databases. Individual adjustments using a single experiment or complete adjustments, using up to 93 criticality mass experiments for which final experimental uncertainty is reported in the ICSBEP Handbook, can be performed. Furthermore, the REWIND methodology has been implemented in DAWN in order to rank experiments to avoid compensation effects. Complete adjustments with non-zero weight experiments predicted by REWIND are recommended when SUMMON is used in conjunction with MCNP, because progressive adjustments are biased due to MCNP not computing the effect of the cross section self-shielding on the sensitivity coefficients in multi-group calculations. However, the complete methodology has been implemented in SUMMON so that the full potential of the data assimilation methodology can be reached when other MC code, with no limitations in the sensitivity coefficient calculation using multi-group cross sections, is used, or more data on correlations of uncertainties in integral experiments are available. Nevertheless, correct results are expected because progressive and complete adjustments yield quite similar results when using k_{eff} experiments for data assimilation.

Recommendations have also been given for covariance data processing with NJOY to ensure that no problems arise with state-of-the-art evaluations due to the presence of zero and/or negative eigenvalues due to rounding or truncations.

It must be stressed that, from a general-purpose library, the adjustment procedure generates a specific-application library, only usable for the reactor concept for which it has been adjusted, or for a system with a representativity factor f_{RE} close to one with the targeted reactor or experiments used in the adjustment.

In order to verify the data assimilation module, ^{235}U , ^{238}U and ^{239}Pu data adjustment with DAWN using JEFF-3.3 state-of-the-art nuclear data library and critical mass experiments from ICSBEP database, considered individually, has been performed and results have been compared with the BMC methodology using TALYS-generated nuclear data. Very good agreement between SUMMON and BMC was observed in the uncertainties *a posteriori*, even if there were significant differences, up to 1000 pcm, between prior uncertainties in systems with intermediate uranium enrichment.

SUMMON's data assimilation module, DAWN, has been used to perform data assimilation for MYRRHA with JEFF-3.3 nuclear data library on ^{238}U , $^{239,240}\text{Pu}$, ^{10}B , Fe and Pb nuclides, aiming to produce a new covariance data set capable of predicting the criticality safety coefficients with uncertainties lower than the established target accuracies. Individual critical mass experiments from ICSBEP that provide information on separated individual physics effects related to the nuclides with highest sensitivity were chosen to perform data assimilation. No progressive or complete adjustments were made due to the limitations of SUMMON's current implementation with MCNP. The implementation in SUMMON of another code that can calculate the sensitivities of elemental parameters such as neutron leakage and reaction rates to nuclear data, as well as capable of using the posterior multi-group cross sections, is needed.

Significant reductions in the uncertainties of the integral experiments *a posteriori* were obtained due to the appearance of strong negative correlations between reaction channels that were not present in the prior covariance matrix. Posterior cross section uncertainties were also constrained. The consistency of the assimilation was checked to ensure that no unphysical adjustments have been produced.

The adjusted covariance matrix was used to re-assess the total uncertainty in k_{eff} , Doppler coefficient and change in coolant density criticality safety coefficients. A significant reduction in k_{eff} uncertainty was observed, but target accuracies for k_{eff} , ρ_T and ρ_p were still not met. To achieve uncertainties lower than the established target accuracies for GEN-IV advanced lead-cooled fast reactors several recommendations are given:

- Elemental experiments highly sensitive to a single nuclide and reaction channel should be preferably used for data assimilation.

- Criticality safety coefficients are governed by very different physical processes and the corresponding sensitivities are also expected to differ. Thus, the use of adjusted nuclear data for UQ may have negligible impact if those data have been adjusted using a different reactor parameter than the one quantified, as seen in this chapter. To cover the whole range of physical processes involved in all reactor parameters, experimental measurements of other integral parameters, such as β_{eff} , Λ_{eff} or reactivity effects should be used in the adjustment to provide further complementary information about nuclides and reaction channels that is missing when only k_{eff} is assessed.
- To perform a consistent and complete adjustment, correlations between the experimental uncertainties of the integral parameters used in the adjustment are needed to avoid bias and compensation errors. Only 93 integral experiments in public databases have correlation data for different criticality cases; therefore, the research community should make further efforts to estimate the correlations between the experimental uncertainties of integral experiments representative of innovative reactor designs that can be used in nuclear data validation, adjustment, and assimilation.
- In particular for MYRRHA, data assimilation using results from the experimental campaign carried out in VENUS-F CC 10 core configuration [Kochetkov et al., 2017] is recommended to achieve target accuracies. Metallic uranium has been used as fuel in VENUS-F, so the assimilation of measurements of reactor parameters sensitive to Pu would not serve to constrain the uncertainty. However, the uncertainties in other criticality safety parameters, such as Λ_{eff} or change in coolant density, which are highly sensitive to reflector or coolant materials, would probably be significantly reduced using these measurements. Furthermore, if Pu were to be available, VENUS-F could be fully used to obtain LFR-specific nuclear data libraries capable of predicting reactor parameters with the requested level of confidence.

