UNIVERSIDAD POLITÉCNICA DE MADRID

E.T.S. DE INGENIEROS INDUSTRIALES

**Análisis de incertidumbres y
optimización de ciclos de combustible
avanzados con reactores de
Generación IV**

**Uncertainty and optimization analysis of
advanced nuclear fuel cycles with Generation IV
reactors**

Tesis Doctoral

Aris Villacorta Skarbeli

Graduated in Physics

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DEPARTAMENTO DE INGENIERÍA ENERGÉTICA

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2020

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Resumen

La introducción de nuevas tecnologías y procesos industriales, y en particular de los reactores de Generación IV, supondrá lograr una energía nuclear más sostenible en términos de eficiencia, gestión de residuos, seguridad y competitividad económica gracias a la adopción de estrategias basadas en la Separación y la Transmutación. No obstante, debido a la gran cantidad de diseños existentes, así como a sus diferentes peculiaridades, esta introducción pasa necesariamente por la evaluación de su impacto en el ciclo de combustible nuclear. De esta forma, será posible determinar, según los objetivos que cada país o región se marque, cual es la mejor manera de pasar de los sistemas actuales a estas tecnologías más avanzadas, así como encontrar e identificar posibles limitaciones que puedan derivarse de su implementación y uso.

Por otro lado, debido a la gran complejidad que entrañan estos análisis, el desarrollo de códigos y herramientas para la simulación de ciclos de combustible está estrechamente ligado a estos análisis. No es de extrañar, por tanto, que estas herramientas estén siendo actualmente utilizadas a lo largo de todo el mundo por expertos y legisladores para el estudio y comprensión de estos nuevos ciclos avanzados. Sin embargo, las conclusiones que se deriven de estos análisis serán tan buenas como la calidad de los resultados que puedan arrojar estas herramientas, lo cual cobra especial importancia en un mundo rodeado por incertidumbres.

Bajo estas premisas, esta tesis se ha centrado en mejorar la confianza de los resultados proporcionados por los códigos simuladores de ciclos; a fecha de hoy, los estudios existentes en este campo son bastante escasos y están limitados por las fuertes hipótesis y suposiciones que emplean. Para ello, se han desarrollado e implementado diversas metodologías que permiten tener en cuenta el efecto de las distintas incertidumbres que aparecen en este tipo de estudios de forma genérica. Todo esto se ha llevado a cabo a través del estudio de diversos escenarios avanzados. De forma más precisa, estos escenarios se han basado en casos propuestos a nivel internacional por diferentes proyectos y colaboraciones debido a su interés desde el punto de vista de la transmutación y la gestión de residuos, entre otros.

El primer paso para lograr alcanzar estos objetivos ha consistido en actualizar TR_EVOL (el código de simulación de ciclos desarrollado por el CIEMAT) con distintas

metodologías tanto para propagar incertidumbres, como para optimizar escenarios nucleares. En paralelo, se ha hecho un gran esfuerzo para mejorar esta herramienta, de forma que sea mas versátil y rápida. Una vez se ha dispuesto de la herramienta necesaria, el trabajo de esta tesis se ha dividido en dos partes. La primera de ellas ha estado enfocada en la cuantificación de los efectos causados por distintas incertidumbres, mientras que la segunda parte se ha dedicado a analizar cómo las incertidumbres pueden afectar a la optimización de escenarios, y, por consiguiente, a la toma de decisiones.

La cuantificación de las incertidumbres se ha realizado a través del estudio de tres escenarios diferentes, cubriendo en cada uno de ellos una familia distinta de fuentes de incertidumbres. En primer lugar, se han estudiado las incertidumbres en los parámetros del ciclo de combustible. Para ello, se ha utilizado una metodología híbrida que combina métodos locales y globales. De este modo, es posible seleccionar de forma rápida aquellas variables más relevantes en términos de propagación de incertidumbre, sobre las cuales se puede posteriormente estudiar de forma detallada su impacto, buscando tanto interacciones como efectos de orden superior. Esta forma de abordar el problema, en combinación con la construcción de un modelo subrogado través de la expansión en Polinomios del Caos, ha permitido reducir de forma muy notable la demanda computacional de las técnicas globales.

En el segundo escenario se ha abordado el efecto de las incertidumbres provenientes de los datos nucleares. En este caso, se ha desarrollado una metodología basada en métodos Monte Carlo a través de la generación de varias librerías perturbadas la cual se ha verificado previamente con el experimento integral GODIVA. Tras ello, se ha aplicado a un ciclo abierto donde sus efectos se han comparado con los efectos debidos a los parámetros más relevantes del ciclo para poder determinar cómo de relevante es su impacto.

En tercer lugar, se han analizado las diferencias debidas al uso de los propios simuladores. Para ello, a través de una colaboración con el SCK · CEN, se ha simulado el mismo escenario avanzado con dos códigos distintos. Las diferencias obtenidas, las cuales han mostrado ser insalvables y por tanto aparecerán en cualquier estudio independientemente de la calidad de los códigos que se utilicen, se han cuantificado comparando de nuevo con los efectos introducidos por las incertidumbres en los parámetros del ciclo de combustible.

Estos análisis han mostrado que tanto las incertidumbres en datos nucleares como las distintas aproximaciones tomadas por los diferentes códigos producen un efecto en la simulación que es comparable al de las incertidumbres en los parámetros del ciclo. Además, este efecto cobra especial relevancia en escenarios avanzados con Separación y Transmutación, donde se persigue el multireciclado de los materiales para su óptimo uso. Por su parte, los efectos de las incertidumbres en parámetros del ciclo han resultado ser

muy dependientes tanto del observable en particular, como del escenario en consideración.

Finalmente, la tesis concluye mostrando la importancia que tienen las incertidumbres en los estudios de optimización. Para ello, se ha planteado un problema multiobjetivo el cual se ha resuelto dos veces: la primera de forma ordinaria sin tener en cuenta ninguna incertidumbre, y la segunda suponiendo que alguno de los parámetros de entrada es incierto. El problema escogido se ha basado en un escenario avanzado focalizado en reducir tanto la masa de transuránicos como los costes mediante el uso de tecnologías avanzadas. Para la optimización, se ha empleado un algoritmo evolutivo que alcanza la solución de forma iterativa sin requerir ninguna hipótesis de entrada. A pesar de que ambos resultados han producido aparentemente las mismas soluciones estando el caso con incertidumbres contenido dentro del caso sin incertidumbres, las configuraciones de parámetros de entrada que dan lugar a dichos resultados han sido diferentes. Además, el estudio detallado de las soluciones sin incertidumbres ha mostrado que, en su presencia, se vuelven inestables. De esta forma, las incertidumbres no solo pueden conducir a soluciones subóptimas, sino que además pueden comprometer la viabilidad del escenario en caso de no considerarse durante el proceso de optimización.

Abstract

The introduction of new technologies and industrial processes, and of Generation IV reactors in particular, will translate into a more sustainable nuclear energy in terms of efficiency, nuclear waste management, safety and economic competitiveness due to the adoption of strategies based on Partitioning and Transmutation. However, as a consequence of the numerous existing designs as well as their different peculiarities, this introduction necessarily requires the evaluation of the impact of these new systems in the nuclear fuel cycle. In this manner, it will be possible to determine, based on the particular objectives of each country or region, the best way for transitioning from the current systems to these advanced technologies, finding and identifying in this process the possible limitations that may appear as a consequence of their implementation and use.

Besides, given the complexity of these analyses, the study of nuclear fuel cycle scenarios is closely linked to the development of computer codes and tools for the simulation of these scenarios. It is therefore not surprising that these tools are currently being used for experts and policy makers around the world for studying and comprehending these new advanced fuel cycles. However, the conclusions that can be derived from these analyses will be as good as the quality of the results provided by the used tools, being this aspect of special importance in a world surrounded by uncertainties.

In this context, this thesis has been focused on improving the reliability of the results provided by the nuclear fuel cycle simulators; to date the existing studies on this topic are scarce and present some limitations as a consequence of the strong hypotheses and assumptions they made. To that end, different methodologies that allow for taking into account the effect of the uncertainties appearing in this kind of studies in a generic way have been developed and implemented. All of this has been carried out through the study of several advanced electronuclear scenarios. More precisely, these scenarios have been inspired in realistic cases proposed at international level through different projects and collaborations given their interest from the point of view of transmutation and waste management, among others.

The first step for meeting these objectives has been to upgrade TR_EVOL code (the nuclear fuel cycle simulator developed by CIEMAT) with different methodologies

that allow for both uncertainty propagation and electronuclear scenario optimization. Meanwhile, a lot of effort has been made for improving this tool in such a way it becomes more versatile and faster. Once the necessary tool has been upgraded, the work of this thesis has been divided in two major parts. The first one is focused on the quantification of the effect produced by the different uncertainties, while the second part has been dedicated to the study of how the uncertainties may affect the optimization of electronuclear scenarios, and consequently, how they can affect decision making.

The uncertainty quantification has been performed through the study of three scenarios, covering in each one of them one different family of uncertainties. Firstly, the uncertainties in the input parameters of the fuel cycle have been studied. To that end, a hybrid methodology making use of local and global methods has been used. In this way, the most relevant variables from the uncertainty propagation point of view can be identified in a quick and efficient manner, and in a second step, over this group of selected variables it is possible to study their detailed impact identifying non-linear effects or interactions. In conjunction with a surrogated model building based on the Polynomial Chaos expansion, this technique has allowed reducing very notably the computational demand of the global uncertainty propagation techniques.

In the second scenario, the effect of the nuclear data uncertainties has been addressed. For this case, a methodology based on Monte Carlo methods and the generation of multiple perturbed nuclear data libraries has been developed and verified with the GODIVA integral experiment. After that, this methodology has been applied to an open fuel cycle in which the effect of the nuclear data has been compared with the effects produced by the most relevant parameters of the cycle in order to determine its relevance.

In third place, the differences due to the fuel cycle simulation tools have been analyzed. Through a collaboration with the SCK · CEN research center, the same electronuclear scenario has been simulated with two different codes. The obtained differences which have been shown to be intrinsic to these tools, and therefore they will appear in any fuel cycle simulation whatever the quality or precision of the codes used, have been quantified through the comparison again with the effects due to the uncertainties in the input fuel cycle parameters.

These analyses have shown that both the uncertainty in the nuclear data and the modeling and approximations made by the different fuel cycle codes, produce an effect in the simulation that is comparable to the uncertainty in the fuel cycle parameters. Additionally, these effects gain special relevance in advanced scenarios using Partitioning and Transmutation in which the multirecycling of the materials is pursued for its optimum use. On another note, the effect of the uncertainties in the fuel cycle parameters have shown to have a strong dependency with both the particular selected observable, and the electronuclear scenario under study.

Finally, the thesis concludes by showing the relevance of the uncertainties in optimization studies. This has been evaluated through a multiobjective optimization problem which has been solved twice: the first one does not take into account the uncertainties while in the second one it has been assumed that some of the input parameters are unknown. The chosen problem has been based on an advanced scenario focused on reducing both the transuranic inventories and the fuel cycle cost with the use of advanced technologies. For the optimization, an evolutionary algorithm which iteratively evolves towards the best solution without making any assumption has been used. Although both solutions seem to produce similar results in the objective space being the case with uncertainties case contained in the case without uncertainties, the configurations leading to these solutions have shown to be different. In addition, the detailed study of the solutions without uncertainties has shown that, in their presence, they are unstable. In this manner, the uncertainties may not only lead to sub-optimal solutions but also can compromise the viability of the scenario if they are not considered during the optimization process.

Chapter 1

Introduction

In 1942, the first sustainable human-made critical reaction was achieved during an experiment led by Enrico Fermi in an early and rudimentary reactor placed in the middle of the Chicago University campus. Since that historic moment, nuclear energy has evolved to provide over 10% of the world's electricity (rising to 18% in advanced economies*), and this trend is expected to be continued in the future: considering the policy intentions and targets, the electricity production in the world is projected to increase from 26 600 TW h in 2018 to 41 400 TW h in 2040 of which 43% it is expected to be supplied by renewable and 8% by nuclear [64]. Nowadays, there are 440 nuclear power reactors in operation, 54 under construction and over 100 order or planned in 42 countries [110, 154].

Although it has always been surrounded by public debate about its risk and benefits, in face of climate change nuclear energy emerges as a part of a clean energy strategy. From 1971 to 2018, it has avoided the emission of 63 Gt of CO₂ worldwide (without nuclear the emissions from electricity generation would have almost 20% higher for the same period) and it is actually responsible of the 40% of low-carbon generation in advanced economies, becoming the largest low-carbon source of electricity in these countries [63].

With the Paris Agreement committed to limiting global warming below 2 °C and pursuing efforts to keep it under 1.5 °C [146], the European Union has targeted itself to cut off greenhouse emissions by at least 40% from 1990 levels with 30.4% to 31.9% of renewable energies by 2030 [35]. A more ambitious goal considers a net-zero greenhouse emissions by 2050 based on 80% renewable and 15% nuclear [34]. Despite the fact that it was delegated to the members the decision on whether to include or not nuclear in their energy mix for achieving those objectives, last year the European parliament adopted a resolution recognizing the importance of nuclear energy in fighting climate change:

*Advanced economies include Australia, Canada, Chile, the 28 members of the European Union, Iceland, Israel, Japan, Korea, Mexico, New Zealand, Norway, Switzerland, Turkey and the United States.

59. Believes that nuclear energy can play a role in meeting climate objectives because it does not emit greenhouse gases, and can also ensure a significant share of electricity production in Europe; considers nevertheless that, because of the waste it produces, this energy requires a medium- and long-term strategy that takes into account technological advances (laser, fusion, etc.) aimed at improving the sustainability of the entire sector; [36]

In this manner, it is clear that nuclear energy will play a key role in conjunction with renewable energy supplying the energy demand while contributing to climate change goals in the future, although more efforts should be made to ensure its sustainability. Nevertheless, with the adoption of P&T (Partitioning and Transmutation) strategies and the development of advanced transmutation systems (Generation IV fast reactors and ADS (Accelerator Driven Subcritical System)) for closing the nuclear fuel cycle, the sustainability can be achieved [93, 125, 94].

Generation IV reactors refer to the next generation systems aimed to guarantee the future development of the nuclear energy. In January 2002, the Generation IV International Forum was created for leading the international collaborative efforts to develop these next generation systems [46]. These reactors must fulfill the goals that were defined in this collaboration: sustainability, safety & reliability, economic competitiveness and proliferation resistance & physical protection. Under these ideas, from nearly 100 concepts six different designs were selected, namely GFR (Gas Fast Reactor), LFR (Lead Fast Reactor), MSR (Molten Salt Reactor), SFR (Sodium Fast Reactor), SCWR (Super Critical Water Reactor) and VHTR (Very High Temperature Reactor). The first four of them (GFR, SFR, MSR, SFR) are devoted to operate with closed fuel cycles while for the SCWR both open and closed cycles can be used (all of them can be designed with fast neutron spectrum); in the case of VHTR, although its original version operates with low-enriched fuel in an open cycle, the flexibility of the system will allow adopting a closed one and offer TRU (Transuranic) burning as well [47].

At the European level, in 2007 with support of the European Commission, the SNETP (Sustainable Nuclear Energy Technology Platform) was created for defining its own priorities and strategies [134]. The SNETP Vision Report set out three major pillars: maintaining the safety and competitiveness of today's technologies; developing a new generation of more sustainable reactor technologies; and developing new applications for nuclear power. In particular, the second one is coordinated under the ESNII (European Sustainable Nuclear Industrial Initiative), which prioritised SFR as reference solution and proposes LFR and GFR systems as alternative technologies [135]. Under these alternatives, MYRRHA a multipurpose hybrid facility dedicated to test both ADS and LFR, is included.

All of these efforts evidence the relevance advanced reactors will have in the future

evolution of the nuclear energy. However, once their feasibility and commercial viability are proven, it will be necessary to study their strategic deployments and how the transition from the current fleets to the new ones is going to occur. More broadly, this transition will be part of a nuclear fuel cycle, which covers all activities involved in the production of energy, starting with the uranium exploration and ending with the disposal [58]. Given the ability of these new reactor to burn and breed, properties that are closely linked to the reprocessing and reutilization of the nuclear fuel, it becomes clear that their introduction, as well as the adoption of P&T strategies, complicates the nuclear fuel cycle analyses in such a way computer codes are required for evaluating their impact. With these codes, known as nuclear fuel cycle simulators, it is possible to model different nuclear facilities and track material flows between them in a simple way. It is not surprising then that they have become an essential tool for researchers and policy makers, being extensively used in scenario modelling and analyses in the recent years [77, 44, 97].

Nonetheless, the definition of a precise electronuclear scenario relies on numerous assumptions about the particular performance and characteristics of present and future technologies as well as the role nuclear energy may have in the forthcoming years. Additionally, fuel cycle simulators strongly depend on experimental and theoretical data for performing the evolution of the nuclear materials, data which is ultimately subject to uncertainties. Furthermore, the codes make use of different approximations to model the reality. Given that fuel cycle studies may contribute to the selection of a particular technology focusing thus research and development in that particular direction, it is crucial to determine how all these uncertainties will affect and impact the simulation outcomes.

Finally, although the previous discussion has closely linked fuel cycle simulators and fast reactors, it should be mentioned that whatever the future of nuclear energy, the development and improvement of these tools is fundamental. For example, in the most pessimistic scenario in which nuclear energy is definitely abandoned, the existing spent nuclear fuel legacy will have to be managed too. Thus, having reliable tools that allow for its precise characterization will translate in a better management and disposal.

Under these ideas, this thesis is aimed to improve the confidence of nuclear fuel cycle studies. This has been carried out with the study and quantification of the uncertainties that appear in fuel cycle simulations, as well as their effect when specific goals are pursued. In this way, different advanced transition fuel cycle scenarios that have been proposed in international projects and collaborations for achieving some particular objectives that will be described in the following chapters, have been analyzed in this work. Excluding this chapter where the motivations of the work have been introduced, this thesis has been divided in five additional chapters:

- In Chapter 2, nuclear fuel cycles and the tools available for their study are presented.

In particular, the TR_EVOL nuclear fuel cycle simulation system is described, outlining the most important modifications introduced during the course of this work focused on speeding up the calculations and that will allow for performing the future studies.