The adjustment performed in this chapter has been severely limited by the impossibility of performing a progressive or complete adjustment due to the current implementation of MCNP, however, it has been proved that the combination of experimental covariance data and integral experiments together with Generalised Least Squares technique, can provide adjusted nuclear data capable of predicting reactor properties with lower uncertainty and consistent with energy dependent data.

Part IV

Conclusions

Chapter 9

Conclusions and future work

9.1. Conclusions

The aim of this Thesis was to analyse and improve the nuclear data required for the development, safety assessment and licensing of lead cooled fast reactors, reducing the uncertainties in the criticality safety parameters due to the uncertainties in nuclear data, in order to reach the target accuracies defined by industry, experts and regulators. For this purpose, SUMMON system and DAWN module have been developed to perform sensitivity and uncertainty analyses of reactor criticality safety parameters and constrain uncertainties by means of data assimilation. JEFF-3.3 state-of-the-art nuclear data library has been thoroughly assessed in order to validate data for coolant materials of lead-cooled fast reactors. Furthermore, nuclear data needs for advanced LFR's have been identified, improvements to reach target accuracies have been proposed and recommendations have been given.

SUMMON

Due to the limitations of existing tools, Sensitivity and Uncertainty Methodology for MONte carlo codes (SUMMON), a general methodology to calculate the sensitivities and uncertainties of the criticality safety parameters, has been developed. SUMMON has been conceived as a tool to perform complete automated sensitivity and uncertainty analyses of the most relevant criticality safety parameters of detailed complex reactor designs from the neutronic point of view, i.e., k_{eff} , β_{eff} , Λ_{eff} and reactivity coefficients, using state-of-the-art nuclear data libraries and corresponding covariance data.

The methodology is based on the use of the KSEN card of MCNP code to perform the eigenvalue sensitivity calculations, although any code that can provide sensitivity coefficients can be used. The sensitivity coefficients of a reactivity response are calculated using the eigenvalue definition of reactivity, which is equivalent to applying the Equivalent Generalized Perturbation

Theory. Moreover, the effective delayed neutron fraction sensitivity coefficients are derived from Bretscher's approximation or employing Chiba's modified method, whereas the sensitivity coefficients of the effective neutron generation time are obtained using the $1/\nu$ insertion method and the Equivalent Generalized Perturbation Theory. Uncertainties are propagated using the "Sandwich Rule" of the "Propagation of Moments" method employing state-of-the-art covariance libraries.

The implementation in SUMMON of the prompt method, the modified method and the $1/\nu$ insertion method has been validated using integral experiments from ICSBEP and IRPhE databases, while the methods for calculating the sensitivity coefficients and propagating uncertainties have been verified against consolidated codes, such as SCALE, SUS3D, SERPENT and XSUSA and good agreement has been obtained.

DAWN

Data Assimilation With summon (DAWN) module has been developed to perform data assimilation using integral experiments from public databases, with the aim of providing adjusted nuclear data, not only capable of predicting reactor properties within the target design accuracy, but also statistically consistent with the various energy dependent measurements.

The implemented methodology is based on the GLS technique and the use of integral experiments from ICSBEP and IRPhE databases. Individual adjustments using a single experiment or complete adjustments, using up to 93 criticality mass experiments for which final experimental uncertainty together with cross-experiment correlations is reported in the ICSBEP Handbook, can be performed. Furthermore, the REWIND methodology has been implemented in DAWN in order to rank experiments to avoid compensation effects. Limitations in the current implementation due to the use of MCNP (i.e., not taking into account self-shielding effects when using multi group cross sections) have been identified.

DAWN has been verified using JEFF-3.3 state-of-the-art nuclear data library and critical mass experiments from ICSBEP database, considered individually, against BMC methodology using TALYS-generated nuclear data. Very good agreement between SUMMON and BMC was observed in the posterior uncertainties.

It has been stressed that, from a general-purpose library, the adjustment procedure generates a specific-application library, only usable for the reactor concept which has been adjusted, or for a system with a representativity factor f_{RE} close to one with the targeted reactor or experiments used in the adjustment.