- Chapter 3 sets the theoretical basis and key concepts that will be used in the forthcoming chapters. Specifically, this chapter has been divided in two major sections in which the state-of-the-art techniques in uncertainty and optimization analyses will be discussed respectively. Their possible implementations by other fuel cycle simulators (and more generally, by any code) are presented in this chapter too.
- Chapter 4 is dedicated to the study of the uncertainties in the nuclear fuel cycle. Three different scenarios have been analyzed, covering, in each case, one different family of uncertainties. The first of them analyzes the effect of the uncertainty in the scenario specifications. In the second one, the uncertainties in the nuclear data are addressed. Finally, the effects introduced by the proper fuel cycle simulators are investigated.
- Chapter 5 extends the effects of the uncertainty to optimization problems, studying another advanced nuclear fuel cycle scenario. More precisely, the chapter shows why uncertainties should be part of the optimization in fuel cycle simulations and the problems derived from not considering them in a first approach.
- Finally, in Chapter 6 the achievements and main conclusions of the thesis are summarized. The thesis closes discussing future lines of work and research.

The original contributions of this thesis have been already published (or will be), partially or completely, in the following journals[†]:

- Skarbeli, A. V. and Álvarez-Velarde, F. “Uncertainty quantification on advanced fuel cycle scenario simulations applying local and global methods”. In: *Annals of Nuclear Energy* 124 (Feb. 2019), pp. 349–356. DOI: [10.1016/j.anucene.2018.10.018](https://doi.org/10.1016/j.anucene.2018.10.018).
- Skarbeli, A. V. and Álvarez-Velarde, F. “Sparse Polynomial Chaos expansion for advanced nuclear fuel cycle sensitivity analysis”. In: *Annals of Nuclear Energy* 142 (July 2020), p. 107430. DOI: [10.1016/j.anucene.2020.107430](https://doi.org/10.1016/j.anucene.2020.107430).

[†]A detailed list of all the scientific contributions can be found in Appendix B.

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- Skarbeli, A. V. et al. “Quantification of the differences introduced by nuclear fuel cycle simulators in advanced scenario studies”. In: *Annals of Nuclear Energy* 137 (Mar. 2020), p. 107160. DOI: [10.1016/j.anucene.2019.107160](https://doi.org/10.1016/j.anucene.2019.107160).
 - Skarbeli, A. V., Álvarez-Velarde, F., and Bécares, V. “Optimization under uncertainty for robust fuel cycle analyses”. Submitted.

More precisely, the first two references corresponds to the studies conducted in Section 4.2, the third to Section 4.4 and the last one to Section 5.2. Additionally, another publication is currently being prepared for its submission:

- Skarbeli, A. V. et al. “Impact of the uncertainties in nuclear data on nuclear fuel cycle parameters”. To be submitted.

which corresponds to Section 4.3. This latter work has been performed as part of the master’s thesis of R. de Eusebio-Yebra.

Chapter 2

TR_EVOL

Studying the feasibility of electronuclear scenarios requires following materials flows between different facilities, that is, studying the nuclear fuel cycle. As more installations are considered the complexity of the cycle grows. In addition, the large number of isotopes that has to be tracked must be considered too. Thus, even for small scenarios, it is almost impossible to solve the problem by hand and computer codes are required. These codes, formerly known as fuel cycle simulators, are used around the world by different experts for addressing the key aspects of these cycles.

This chapter presents the TR_EVOL fuel cycle simulator, which was created by CIEMAT's Nuclear Innovation Unit in 2010 and whose main developer has been the present writer during the last years. Its current capabilities will be introduced, and the main improvements and modifications done to the code over the course of this thesis will be briefly discussed.

2.1 The nuclear fuel cycle

Nuclear fuel cycle refers to all the activities involved in the production of energy in the nuclear power plants by fission, starting with the uranium exploration and ending with the disposal of the spent nuclear fuel. The different activities are usually classified in two stages, the front end activities and the back end ones, which are separated by the irradiation in the reactors in which the energy of the nuclear materials is extracted [58]. In this way, the front end process includes activities such as uranium exploration and mining, conversion, enrichment and fuel fabrication, while in the back end the irradiated fuel storage, reprocessing, conditioning and disposal can be found. Depending on how the material flows move through these processes, two major classifications can be performed:

- Open fuel cycles (or once-through)

No material recycling is performed; after the first irradiation the nuclear fuel is

directly prepared for its final disposal. In this way, the nuclear materials move forward from the mining to the final disposal.

– Closed fuel cycles

After the irradiation, some elements are separated and reintroduced in previous stages of the cycle again for its future reutilization in nuclear power plants. In this way, backwards loops appear in the cycle and the materials can move from back end activities to front end ones (in particular from the reprocessing to the fabrication). Depending on how the recycling is implemented, this group can be further subdivided in three categories [94]:

– Single recycling

The Pu is recycled once in LWR (Light Water Reactor) with the use of MOX (Mixed Oxides) fuels. Additionally, Np can go with the Pu thereby avoiding the separation of pure plutonium. Alternatively, it is possible to recycle the U after its re-enrichment and/or blending with low enriched uranium, being especially noteworthy the option of its direct use in CANDU reactors* [59].

– Partially closed

The Pu (an eventually Am and Cm) is continuously recycled, either in PWR or FR (Fast Reactor) systems. The use of PWR for multirecycled Pu requires the utilization of advanced MOX fuels with enriched uranium that compensates for the Pu quality degradation by the successive irradiations.

– Fully closed

All actinides are continuously recycled until their fission in advanced reactors. Therefore, only reprocessing losses are sent to the final disposal.

This classification focuses on waste management, without specifying particular implementations. For example, a fully closed scheme could be either achieved with a *double-strata* approach[†], with a mixture of LWR and fast systems, or considering only fast reactors.

To date, only France, India, Italy, Japan, Netherlands and Russia are positioned in favour of reprocessing, China seems to be in favour too while United Kingdom has announced its discontinuity from these activities in the next years [86]. With that decision UK joins other countries such as Belgium, Canada, Finland, Germany, Switzerland, Sweden, Spain, South Korea or US that have an open fuel cycle strategy, despite some of them have reprocessed in the past.

*This particular fuel cycle scheme is referred as DUPIC (Direct Use of spent PWR (Pressurized Water Reactor) fuel in CANDU) [89].

[†]The *double-strata* concept, proposed by the Japan Atomic Energy Research Institute back in the 80's, considers two differentiated stages: one is dedicated to energy production while the other focuses on TRU burning [88].

2.1.1 The role of ADS and Generation IV reactors

Advanced fuel cycles described in the previous section require the transmutation of Pu and MA (Minor Actinides) in the reactors. Although multiple fuel assemblies designs have been proposed for incinerating those elements in the existing thermal LWR systems (see for example APA, CORAIL or DUPLEX concepts [149]) as well as in thorium-based fuels [132], serious limitations appear due to their accumulation through recycling and their impact on the safety of the plants [98, 132]. From the physics point of view, in order to burn actinides fission must dominate capture, and given the energy dependence of these processes, thermal systems are penalized when compared to fast ones [126]. Additionally, the better neutron economy of fast systems allows the surplus neutrons to transmute actinides. Hence, in order to achieve the hundredfold reduction in the long term radiotoxicity goal of the P&T strategy, fast systems (ADS and/or FR) are required [93, 94].

On the other hand, the utilization of fast reactors also presents challenges. The design of TRU burner cores is constrained by its performance and safety parameters such as reactivity swing, coolant void reactivity, Doppler effect and effective delayed neutrons [93]. This limits the amount of MA that can be loaded in FR, although recent studies have shown that the core design can potentially mitigate these effects [104]. In the case of ADS systems, they are less affected by these issues due to the large flexibility offered by the accelerator component.

2.1.2 Nuclear fuel cycle simulators

Nuclear fuel cycle simulators emerged to be versatile and powerful tools for experts and policy makers in order to address, analyze and study the key aspects of the different options in nuclear fuel cycles. Schematically, these tools track the materials flows between the different facilities propagating the masses or isotopic content through the fuel cycle, providing multiple metrics predefined by the user.

Motivated by different scientific and industrial questions multiple institutions around the world have developed (or are currently developing) their own tools for studying the multiple aspects of the fuel cycle they consider to be the most relevant according to their own interests. Those interests are commonly related to resources and economic analyses, or related to the impact on the cycle when applying a new technology or advanced strategy. Table 2.1 collects the fuel cycle codes that have been used worldwide during the last two decades. Most of the listed simulators are only used internally by its developing institution, so in general the codes are not accessible to the public. Note that due to this lack of transparency, as there are no official communication channels some of the listed projects may no longer be continued. This obscurity has motivated in the recent years the development of open source tools such as CLASS and CYCLUS which aim to be

Table 2.1: Fuel cycle simulators used over the last two decades.

Code	Main Institution	Country	Ref.
ANICCA	SCK-CEN	Belgium	[119]
CAFCA	MIT	US	[15]
CEPMNFC	Cornel Univ.	US	[131]
CLASS	CNRS/IRSN	France	[87]
COSAC	AREVA	France	[20]
COSI6	CEA	France	[24]
CYCLE	IPPE	Russia	[66]
CYCLUS [‡]	UW	US	[56]
DANESS	ANL	US	[147]
DESAE 2.2	Kurchatov Inst.	Russia	[145]
DYMOND	ANL	US	[158]
FANCSEE	KTH	Sweden	[22]
FAMILY 21	JAEA	Japan	[95]
FUTURE	KAERI	South Korea	[67]
GENIUS	UW	US	[103]
JOSSETE	BME	Hungary	[50]
MARKAL	BNL	US	[39]
NFCSim	LANL	US	[130]
NFCSS [§]	IAEA	—	[62]
NUWASTE	NWTRB	US	[92]
NMB	JAEA	Japan	[91]
ORION	NNL	UK	[49]
SITON	BME	Hungary	[13]
TIRELIRE-STRATEGIE	EDF	France	[78]
TR_EVOL	CIEMAT	Spain	[1]
VISION	INL	US	[65]

[‡] CYCLUS is a successor of GENIUS.

[§] Formerly known as VISTA [57].

more accessible to the community and potential new users while increasing the software robustness and reproducibility of the calculations.

Since each institution has created the tool on its own, each simulator makes use of different assumptions and considerations, covering different degrees of approximations that can be assumable or not depending on the desired accuracy of the results. For example, for certain applications having an estimated mass balance could be enough. This is the case of some simple codes as for example DYMOND which does not have implemented radioactive decay. On the other hand, in studies in which the radiotoxicity at a given point of the cycle is desired, the precise isotopic composition has to be provided. The number of isotopes that can be tracked depends on the code too, ranging from no isotopic tracking (DYMOND) to only the major actinides and fission products (DESAE)

or all the isotopes available in the nuclear data libraries (ANICCA). Fuel cycle facilities and material flows can either be described in a continuous manner (VISION) or as discrete entities (CYCLUS), allowing the second approach a greater flexibility since each component can be individually modeled. Regarding fuel irradiation, there are a wide range of options among the community too. The most basic ones does not perform depletion (DESAE), while others make use of burn-up tables (VISION), interpolate with artificial neural networks (CLASS), or are directly coupled with a depletion code (COSI). This rich diversity of implementation options is illustrated in Table 2.2, in which the most relevant characteristics of some of the codes that have been used under NEA (Nuclear Energy Agency) studies are shown.

Given this wide range of physics models, hypotheses, approximations and simulation techniques it is natural to wonder how the results compare when the same scenario is assessed with different codes. In this area, multiple benchmarking exercises have been done in the past, leading to the acceptance of some discrepancies in the results [95, 37, 6, 119]. In Section 4.4 we will go one step further and the quantification of such differences will be estimated. Additionally, in order to understand and analyze the effect of each different implementation, an international collaboration has recently emerged. More details will be given in Section 2.3.2.

2.2 The TR_EVOL fuel cycle simulation system

In 2010, from the need of studying mass balances of advanced transition electronuclear scenarios, CIEMAT started with the development of the TR_EVOL (Transition Evolution code) fuel cycle simulator, code which has been verified with the experimental data of the Spanish nuclear fuel cycle [1, 83]. It is an extension of the burn-up simulation system EVOLCODE which still constitutes the cornerstone of the code for the simulation of the different reactors involved in the studied cycle as it will be explained in Section 2.2.1. The irradiation and decay of the nuclear materials are calculated through ORIGEN2.2 code (also described in Section 2.2.1) which has been embedded in the TR_EVOL sources in order to improve the performance. For the irradiation process, specific cross-section libraries can be used depending on the reactor design. They are obtained from a detailed and exhaustive study with EVOLCODE. Hence, any kind of reactor using any fuel can be modelled in TR_EVOL. Nuclear fleets can be modeled either considering each single reactor individually or with macroreactors averaged by kind of technology, demanding the latter much less computational resources.

The different material storages are represented in TR_EVOL by means of buffers that store the isotopic contents averaged at the time intervals defined by the user, like weeks, months or years, although arbitrary times can be used too. This time scale also implies that the parameters of the facilities are averaged over this period. The number

Table 2.2: Main characteristic of some of the codes actively used under the NEA studies [95, 133].

Feature	ANICCA	COSI6	DESAE 2.2	FAMILY 21	TR_EVOL	VISION
Language	Python	Java	—	Visual Basic	Fortran	System Dynamics/PowerSim
Simultaneous advanced technologies	Any combination + different fuel types	Any combination + different fuel types	Yes	Any combination + different fuel types	Any combination + different fuel types	One-tier, two-tier scenarios
Isotopes tracked in irradiation and decay	All available in the nuclear data libraries (~3800)	U/Pu/MA/200 FP	U/Pu/MA/FP	U/Pu/MA/880 FP	All available in the nuclear data libraries (~3800)	81
Irradiation solver	CRAM16 (ALEPH2 libraries)	CESAR or direct coupling with ERANOS	No	Stored depletion matrix based on ORIGEN2	ORIGEN2.2 (EVOLCODE libraries)	Burn-up tables with interpolation
Start-up/Shut-down fuel loading	Yes	Yes	Start-up only	Yes	Yes	No
Spent fuel reprocessing strategy	FIFO, LIFO, Homogeneous	FIFO, LIFO	FIFO	FIFO, LIFO	FIFO, LIFO, Homogeneous	FIFO, LIFO
Waste Radioactivity/Radiotoxicity/Decay heat	No/Yes/Yes	Yes/Yes/Yes	No/Yes/Yes	Yes/Yes/No	Yes/Yes/Yes	Yes/Yes/Yes
Economic module	No	Yes	Yes	No	Yes	Yes

of isotopes that can be tracked is only limited by the existence of database information (isomers can be tracked too). Buffers are connected to each other by the different rules that define a particular action over a specific buffer (for example decay, fuel fabrication or irradiation, material movement, reprocessing...). Also the material can be moved from one facility to another, always maintaining the total and isotopic composition of the buffer. In this way, any kind of facility can be modelled in a flexible way according to a series of basic instructions. A detailed list of all the available rules can be found on [82], while examples of facilities that can be modelled include:

- External or initial inventory

External nuclear material coming from a different fuel cycle or an initial legacy can be added to the cycle. That material can be separated into plutonium and minor actinides, spent fuel, depleted or reprocessed uranium, etc.

- Mining

A facility devoted for creating all the material required for the cycle, that is, from natural uranium (U_{nat}) to the metal alloy for fuel fabrication, if required.

- Fabrication plant

This component groups the different processes to produce nuclear fuel from raw material. Different fuel types can be produced, such as: UOX (Uranium Oxide), MOX for LWR or FR and ADS fuels. Equivalence models to maintain reference reactivity have been implemented in the code.

- Reactor plant

This facility produces the electricity required according to the plant specifications and the burnup of the nuclear fuel. After the irradiation, the spent fuel is stored in the reactor pool for the time defined by the user.

- Reprocessing Plant

Its purpose is to separate the required elements or materials for the cycle from the rest of the spent fuel. The process includes different strategies of reprocessing (according to the residence time of the spent fuel) and elements or isotopes released into the environment.

- Repositories

These facilities store the nuclear material temporarily or indefinitely, subjecting it to the different processes that happen, such as: radioactive decay, extraction or addition of new material. The number of repositories can be as many as the cycle requires.

Figure 2.1: Flowchart of TR_EVOL fuel cycle simulator.

Fig. 2.1 presents the flowchart of a TR_EVOL fuel cycle simulation. Communication with the program is made through the highlighted elements, and the dashed lines represent optional steps. The scenario description is embedded in two input files, being three in the case the cost module is enabled. These inputs are represented with the blue color. In one of the mandatory files the reactor fleet characteristics are described (reactor properties and energy production), while in the other the particular rules that have to be applied are defined, indicating what results have to be printed in the output file. Additionally, the specific reactor libraries for the irradiation containing averaged one-group cross sections and fission yields as well as a library containing the tracked isotopes and their nuclear data properties must be available by the code (red elements). Hence, if a new reactor is simulated, its corresponding nuclear data has to be previously calculated with EVOLCODE system. Once TR_EVOL simulation is completed, different observables can be obtained. These include mass inventories, isotopic contents, radiotoxicity, decay heat, gallery length at the repository or, after the last upgrade before the commence of this thesis, even costs. These costs are estimated by means of the Levelized Cost of Electricity, breaking them down in four different components namely investment, fuel, O&M (Operation & Maintenance) and decommissioning, dismantling & disposal costs [82, 120].

2.2.1 Approximating the irradiation

From all the processes involved, the key part of the fuel cycle simulation is undoubtedly the irradiation of the nuclear fuel. Since a detailed and accurate study of the evolution of a single batch in the reactor core requires large computational resources (taking hours of execution time), this process has to be approximated by the fuel cycle code in order to be able to simulate the thousands of loads a complete electronuclear scenario description has in a feasible time. In TR_EVOL, this approximation is carried out by solving the one-group depletion equations that describe the evolution of the isotopes in a neutron field. This strategy requires the help of two additional tools that are described

hereunder[¶].

ORIGEN2.2

ORIGEN is a point depletion code developed by Oak Ridge National Laboratory which calculates the buildup, decay and processing of radioactive materials [25, 112]. The rate of change in the abundance of an isotope N_i in a neutron field can be estimated from the balance between the formation and disappearance due to nuclear decay and transmutation reactions

$$\frac{dN_i}{dt} = \sum_j \left(l_{ij} \lambda_j + \bar{\phi} f_{ij} \sigma_j \right) N_j - \left(\lambda_i + \bar{\phi} \sigma_i \right) N_i, \quad (2.1)$$

where λ_i and σ_i are the decay constant and one-group neutron absorption cross section respectively of the isotope i , l_{ij} and f_{ij} are the branching ratios of decay and neutron absorption with leads to the formation of the isotope i from j , and $\bar{\phi}$ is the neutron flux averaged in space, time and energy. Since the decay and branching ratios are read from the nuclear libraries and the neutron flux is estimated by ORIGEN given a certain power density which in turn is calculated by TR_EVOL from the reactors input file, the only unknowns in the previous equation are the one-group cross sections. The process of obtaining this values is described in the following subsection. Assuming that the neutron flux $\bar{\phi}$ is constant over the time interval, Eq. (2.1) describe a homogeneous set of simultaneous first-order ordinary differential equations of constant coefficients which are solved by ORIGEN using the matrix exponential method.