JEFF-3.3

The coolant materials of advanced LFRs (i.e., lead and bismuth) present in the latest version of the JEFF nuclear data library, JEFF-3.3, have been thoroughly studied. First, the origin of each evaluation has been analysed; then, JENDL-4.0, JEFF-3.3T1 and JEFF-3.3 lead and bismuth files have been validated using time-of-flight transmission and integral experiments; and finally, a benchmarking has been carried out using ALFRED and MYRRHA advanced reactor designs in order to analyse the impact of the differences between the previous lead and bismuth evaluations and the new ones on the criticality and neutronics of both reactors.

Several problems were found in the RRR of JEFF-3.3T1 lead and bismuth evaluations, which have an impact in the experimental integral parameters when the data is validated using integral benchmarks, and in the criticality and neutronics of ALFRED and MYRRHA reactor designs when JEFF-3.3T1 library is used for benchmarking.

These problems, as well as the recommendation to employ the RRR from JENDL-4.0 for cross sections for these nuclides in the final version of JEFF-3.3, were communicated to the JEFF collaboration. The recommendations were adopted in the production version of JEFF-3.3 nuclear data library, except for ^{204}Pb which is still based on JEFF-3.2 evaluation.

Nuclear data needs and recommendations for advanced LFR

A target accuracy assessment of the latest MYRRHA design has been performed with the SUMMON system and JEFF-3.3 nuclear data library. Integrated sensitivity coefficients, total uncertainties and main contributors to the uncertainty in the criticality safety coefficients (i.e., k_{eff} , β_{eff} , Λ_{eff} , change in fuel temperature, change in coolant density and control rod worth) have been obtained. Strong reliance of uncertainty quantification analyses on initial covariance data has been observed. Significant differences between JEFF-3.3, ENDF/B-VIII.0 and JENDL4.0u2 covariance evaluations have been found. ^{238}U , $^{239,240}\text{Pu}$, $^{10}\text{B}(n,n')$, $^{54,56,57}\text{Fe}(n,n)$ and $^{208}\text{Pb}(n,n)$ have been identified as major contributors to the uncertainty in the criticality safety parameters. Target accuracies defined by industry and experts for k_{eff} , change in fuel temperature and change in coolant density scenarios are exceeded.

Aiming to produce a new covariance data set capable of predicting the criticality safety coefficients with uncertainties lower than the established target accuracies, SUMMON's data assimilation module, DAWN, has been used to perform data assimilation with JEFF-3.3 nuclear data library on ^{238}U , $^{239,240}\text{Pu}$, ^{10}B , Fe and Pb nuclides. Individual critical mass experiments from ICSBEP that provide information on separated individual physics effects related to the nuclides with highest sensitivity were chosen to perform data assimilation. No progressive or complete adjustments were made due to the limitations of SUMMON's current implementation with MCNP.

Significant reductions in the uncertainties of the integral experiments *a posteriori* were obtained due to the appearance of strong negative correlations between reaction channels that were not present in the prior covariance matrix. Posterior cross section uncertainties were also constrained. The consistency of the assimilation was checked to ensure that no unphysical adjustments have been produced.

The adjusted covariance matrix was used to re-assess the total uncertainty in k_{eff} , Doppler coefficient and change in coolant density criticality safety coefficients. A significant reduction in k_{eff} uncertainty was observed, but k_{eff} , ρ_T and ρ_p target accuracies were still not met. However, it was proved that the combination of experimental covariance data and integral experiments together with Generalised Least Squares technique, can provide adjusted nuclear data capable of predicting reactor properties with lower uncertainty and consistent with energy dependent data.

The following nuclear data needs in JEFF-3.3 nuclear data library have been identified during the course of this Thesis:

1. Adoption of JENDL-4.0 evaluation for ^{204}Pb or re-evaluation in the RRR and URR.
2. Covariance evaluation for ^{209}Bi elastic scattering cross section.
3. Covariance evaluations for the average number of prompt and delayed neutrons emitted per fission in ^{240}Pu and for the number of delayed neutrons emitted per fission in ^{235}U , ^{238}U , ^{239}Pu and ^{242}Pu .
4. Reduction of the uncertainty in $^{240}\text{Pu}(\text{n},\text{f})$ cross section.
5. $^{10}\text{B}(\text{n},\text{n}')$ has an unphysical relative uncertainty of 500000% in the threshold of the reaction, while from 0.82 to 4 MeV the uncertainty highly exceeds 100%. New evaluation of this uncertainty is needed.
6. Reduction of the uncertainty in ^{54}Fe and ^{57}Fe elastic scattering cross sections.
7. New evaluation of the ^{57}Fe inelastic scattering cross section.
8. Reduction of the uncertainty in ^{208}Pb elastic scattering cross section.
9. Reduction of the uncertainty in ^{238}U inelastic scattering cross section.

To achieve uncertainties lower than the established target accuracies for GEN-IV advanced lead-cooled fast reactors several recommendations have been given:

1. Elemental experiments highly sensitive to a single nuclide and reaction channel should be preferably used for data assimilation.
2. When using integral benchmarks for data assimilation, experimental measurements of other integral parameters, such as β_{eff} , Λ_{eff} or reactivity effects should be used in the adjustment to provide further complementary information about nuclides and reaction channels that is missing when only k_{eff} is assessed.

3. Correlations between the experimental uncertainties of integral experiments representative of innovative reactor designs that can be used in nuclear data validation, adjustment, and assimilation, should be determined.
4. Data assimilation using results from the experimental campaign carried out in VENUS-F experimental reactor is recommended to achieve target accuracies in LFRs.
5. Public integral benchmarks for bismuth data validation are needed.

Recommendations have also been given for covariance data processing with NJOY to ensure that no problems arise with state-of-the-art evaluations due to the presence of zero and/or negative eigenvalues due to rounding or truncations.

9.2. Future work

The following lines of research are proposed as continuation of this Thesis.

Experiments

Due to the studies performed in Chapter 6, improvements in the resolved and unresolved energy regions of lead and bismuth files were made in the JEFF-3.3T2 evaluation [Kodeli et al., 2016b], which were carried on to the final version of the library. This illustrates the importance of well documented high-resolution experiments for nuclear data validation.

Unfortunately, transmission data for lead and bismuth are scarce and, in some cases, discrepancies have been found between experimental datasets available in EXFOR (e.g., ^{206}Pb in Section 6.3.2). Measurements to produce experimental transmission data that can be used to validate evaluated cross sections for neutron induced reactions on $^{\text{nat}}\text{Pb}$ and ^{209}Bi in the resonance region were proposed under the framework of the EUFRAT programme. While the proposal was accepted by the Programme Advisory Committee, regrettably, due to time constraints the experiments could not be performed. Consequently, a re-submission of this proposal within a new experimental campaign is proposed.

Nuclear data validation

Integral experiments are widely used by the nuclear data community to validate new nuclear data evaluations and simulation tools. Several databases are publicly available such as ICSBEP, IRPhE, SINBAD and SFCOMPO [Michel-Sendis et al., 2017], however, not all information available in these databases is used for validation purposes, e.g., usually only the experimental k_{eff} of the critical configurations available in ICSBEP is used. However, other experimental parameters such as β_{eff} , Λ_{eff} , reaction rates and energy-dependent data should also be used to provide further complementary information about nuclides and reaction channels that is missing when only k_{eff} is assessed.

The development of a new evaluated database for validation purposes, composed of publicly available experiments that contain kinetic, reaction rate and energy-dependent experimental data and that can be used by the nuclear data community and code-developers to further validate nuclear data and tools and perform adjustment, and assimilation studies, is proposed.

Furthermore, to perform consistent adjustments, correlations between the experimental uncertainties of the integral parameters used in the adjustment are needed, though they are scarcely found in the experiment reports. Correlation between experiments is also vital for nuclear data evaluation because missing correlations can introduce bias and compensation effects in evaluated nuclear data. In spite of its importance, correlation coefficient data of uncertainties for criticality cases are publicly available for only 93 integral experiments of the DICE database associated with the ICSBEP Handbook. Consequently, detailed analyses in order to establish correlations between the experimental uncertainties of integral experiments representative of innovative reactor concepts such as MYRRHA or ALFRED, are also proposed.

Code development

When SUMMON is used in conjunction with MCNP, progressive adjustments are biased due to the fact that MCNP does not compute the effect of the cross section self-shielding on the sensitivity coefficients in multi-group calculations. Another code that can calculate the sensitivities of elemental parameters, such as neutron leakage and reaction rates, and that is capable of using the posterior multi-group cross sections, is needed.

Therefore, the implementation in SUMMON of MCSSEN [Perel et al., 1996] or SERPENT codes is proposed. Additionally, in order to use posterior cross sections, the creation of a new computer tool for the replacement of the cross section values included in the library in ACE format by the posterior cross sections values is also proposed. In this way, all the reactor parameters for the specific application as the criticality constant or the adjusted sensitivity coefficients could be recalculated using the adjusted cross sections. The implementation of MCSSEN and such program would allow SUMMON to continue using MCNP without any bias in the adjustment analyses.