EVOLCODE

The EVOLCODE 2.0 simulation system was developed at CIEMAT with the aim of providing a computer code able of making simulations of current and future reactors in any range of operation and to provide detailed spatial distribution and time evolution of the isotopic composition of fuels and activated materials [3, 2]. It is a combination of a neutronic and burn-up evolution codes that uses for the neutron transport the MCNP6.2 code [151] (although previous releases can be used too) and for the depletion part either ORIGEN or ACAB [129].

Schematically, the code considers that the irradiation is divided in several time steps in which constant neutronic parameters are assumed. The reactor design is also geometrically subdivided in multiple cells in which the neutron parameters are estimated with the transport code at each time interval. With them, the effective one-group cross sections are obtained and the depletion of each cell is estimated. In this way, given a

[¶]ORIGEN and EVOLCODE are the two particular codes used by TR_EVOL for solving the one-group depletion equations. In general any other tool could be used.

complete simulation with EVOLCODE, multiple one-group cross sections as well as fission yields (one per cell and time step) are obtained. In order to obtain representative values of the reactor cross sections for their use in TR_EVOL, they have to be homogenized in time and space with an external program. Since the new version of TR_EVOL can perform the irradiation in several steps, the time averaging can be divided in multiple intervals.

2.2.2 Major improvements

Previous versions of TR_EVOL were completely written in Fortran, but after the modifications described in this section, the sources now contains small functions in C++ too. Algorithms described in Chapter 3 have been externally implemented in C++ and Python. Data processing depends on C++ (relying heavily on ROOT framework [14] as it will be described in the following), and the analysis programs are either in C++ or Python, depending on the functionality and requirements of each one. In this manner, the TR_EVOL fuel cycle simulator (mainly developed in Fortran with small functionalities in C++) is surrounded by an ecosystem of C++ and Python independent applications interconnected through Bash scripts. As a result, these applications can be easily extended to any other program.

Aside from the uncertainty and optimization algorithms that were implemented in TR_EVOL and that will be described in next chapter as it has been already mentioned, since the commence of this thesis multiple modifications have been introduced in the source code. These modifications have been focused on improving the execution speed without degrading the quality of the results. The main motivation beyond having a faster version was the huge amount of executions expected to be needed by the uncertainty and optimization analyses and that will be described in the following chapters. Although most of the modifications included minor bug fixes and small changes for making a more versatile and flexible code, in the following the major improvements will be discussed. The list is provided in alphabetical order.

Allocatable matrices

In the previous version, the size of all the matrices used by the program was determined at compiling time given some predefined maximum limits. This implied that for very complex scenarios with many rules these bounds could be exceeded resulting in the abnormal execution of the program in the case these limits were not increased and the sources recompiled beforehand. Also, when the requirements of the scenario were lower than the predefined limits, the reserved memory exceeded the real needs. In the current version, the size of the matrices is determined at execution time.

Automatic data processing

The results obtained with TR_EVOL are automatically processed with the ROOT framework, producing TTree's objects. This allow the fast plot of the results as well as a handy way of managing thousands of results in order to obtain statistical information. Also, other auxiliary codes for performing uncertainty and optimization studies (which details will be described in the next chapter) have been created.

Averaging time step

Traditionally TR_EVOL averages the different quantities in year-time intervals. In the new version, this averaging can be performed at the arbitrary time intervals defined by the user, like for example days, weeks or months. This implementation will allow, for example, for study scenarios with load following in a energy mix with renewable energies.

Broken scenarios

If there is not enough material for fuel fabrication (see Section 2.2.3 on page 19), a new execution flag allows for increasing artificially the inventories so the simulation can be finalized. The exact mass required for fabrication is added with the same isotopic content as the insufficient stock. The accumulated additional mass at each time step is provided in the output file.

Decay chains

Instead of calling ORIGEN each time step for decaying the materials, a general file containing the daughter production of all the tracked isotopes after the particular time scale of the simulation is used. Then, the decay can be calculated with a single vector product bypassing thus the ORIGEN calculation.

Multiple irradiation steps

The irradiation can now be divided in several time intervals using for each one a different set of one-group cross sections. This is of special interest on those reactors where the isotopic composition changes too much during the irradiation and a single set of cross sections is not a valid representation of the fuel behaviour.

ORIGEN embedding

Traditionally, the irradiation and decay calculations have been performed with external calls to ORIGEN code sharing the data through text files. In the updated version, the ORIGEN sources have been embedded in the TR_EVOL sources, avoiding the use of

system calls. Furthermore, the results provided by ORIGEN are not longer written to text files but directly to memory, reducing thus I/O operations.

Reduced library

Depending on the desired outcomes of the cycle, it is not necessary to track all the isotopes available in the nuclear data libraries (for example, if neither heat nor radiotoxicity are required). In the new version of the code, a reduced list containing only the main actinides can be chosen. This makes the ORIGEN executions much faster (see Table 2.3).

Refactoring

The sources have been refactored with the intent of improving the readability, debuggability, robustness and efficiency of the code. For example, all the shared variables as well as the stand-alone functions and subroutines have been included or grouped into modules. In this manner, it is possible to share allocatable arrays between the different parts of the code. Additionally, this approach generates explicit interfaces for the functions and subroutines which allows the compiler to perform argument checks detecting thus potential programming errors.

Scratch files

All the temporary external files produced by TR_EVOL were marked as *scratch*. Apart from the fact that they are automatically deleted when closed, the main advantage of this approach is that they are created under the path determined by the environment variable \$FOR_TMPDIR or \$TMPDIR (on UNIX systems and Intel compilers). In this manner, if a ramdisk is selected, the I/O operations will be boosted.

Simplified input files

The input files syntaxes have been simplified and made more human readable.

Table 2.3 shows the computational resources employed by the first and latest TR_EVOL versions for three different test scenarios when executed in an Intel Xeon E5430 processor. The scenarios include an open cycle with PWR(UOX) technologies and a fully closed one consisting of PWR(UOX), PWR(MOX) and ADS systems. For all of them the scenario extends over 200 years, while for the latter, both homogeneous and FIFO (First In First Out) reprocessing strategies have been considered. Note that FIFO (and LIFO (Last In First Out)) strategy increases notably the computational effort of the simulation given that the historical record of the stocks has to be stored in TR_EVOL methodology in order to decay the specific time between their production

2.2. The TR_EVOL fuel cycle simulation system

Table 2.3: Comparison between the execution resources demanded by the different TR_EVOL versions for three test scenarios.

Scenario	Old version			Full library			Reduced library		
	Time (s)		Mem. (kB)	Time (s)		Mem. (kB)	Time (s)		Mem. (kB)
	CPU	Total		CPU	Total		CPU	Total	
Open	519.1	643.5	1578.6	1.5	1.7	—	0.3	0.4	—
Closed (none)	1296.0	1959.6	1579.1	86.2	87.2	695.4	7.4	8.3	—
Closed (FIFO)	5471.2	12 267.7	1579.2	1239.6	1259.6	733.6	40.8	45.2	116.8

and the reprocessing. Each case was run multiple times (ten executions in an 8-core node) in order to diminish differences caused by scheduling and averaged quantities are reported. The difference between the full and reduced library versions is that the former tracks all the isotopes defined in the JEFF-3.2 (Joint Evaluated Fission and Fusion) decay data library while the latter only the actinides. The CPU and total execution times are reported (the difference between them gives an estimation of the elapsed time in I/O operations), as well as the peak memory usage. It must be pointed out that in the environment the test were run, the jobs are monitored each 45 seconds so for the fastest cases for which the execution time is below this number, no memory usage can be reported.

According to the tests, the new version with the full library is roughly $\times 380$, $\times 20$ and $\times 10$ times faster in the open and closed homogeneous and FIFO scenarios respectively. When the reduced library is chosen, speed gains of $\times 1600$, $\times 240$ and $\times 270$ are achieved. Furthermore, apart from a much faster execution the memory consumption is also notably reduced although it has now a dependency with the complexity of the scenario. This is in contrast with the previous version, in which the memory usage is constant as a consequence of the fixed matrices size.

Finally note that the changes summarized in this section represents nearly four years of development. The final version of TR_EVOL was not available for some of the results provided in this thesis and hence intermediated versions have been used, having impact only on execution time, but not on the quality of results.

2.2.3 Broken scenarios

The availability of nuclear materials for fuel fabrication imposes a restriction in the amount of energy that can be produced. Therefore, given a detailed electronuclear scenario description, it could happen that at certain point the energy demand is not satisfied due to shortage of nuclear material. In this case, the scenario will be *broken* and it will not be possible to complete the simulation for the whole period with the original input specifications. As it will be shown in next chapters, this issue is of special

interest in uncertainty and optimization analyses because, starting from a well-defined non-broken input scenario, perturbations in the parameters could disturb the delicate equilibrium balance of certain material flows between different facilities producing thus this effect.

Multiple approaches could be considered in order to overcome this problem. The most trivial one consist in simply adding a constant legacy inventory stock that can be understood as borrowing the material from an external supplier. Until the introduction of the *Broken scenarios* change (Section 2.2.2) this was the methodology followed by TR_EVOL. With this new flag the flexibility of the simulations is enhanced since it is not necessary to known in advance how much mass has to be added and to which inventory. Other different options include modifying the reprocessing capacity, the introduction dates of the critical facilities or even the electricity profile. However, they will change the specifications and therefore it would not be feasible to study the stability of the broken scenario. Furthermore, these methods can only solve the problem to a certain extent; if the material shortage is too strong it may not be possible to readapt the scenario.

Finally, one advantage of adding an external mass to the scenario instead of modifying the specifications is that it naturally provides a measurement of the feasibility of the scenario: the more additional mass required, the less feasible the scenario. This will be very helpful in optimization studies as it will be explained in Chapter 5.

2.3 Participation in international projects

The development of TR_EVOL has allowed CIEMAT to participate in multiple projects during the last years. These past projects include international projects (IAEA INPRO-SYNERGIES and OECD/NEA Expert Group activities) [61, 95], national programs (SYTRAD-2) as well as collaborations with ENRESA. Furthermore, CIEMAT is going to lead the Work Package dedicated to fuel cycle activities in the already accepted Horizon 2020 PUMMA (Plutonium Management for More Agility) project. Additionally, there are actually two different ongoing activities among the nuclear fuel cycle community in which TR_EVOL is taking part. In the following, the work being done under these collaborations is briefly described.

2.3.1 EG-AFCS

Under the NEA nuclear science committee and the mandate of the Working Party on Scientific Issues of the Fuel Cycle, the EG-AFCS (Expert Group on Advanced Fuel Cycle Scenarios) was born for studying advanced nuclear fuel cycles and their associated needs. The specific objectives and scope of the group can be found on its website at [33]. CIEMAT has been present since the creation of the group in 2010 when it replaces the

Expert Group on Fuel Cycle Transition Scenarios Studies, and multiple reports accessible from the website have been produced since then.

One of the activities that is currently being elaborated is the study of advanced transition scenarios and the possibility of managing legacy inventories from other countries. The scenario considers an initial fleet of LWR that is replaced by burner technologies with the objective of burning the TRU inventories and achieving a sustainable state in which the inventories does not increase nor decrease. Each participant has freedom for choosing the burner reactors they want, and the purpose of the study is to benchmark the different scenarios that will emerge from the different designs. In particular, CIEMAT studies a burner fleet based on high Pu content PWR(MOX) reactors and ADS systems. This scenario (with some minor changes) has been used in the work described in Section 4.4, so more details can be found there.

2.3.2 FIT

The FIT (Functionality Isolation Test) project is an international collaboration between the nuclear fuel cycle community coordinated by CNRS/IN2P3. Originally started in 2016 as a cooperation between France and US, in 2018 it was presented to the international community. Its main goal is to improve the confidence provided by the nuclear fuel cycle simulators, focusing in the comparison between different isolated functionalities. In this manner, it is possible to study the single effect a given approach or method introduces in the fuel cycle and thus to characterize the relationship between the model fidelity and the confidence of the obtained simulation results.

The first functionality that is being studied is the comparison between using a fixed fraction of Pu in fuel fabrication versus more complex methods that change the amount of fissile content depending on the isotopic composition (for example, with the use of recipes, equivalence models or approximations such as artificial neural networks). Other functionalities planned to be analyzed include the response to a fuel shortage (see Section 2.2.3), variable vs constant capacity factor and the effect of the reprocessing, among others. More details can be found on the official repository at GitHub [40].

2.4 Computational environment

All the executions performed during the development of this thesis have been carried out in CIEMAT supercomputers. By the end of 2019, a new HPC (High Performance Cluster) called XULA was acquired, replacing the one used at the commence of this thesis. Until this date the different calculations were performed in the former suupercomputer (EULER) which consist of Intel Xeon processors series as it can be read in Table 2.4, and then, in the new machine. The main characteristics of both EULER and XULA

Table 2.4: Description of the HPC systems available at CIEMAT.

Feature	EULER	XULA
Processors	144 Intel Xeon E5450 96 Intel Xeon X5570	44 Intel Gold 6148 66 Intel Gold 6254
Total num. of cores	1920	3376
R_{peak} (TFLOPS)	23.0	335.2
RAM memory (TB)	3.8	19.2
Storage (TB)	120	440
Other	Lustre filesystem Interconnected by InfiniBand	

are outlined in Table 2.4. In particular, the simulations of Chapter 4 were performed in EULER while the results of Chapter 5 have been obtained in XULA. Both clusters have been checked to perform equal with TR_EVOL so the consistency of the results it is ensured.

Chapter 3

Mathematical background

The complexity of the nuclear fuel cycle makes that it cannot be expressed in an analytical closed form. Hence, the simulators can be treated as a black-box functions in which a given input embedding the scenario description leads to certain solutions corresponding to the scenario outcomes. Thus, the only way of obtaining information from the system is through computer simulations. The objective of this thesis is to answer multiple questions that can arise in these matters such as *how will the scenario response to perturbations?* *are all the input parameters equally relevant?* or *which are the best possible scenarios given a precise set of considerations?* Under this topic, different theories can be applied in order to extract useful information from the simulation results. The first two questions can be answered with the use of uncertainty and sensitivity analyses, while the last one involves an optimization problem.

In this chapter, the theories that will serve as the basis for answering these particular questions are briefly introduced. In addition, their possible implementation in a nuclear fuel cycle code are shown. The first section aims to describe different strategies for performing uncertainty and sensitivity analyses, focusing on the computational efficiency and the strengths and weaknesses of each method. The second part of the chapter is dedicated to black-box function optimization. The key concepts are firstly introduced, and after that the algorithms implemented in TR_EVOL are described.

3.1 Uncertainty and sensitivity analyses

Uncertainty analyses aims to study the probabilistic response of a given model in the presence of uncertainties in the input parameters and, in particular, sensitivity analyses address the problem of how the uncertainty of the model can be expressed as a function of the input uncertainties. In the following, multiple approaches for performing these studies are presented, covering different degrees of approximation. The simplest techniques, involving parametric studies and local methods, have a narrow range of validity since they

make strong assumptions about the nature of the underlying mathematical dependence that the input parameter space has with a certain output indicator [17]. In the case of parametric studies, linear dependency is assumed between the input and the output parameters, while results of local methods, based on a first order approximation, are constrained to the vicinity of the reference values. The obvious benefit of these techniques is that their calculation only require a few evaluations. On the other hand, global theories (like the Sobol's variance decomposition) do not impose any restriction, allowing the capture of non-linear relationships along the whole input parameter space as well as interactions at the expense of a large computational effort [123].

3.1.1 Monte Carlo estimates

In general, nuclear fuel cycle simulators can be treated as a black-box function where an input vector $\mathbf{x}$ of dimension d yields the solution $y := \mathcal{F}(\mathbf{x})$. When uncertainties are considered, the input will be a random vector $\mathbf{X}$ whose values will be drawn from a probabilistic density function $f_{\mathbf{X}}(\mathbf{x})$, and therefore, the response will be now a random function $Y = \mathcal{F}(\mathbf{X})$ whose values will follow a certain distribution. Such distribution will be characterized by its moments, and they can be estimated via MC (Monte Carlo) integration methods in which the integrals are numerically solved with the use of random sampling. In particular, if a random input sample of size n has been generated, *i.e.* $\{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(n)}\}$, the mean of $Y = \mathcal{F}(\mathbf{X})$ can be approximated as

$$\mathbb{E}[Y] \approx \frac{1}{n} \sum_{i=1}^n \mathcal{F}(\mathbf{x}^{(i)}), \quad (3.1)$$

while the variance takes the following form

$$\sigma_Y^2 := \text{Var}[Y] \approx \frac{1}{n-1} \sum_{i=1}^n \left(\mathcal{F}(\mathbf{x}^{(i)}) - \mathbb{E}[Y] \right)^2, \quad (3.2)$$

being σ_Y the standard deviation.

The convergence of the MC methods goes as $\propto n^{-1/2}$. In order to improve this convergence, instead of pseudo-random sampling other alternatives can be used, such as LHS (Latin Hypercube Sampling), a stratified sampling technique [80], or QMC (Quasi-Monte Carlo) methods which are based on low-discrepancy sequences [90]. The latter approach is further discussed in Appendix A.

3.1.2 Sensitivity coefficients

Although the uncertainty quantification via MC estimation is straightforward, this approach does not provide any further information about which variable (or subset

of them) are responsible and to which degree of the final uncertainty. The simplest approach to the problem of sensitivity analysis is to perform a Taylor expansion around the reference value $\hat{\mathbf{x}}$

$$Y = \mathcal{F}(\mathbf{X}) = \mathcal{F}(\hat{\mathbf{x}}) + \sum \left. \frac{\partial \mathcal{F}}{\partial x_i} \right|_{\hat{x}_i} (X_i - \hat{x}_i) + \mathcal{O}(\mathbf{x}^2), \quad (3.3)$$

so the variance of the random function will read

$$\text{Var}[Y] \approx \sum_{i,j} \text{Cov}_{ij} \left. \frac{\partial \mathcal{F}}{\partial x_i} \right|_{\hat{x}_i} \left. \frac{\partial \mathcal{F}}{\partial x_j} \right|_{\hat{x}_j} = \text{Var}[X_i] \left(\left. \frac{\partial \mathcal{F}}{\partial x_i} \right|_{\hat{x}_i} \right)^2, \quad (3.4)$$

where the assumption of uncorrelated inputs has been done in the last step so the covariance matrix only contains diagonal terms. Normalizing the previous equation, the relative importance of each parameter can be defined as

$$\eta_i := \left(\left. \frac{\partial \mathcal{F}}{\partial x_i} \right|_{\hat{x}_i} \right)^2 \frac{\text{Var}[X_i]}{\text{Var}[Y]}. \quad (3.5)$$

If now the coefficients are ordered based on their contribution to the variance

$$\boldsymbol{\eta} := \{\eta_1, \eta_2, \dots, \eta_d\} \mid 1 \geq \eta_1 \geq \eta_2 \geq \dots \geq \eta_d \geq 0, \quad (3.6)$$

it is possible to introduce the notion of the k -largest contributors, which will be the sum of the first k -elements of this ordered vector

$$H_k := \sum_{i=1}^k \eta_i, \quad (3.7)$$

measuring how much of the variance could be explained by the k -most relevant variables. Note that with this definition $H_d = 1$.