Uncertainty quantification

Nuclear data uncertainty quantification in transient scenarios such as ULOF and UTOP for LFR reactors is proposed. SUMMON capabilities allow calculating the uncertainties in the criticality safety coefficients (effective neutron multiplication factor, effective delayed neutron fraction, effective neutron generation time and reactivity coefficients) of present and innovative reactor designs. Therefore, SUMMON can be coupled with a thermal-hydraulic code in order to provide the uncertainties due to nuclear data of the input parameters. The propagation of these uncertainties to transient scenarios will provide an exhaustive picture of the influence of nuclear

data on core performance, identifying key parameters and allowing proposing specific actions to achieve an improved safety level.

Furthermore, after an assessment of the performance of the transient scenarios employing state-of-the-art nuclear data, target accuracies can be redefined for these reactor concepts. The most recent target accuracies published by expert groups date from 2008 [Salvatores and Jacqmin, 2008].

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Annex A

1.0000E-11 1.0000E-10 5.0000E-10 7.5000E-10 1.0000E-09 1.2000E-09 1.5000E-09 2.0000E-09
2.5000E-09 3.0000E-09 4.0000E-09 5.0000E-09 7.5000E-09 1.0000E-08 2.5300E-08 3.0000E-08
4.0000E-08 5.0000E-08 6.0000E-08 7.0000E-08 8.0000E-08 9.0000E-08 1.0000E-07 1.2500E-07
1.5000E-07 1.7500E-07 2.0000E-07 2.2500E-07 2.5000E-07 2.7500E-07 3.0000E-07 3.2500E-07
3.5000E-07 3.7500E-07 4.0000E-07 4.5000E-07 5.0000E-07 5.4000E-07 5.5000E-07 6.0000E-07
6.2500E-07 6.5000E-07 7.0000E-07 7.5000E-07 8.0000E-07 8.5000E-07 9.0000E-07 9.2500E-07
9.5000E-07 9.7500E-07 1.0000E-06 1.0100E-06 1.0200E-06 1.0300E-06 1.0400E-06 1.0500E-06
1.0600E-06 1.0700E-06 1.0800E-06 1.0900E-06 1.1000E-06 1.1100E-06 1.1200E-06 1.1300E-06
1.1400E-06 1.1500E-06 1.1750E-06 1.2000E-06 1.2250E-06 1.2500E-06 1.3000E-06 1.3500E-06
1.4000E-06 1.4500E-06 1.5000E-06 1.5900E-06 1.6800E-06 1.7700E-06 1.8600E-06 1.9400E-06
2.0000E-06 2.1200E-06 2.2100E-06 2.3000E-06 2.3800E-06 2.4700E-06 2.5700E-06 2.6700E-06
2.7700E-06 2.8700E-06 2.9700E-06 3.0000E-06 3.0500E-06 3.1000E-06 3.1500E-06 3.2000E-06
3.5000E-06 3.7300E-06 4.0000E-06 4.1000E-06 4.7000E-06 4.7500E-06 5.0000E-06 5.4000E-06
6.0000E-06 6.2500E-06 6.5000E-06 6.7500E-06 6.8750E-06 7.0000E-06 7.1500E-06 8.1000E-06
8.3153E-06 9.1000E-06 1.0000E-05 1.1500E-05 1.1900E-05 1.2900E-05 1.3710E-05 1.3750E-05
1.4400E-05 1.5100E-05 1.6000E-05 1.7000E-05 1.8500E-05 1.9000E-05 1.9400E-05 2.0000E-05
2.0500E-05 2.1000E-05 2.1200E-05 2.1750E-05 2.2500E-05 2.2603E-05 2.5000E-05 2.7500E-05
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3.6000E-05 3.7000E-05 3.7130E-05 3.7270E-05 3.7630E-05 3.8000E-05 3.9100E-05 3.9600E-05
4.0169E-05 4.1000E-05 4.2400E-05 4.4000E-05 4.5200E-05 4.7000E-05 4.8300E-05 4.9200E-05
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1.1600E-04 1.1750E-04 1.1900E-04 1.2200E-04 1.4300E-04 1.4863E-04 1.7000E-04 1.8000E-04
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1.5000E-03 1.5500E-03 1.8000E-03 2.0347E-03 2.2000E-03 2.2500E-03 2.2900E-03 2.5000E-03