Since this approximation only requires knowing the derivative appearing in Eq. (3.5), and it can numerically be computed with finite difference formulas, the number of function evaluation required for estimating the sensitivity coefficients has a linear dependence with the number of variables, depending on the target accuracy of the differentiation. This makes this approximation very cheap computationally speaking, although the range of validation will be constrained to a small region around the reference value unless true linear dependence exists between the input and the observable.

3.1.3 Sobol indices

Assuming that $Y = \mathcal{F}(\mathbf{X})$ is an integrable function over the d -dimensional hypercube $[0, 1]^d$, and that the input variables X_i are independently distributed, its variance can be

uniquely decomposed into increasing order summands [136]

$$\text{Var}[Y] = \sum_{i=1}^d V_i + \sum_{1 \leq i < j \leq d} V_{ij} + \dots + V_{1,\dots,d}, \quad (3.8)$$

being the different terms

$$\begin{aligned} V_i &:= V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y|X_i)), \\ V_{ij} &:= V_{X_{ij}}(E_{\mathbf{X}_{\sim ij}}(Y|X_i, X_j)) - V_i - V_j, \\ V_{ijk} &:= V_{X_{ijk}}(E_{\mathbf{X}_{\sim ijk}}(Y|X_i, X_j, X_k)) - V_{ij} - V_{ik} - V_{jk} - V_i - V_j - V_k, \\ &\vdots \\ V_{1,\dots,d} &:= \text{Var}[Y] - \sum_{i=1}^d V_i - \sum_{1 \leq i < j \leq d} V_{ij} - \dots - \sum_{1 \leq i_1 < \dots < i_{d-1} \leq d} V_{i_1 \dots i_{d-1}}, \end{aligned} \quad (3.9)$$

where $V/E_{X_i}(\dots)$ denotes the variance/expected value of the argument $(\dots)$ taken with respect to the factor X_i , while $V/E_{\sim \mathbf{X}_i}(\dots)$ is taken over all factors but X_i^* . The Sobol indices are therefore defined as the sensitivity estimators of each factor

$$S_{i_1 \dots i_s} := \frac{V_{i_1 \dots i_s}}{\text{Var}[Y]}. \quad (3.10)$$

The Sobol indices provide a measurement of the contribution of the selected group of variables $\{i_1, \dots, i_k\}$ to the total variance. The number of terms in the expansion of Eq. (3.8) is equal to $2^d - 1$, leading to the same number of Sobol indices, so in order to reduce the calculation cost, the total order indices are usually introduced [55]

$$ST_i := \frac{E_{\mathbf{X}_{\sim i}}(V_{X_i}(Y|\mathbf{X}_{\sim i}))}{\text{Var}[Y]}, \quad (3.11)$$

which includes the fraction of the variance accounted by X_i alone as well as the contribution of every group of variable where it is included. In this way, only first and total order Sobol indices are traditionally estimated. In addition, these definitions imply that $\sum S_i \leq 1$, $ST_i \geq S_i$ and $\sum ST_i \geq 1$, with the equality being fulfilled when no correlations exists.

The computation of both S_i and ST_i indices can be done via MC or any other sampling technique. From two independent sampling matrices $\mathbf{A}$ and $\mathbf{B}$ of dimension $n \times d$, they can be estimated via the formulas proposed at [124]

*Note that with this notation $\mathbf{X} = (X_i, \mathbf{X}_{\sim i})$.

$$\begin{aligned}
V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y|X_i)) &= \frac{1}{n} \sum_{j=1}^n \mathcal{F}(\mathbf{B})_j \left(\mathcal{F}(\mathbf{A}_B^{(i)})_j - \mathcal{F}(\mathbf{A})_j \right), \\
E_{\mathbf{X}_{\sim i}}(V_{X_i}(Y|\mathbf{X}_{\sim i})) &= \frac{1}{2n} \sum_{j=1}^n \left(\mathcal{F}(\mathbf{A})_j - \mathcal{F}(\mathbf{A}_B^{(i)})_j \right),
\end{aligned} \tag{3.12}$$

where $\mathbf{A}_B^{(i)}$ is the matrix where all columns are from $\mathbf{A}$ except the i -th column which is from $\mathbf{B}$. This approach will require $n \times (d + 2)$ function evaluations, so only a small subset of variables can be practically studied. The variable selection can be performed with the help of sensitivity coefficients (see Eq. (3.5)) in a hybrid methodology: from the whole input parameter space, a sensitivity analysis is performed, and from those subset of input variables which contributes the most to the variance, the Sobol indices are computed in order to search for interactions and higher order dependencies.

3.1.4 Polynomial Chaos expansion

General remarks

The Polynomial Chaos expansion, originally introduced by Wiener for studying Gaussian variables back in the 30' [152] and lately extended to other families of random variables [156], has in the last decades gained attention in the field of uncertainty quantification given its ability for modeling random responses [45, 157, 140]. Since a detailed description of the mathematical background can be found on the mentioned references, in the following only the key points of the theory will be introduced following the discussion of [140, 10].

The main idea of this approach is to decompose the response function in a basis that is orthogonal within the probability density function of the input parameters, *i.e.*

$$Y = \mathcal{F}(\mathbf{X}) = \sum \alpha_{\boldsymbol{\mu}} \Psi_{\boldsymbol{\mu}}(\mathbf{X}), \tag{3.13}$$

where $\Psi_{\boldsymbol{\mu}}(\mathbf{x})$ is a d -dimensional polynomial of d -dimensional index $\boldsymbol{\mu}$ and $\alpha_{\boldsymbol{\mu}}$ is the set of expansion coefficients. The polynomials are constructed in such a way that the inner dot product verifies

$$\langle \Psi_{\boldsymbol{\mu}} | \Psi_{\boldsymbol{\nu}} \rangle := \int d\mathbf{x} \Psi_{\boldsymbol{\mu}}(\mathbf{x}) \Psi_{\boldsymbol{\nu}}(\mathbf{x}) f_{\mathbf{X}}(\mathbf{x}) = \delta_{\boldsymbol{\mu}\boldsymbol{\nu}}, \tag{3.14}$$

being $f_{\mathbf{X}}(\mathbf{x})$ the probability density function of the random vector $\mathbf{X}$ and $\delta_{\boldsymbol{\mu}\boldsymbol{\nu}}$ the Kronecker delta. Note that the polynomials constructed here are not only orthogonal but also orthonormal; although the latter is not required it simplifies the notation since no multiplicative factors will appear each time inner products are calculated. For the uncorrelated case, $f_{\mathbf{X}}(\mathbf{x})$ can be expressed as the product of marginal distributions and thus the multidimensional polynomial will be just the product of one-dimensional

polynomials

$$\Psi_{\boldsymbol{\mu}}(\mathbf{X}) = \prod_{i=1}^d \psi_{\mu_i}^{(i)}(X_i), \quad (3.15)$$

being now the multidimensional index $\boldsymbol{\mu} \in \mathbb{N}^d$ the order of the individual polynomials $\boldsymbol{\mu} = \{p_1, p_2, \dots, p_d\}$. The most common continuous distributions and the associated family of polynomials verifying Eq. (3.14) include the Hermite polynomials for Gaussian distributions, Legendre for Uniform, Laguerre for Gamma and Jacobi for Beta. For other distributions for which a correspondence is not explicitly known, although the convergence may be degraded, one possible approach for generating the basis is to project the input on certain polynomials after transforming the probability space [156].

Exploiting the orthogonality properties of the basis, all the statistical moments can be derived from the coefficients, so once the model is constructed, all indicators can be trivially computed. In particular, the mean and the variance can be obtained as

$$\begin{aligned} \mathbb{E}[Y] &= \alpha_0, \\ \text{Var}[Y] &= \sum_{\boldsymbol{\mu} \neq \mathbf{0}} \alpha_{\boldsymbol{\mu}}^2, \end{aligned} \quad (3.16)$$

while the Sobol indices take the following form [140]

$$\begin{aligned} S_i &= \sum_{\boldsymbol{\mu} \in \mathcal{A}_i} \alpha_{\boldsymbol{\mu}}^2 / \text{Var}[Y] & A_i &:= \left\{ \boldsymbol{\mu} \in \mathbb{N}^d \mid \mu_i > 0, \mu_{i \neq j} = 0 \right\}, \\ ST_i &= \sum_{\boldsymbol{\mu} \in \mathcal{A}_i} \alpha_{\boldsymbol{\mu}}^2 / \text{Var}[Y] & A_i &:= \left\{ \boldsymbol{\mu} \in \mathbb{N}^d \mid \mu_i > 0 \right\}, \\ S_{i_1 \dots i_s} &= \sum_{\boldsymbol{\mu} \in \mathcal{A}_{i_1 \dots i_s}} \alpha_{\boldsymbol{\mu}}^2 / \text{Var}[Y] & A_{i_1 \dots i_s} &:= \left\{ \boldsymbol{\mu} \in \mathbb{N}^d \mid k \in \{i_1, \dots, i_s\} \Leftrightarrow \mu_k > 0 \right\}. \end{aligned} \quad (3.17)$$

Building a sparse basis

Although the expansion in Eq. (3.13) extends to infinity, for practical purposes the series must be truncated at certain order. Considering only those polynomials whose indices are included in the subset $\mathcal{A} \subset \mathbb{N}^d$, the expression becomes

$$Y = \mathcal{F}(\mathbf{X}) = \sum_{\boldsymbol{\mu} \in \mathcal{A}}^{\infty} \alpha_{\boldsymbol{\mu}} \Psi_{\boldsymbol{\mu}}(\mathbf{X}) \approx \sum_{\boldsymbol{\mu} \in \mathcal{A}} \alpha_{\boldsymbol{\mu}} \Psi_{\boldsymbol{\mu}}(\mathbf{X}) = \boldsymbol{\alpha}^T \boldsymbol{\Psi}(\mathbf{X}), \quad (3.18)$$

where vector notation has been introduced in the last part of the equation. Trivially, the dimensions of these vectors *i.e.*, the number of terms in the expansion, will be determined by the cardinality of the set $\mathcal{A}$. For example, one natural choice for $\mathcal{A}$ is to retain only

those polynomials whose sum of each individual component is below a certain degree p

$$\mathcal{A}^p := \left\{ \boldsymbol{\mu} \in \mathbb{N}^d \mid \sum \mu_i \leq p \right\}, \quad (3.19)$$

which has a cardinality

$$\#\mathcal{A}^p = \binom{d+p}{p}. \quad (3.20)$$

Given n observations, the straightforward approach for obtaining the vector coefficients $\boldsymbol{\alpha}$ is by solving the OLS (Ordinary Least Squares) problem

$$\hat{\boldsymbol{\alpha}} = \arg \min \mathbb{E} \left[\left(\mathcal{F}(\mathbf{X}) - \boldsymbol{\alpha}^\top \boldsymbol{\Psi}(\mathbf{X}) \right)^2 \right] = (\boldsymbol{\Phi}^\top \boldsymbol{\Phi})^{-1} \boldsymbol{\Phi}^\top \mathcal{Y}, \quad (3.21)$$

where by $\mathcal{Y} := \left\{ \mathcal{F}(\mathbf{x}^{(1)}), \dots, \mathcal{F}(\mathbf{x}^{(n)}) \right\}^\top$ we denote the computation results vector obtained from n different samples $\mathbf{x}^{(i)}$ and $\boldsymbol{\Phi}_{ij} := \boldsymbol{\Psi}_j(\mathbf{x}^{(i)})$ is an $n \times \#\mathcal{A}$ matrix. Note that the product $\boldsymbol{\Phi}^\top \boldsymbol{\Phi}$ is assumed to be invertible which does not hold when $\text{rank}(\boldsymbol{\Phi}) < \#\mathcal{A}$, *i.e.* when the number of evaluated points n is below the number of coefficients to determine or when linear dependence exists between different $\mathbf{x}^{(i)}$.

Following the truncation scheme of Eq. (3.19), since p is desired to be as large as possible in order to have an accurately approximation to the true model, when the number of variables increases the number of terms become prohibitively large from a computational point of view given that $n \geq \#\mathcal{A}^p$ in order to have a non-singular product in the right-hand side of Eq. (3.21). However, it is reasonable to assume that not all the terms in the expansion are relevant; most of them will be zero. In this way, if only the most relevant variables are selected (and the others are set to zero), a sparse solution will be constructed. This can be done with the LASSO (Least Absolute Shrinkage and Selection Operator) regression, which consists in including a penalty term in the OLS problem [52]. This penalty, which is proportional to the ℓ^1 norm of the coefficients, is used for performing the regularization and the variable selection (see Fig. 3.1).

$$\hat{\boldsymbol{\alpha}}^{\text{lasso}} := \arg \min \mathbb{E} \left[\left(\mathcal{F}(\mathbf{X}) - \boldsymbol{\alpha}^\top \boldsymbol{\Psi}(\mathbf{X}) \right)^2 \right] \quad \text{subject to} \quad \|\boldsymbol{\alpha}\|_1 \leq t. \quad (3.22)$$

In this way, a sparse solution $\hat{\boldsymbol{\alpha}}^{\text{lasso}}(t) := \left\{ \hat{\alpha}_1^{\text{lasso}}, \hat{\alpha}_2^{\text{lasso}}, \dots, \hat{\alpha}_m^{\text{lasso}} \right\}$ with $0 \leq m \leq p$ non-zero terms can be obtained depending on the strength of the penalty factor t .

Note that in the limit $t = \infty$ the OLS solution is recovered, while $t = 0$ shrinks all the coefficients towards zero. In this work, the LARS implementation available in the Scikit-learn Python machine learning library has been used [32, 106]. However, LASSO tends to shrink the non-zero coefficients too, so in order to debiasing them, LASSO could be applied again with a soft penalty factor in such a way no more variable selection is

Figure 3.1: Geometric interpretation of the LASSO regularization for a two-dimensional case. The ellipses, centered on the OLS solution, represent the contour plots of the residual sum of squares $(\mathcal{F}(\mathbf{X}) - \boldsymbol{\alpha}^\top \boldsymbol{\Psi}(\mathbf{X}))^2$ while in red the constraint region is drawn. The LASSO solution will be placed in the point where both regions meet; if it happens in one corner, only a variable will be selected since the other will be zero. More details can be found on [52].

performed. This two stage LASSO estimation, referred as hybrid-LASSO, is known to outperform regular LASSO [32, 81]. In this work we will consider the special case where no penalty term is included the second time, so the solution is equivalent to applying OLS to the LASSO selected variables.

At this point, given a certain maximum polynomial order, several models are constructed by means of the LASSO-OLS solution. In order to measure the performance of each one, the predicted sum of residuals is computed using the repeated k -Fold CV (Cross-Validation) technique [51]. The idea consists in partitioning the data in k subsets, validating each one against the model trained with the remaining $k - 1$. Finally, in order to reduce the possible dissimilarities between different partition schemes, the process is repeated multiple times. Therefore, the prediction error of the model can be estimated as

$$\varepsilon_{\text{CV}} := \frac{1}{\text{Var}[Y]} \cdot \mathbb{E} \left[\left(\mathcal{F}(\mathbf{x}^{(i_k)}) - \mathcal{F}'_k(\mathbf{x}^{(i_k)}) \right)^2 \right], \quad (3.23)$$

where $\mathcal{F}'_k(\mathbf{x}^{(i_k)}) := \hat{\boldsymbol{\alpha}}_k^\top \boldsymbol{\Psi}_k(\mathbf{x}^{(i_k)})$ denotes all the different k models that are built and i_k are the indexes of the validation subset. The result has been divided by the variance of the data with the purpose of having a dimensionless number.

In the following, the methodology proposed in [10] is used in order to build the sparse basis. Let us denote by $\mathcal{F}_p$ the best polynomial of degree p and by $\varepsilon_{\text{CV}}(\mathcal{F}_p)$ its associated error computed by means of the cross validation methodology in Eq. (3.23). The best polynomial is denoted by $\mathcal{F}^*$. Then, the sparse model can be obtained with the procedure described in Algorithm 1.

Algorithm 1: Adaptive sparse Polynomial Chaos expansion:

```

initialize
   $n$  points
   $p = 0$  // so  $\mathcal{F}^* = \mathcal{F}_0$ 
   $\varepsilon_{CV}(\mathcal{F}^*) = \infty$ 
while  $\varepsilon_{CV}(\mathcal{F}^*) > \text{target error}$  do
   $p += 1$ 
  Build a full basis following the truncation scheme of Eq. (3.19)
  foreach  $m$  different basis given the outcomes of the LASSO regularization
     $path$  do
    Recompute the coefficients with OLS and calculate the error
     $\mathcal{F}_p$  = polynomial with the lowest error
  if  $\varepsilon_{CV}(\mathcal{F}_p) < \varepsilon_{CV}(\mathcal{F}_{p-1})$  then
     $\mathcal{F}^* = \mathcal{F}_p$ 
  else if  $\varepsilon_{CV}(\mathcal{F}_p) > \varepsilon_{CV}(\mathcal{F}_{p-1}) > \varepsilon_{CV}(\mathcal{F}_{p-2})$  then // overfitting
     $n += 1$ 
     $p = \text{degree}(\mathcal{F}^*) - 1$ 

```

3.2 Optimization

As it has been shown in the previous chapters, the implementation of advanced nuclear fuel cycles requires the consideration of multiple facilities and hypotheses that depends on a large number of variables mixed through non-trivial relationships between them. Hence, given a precise desired outcome of the simulation, it is not trivial which configuration of input parameters is able to achieve it, that is, how to optimize the scenario. In this section, the optimization problem is discussed and the algorithm chosen for its implementation in TR_EVOL is presented. There exists a vast literature on this topic, so only key concepts required for understanding the main ideas will be introduced. For a deeper insight, additional details can be found in specific references such as [141, 84, 122] on constrained, multiobjective and stochastic optimization respectively.

3.2.1 General problem and key concepts

A non-linear general optimization problem can be expressed mathematically as

$$\min_{\mathbf{x} \in \mathbb{R}^d} f(\mathbf{x}), \quad (3.24)$$

where $f(\mathbf{x})$ is the objective function to be minimized over the input parameter space of dimension d which has been assumed to be real. In order to perform maximization, the function is simply multiplied by minus one so the problem can be transformed into a minimization one.

Constrained optimization

More general problems involve the inclusion of certain conditions in the target solution, *i.e.*

$$\min_{\mathbf{x} \in \mathbb{R}^d} f(\mathbf{x}) \quad \text{subject to} \quad \begin{cases} g_i(\mathbf{x}) < 0 & \text{for } 0 \leq i \leq r, \\ h_j(\mathbf{x}) = 0 & \text{for } 0 \leq j \leq s, \end{cases} \quad (3.25)$$

where $g_i(\mathbf{x})$ and $h_j(\mathbf{x})$ define a set of inequality and equality constraints respectively. In this way the solution space will be split in two regions: the feasible one in which the constraints are satisfied, and the unfeasible region where they are not. With these considerations, it is possible to express the problem in a more compact form

$$\min_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x}), \quad (3.26)$$

in which $\mathcal{X} := \{ \mathbf{x} \in \mathbb{R}^n \mid g_i(\mathbf{x}) < 0, h_j(\mathbf{x}) = 0 \forall i, j \}$ represents the feasible set. Anyway, in general the problem can be defined such that $\mathcal{X} = \emptyset$. Hence, the problem is said to be infeasible and no solution can fulfill all the imposed constraints.

One approach for solving these problems are penalty methods in which all the constraints are embedded in a penalty function that measures the degree of constraint violation of the solutions, being zero in the feasible region

$$\phi(\mathbf{x}) := \sum_i \max(0, g_i(\mathbf{x}))^p + \sum_j \|h_j(\mathbf{x})\|^p, \quad (3.27)$$

with p a positive number that traditionally is taken as $p = 1$ (the simple sum of constraints) or $p = 2$ (quadratic sum).

Multiobjective optimization: the Pareto front

Another class of problems considers the optimization where several objectives must be minimized simultaneously

$$\min_{\mathbf{x} \in \mathcal{X}} f_1(\mathbf{x}), f_2(\mathbf{x}), \dots, f_n(\mathbf{x}). \quad (3.28)$$

As in general no single solution will optimize all of them, there is a trade-off between improving one objective and degrading the others. Under this consideration, a solution $\mathbf{x}_1$ is said to dominate another solution $\mathbf{x}_2$ if it improves at least one objective without degrading the others:

$$f_i(\mathbf{x}_1) \leq f_i(\mathbf{x}_2) \quad \forall \quad i \in \{1, \dots, n\} \quad \text{and} \quad f_j(\mathbf{x}_1) < f_j(\mathbf{x}_2) \quad \text{for some } j \in \{1, \dots, n\}. \quad (3.29)$$

All the dominant solutions, which will define an hypersurface, form the so-called Pareto front [84].

Stochastic optimization

Finally, in the presence of uncertainties, the evaluation of a set of input parameters does not produce a single value. Therefore, the optimization problem of Eq. (3.24) will be transformed to

$$\min_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x}, \boldsymbol{\xi}), \quad (3.30)$$

being $\boldsymbol{\xi}$ a random vector. For the sake of simplicity, it has been assumed that the uncertainty only affects to the objective function although in general it could also be present in the constraints. In order to be able to solve the problem, it is necessary to transform it to a deterministic one. The most trivial approach is to replace the random variables by their expected value $\hat{\boldsymbol{\xi}}$ so the problem is equivalent to Eq. (3.24). However, this approach will solve the expected case without accounting for the variability of the random variables, and thus the solutions obtained in this way could not be stable. Instead, it is a better option to optimize the expected value of the random response

$$\min_{\mathbf{x} \in \mathcal{X}} \mathbb{E}_{\boldsymbol{\xi}} [f(\mathbf{x}, \boldsymbol{\xi})]. \quad (3.31)$$

The problem now is how to calculate the expected value. In the following, the SAA (Sample Average Approximation) will be used [122]. For a given $\mathbf{x}$, multiple samples from $\boldsymbol{\xi}$ are drawn and the expected value is replaced by its MC estimate (see Eq. (3.1))

$$\mathbb{E}_{\boldsymbol{\xi}} [f(\mathbf{x}, \boldsymbol{\xi})] \approx \sum_{i=1}^n f(\mathbf{x}, \boldsymbol{\xi}^{(i)}). \quad (3.32)$$

3.2.2 Choosing the right algorithm

Dozens of different algorithms for global optimization can be found in the literature as Fig. 3.2 shows. Since there is not a general method that outperforms all cases in all situations, the election should be based on the characteristics of the problem and the resources available. As it has been previously mentioned, in fuel cycle simulations the analytic form of the problem is unknown so it is not possible to exploit the underlying structure of the function that is going to be optimized. In this way, we have a black-box function in which information can be only gained through evaluations. On the other side, the latest TR_EVOL version has a fast execution speed (Table 2.3) and additionally the calculations can be run using massive parallelization at the CIEMAT supercomputing environment (Section 2.4). Hence, it becomes clear that the most suitable family of algorithms fall in the category of evolutionary ones.

Figure 3.2: Taxonomy of global optimization algorithms, data from [150]. In red, the classification of the DE (Differential Evolution) algorithm.

Figure 3.3: Generation of a new candidate solution with the DE/rand/1/bin algorithm in a 2-dimensional space. Once the mutant vector $\mathbf{m}_i^{G+1}$ is obtained (red), the crossover operator (in blue) produces three different candidates $\mathbf{c}_i'^{G+1}$, $\mathbf{c}_i^{G+1}$ and $\mathbf{c}_i''^{G+1}$ from which one will be randomly picked.

This kind of methods generates a set of candidate solutions which are iteratively updated according to a series of stochastic operators. With these operators, at each step a new set of candidate solutions is generated after selecting the most promising ones while rejecting the worst ones. In this way, the solutions move randomly through the search-space but focusing on those regions that have produced the best results.

In the following, the DE algorithm as well as their extensions for handling constrained multiobjective stochastic optimization are discussed. This election has been done based on the previous considerations and the extreme simplicity of this algorithm.

The Differential Evolution algorithm

The DE algorithm was developed by Storn and Price in 1995 [138, 139]. It is a stochastic population based strategy where the new individuals are chosen using the distance and direction information from the current population members: the parameters to be optimized are embedded in a vector and a series of operators are applied to them in order to generate new solutions. The key steps, illustrated on Fig. 3.3, are:

1. Initialization

In the first call, for each member of the population (of size N) an input vector of dimension d (the number of variables) is randomly chosen in order to cover all the parameter space.

2. Mutation

For each individual, a mutant vector is generated from other members in the generation as

$$\mathbf{m}_i^{G+1} = \mathbf{x}_{r1}^G + F(\mathbf{x}_{r2}^G - \mathbf{x}_{r3}^G), \quad (3.33)$$

where G denotes the current generation, $G + 1$ the new one, $r_1 \neq r_2 \neq r_3 \neq i$ are three random indices different between them and from the running index i and $F \in [0, 2]$ is a positive scale factor which controls the amplification of the differential variation.

3. Crossover

In the next step, parameter mixing is performed according to the following criteria:

$$c_{i,k}^{G+1} = \begin{cases} m_{i,k}^{G+1} & \text{if } (\text{rand}_{i,k}^{\mathbb{R}} \leq CR \text{ or } k = \text{rand}_i^{\mathbb{N}}) \\ x_{i,k}^G & \text{otherwise} \end{cases} \quad \text{for } k = 1, \dots, d. \quad (3.34)$$

Here $CR \in [0, 1]$ is the crossover constant, $\text{rand}_{i,k}^{\mathbb{R}} \sim \mathcal{U}(0, 1)$ is a random number generated for each (i, k) pair and $\text{rand}_i^{\mathbb{N}} \sim \mathcal{U}\{1, d\}$ is a random integer that ensures that at least one mutated parameter is included in the new vector guaranteeing that no duplication occurs.

4. Selection

Finally, the new generation is evaluated and the best individuals are retained for the next generation, *i.e.* $x_i^{G+1} = \text{Best}(c_i^{G+1}, x_i^G)$. The process is iteratively repeated from Step 2 until the convergence criterion is reached.

Note that the definition of Eq. (3.33) implies that the mutation rate decreases as the individuals approach to the solution since the differences will be smaller. Therefore, for the future generations the individuals will get closer and eventually, all of them will converge to the same solution.

The strategy summarized in the previous lines is known as DE/rand/1/bin, where *rand* refers to how the target vector was chosen, 1 is the number of difference vectors used and *bin* means binomial crossover because the number of parameters donated by the mutant vector closely follows a binomial distribution. Other variants of the algorithm include different mutation schemes such as DE/rand/1/exp, DE/best/1/bin or DE/best/2/bin (see for example [27]).

Finally, some authors have shown that randomizing the differential weight F (known as *dithering*) can help speed the convergence [109, 26]. This approach will be chosen in this implementation too.

Including constraints: the ε level comparison

Once the problem is transformed into a non constrained one by defining a penalty function as it was indicated in Section 3.2, it is necessary to introduce a new metric in order to evaluate the goodness of a solution. Under this idea, the ε level comparison defines a lexicographic order in which the comparison of the penalty proceeds the differences

in the function values [142]. Therefore, the comparison operators are replaced by the following ones

$$\begin{aligned}
(f(\mathbf{x}_1), \phi(\mathbf{x}_1)) &<_{\varepsilon} (f(\mathbf{x}_2), \phi(\mathbf{x}_2)) \\
&\iff \begin{cases} f(\mathbf{x}_1) < f(\mathbf{x}_2) & \text{if } (\phi(\mathbf{x}_1), \phi(\mathbf{x}_2) \leq \varepsilon \text{ or } \phi(\mathbf{x}_1) = \phi(\mathbf{x}_2)), \\ \phi(\mathbf{x}_1) < \phi(\mathbf{x}_2) & \text{otherwise,} \end{cases} \\
(f(\mathbf{x}_1), \phi(\mathbf{x}_1)) &\leq_{\varepsilon} (f(\mathbf{x}_2), \phi(\mathbf{x}_2)) \\
&\iff \begin{cases} f(\mathbf{x}_1) \leq f(\mathbf{x}_2) & \text{if } (\phi(\mathbf{x}_1), \phi(\mathbf{x}_2) \leq \varepsilon \text{ or } \phi(\mathbf{x}_1) = \phi(\mathbf{x}_2)), \\ \phi(\mathbf{x}_1) \leq \phi(\mathbf{x}_2) & \text{otherwise.} \end{cases}
\end{aligned} \tag{3.35}$$

In this way, the solutions with the lowest penalties are always preferred.

Differential Evolution for Multiobjective Optimization

In 2005, in order to extend DE for handling MO (Multiobjective Optimization), Robič and Filipič proposed the DEMO (Differential Evolution for Multiobjective Optimization) algorithm [116]. It replaces the selection operator with a new mechanism based on Pareto ranking and crowding distance sorting that will be briefly explained in the following lines. In pseudocode, the new selection is provided in Algorithm 2.

Algorithm 2: DEMO selection operation:

```

foreach individual do
    if Candidate dominates the parent then
        | Candidate replaces the parent
    else if Parent dominates then
        | Candidate discarded
    else
        | Candidate added to population
if Population size has increased then Truncate it
Randomly enumerate the individuals of the population

```

The truncation is derived from the MO genetic algorithm NSGA-II [28]. In a first place, the individuals are ranked into non-dominated Pareto front levels, and then, for each individual in the same front, the crowding distance, *i.e.* a measurement of how closed are the neighbors solutions, is calculated. Those solutions having the lower rank are selected, and between two solutions with the same rank, the less crowded one is chosen. The pseudocodes for calculating both the rank level and the crowding distance are provided in Algorithms 3 and 4 and they have been extracted from the above mentioned reference.

Algorithm 3: Fast non-dominated sorting (P):

```

foreach  $p \in P$  do
     $S_p = \emptyset$ 
     $n_p = 0$ 
    foreach  $q \in P$  do
        if  $p \prec q$  then                                     // if  $p$  dominates  $q$ 
             $S_p = S_p \cup \{q\}$  // add  $q$  to the set of sols. dominated by  $p$ 
        else
             $n_p += 1$  // increment the domination counter of  $p$ 
    if  $n_p = 0$  then //  $p$  belongs to the first front
         $p_{\text{rank}} = 1$ 
         $\mathcal{F}_1 = \mathcal{F}_1 \cup \{p\}$ 
     $i = 1$  // initialize the front counter
while  $\mathcal{F}_i \neq \emptyset$  do
     $Q = \emptyset$  // for storing the members of the next front
    foreach  $p \in \mathcal{F}_i$  do
        foreach  $q \in S_p$  do
             $n_q -= 1$ 
            if  $n_q = 0$  then //  $q$  belongs to the next front
                 $q_{\text{rank}} = i + 1$ 
                 $Q = Q \cup \{q\}$ 
     $i += 1$ 
     $\mathcal{F}_i = Q$ 

```

Algorithm 4: Crowding distance assignment ($\mathcal{I}$):

```

 $l = |\mathcal{I}|$  // number of solutions in  $\mathcal{I}$ 
foreach  $i$  do  $\mathcal{I}[i]_{\text{distance}} = 0$  // initialize distance
foreach objective  $m$  do
     $\mathcal{I} = \text{sort}(\mathcal{I}, m)$  // sort using each objective value
     $\mathcal{I}[1]_{\text{distance}} = \mathcal{I}[l]_{\text{distance}} = \infty$  // boundaries always selected
    for  $i = 2$  to  $(l - 1)$  do // for all other points
         $\mathcal{I}[i]_{\text{distance}} = \mathcal{I}[i]_{\text{distance}} + \frac{\mathcal{I}[i+1].m - \mathcal{I}[i-1].m}{f_m^{\max} - f_m^{\min}}$ 

```

Chapter 4

Uncertainties in the nuclear fuel cycle

As it has been pointed out in previous chapters, fuel cycle simulations are nowadays extensively used in scenario evaluation. However, the input parameters that feed the simulations are not exactly determined, maybe due to experimental precision or just because of lack of knowledge or ignorance. In addition these tools make use of different assumptions and approximations in order to solve the associated problem. All of this has an impact on the obtained outcomes, and thus, it is crucial to determine their effect in order to provide reliable results. Under this topic, uncertainty analyses emerge as powerful techniques due to their ability not only for propagating the uncertainties, but also for measuring the relevance or importance of each input.

In this chapter, the uncertainties that can affect fuel cycle simulations are investigated. Three different scenarios have been chosen for studying their effects, each one of them covering one different category of uncertainties that will be defined in the forthcoming section.

4.1 Introduction

Nuclear fuel cycle simulations, as any representation of the real world, involve uncertainties. Consequently, it is vital to study and understand how these uncertainties propagate and impact (and to which extent) the results of the fuel cycle analyses. Taking into account the nature of these tools (see for example the TR_EVOL simulation flowchart depicted on Fig. 2.1), it is possible to classify the uncertainties under three different categories depending on their origin:

- Fuel cycle parameters
- Nuclear data

– Simulator

The fuel cycle parameters refer to the set of input parameters required for modeling the particular scenario under study. They include technological and industrial parameters of the fuel and the nuclear facilities (*e.g.* fuel enrichment, burn-up, reprocessing efficiency) as well as hypotheses and assumptions about the future such as introduction and decommission dates of these facilities or the predicted energy demand. Uncertainties can be represented with a particular probability density function which can be chosen by expert judgment or industrial feedback and experimental results, and their impact can be directly addressed with the techniques described in the previous chapter.

Nuclear data consists of data describing neutron (and sometimes other particle) interactions with the nuclei conforming the system, as well as data describing nuclear changes in system constituents, as a result of fission, activation or decay. Nuclear data includes hence reaction cross sections, fission products yields, branching ratios and decay data. In this manner, they play a fundamental role in nuclear fuel cycle simulations since they govern the evolution of the nuclear materials. The values of these data which can be obtained either through experimental results or by the application of theoretical models, are collected in nuclear data libraries after a validation process. Additionally, their uncertainty (when available) are also included in these libraries through the covariance matrices. However, the impact of these covariance matrices has to be considered carefully (requiring thus an special methodology) because two reasons: the libraries are not directly used by the nuclear fuel cycle simulators and the presence of numerous correlations. This will be detailed in Section 4.3.

Finally, the effect of the simulator embraces all methodologies, approximations and simplifications made by the codes for modelling the reality and solve the electronuclear scenarios in a feasible amount of time. Hence, they are intrinsic to the fuel cycle simulator. Nevertheless, due to the lack of analytical solutions, their impact can not be directly estimated and the comparison with other methods and models is required in order to infer their effect.

In the following sections, the impact of each category will be addressed with the study of a different nuclear fuel cycle scenario. As the first category is the easiest to calculate since it does not require any further methodology, the uncertainty in the cycle parameters will serve as a basis against which the other two groups will be compared in order to estimate their relevance. In this way, it will be possible to determine if they are negligible and thus they can be disregarded in future analyses, or on the contrary, they should be considered due to their relevance.

4.2 Uncertainties in the fuel cycle parameters

The uncertainty propagation from the input specifications to the desired observables, as well as the quantification of the impact of each variable has been recently investigated by the fuel cycle community covering different degrees of approximation. For example, [100] considers parametric variations while [144] is based on Sobol variance decomposition. Nevertheless, as it was indicated in Section 3.1, parametric studies and local method considers linear dependence between inputs and outputs. This assumption constraints their range of validity to the vicinity of the reference values unless true linear dependence exists which does not hold when the nuclear fuel is irradiated. On the other hand, the Sobol's variance decomposition (a global theory) does not impose any restriction allowing the capture of non-linear relationships along the whole input parameter space as well as interactions at the expense of large computational cost. In this way, in order to be affordable from a practical point of view, only a small subset of variables can be selected for this kind of studies although the computational demand for estimating Sobol indices for this reduced parameter space could be still too high if several variables are chosen.

One possibility for dealing with this situation is to approximate the computational exhaustive simulation system with a simpler model. This approach, known as surrogate model or metamodel, include splines, artificial neural networks and support vector machine approximations, among others (see for example [11, 9, 23]). Another way of generating the surrogate model is by using the Polynomial Chaos expansion as introduced in Section 3.1.4. The advantage of this choice, as explained in the referred section, is that it allows for the easy deduction of the statistical information as it has already been proven by previous works within the nuclear community. In [153], they are used for solving a stochastic transport equation. Transient scenarios have also been studied with this methodology by means of the point kinetics approximation. For example, [48] studies a reactivity insertion which was lately explored by [155] too but for performing inverse uncertainty quantification. In [107], the case of an unprotected loss of flow is analyzed by using an adaptive basis which is constructed depending on the contributions to the variance.

In this section, a hybrid uncertainty quantification strategy has been applied to an advanced European collaborative scenario positioned on a closed fuel cycle strategy in order to establish the most relevant input parameters. To that end, in a first approach a first order approximation has been conducted with the purpose of reducing the input parametric space and avoiding the excessive computational cost the global techniques demand. After that, the Sobol analysis of variance was applied following the two different approximations described in Sections 3.1.2 and 3.1.4 (direct integration vs Polynomial Chaos expansion). The results have been compared in order to show the improvements of the latter methodology.