2.5800E-03	3.0000E-03	3.3546E-03	3.7400E-03	3.9000E-03	5.5308E-03	5.7000E-03	6.0000E-03
8.0300E-03	9.1188E-03	9.5000E-03	1.3000E-02	1.5034E-02	1.7000E-02	2.0000E-02	2.4788E-02
2.5000E-02	3.0000E-02	4.0868E-02	4.5000E-02	5.0000E-02	5.2000E-02	6.0000E-02	6.7380E-02
7.3000E-02	7.5000E-02	8.2000E-02	8.5000E-02	1.0000E-01	1.1109E-01	1.2830E-01	1.4900E-01
1.5000E-01	1.8316E-01	2.0000E-01	2.7000E-01	3.0197E-01	3.3000E-01	4.0000E-01	4.2000E-01
4.4000E-01	4.7000E-01	4.9200E-01	4.9787E-01	4.9952E-01	5.5000E-01	5.7300E-01	6.0000E-01
6.7000E-01	6.7900E-01	7.5000E-01	8.2000E-01	8.2085E-01	8.6110E-01	8.7500E-01	9.0000E-01
9.2000E-01	1.0100E+00	1.1000E+00	1.2000E+00	1.2500E+00	1.3170E+00	1.3534E+00	1.3560E+00
1.4000E+00	1.5000E+00	1.8500E+00	2.2313E+00	2.3540E+00	2.4790E+00	3.0000E+00	3.6788E+00
4.3040E+00	4.8000E+00	6.0653E+00	6.4340E+00	8.1870E+00	1.0000E+01	1.2840E+01	1.3840E+01
	1.4550E+01	1.5680E+01	1.7330E+01	1.9640E+01	2.0000E+01		

Figure A1. SUMMON 308 energy group structure

Curriculum Vitae

DATOS PERSONALES

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EXPERIENCIA PROFESIONAL

Titulado Superior de Investigación (Marzo 2019 – Actualidad)
Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas
Titulado Superior de Investigación (Abril 2017 – Diciembre 2018)
Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas
Becario (Marzo 2014 - Abril 2017)
Universidad Politécnica de Madrid

FORMACIÓN ACADÉMICA

Doctorado en Energía Sostenible, Nuclear y Renovable (2015 - 2019)
Universidad Politécnica de Madrid
Máster en Ciencia y Tecnología Nuclear (2014 - 2015)
Universidad Politécnica de Madrid
Ingeniero Industrial (especialidad en Técnicas Energéticas) (2006 - 2014)
Universidad Politécnica de Madrid

CURSOS Y SEMINARIOS

ESFR-SMART workshop on liquid metal thermal hydraulics (2019)
UPM, CIEMAT Y CEA
Sensibilización en igualdad de oportunidades - 30 horas (2019)
Instituto de la mujer y para la igualdad de oportunidades
2nd 7FP GENTLE Intersemester Course on Nuclear Data - 1 semana (2016)
EC-JRC Geel y SCK·CEN
Curso Superior en Dirección y Gestión de Proyectos - 270 horas (2015)
Universidad Politécnica de Madrid

La transición energética en Europa y el cambio climático - 18 horas (2014)

Universidad Complutense de Madrid

1st 7FP GENTLE Intersemester Course on Nuclear Data - 1 semana (2014)

EC-JRC Geel, SCK·CEN y UPM

ESTANCIAS

European Commission Joint Research Centre Geel – JRC Geel

Objetivo: Transmission experiments to validate nuclear data for neutron induced reactions on Pb and Bi

País: Bélgica Duración: 20/03/2017 – 24/03/2017

European Commission Joint Research Centre Geel – JRC Geel

Objetivo: Analysis of nuclear data in MYRRHA: impact of nuclear data uncertainties