4.2.1 Scenario description

The scenario chosen for the study is based on the first one defined in the PATEROS (Partitioning and Transmutation European Roadmap for Sustainable Nuclear Energy) project framed on the 6th Framework Program of Euratom [77, 127]. Four different scenarios were defined in the project. Three of them were assumed to be the most realistic implementation of the P&T strategy, while the fourth assumed a nuclear energy resurgence in some countries. From the conservative ones, two of them considered that a shared ADS fleet would be built collaboratively between all countries with the purpose of managing the SNF (Spent Nuclear Fuel) (they differ in the mono/multirecycling of the Pu), while the latter assumed that a FR fleet was built but only for a selected group of countries with the same objective. In this work the first of these scenarios has been selected.

Schematically, the selected scenario considers two different groups of countries, namely Groups $\mathcal{A}$ and $\mathcal{B}$, that have a legacy SNF stock (see Table 4.1). Group $\mathcal{A}$ is at a standstill for nuclear energy but has to manage its own SNF, while Gr. $\mathcal{B}$ is in a continuation scenario that optimizes its Pu stocks in order to replace in the future its current fleet of PWR by FR, while managing the MA. Both of them collaborate in the deployment of a shared group of ADS facilities that are fed with the Pu of Gr. $\mathcal{B}$ and transmutes the entire MA inventory available in the cycle. Therefore, the main objectives of this scenario are to decrease the SNF stock of Gr. $\mathcal{A}$ down to zero and to stabilize the MA inventory of Gr. $\mathcal{B}$ while storing its Pu for the future deployment of FR. In this way, the different phases depicted in Fig. 4.1 read:

1. Initial phase (2010–2045)

The electricity is produced in LWR PWR systems using either UOX or MOX fuels. There exists an initial legacy of SNF that has to be managed.

2. Burning phase (2045–2105)

From year 2045, ADS are deployed with the purpose of burning down the SNF stock of Group $\mathcal{A}$ as well as the MA of the cycle. The Pu recovered from Gr. $\mathcal{B}$ is kept as resource for future deployment of FR.

3. Stabilization phase (2105–2300)

After 60 years of lifetime, some ADS units are decommissioned in order to reach a sustainable state in which the MA inventories neither increase nor decrease with time.

During the whole scenario the electricity produced by Group $\mathcal{B}$ consisting of a PWR fleet is fixed at 430 TWh_e, with a ratio of 90/10 for the UOX and MOX technologies. In the case of the ADS fleet, its energy is set as high as possible in each phase in

Table 4.1: Initial SNF inventories per group of countries. Part of the SNF of Group $\mathcal{A}$ is added in year 2022, while the SNF of Gr. $\mathcal{B}$ (all of them added in 2022) was broken down in UOX and MOX types because the Pu generated in PWR will be reused in MOX fuels.

	Group $\mathcal{A}$ (t)		Group $\mathcal{B}$ (t)	
	2010	2022	UOX	MOX
^{234}U	2.9	0.4	2.5	0.2
^{235}U	128.4	81.2	79.5	1.6
^{236}U	87.2	40.7	61.4	0.3
^{238}U	16 736.8	9167.3	10 778.1	1177.5
^{237}Np	11.5	6.0	7.6	0.3
^{238}Pu	4.7	3.0	3.5	2.1
^{239}Pu	105.5	68.5	67.6	27.7
^{240}Pu	45.1	35.6	31.9	18.6
^{241}Pu	26.0	9.7	14.3	8.8
^{242}Pu	14.3	10.0	9.9	6.6
^{241}Am	6.9	11.9	5.5	4.0
^{243}Am	3.9	2.3	2.3	1.7
^{242}Cm	0.2	—	—	—
^{244}Cm	1.3	0.6	0.7	0.7
^{245}Cm	—	0.1	0.1	0.1
FP	799.6	403.0	535.2	49.9
Total	17 974.3	9840.3	11 600.1	1300.1

Figure 4.1: Basic components of the simulated scenario. Circles represents the reactors, the diamonds the stocks of materials and the rectangles the different facilities. Note that there are four different reprocessing facilities (UOX and MOX SNFs of Gr. $\mathcal{B}$, SNF of Gr. $\mathcal{A}$ and ADS SNF).

Figure 4.2: Energy of the ADS fleet. The burning phase runs out until year 2105, and after that for a period of 18 years the fleet is adjusted to reach the stabilization objectives. This period has been selected to provide a decommissioning rate closest to the construction rate taking into account the 60 years lifetime of each ADS unit.

Table 4.2: Energy input for the scenario.

Parameter	Value
PWR MOX ratio	10%
PWR Park energy	430.00 TWh _e
ADS burning phase energy	24.66 TWh _e
ADS stabilization phase energy	15.27 TWh _e

order to match the scenario objectives. In particular, during the burning phase the production is almost 25 TWh_e while in the stabilization it is close to 15 TWh_e (see Fig. 4.2 and Table 4.2). In the following, the main scenario parameters are described. Since not all the information required for running the simulation with TR_EVOL can be found in the bibliography, some additional assumptions were done. Also, for technical reasons that will be explained in Section 4.2.2, the initial SNF inventories were increased.

Reactor technologies

Each PWR unit has an output of 1000 MW_e while for the ADS, based on the EFIT (European Facility for Industrial Transmutation) design [4] is 154 MW_e. The main parameters of the reactors are collected in Table 4.3.

Table 4.3: Reactor features.

Reactor	Power (GW_e)	Thermal eff. (%)	Load factor (%)	Core mass (t_{HM})	Burn-Up ($\text{GW d } t_{\text{HM}}^{-1}$)
PWR(UOX)	1.000	33.0	80.0	78.545	50.0
PWR(MOX)	1.000	33.0	80.0	78.545	50.0
ADS	0.154	40.0	87.0	5.325	78.3

Table 4.4: Fuel specifications.

Parameter	Value
^{235}U enrichment for UOX	4.20%
^{235}U enrichment tails	0.25%
Pu content for MOX	8.50%
Pu/MA content for ADS	45/55%

Fuel specification

The fuel specifications are detailed in Table 4.4. The PWR are fueled with UOX (enrichment of 4.2%) or MOX (8.5% of Pu), depending on the technology. In the case of the ADS systems, the fuel contains a mixture of Pu/MA at a ratio 45/55%. The Pu of Group $\mathcal{B}$ is monorecycled in the MOX fuels, while the Pu used in future cycles as well as the MA of the cycle are continuously recycled in the ADS. Fabrication time and cooling period are set to two and five years respectively.

Reprocessing

The main parameters of the reprocessing plants can be found in Table 4.5. The reprocessing plants of Gr. $\mathcal{B}$ start their operation in 2010 with a capacity of 1700 t y^{-1} for UOX and 120 t y^{-1} for MOX SNF. Group $\mathcal{A}$ starts its reprocessing strategy in 2040 (850 t y^{-1}) and the ADS in 2050 with infinite reprocessing capacity assumed (but always lower than 40 t y^{-1}). Two different processes have been considered. The hydrometallurgical process is used for the UOX and MOX irradiated fuel, while the pyrometallurgical process is applied to the ADS fuel. In addition, an homogeneous reprocessing strategy has been employed for all of them.

4.2.2 Methodology

The uncertainty in the input parameters described in the previous tables (they have been gathered again in Table 4.6) has been modelled following a symmetric uniform distribution centered on the reference value. With the exception of the reprocessing efficiencies, the support of such distribution was chosen as an arbitrary range of 10%

4.2. Uncertainties in the fuel cycle parameters

Table 4.5: Main parameters of the reprocessing plants.

Spent Fuel	Max. amount (t_{HM})	First year	Process	Separation eff. (%)
UOX	1700	2010	Hydrometallurgical (Pu)	99.99
MOX	120	2010	Hydrometallurgical (MA)	99.99
Gr. $\mathcal{A}$	850	2040	Pyrometallurgical (Pu)	99.99
ADS	∞	2050	Pyrometallurgical (MA)	99.99

of variation around the reference value $\hat{x}$ in order to assign the same relative standard deviation to each input, *i.e.* $\mathcal{U}(\hat{x} \cdot 0.95, \hat{x} \cdot 1.05)$. For the reprocessing efficiency, the range was set to only 0.1% to ensure that the maximum possible value is lower than a hundred percent. For the reactor parameters, the variation was performed over the entire fleet since the uncertainty achieved on this way is more conservative than performing variations over single reactors given the fact that the sum of multiple random variables tends to a normal distribution.

Please note that no uncertainty over the initial SNF legacy was assumed. As it was explained in Section 2.2.3, perturbations around the reference values could lead to broken scenarios. In the scenario studied here, this issue is produced by lack of the necessary TRU elements for ADS or MOX fabrication. Since a region of the initial input space is lost if this happens, the estimated variance would be underestimated. However, this effect is only relevant in global uncertainty analysis; sensitivity coefficients are computed by finite difference so the solution is close enough to the reference case, and in this region scenarios are stable. In order to avoid this problem, an additional mass of 200 t of Pu and 100 t of MA has been artificially added at the first year of the cycle (2010). This auxiliary mass can be understood as an increment of the initial SNF legacy so, in this way, it makes no sense to assign an uncertainty to Groups $\mathcal{A}$ and $\mathcal{B}$ SNF inventories since their value will be masked by this extra mass.

A hybrid methodology relying on both local and global methods has been used for the uncertainty and sensitivity analyses. In a first step, the sensitivity coefficients of the selected variables will be estimated. With that information, the variables showing the largest contribution to the variance will be chosen for the Sobol analysis. At this point, two different methodologies will be used in order to estimate the Sobol coefficients: the direct integration and the Polynomial Chaos expansion in order to compare their performance.

In addition, the input parameter space has been sampled with the Sobol quasi-random sequence (see Appendix A), which is justified as follows. In fuel cycle simulations, the generation/decay of the isotopes is governed by a non-homogeneous first-order ordinary differential equations (*i.e.* smooth functions), and it is also a reasonable assumption that not all the input parameters will have the same impact over a specific output variable.

Table 4.6: List of the input parameters used for the uncertainty analyses and their bounds. Labels to the left indicate the ones being used for Sobol analysis.

Label	Parameter	Units	Min.	Max.
E_{PWR}	PWR Park energy	TWh _e	408.500	451.500
	ADS burning phase energy	TWh _e	23.427	25.893
	ADS estabilization phase energy	TWh _e	14.507	16.034
r_{MOX}	PWR MOX ratio	%	9.500	10.500
	Power PWR(UOX)	GW _e	0.950	1.050
	Power PWR(MOX)	GW _e	0.950	1.050
	Power ADS	GW _e	0.146	0.162
ε_{UOX}	Thermal eff. PWR(UOX)		0.314	0.347
ε_{MOX}	Thermal eff. PWR(MOX)		0.314	0.347
ε_{ADS}	Thermal eff. ADS		0.380	0.420
	Load factor PWR(UOX)		0.760	0.840
	Load factor PWR(MOX)		0.760	0.840
	Load factor ADS		0.827	0.914
Q_{UOX}	Core mass PWR(UOX)	t _{HM}	74.618	82.472
	Core mass PWR(MOX)	t _{HM}	74.618	82.472
	Core mass ADS	t _{HM}	5.059	5.591
	Burn-up UOX	GW d t _{HM} ⁻¹	47.500	52.500
	Burn-up MOX	GW d t _{HM} ⁻¹	47.500	52.500
	Burn-up ADS	GW d t _{HM} ⁻¹	74.385	82.215
	UOX enrichment	%	3.990	4.410
	Enrichment tails	%	0.238	0.263
	Pu in MOX fuel	%	8.075	8.925
	Pu in ADS fuel	%	42.750	47.250
Pu_{ADS}	Reprocessing capacity (UOX)	t y ⁻¹	1615.000	1785.000
	Reprocessing capacity (MOX)	t y ⁻¹	114.000	126.000
	Reprocessing capacity ($\mathcal{A}$)	t y ⁻¹	807.500	892.500
	Hydrometallurgical sep. eff. (Pu)	%	99.850	99.950
	Hydrometallurgical sep. eff. (MA)	%	99.850	99.950
	Pyrometallurgical sep. eff. (Pu)	%	99.850	99.950
	Pyrometallurgical sep. eff. (MA)	%	99.850	99.950

Figure 4.3: Comparison between Monte Carlo sampling (dashed line) and Sobol quasi-random sequence (continuous). Both results have been smoothed.

Under these conditions, it is expected that QMC sampling has better convergence than MC methods as described in the appendix. This is represented for one of the estimators from Eq. (3.12) in Fig. 4.3, where the generator available at the GNU Scientific Library for the Sobol Sequence [42] has been used. From the figure, it is clear that QMC convergence outperforms MC. In any case, as Sobol sequence is of open type, points can be added until the convergence criteria is reached without having to discard the previous results.

As the upper bound of the QMC integration error is in general not meaningful since it does not provide a realistic error, we will use as criterion for its estimation that all the values for the Sobol indices obtained with the last k -points converge to the same number up to some decimal place. If $f^{(i)}$ denotes the integral estimated with $\{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(i)}\}$ points, then

$$\varepsilon_f = \max \left(|f^{(n)} - f^{(i)}| \right) \leq \delta \quad \forall \quad k \leq i \leq n, \quad (4.1)$$

where δ is the desired precision for all the integrals.

4.2.3 Results

In the following, the results of the scenario are discussed. Firstly, the reference calculation is presented. In the next sections, the analysis of variance is performed using two different approaches. In this way, the direct integration method can be compared with the Polynomial Chaos expansion in order to show the strengths and weaknesses of both

(a) Minor Actinides

(b) Plutonium

Figure 4.4: Separated mass in pools (red color) and in the whole cycle (blue) for the MA and Pu stocks. Note the green line in Fig. 4.4b representing the available Pu for FR deployment. The line shows the reference case scenario and the shaded area represents the uncertainty calculated as 1σ from the average value.

techniques when applied to fuel cycle simulation studies.

Reference calculation

As the main objective of the scenario is the minimization of the TRU contents and its posterior stabilization, the output variables selected for this study were the final MA and Pu separated masses, corresponding to the stocks of materials that are available for fuel fabrication, and the final MA and Pu masses in the whole fuel cycle which is the sum of the masses in every facility without considering the waste (see Fig. 4.1). The results are provided at Fig. 4.4 (see caption for curves information). The fact that graphs do not start from zero, and the discontinuity observed in year 2022, is explained by the initial SNF legacy that is added to the scenario in years 2010 and 2022, as it was indicated previously in Table 4.1. Notice that this initial SNF also includes the additional 200 t of Pu and 100 t of MA that were artificially added the first year in order to avoid scenario breaking: all the scenarios below the dashed line representing this additional mass in the MA Fig. 4.4a would be broken. In the case of the Pu in Fig. 4.4b, this effect cannot be appreciated since part of the material in the separated stocks is not available for MOX/ADS fuel fabrication due to the fact that it is reserved for the future deployment of FR.

At the beginning of the scenario, there is an increase in both the separated Pu and the separated MA curves. This is an effect of reprocessing, starting in 2010, of both PWR fleet SNF (UOX and MOX) coming from Group $\mathcal{B}$ and the initial legacy. At year 2018, the increase rate of both curves of separated material slightly decreases due to the ending of the stock of PWR(UOX) from the initial legacy. At year 2040, the increase rate grows again because of the start of Gr. $\mathcal{A}$ reprocessing. The separated MA curve changes from increasing to decreasing due to the commissioning of the first ADS units in year 2046. The MA consumption increases as more ADS units are deployed, until year 2105 where the burner fleet is adjusted to achieve the stabilization of the separated MA inventory, which takes place at years 2105–2123 (see Fig. 4.2 on page 45). Before, at year 2072, the stock of PWR(MOX) from the initial legacy is exhausted (completely reprocessed) causing that both the separated Pu and the separated MA curves have a sharp change in the variation rate. In addition, as the ADS was designed to be neither a Pu burner nor a breeder [4], the Pu is only consumed by the MOX reactors. As the UOX/MOX ratio remains constant, the Pu inventory in cycle grows steadily along the simulation. In both cases, it is noticeable in the separated pool the greater TRU demand during the ADS deployment (that concludes at year ~ 2090) related to the new cores that must be created.

The maximum installed ADS power is constrained by the MA available for fuel fabrication. As seen in Fig. 4.2, this number is maximal when all the separated MA

(Fig. 4.4a) is exhausted. Note that as abovementioned, the minimum value is 100 t instead of zero to avoid scenario break. After that year, the decommission for readapting to the last phase starts. Following this, during the phase-out of some ADS to reach the stabilization phase, the available MA inventory rises because of the additional mass that is coming from the ADS spent cores that are being decommissioned. The recuperated Pu follows the same slope changes excepting that in this case the demand for fuel fabrication is lower than the separation rate. Furthermore, since the stored Pu pool for the future FR deployment is fed by MOX reactors, and along the simulation their energy remains constant, it grows continuously. Note that the slope of Pu in cycle follows the same trend than the Pu storage for FR reactors, meaning that with those technologies the stabilization of the Pu inventory (and thus of all the TRU) can be achievable.

Sensitivity & Sobol indices

As abovementioned, the computational cost of a pure Sobol analysis is non-affordable. To reduce it to viable levels, only a subset of the input parameters whose contribution to the variance was larger than 10% were selected for each studied output. This selection was made by means of the sensitivity analysis approximation, obtaining that a total of seven parameters matched this criterion (labeled in Table 4.6). The variance obtained by the sensitivity approximation was recalculated again only considering this subset and each individual contribution is shown in Table 4.7. The sign of the sensitivity coefficient was also included to show if in a first order approximation the observable is an increasing or decreasing function. Finally, Sobol first and total indices, as well as their difference, were printed too after their estimation via the integral forms. Following the criterion introduced in Section 4.2.2, we fixed for this study $\delta = 0.01$ and $k = 1000$ in all the calculated integrals, so $n = 12\,500$ points were required for the worst of the integrals in order to match the selected criterion. Therefore, a total of $12\,500 \times 9 = 112\,500$ simulations (see Eq. (3.12)) were computed. Note that a variation of ± 0.01 in the Sobol indices translates into uncertainties of 1% in the contributions to the variance. Also, by definition $ST_i \geq S_i$ so all the negative values appearing in the table are consistent with the assigned uncertainty.

According to the sign of the sensitivity coefficients, two input parameters (E_{PWR} , positive; ε_{UOX} , negative) have the same behavior in all the TRU. Higher PWR fleet energy implies a large number of reactors in the park, so TRU production increases. On the other hand and whatever the technology, the less efficient a reactor is, the more mass is needed each refueling. In the case of UOX, TRU inventories at discharge will increase, while the effect of lowering MOX or ADS efficiency will translate in less Pu or MA burnt respectively in those reactors.

In the case of Pu streams, it was found that the variable with the largest impact

Table 4.7: Sensitivity normalized indices (recalculated) and Sobol indices for the selected input variables ordered by importance.

Variables		Sensitivity		Sobol		
		Sign	η_i	S_i	ST_i	ΔS_i
MA pool	Pu _{ADS}	+	0.33	0.30	0.30	0.00
	E_{PWR}	+	0.25	0.27	0.27	0.01
	ε_{ADS}	+	0.21	0.20	0.20	0.00
	ε_{UOX}	−	0.09	0.08	0.08	0.00
	Q_{UOX}	+	0.06	0.05	0.05	0.00
	ε_{MOX}	−	0.03	0.05	0.06	0.01
	r_{MOX}	+	0.03	0.04	0.05	0.01
MA cycle	E_{PWR}	+	0.32	0.33	0.35	0.02
	Pu _{ADS}	+	0.27	0.23	0.23	0.00
	ε_{ADS}	+	0.16	0.15	0.15	0.00
	ε_{UOX}	−	0.11	0.10	0.10	0.00
	Q_{UOX}	+	0.07	0.06	0.06	0.00
	ε_{MOX}	−	0.04	0.06	0.08	0.02
	r_{MOX}	+	0.03	0.05	0.07	0.02
Pu pool	ε_{UOX}	−	0.44	0.42	0.41	−0.01
	r_{MOX}	−	0.19	0.22	0.22	0.00
	ε_{MOX}	+	0.13	0.16	0.16	0.00
	Q_{UOX}	−	0.12	0.12	0.12	−0.01
	E_{PWR}	+	0.09	0.07	0.07	0.00
	Pu _{ADS}	−	0.03	0.03	0.03	−0.01
	ε_{ADS}		0.00	0.01	0.00	−0.01
Pu cycle	ε_{UOX}	−	0.45	0.45	0.44	−0.01
	r_{MOX}	−	0.17	0.19	0.18	0.00
	Q_{UOX}	−	0.13	0.13	0.13	−0.01
	ε_{MOX}	+	0.12	0.13	0.13	0.00
	E_{PWR}	+	0.12	0.11	0.11	−0.01
	Pu _{ADS}	−	0.02	0.03	0.02	−0.01
	ε_{ADS}		0.00	0.01	0.00	−0.01

on its variance is ε_{UOX} . The next one (but half important) is r_{MOX} : the more MOX reactors, the more Pu can be burnt. For the MA, two streams (E_{PWR} and Pu_{ADS}) carry around $\sim 60\%$ of the variance. Pu content in ADS fuel (or equivalently MA content) plays now an important role because, as MA streams are minimized (while Pu streams are not), relative changes are more significant.

Sobol indices indicate that there is no relevant interaction among the input parameters. The maximum interaction observed is in the case of the MA in cycle, and is caused by three variables ($E_{\text{PWR}}, \varepsilon_{\text{MOX}}, r_{\text{MOX}}$). Without higher order indices, it is not possible to differentiate if it is caused by a second-order interaction, a third-order one, or both of them. Whatever the case, the contribution to the variance will be bounded between the extreme cases where it is a third-order interaction (contribution of 2%) or a second-order interaction between all pairwise combinations (3%), being 10 times smaller than the most relevant variable. Moreover, as interactions are negligible, first Sobol indices are equivalent to η_i making possible the comparison between the two approaches. Differences will point out a non linear relationship between the input parameters and the studied output. In the worst-case, found in MA cycle stream for the Pu in ADS fuel, the difference is only of 4%, so linear dependence can be assumed.

Finally, the effect of the uncertainties along the simulation has been shown in Fig. 4.4 with the shaded areas. This area represents the uncertainty estimated as 1σ from the average value that was obtained with the QMC sampling. It becomes clear that the effect of the uncertainties, present in all the observables, accumulates over time growing with the simulation.

Sparse Polynomial Chaos expansion

The estimation of the Sobol indices in the previous section via the integral expressions of Eq. (3.12) required the use of 112 500 simulations, despite of the use of QMC sampling. This translates to around two weeks of calculations in the EULER cluster available at CIEMAT Section 2.4. In this section, the problem will be tackled using the Polynomial Chaos Expansion. Considering that the probability density function used was a uniform one, as it was introduced in Section 3.1.4 the family of polynomials satisfying the orthogonality properties required by the Polynomial Chaos expansion in Eq. (3.14) are the Legendre functions. Although they are defined over the interval $x \in [-1, 1]$, with a change of variable their domain can be extended to the input parameters one. Once the set of polynomials are determined, the expansion is performed following the steps described in Algorithm 1. The target predicted error, which was estimated following the 100-repeated 10-Fold CV (see Eq. (3.23)), was set to 10^{-3} . Finally, the number of initial points for performing the expansion was arbitrarily set to 100 (and if overfitting occurs, 25 more points will be added each time).

4.2. Uncertainties in the fuel cycle parameters

Table 4.8: Basis properties for each observable. As reminder, n is the number of initial points, p the maximum degree of the polynomial expansion, m and $\#\mathcal{A}^p$ the number of non-zero and total terms of the basis $\mathcal{A}^p$ respectively, and finally ε_{CV} is the prediction error of the model.

Observable	n	p	m	$\#\mathcal{A}^p$	ε_{CV}
MA pool	100	4	64	330	7.42×10^{-4}
MA cycle	100	5	38	792	9.52×10^{-4}
Pu pool	100	3	44	120	9.97×10^{-4}
Pu cycle	100	2	17	36	9.69×10^{-4}

For the sampling points, the Sobol quasi-random sequence was used too. On Table 4.8, the expansion details for each observable is shown. It was found that for these cases, with the initial set of 100 simulations, the target error was reached. In general, all the observables are well described with low order polynomials, from which the LASSO regularization selects a small subsets of relevant terms reducing notably the computational cost. Finally, it is important to notice that the polynomial order fixes the maximum degree of interaction between variables. In any case, with such reduced number of points, all the fuel cycle scenarios can be executed in less than half an hour instead of the two weeks of the previous section.

The total and first Sobol indices computed with this approximation are shown in Table 4.9, while a graphical comparison with the values obtained in the previous section (Table 4.7) is provided in Fig. 4.5. In this plot, for each indicator, the first and total Sobol indices are shown. The first coordinates of the points are the values obtained by direct integration while the second corresponds to the Polynomial Chaos expansion approach. In this way if both approximations provide the same value, the point must lie on the dashed line $y = x$, being the deviations a measurement of the discrepancy. Moreover, for a given input, the closest the first and total indices are, the smallest interactions this parameter has as previously indicated. Finally note that with this representation, the variables with the largest contribution to the variance are located in the upper right corner.

When the results are compared, it is found that both approaches provide approximately the same results. However, it must be pointed out that although the prediction error of the model is estimated, it can not be related for quantifying the uncertainty of the derived estimators. This is evidenced by the value of the sum of the total order coefficients in the Pu pool indicator in Table 4.9, which by definition cannot be lower than one. The largest discrepancies, appearing in the effect of the ε_{UOX} in the Pu pool, are below a 3% of the total variance. Although in general there is no interaction between the input variables since $ST_i \approx S_i$ and both sums are very close to one, the results of the MA in cycle indicates the existence of higher order terms, despite the fact that their contribution will be negligible. Nevertheless, the Polynomial Chaos expansion allows for

Table 4.9: Sobol first and total indices computed within the sparse Polynomial Chaos Expansion. Again, only coefficients greater than 0.01 are shown for consistency with the previous table.

Variable	MA pool			MA cycle			Pu pool			Pu cycle		
	S_i	ST_i	ΔS_i	S_i	ST_i	ΔS_i	S_i	ST_i	ΔS_i	S_i	ST_i	ΔS_i
E_{PWR}	0.27	0.28	—	0.34	0.36	0.02	0.06	0.07	0.01	0.10	0.10	—
r_{MOX}	0.04	0.04	—	0.05	0.07	0.02	0.21	0.22	0.01	0.17	0.18	—
ε_{ADS}	0.20	0.20	—	0.14	0.14	—	—	—	—	—	—	—
ε_{UOX}	0.08	0.08	—	0.09	0.09	—	0.39	0.39	—	0.43	0.43	—
ε_{MOX}	0.05	0.05	—	0.05	0.07	0.01	0.14	0.15	—	0.12	0.13	—
Q_{UOX}	0.05	0.06	—	0.06	0.06	—	0.11	0.11	—	0.12	0.12	—
Pu_{ADS}	0.31	0.31	—	0.23	0.23	—	0.02	0.02	—	0.02	0.02	—
Sum	1.01	1.03		0.96	1.01		0.94	0.97		0.97	0.98

Figure 4.5: Comparison between the first (in blue) and total (red) Sobol indices estimated by direct integration with Sobol quasi-random sequence and by the sparse Polynomial Chaos expansion (results from Table 4.7 and Table 4.9) for each observable.

Table 4.10: Sobol higher order for the MA inventories in cycle.

Second Order		Third Order	
$S(E_{\text{PWR}}, r_{\text{MOX}})$	0.008	$S(E_{\text{PWR}}, r_{\text{MOX}}, \varepsilon_{\text{MOX}})$	0.005
$S(E_{\text{PWR}}, \varepsilon_{\text{MOX}})$	0.006		
$S(r_{\text{MOX}}, \varepsilon_{\text{MOX}})$	0.004		

the estimation of any order coefficient without extra computational cost (see Eq. (3.17)). The second and third Sobol indices are shown in Table 4.10 for this observable. Again, the uncertainty of these values has not been derived so given their lower values, they must be considered carefully.

Besides, the presence of interactions is an indicator of the existence of a relationship between the input variables. For example, the MA in the cycle depend on the production/burning rate in the reactors, and therefore they are also related with the fabricated mass for refuelling. This mass can be estimated as $m = P_{\text{th}} \cdot t/Q$, where $P_{\text{th}} = P_{\text{th}}(E, \varepsilon)$, and thus MA cycle $\propto (E, \varepsilon)$ as inferred from Table 4.10. Note that for this case, this dependence can be trivially deduced, but for more complicated observables, this methodology will provide a deeper insight in the understanding of the physics. Note that although this interaction will exist for the other observables as well, its effect is not strong enough to be noticeable.

4.2.4 Conclusions

Analysis of variance is a strong technique that can be very useful for understanding the underlying physics of fuel cycle simulations. Although global methods appear to be the desirable option, different issues show up as it has been shown in this work when applied to fuel cycle simulations. The main drawback occurs when the goals of the studied scenario include minimization; as the reference case has been pushed to the edges, when large variations in the input space occurs the scenario may fail by lack of crucial material. The other limitation is related to the computational cost when large number of variables are involved. On the other hand, these are the strengths of local methods, they are stable and very cheap computationally speaking, so it is clear that one method complements another. It is possible then to make an initial guess with the sensitivity coefficients, and based on the observed results to perform Sobol decomposition. Nevertheless, as it has been proven, although this hybrid methodology can be used for reducing the dimension of the problem, the exhaustive computational cost the direct Sobol indices estimation demands as a consequence of the high-multidimensional integrals that emerge from their definitions, makes them generally unaffordable for nuclear fuel cycle global sensitivity analyses. In order to reduce that effort, an alternative approach to deduce the Sobol indices with smaller cost has been applied. It consists in expanding the desired

observables in a set of orthonormal polynomials that allows for the easy deduction of the indices. The expansion coefficients are then obtained by solving the OLS problem, in which LASSO regularization is introduced in order to reduce the effective dimension of the basis.

In this work these methodologies have been applied to a European collaborative advanced nuclear fuel cycle scenario. Within its objectives the minimization of the MA pools is pursued, meaning that the available stock for fuel fabrication in the reference scenario must be as low as possible. In order to overcome the lack of material when the input parameters are perturbed, an additional mass was added at the beginning of the simulation. The reference case shows that the minimization and posterior stabilization the MA pools is possible as well as the stabilization of the Pu streams of Group $\mathcal{B}$. That means that with the future incorporation of FR, all the TRU of the cycle can be efficiently managed. In addition, analysis of variance shows that the most relevant parameters are $(\text{Pu}_{\text{ADS}}, E_{\text{PWR}})$ for the MA streams and $(\varepsilon_{\text{UOX}})$ for the Pu ones. By comparing local and global approaches, it can be concluded that there is no noticeable interaction between the input parameters nor higher-order effects, so in this case, the response model can be approximated by a multivariable lineal function. Also, sensitivity coefficients signs are provided. All this information can be exploited in optimization studies; with the knowledge that the selected parameter is an increasing/decreasing function and that linear dependence can be assumed the input parameters can be changed towards the desired case. The optimization analyses are planned to be developed in the near future, as well as decomposition of variance with realistic uncertainties.

Regarding the comparison between direct and Polynomial Chaos Sobol estimation, both methods have shown to provide compatible results. In addition, the latter has shown its outperformance since it only required 100 fuel cycle simulations for achieving the target prediction error chosen instead of the 112 500 executions of the integration technique. In this way, analyses that took days now can be done in a few minutes. However, the main drawback of this model is that the prediction error can not be used for addressing the uncertainty of the obtained estimators. This should be deeper investigated in future works. In any case, the computational reductions are expected to be also found for other scenarios, allowing the consideration of more input parameters in the sensitivity analysis. This computational cost reduction will also allow other institutions having limited computational capabilities, for whom it is not possible to execute a large amount of simulations, to investigate with their own fuel cycle codes the propagation of variance in fuel cycle scenario analyses.

4.3 Uncertainties in the nuclear data

As it has been shown in the previous section, the studies conducted for propagating and quantifying uncertainties in the nuclear fuel cycle have been traditionally focused on the effects caused by the scenario input parameters such as the number of facilities, introduction rates or burn-up of the reactors, leaving aside the effect of the nuclear data. This data, understood as data describing neutron (and sometimes other particle) interactions with the nuclei conforming the system, as well as data describing nuclear changes in system constituents, as a result of fission, activation or decay, have been usually neglected in these studies due to the complexity of integrating their uncertainty in a fuel cycle simulation. Nevertheless, nuclear data have been reported to be one of the most important sources of uncertainty in reactor physics calculations [69], producing too a non-negligible impact on the isotopic composition of the spent fuel (as studied, among others, by [118, 30]). This effect is even more important in advanced reactors [85]. Moreover, [117] revealed that these uncertainties are comparable to the uncertainties produced by technological parameters of the reactor (*e.g.* boron concentration, pellet size or fuel/moderator densities). Hence, it is not unreasonable to expect that the nuclear data plays an important role in fuel cycle simulations too. This was studied in [71], showing that nuclear data seem to have a significant impact on Pu and MA inventories but it has been reported that the effect is probably small when compared to other uncertainty sources [143].

In this section, the relevance of the nuclear data uncertainties in fuel cycle analyses will be deeply studied. To that end, the uncertainties in the final composition due to the uncertainties in nuclear data have been firstly estimated with a Monte Carlo methodology. Then, the results have been compared against other classical sources of uncertainties that typically take part in fuel cycle simulations in order to measure their relevance.

4.3.1 Scenario description

The scenario chosen for this study considers an open fuel cycle with only LWR or PWR type. Despite its simplicity, this decision was made based on multiple criteria:

- Many of the countries with an ongoing nuclear energy program are currently positioned on an open fuel cycle strategy [60]. In particular, the PWR assumption is representative of the Spanish case in which six of the seven reactors currently in operation use this technology.
- Nuclear data in the thermal range for the major fissile isotopes in a PWR have been extensively studied because of their relevance, achieving low uncertainties due to the high precision of the experiments [21, 76]. Therefore, if the nuclear data play

Table 4.11: PWR pin-cell configuration data.

Parameter	Value
Pin radius	0.465 cm
Pin side length	1.498 cm
Cladding thickness	0.070 cm
Fuel density	0.0681 at/cm b
Cladding density	0.0432 at/cm b
Moderator density	0.0721 at/cm b
Fuel temperature	1200 K
Cladding temperature	600 K
Water temperature	600 K
Pin-cell power	0.2196 kW
Initial ^{235}U enrichment	3.1%
Total residence time	1665.7 d

an important role in this open cycle scenario, for other reactors/scenarios having isotopes and reactions with larger uncertainties (as it is the case of fast reactors using Pu or even MA in the fuel which will have a harder neutron spectrum), nuclear data uncertainties will also have an important impact.

- For the irradiation, the EVOLCODE 2.0 burn-up simulation system will be used. This tool has been validated against thermal spectrum reactors [2].

As the nuclear fleet will be only composed of PWRs, one reactor has been selected as representative of the whole fleet. The results for the scenario will be proportional to the energy produced by the representative facility. In addition, in order to reduce the computational effort, a single pin-element has been selected as representative of the full reactor core. This approach is based on previous studies reporting that this methodology provides a proper description of the PWR system [2]. Finally, the reactor chosen for the simulation is the German Obrigheim nuclear power plant since it was used for the EVOLCODE validation (more details can be found on the previous reference).

The irradiation history of the reactor, the model geometry, as well as the boron concentration in water are available in the bibliography [68, 12]. The burn-up was divided into three operational cycles (with a decay period between them) reaching a final total burn-up close to 30 GWd/t_U after 830 days of irradiation. During this time, refueling periods and unscheduled shutdowns were produced too, so the total residence time of the fuel was close to 1700 days. The pin-cell element made of uranium oxide is embedded in a zirconium cladding and surrounded by light water (with a small concentration of boron) that act as coolant and moderator. Also reflecting boundary conditions have been imposed. The main parameters are given in Table 4.11.

4.3.2 Methodology

The following methodology has been used for propagating the uncertainties from the nuclear data:

- The stochastic nuclear data sampling code SANDY [38] has been used. SANDY retrieves nuclear data (*i.e.*, cross sections, resonance parameters, fission yields and decay data) and their covariances from nuclear data files and samples the nuclear data according to a log-normal probability density function. Random nuclear data are then written in ENDF-6 (Evaluated Nuclear Data File) format [54] files (the so called perturbed files), which can be used by any code compatible with this format.
- For the nuclear data, the state-of-the-art JEFF-3.3 nuclear data library [108] has been used since it has one of the most complete sets of covariance matrices.
- In this work, the cross sections of ^{235}U , ^{238}U , ^{238}U , ^{239}U , ^{240}U , ^{241}Pu and ^{241}Am from JEFF-3.3 have been sampled with SANDY as a first step using this methodology, as they are the main fissile/fertile materials in UO_2 fuel and thus their uncertainties should be the main contributors to the uncertainty in the resulting isotopic vector after burn-up. ^{242}Pu has been neglected since no covariances for this nuclide are available in JEFF-3.3. Other superior actinides have been neglected due to its relatively small impact in a PWR irradiation with low burn-up. Multiple perturbed nuclear data libraries have been produced.
- The required number of perturbed libraries will be determined by the convergence criterion. The convergence has been considered reached when the error in the standard deviation is two orders of magnitude smaller than the value of the proper estimator. Therefore, we will impose in this work that the relative standard error of the standard deviation has to be below 3%.
- The correct generation of the perturbed files has been verified with the SUMMON code [121]. This code is based on deterministic First Order Perturbation Theory to derive the sensitivities, and on the Propagation of Moments Method (Sandwich Rule) to propagate the uncertainties in nuclear data. GODIVA integral experiment [101], the reference experiment for ^{235}U nuclear data validation, has been chosen to verify this methodology because it allows comparing the nuclear data uncertainties coming from stochastic sampling and a deterministic methodology with experimental results.
- The reference JEFF-3.3 nuclear data library and stochastically perturbed files have been processed with NJOY2016 [75] and converted from the ENDF-6 to the ACE format used by the simulation code MCNP6.2 [151].