País: Bélgica Duración: 01/02/2016 – 04/05/2016

MENCIONES

1. Finalista 13th ENEN PhD Event&Price 2019
2. Finalista Premio SNE al mejor Trabajo o Proyecto Fin de Máster 2016

PUBLICACIONES

1. E. Mendoza et al. *Neutron production induced by α -decay with Geant4*. Submitted to Journal of Cosmology and Astroparticle Physics
2. P. Dimitriou et al. *Development of a Reference Database for Beta-Delayed Neutron Emission*. Submitted to Nuclear Data Sheets
3. P. Romojaro et al. *Sensitivity methods for effective delayed neutron fraction and neutron generation time with SUMMON*. Ann. Nucl. Energy 126 (2019) 410-418
4. G. Grasso et al. *Stress-testing the ALFRED design - Part I: Impact of Nuclear Data Uncertainties on Design Extension Conditions Transients*. Prog. Nucl. Energ. 106 (2018) 372-386
5. P. Romojaro et al. *Nuclear data sensitivity and uncertainty analysis of effective neutron multiplication factor in various MYRRHA core configurations*. Ann. Nucl. Energy 101 (2017) 330-338
6. R.W. Mills et al. *Extended Procedure for Experimental and Theoretical Uncertainty Handling*. Deliverable D9.5 CHANDA EU Project (2018)
7. U. Díaz-Chirón et al. *Preliminary calculations of the ESFR core catcher*. Informe interno CIEMAT DFN/IN-01/II-18 (2018)
8. G. Žerovnik et al. *Recommendations for MYRRHA relevant cross section data to the JEFF project*. JRC Technical Report EUR 28957 EN (2017)
9. I. Kodeli et al. *Report on the validation of improved data libraries*. Deliverable D10.4 CHANDA EU Project (2017)
10. G. Žerovnik et al. *Report with recommendations for the JEFF project*. Deliverable D10.5 CHANDA EU Project (2017)
11. G. Grasso et al. *ALFRED core safety parameters and influence of model uncertainties on transients*. Deliverable D6.1.6-1 ESNII PLUS EU Project (2017)
12. F. Álvarez-Velarde et al. *Contribution of CIEMAT to CHANDA Task 9.5: Development of SUMMON, a methodology for Sensitivity/Uncertainty analyses for the criticality safety parameters with MCNP*. Informe interno CIEMAT DFN/IN-01/II-17 (2017)
13. G. Žerovnik et al. *Assessment of evaluations for MYRRHA*. JRC Technical Report EUR 28240 EN (2016)
14. I. Kodeli et al. *Summary report of available and new data for library validation*. Milestone MS10.1 CHANDA EU Project (2016)
15. P. Romojaro et al. *Report on improvements made to existing evaluations*. Deliverable D10.3 CHANDA EU Project (2016)

16. A. Stankovskiy et al. *Report on comparison of evaluated libraries and identification of existing experimental data*. Deliverable D10.2 CHANDA EU Project (2016)
17. P. Romojaro et al. *Report on sensitivity analysis of MYRRHA with list of key reactions*. Deliverable D10.1 CHANDA EU Project (2015)

CONGRESOS

1. P. Romojaro et al. *Joint CIEMAT and UPM contribution: ASTRID, ESFR, ALFRED and MYRRHA*. OCDE/NEA SG-46 31st WPEC meeting, París, Francia, Junio (2019)
2. P. Romojaro. *Nuclear Data Analyses for Improving the Safety of Advanced Lead-cooled Reactors*. FISA 2019 · EURADWASTE'19 – 9th European Commission Conferences on Euratom Research and Training in Safety of Reactor Systems and Radioactive Waste Management. Pitesti, Rumanía, 4-7 Junio (2019)
3. P. Romojaro et al. *Evolution of the importance of neutron-induced reactions along the cycle of an LFR*. ND2019: International conference on nuclear data for science and technology. Beijing, China, 19-24 Mayo (2019)
4. P. Romojaro et al. *Impact of Nuclear Data Evaluations on Data Assimilation for an LFR*. ND2019: International conference on nuclear data for science and technology. Beijing, China, 19-24 Mayo (2019)
5. A. Jiménez-Carrascosa et al. *About the impact of the Unresolved Resonance Region in Monte Carlo simulations of Sodium Fast Reactors*. ICAPP 2019 - International Congress on Advances in Nuclear Power Plants. Juan-les-pins, Francia, 12-15 Mayo (2019)
6. F. Álvarez-Velarde et al. *TR_EVOL: a fuel cycle scenario code for energy policy planning*. Technical Meeting on Nuclear–Renewable Hybrid Energy Systems for Decarbonized Energy Production and Cogeneration. Viena, Austria, 22-25 Octubre (2018)
7. P. Romojaro et al. *Nuclear data analyses for improving the safety of advanced lead-cooled reactors*. WONDER 2018: 5th International Workshop On Nuclear Data Evaluation for Reactor applications. Aix-en-Provence, Francia, 8-12 Octubre (2018)
8. A. Jiménez-Carrascosa et al. *Spanish contribution to the Superphénix reactor benchmark for neutronics validation*. 44 Reunión Anual Sociedad Nuclear Española, Ávila, España, Septiembre (2018)
9. U. Díaz-Chirón et al. *Conceptual design of the ESFR reactor core catcher in the ESFR-SMART project*. 44 Reunión Anual Sociedad Nuclear Española, Ávila, España, Septiembre (2018)
10. F. Álvarez-Velarde et al. *Impact of state-of-the-art covariance evaluations in GEN-IV concepts UQ*. OCDE/NEA SG-44 30th WPEC meeting, París, Francia, Mayo (2018)
11. P. Romojaro et al. *Analysis of the JEFF-3.3 library for the UQ of Gen-IV reactor concepts*. OCDE/NEA Nuclear Data Week, Madrid, España, Abril (2018)
12. A. Sánchez-Caballero et al. *Summation calculations and validation with integral experiments*. OCDE/NEA Nuclear Data Week, Madrid, España, Abril (2018)
13. P. Romojaro et al. *Sensitivity and Uncertainty Methods for Effective Delayed Neutron Fraction and Neutron Generation Time With Summon*. PHYSOR 2018: Reactor Physics paving the way towards more efficient systems, Cancún, México, 22-26 Abril (2018)
14. P. Romojaro et al. *SUMMON: Sensitivity and Uncertainty Methodology for MONte carlo codes*. 43 Reunión Anual Sociedad Nuclear Española, Málaga, España, Octubre (2017)
15. N. García-Herranz et al. *Impact of nuclear data uncertainties on the reactivity coefficients of ALFRED*. International Conference on Fast Reactors and Related Fuel Cycles: Next Generation Nuclear Systems for Sustainable Development (FR17). Yekaterinburg, Rusia, Junio (2017)
16. P. Romojaro et al. *SUMMON: A Sensitivity And Uncertainty Methodology For MONte Carlo Codes*. M&C 2017: International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering. Jeju, Korea, 16-20 Abril (2017)
17. P. Romojaro et al. *Nuclear Data for the Safety of Lead-based Cooled Facilities*. Industriales Research Meeting '17, Madrid, España, Abril (2017)

18. P. Romojaro et al. *Coolant materials description in the new JEFF-3.3T1 for GEN-IV reactors*. 42 Reunión Anual Sociedad Nuclear Española, Santander, España, Septiembre (2016)
19. P. Romojaro et al. *Sensitivity and Uncertainty Analysis of the ALFRED Lead-cooled Fast Reactor using SCALE system*. 42 Reunión Anual Sociedad Nuclear Española, Santander, España, Septiembre (2016)
20. P. Romojaro et al. *Neutron-induced nuclear data for the MYRRHA fast spectrum facility*. ND2016: International conference on nuclear data for science and technology. Brujas, Bélgica, 11-16 Septiembre (2016)
21. O. Cabellos et al. *Benchmarking and Validation Activities within JEFF Project*. ND2016: International conference on nuclear data for science and technology. Brujas, Bélgica, 11-16 Septiembre (2016)
22. P. Romojaro et al. *JEFF-3.3T1 processing & testing for ASTRID and MYRRHA*. OCDE/NEA Nuclear Data Week, París, Francia, Abril (2016)
23. P. Romojaro et al. *Spanish contribution in the design of the ALFRED reactor inside the ESNII+ Project*. 41 Reunión Anual Sociedad Nuclear Española, A Coruña, España, Septiembre (2015)
24. A. Martínez et al. *Impact of nuclear data uncertainties on the reactivity of an ASTRID-like sodium fast reactor*. 41 Reunión Anual Sociedad Nuclear Española, A Coruña, España, Septiembre (2015)
25. F. Álvarez-Velarde et al. *Spanish contribution in the design of the ASTRID reactor inside the ESNII+ Project*. 41 Reunión Anual Sociedad Nuclear Española, A Coruña, España, Septiembre (2015)
26. P. Romojaro et al. *Sensitivity and Uncertainty analysis of nuclear data for MYRRHA*. Joint JEFF-CHANDA ND Workshop, París, Francia, Abril (2015)

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1. R. de Eusebio Yebra. *Impact of Uncertainties in Nuclear Data on Nuclear Fuel Cycle Parameters*. Trabajo Fin de Máster, CIEMAT – UAM (2019)
2. A. Sánchez-Caballero. *Validación de librerías de neutrones diferidos con aplicaciones a la seguridad de reactores nucleares avanzados*. Trabajo Fin de Máster, CIEMAT – UAM (2018)

IDIOMAS

Inglés: Nivel C1. TOEFL IBT puntuación: 103 (2011)

Francés: Nivel B1. DELF A2 (2004)