- The burn-up model has simulated the 3 operational cycles into 53 different irradiation steps.
- A complete Monte Carlo simulation of the burn-up evolution has been performed with EVOLCODE burn-up system for each different perturbed nuclear data library to simulate the irradiation of the PWR pin. The uncertainty in the mass of each relevant actinide present in the irradiated fuel has been estimated from the different simulations.

Several uncertainty propagation codes based on the stochastic sampling of nuclear data exist such as SAMPLER, XSUSA, TMC, Kiwi, Hybrid Method, NUSS and NUDUNA [113, 161, 70, 79, 43, 160, 16]; however SANDY differs from them in being independent of the model and numerical solver, interacting only with the ENDF-6 nuclear data files, which can then be processed to compatible formats for specific codes, therefore allowing the use of any state-of-the-art nuclear data library. Furthermore, it can not only quantify the uncertainty in the model responses, but also estimate the importance of the nuclear data to the response uncertainty.

Finally, with the purpose of quantifying the relevance of the nuclear data uncertainties, the obtained results have been compared with the uncertainties that typically take part in a fuel cycle simulation. For an open fuel cycle like the one studied, these parameters include the initial enrichment, the residence time and the thermal power extracted. As the last two parameters have an impact in the burn-up, an additional case where the time and power have been varied in an anticorrelated way (so that the burn-up remains unchanged) has also been considered. In this way, the space-location effects in the reactor core of different fuel assemblies that reach the same burn-up but with different operational history can be studied. As the scope of this work is to check if the nuclear data uncertainties play an important role when compared to the fuel cycle ones (not to provide a detailed calculation of them), the estimation will be as conservative as possible. For this reason, large deviations from the reference values will be assumed (10% in total, plus 5% and minus 5%). In addition, the Popoviciu's inequality on variances will be used in order to provide an upper limit to the variance produced by these parameters. According to this inequality, for a given input parameter x_i , the variance of the random function $y(x_i)$ is constrained by

$$\sigma_i^2 \leq \frac{1}{4} \left(y_i^{\max} - y_i^{\min} \right)^2, \quad (4.2)$$

where $y_i^{\max/\min}$ corresponds to the upper/lower bounds of $y(x_i)$. In order to reduce the computational cost, these bounds will be estimated with a quadratic approximation between the values obtained from the limits of the input parameter intervals and the

reference one

$$y_i^{\max/\min} = \text{Max/Min} [y(x_i)] \approx \text{Max/Min} [P_2(x; y(x_i - 5\%), y(x_i), y(x_i + 5\%))], \quad (4.3)$$

being $P_2(x)$ the polynomial approximation of $y(x)$. Note that the upper limit on the variance obtained with this methodology holds for any probability distribution whose bounds are included in the range of the interpolation polynomial, which in the worst case is based on a second order approximation.

4.3.3 Results

Verification of the methodology with the GODIVA reference case

As stated in the previous section, the consistency of the perturbed files generated with the SANDY code has been verified with SUMMON. For this purpose, the GODIVA integral experiment from the International Criticality Safety Benchmark Evaluation Project database [101] has been chosen. GODIVA was an integral experiment located at Los Alamos, and was performed in the 1950's to determine the critical mass of a bare sphere of highly enriched uranium (94% of ^{235}U). Since GODIVA is the reference system for ^{235}U nuclear data validation, this experiment has been chosen in this work as the reference case to calculate the uncertainty in k_{eff} due to nuclear data using the proposed methodology. The experimental k_{eff} for GODIVA is 1.000 ± 0.001 . The uncertainty in k_{eff} of GODIVA due to the uncertainties in the ^{235}U cross sections has been calculated in a first step by creating 1000 random perturbed libraries in which ^{235}U cross section values have been modified within their evaluated uncertainty, leaving the cross sections of the rest of the U isotopes unchanged. GODIVA calculations (each with a different library) have been performed with MCNP code, using a simulation with 800 000 particles per neutron generation (or cycle) and 300 cycles (250 of them active), which ensures a statistical error of 4 pcm in k_{eff} , negligible when compared to the rest of the analysis. As a result, the mean ($\bar{k}_{\text{eff}} = 1.00009$) and the standard deviation are calculated throughout the 1000 simulations, as well as relative standard error of the second estimator for measuring the convergence, which is represented in Fig. 4.6.

The figure shows that the convergence criteria is achieved after around 600 simulations. With the 1000 libraries the relative standard error of the standard deviation is close to 2%. At this point, the k_{eff} uncertainty is 1.18%, which corresponds to the uncertainty of nuclear data using stochastic sampling.

The total uncertainty derived by SUMMON code due to ^{235}U cross section uncertainties, as well as the five major contributors to the uncertainty, is presented in Table 4.12. It can be seen that the total uncertainty in k_{eff} due to ^{235}U uncertainties is 1.22%, which is in very good agreement with the value obtained with MCNP using SANDY perturbed

Figure 4.6: Evolution of the relative standard error of the standard deviation with the number of samples (in black) and the target convergence criteria (dashed red line).

Table 4.12: k_{eff} uncertainty and main contributors for GODIVA with SUMMON.

Quantity	Uncertainty (%)
$^{235}\text{U}(\text{n,n}') - ^{235}\text{U}(\text{n,n}')$	0.699
$^{235}\text{U}(\text{n,n}') - ^{235}\text{U}(\text{n,f})$	0.697
$^{235}\text{U}(\text{n,f}) - ^{235}\text{U}(\text{n,f})$	0.657
$^{235}\text{U}(\text{n,n}') - ^{235}\text{U}(\text{n},\gamma)$	-0.424
$^{235}\text{U}(\text{n},\gamma) - ^{235}\text{U}(\text{n},\gamma)$	0.400
Total	1.220

files, while both are also in agreement with the experimental results. Consequently, the stochastic methodology and the convergence of the calculations have been successfully verified.

Uncertainties due to nuclear data

For studying the nuclear data uncertainties in LWRs, different perturbed libraries with variations in the cross sections of the main actinides (from ^{235}U to ^{241}Am) have been produced. As in the previous section, 1000 different perturbed libraries have been generated for running the same number of simulations. With this number of samples the convergence criterion is met since it is reached before ~ 900 simulations, depending on the isotope. Average values and their relative uncertainties for the isotopes with a contribution to the final isotopic composition larger than $1 \times 10^{-5}\%$ are provided

4.3. Uncertainties in the nuclear data

Table 4.13: Average masses of the main elements and isotopes and their associated relative uncertainty due to the nuclear data.

Element/nuclide	Mass (g)	σ_{rel} (%)
U	5.85	1.16×10^{-2}
Np	2.05×10^{-3}	2.21
Pu	5.45×10^{-2}	1.03
Am	9.17×10^{-4}	1.82
Cm	1.25×10^{-4}	2.31
^{235}U	4.91×10^{-2}	8.15×10^{-1}
^{236}U	2.23×10^{-2}	1.67
^{238}U	5.78	1.48×10^{-2}
^{238}Pu	7.32×10^{-4}	2.11
^{239}Pu	3.28×10^{-2}	1.37
^{240}Pu	1.23×10^{-2}	2.26
^{241}Pu	6.39×10^{-3}	1.71
^{242}Pu	2.33×10^{-3}	1.70
^{241}Am	5.52×10^{-4}	1.79
^{243}Am	3.60×10^{-4}	2.03
^{244}Cm	9.41×10^{-5}	2.44

in Table 4.13. Note that correlations between different isotopes may occur, in such a way that the uncertainty of a single element cannot be estimated from the individual uncertainties of its components without considering the correlations. Also notice that no isotopes of neptunium are reported because only ^{237}Np is produced in a significant amount.

With the exception of the uranium, the results obtained show that the relative uncertainties are quite similar for all the elements and isotopes reported in the table with a value close to 2% in spite of their abundance. For the ^{238}U isotope, this figure is almost two orders of magnitude lower as a consequence of the large mass that is present in the fuel before the irradiation. Considering instead the difference between the final and the initial amount of this isotope as indicator (instead of the mass after irradiation), the relative uncertainty is $6.6 \times 10^{-1}\%$. For ^{235}U , using the latter indicator, the relative uncertainty is of $2.9 \times 10^{-1}\%$.

Uncertainties from fuel cycle parameters

Finally, the maximum uncertainty in the fuel cycle parameters has been estimated with parametric calculations with the purpose of establishing the upper bound on the uncertainties in the inventories as it was introduced in Section 4.3.2. The results for each variable are collected in Table 4.14. As shown in the table, the parameters whose uncertainty has been propagated include the initial enrichment, the residence time and

Table 4.14: Relative uncertainties of the main elements and isotopes in the parametric studies.

Element/nuclide	Enrichment	Power	Time	Time/Power
U	6.30×10^{-3}	1.96×10^{-1}	1.96×10^{-1}	1.97×10^{-2}
Np	8.54×10^{-1}	6.49	6.56	3.28×10^{-1}
Pu	3.78×10^{-1}	2.84	2.74	1.37×10^{-1}
Am	3.64	9.12	1.19×10^1	2.98
Cm	9.79	2.16×10^1	2.13×10^1	1.24
^{235}U	1.13×10^1	8.02	8.11	2.87×10^{-1}
^{236}U	3.58	2.26	2.26	4.48×10^{-2}
^{238}U	1.04×10^{-1}	1.39×10^{-1}	1.39×10^{-1}	1.77×10^{-2}
^{238}Pu	2.49	1.16×10^1	1.34×10^1	1.74
^{239}Pu	9.92×10^{-1}	7.78×10^{-1}	6.56×10^{-1}	1.07×10^{-1}
^{240}Pu	2.28	4.81	4.85	1.66×10^{-1}
^{241}Pu	1.27	5.21	4.73	3.44×10^{-1}
^{242}Pu	6.51	1.22×10^1	1.22×10^1	4.08×10^{-1}
^{241}Am	5.43×10^{-1}	3.83	8.48	4.77
^{243}Am	8.46	1.73×10^1	1.72×10^1	6.03×10^{-1}
^{244}Cm	1.12×10^1	2.43×10^1	2.39×10^1	8.40×10^{-1}

the thermal power extracted as well as the combination between these two last.

Results show, for the case of a variation in the initial ^{235}U enrichment, that for the ^{235}U , the uncertainty is very similar to the 10% input variation, although if the difference between the initial and final concentration indicator is chosen, this value is approximately halved. For the other actinides (in particular for Pu isotopes), this uncertainty should be similar, since a larger initial amount of ^{235}U should generate a smaller amount of actinides from ^{238}U . However, a correlation between the fissile isotopes has to be considered since the burn-up (hence the number of fissions) is fixed. Due to this correlation the uncertainty for the Pu isotopes is reduced: a larger initial amount of ^{235}U (and hence a smaller amount of ^{238}U and their transmutation descendants) causes more fissions from this former isotope and less from Pu fissile isotopes, leading to their accumulation (and reduction of the uncertainty).

The cases of the thermal power and the cycle length are the ones with the largest contribution to the uncertainty since they are related with the electricity produced in the park, reported to provide one of the largest uncertainties in fuel cycle analyses [100]. Both parameters can be considered similar since both are directly proportional to the burn-up. Considering each actinide separately, the uncertainties propagated from these parameters are very similar except for those isotopes that have a decay period of the order of magnitude of the irradiation time, which is the case of ^{241}Pu and its daughter ^{241}Am , which have a special behaviour not depending on the burn-up.

For the combination of the residence time (and thus of the irradiation time) and

thermal power maintaining the same burn-up, the isotope showing the largest relative uncertainty is ^{241}Am (around three times larger than the relative uncertainty of the ^{238}Pu) due to the already discussed reasons.

Fig. 4.7 shows the comparison of the maximum bound on the uncertainties propagated from these input parameters with the uncertainties due to the nuclear data that were estimated in the previous section. Uncertainties are represented as $1 \pm \sigma_{\text{rel}}$ for each variable and element/nuclide. For the case of the parametric variation of the initial ^{235}U enrichment, it can be observed that the uncertainty in the actinides is similar or smaller than the one propagated from the nuclear data, excepting for Cm, for which no nuclear data uncertainty was considered. Considering the isotopes, some of them (mainly most isotopes of Pu and ^{241}Am) have a maximum uncertainty from the parametric variation similar to or smaller than the one propagated from the nuclear data.

For the cases of change in the time and power separately (meaning a change in the final burn-up), some actinides (mainly Pu and Np) and isotopes (mainly $^{239, 240, 241}\text{Pu}$) have an uncertainty of the same order of magnitude as the one obtained from nuclear data, while for the rest, the maximum uncertainty propagated from the parametric change is larger than the one propagated from the nuclear data.

Finally, for the combination of residence time and thermal power maintaining the same burn-up, U, Np and Pu have smaller uncertainties than those propagated from the nuclear data (even more than one order of magnitude), while for Am, both uncertainties are similar. For the main isotopes, all of them have an uncertainty smaller than the nuclear data propagated uncertainty (again, sometimes even more than an order of magnitude) except for ^{238}Pu , which has similar values, and ^{241}Am with a smaller uncertainty propagated from the nuclear data. With this parameter involving no change in the burn-up, the impact and the importance of the nuclear data uncertainty in the fuel cycle becomes clearer than for the other parameters.

4.3.4 Conclusions

With the spread of the nuclear fuel cycle simulations for scenario evaluations, uncertainty studies have gained attraction. Nevertheless, the recent works performed under this topic have been usually focused on the impact of fuel cycle parameters, leaving aside the effect of the nuclear data which has been shown to be critical in other fields like reactor physics calculations or safety assessments.

In this work, the importance of the nuclear data in fuel cycle simulations is addressed. The uncertainties in nuclear data (*i.e.*, cross sections) have been propagated with a Monte Carlo approach, which has been also verified against a deterministic sensitivity/uncertainty methodology with GODIVA integral experiment. Once the procedure has been verified, the nuclear data uncertainties have been studied in an open fuel cycle

(a) By element

(b) By isotope

Figure 4.7: Comparison between the relative uncertainties for major elements and isotopes. The uncertainty due to the nuclear data has been estimated with the Monte Carlo methodology while for the others parameters it is the maximum one according to the Popoviciu's inequality of variances (see Eq. (4.2)).

consisting of a PWR system representing the nuclear fleet. Results in terms of the relative uncertainty for the major elements and actinides produced have been provided. After that, the uncertainties on parameters of the fuel cycle have been estimated. In order to be as conservative as possible, a large deviation of $\pm 5\%$ from the reference values (total variation of 10%) was considered, and with the extreme values the maximum variance achievable was calculated. In this way, an upper limit on the uncertainty was obtained for the fuel cycle parameters.

The results show that for certain isotopes the uncertainties due to nuclear data are of the same order of magnitude than the maximum bound on the uncertainties when parametric variations in the fuel cycle parameters are performed. This is the case of ^{236}U and $^{240}, ^{241}\text{Pu}$ isotopes, while for the ^{239}Pu it is not only of the same order but dominates. In the other observables, the nuclear data uncertainties are comparable in order of magnitude to at least one of the fuel cycle parameters for relevant isotopes, indicating that they should not be neglected.

This work has shown the relevance of the nuclear data in fuel cycle simulators. Although the variance due to the fuel cycle parameters has been maximized in a very conservative way for an open fuel cycle for which the nuclear data is well known, its effects cannot be disregarded. Even more, only a few reactions have been considered, leaving the rest of them as well as the fission yields as best estimate parameters without uncertainties. Therefore, as the complexity of the fuel cycle grows, with the multirecycling of the spent fuel and with the use of advanced reactors, it is expected that the nuclear data will gain even more relevance in the advanced fuel cycle analyses.

4.4 Effect of the simulator

At this point, we have studied the effect that the uncertainties in the input parameters have in the fuel cycle simulation. However, the simulators themselves are very complex tools that have to cope with a wide range of physics models, and in order to solve the problem in a feasible time, multiple hypotheses, approximations and simplifications must be introduced in the codes. With this in mind, as many codes are actually used in fuel cycle estimations (see Section 2.1.2), it is natural to wonder if given a fixed set of hypotheses for describing a certain electronuclear fuel cycle scenario, they provide the same results and up to what degree. In this area, multiple benchmarking exercises have been done in the past by the community leading to the acceptance of some discrepancies in the results [95, 37, 6, 119].

This section aims to improve the fuel cycle uncertainty quantification by assessing the impact that the simulation code has on the output parameters, as well as comparing it with other sources of uncertainty with the purpose of knowing if the effect introduced by the code is negligible or not. A benchmark of a complex nuclear fuel cycle scenarios has been

carried out with ANICCA and TR_EVOL nuclear fuel cycle codes. The quantification of the discrepancies between them, based on reference/best estimate values, has been used for the estimation of the impact of the simulation tools, and after that, such impact has been compared with the uncertainty produced by the input parameters which has been calculated following the Monte Carlo and sensitivity coefficients approaches.

4.4.1 ANICCA

ANICCA is an SCK·CEN homemade fuel cycle analysis code that has been in development since 2012 in response to the necessity to answer particular questions about the Belgian nuclear fuel cycle, advanced cycles or scenarios at a regional level. The code is intended to be a flexible and accurate tool for scenario studies, and considers all the strategies that can be applied in a nuclear fuel cycle, from once-through to fully closed cycle strategies. ANICCA is being designed as a stand-alone code and therefore, it does not depend directly on other codes. In this way, the radioactive decay of the nuclear material and the burnup process associated to the nuclear fuel, can be quickly and accurately executed in the code. For the irradiation process, each fuel is simulated by means of an associated prebuilt library. This library is obtained by the post-processing of an exhaustive calculation carried out by the SCK·CEN homemade burn-up code ALEPH2 [137]. The library created has enough information to allow ANICCA to perform the burnup process in one step with CRAM16 [111]. All the facilities involved in the cycle can be generically modeled, but they differ from each other in their processes.

The main results that can be obtained by the code are: mass balances (such as fuel production, material stored, material separated, uranium required, etc.), composition vectors in facilities per isotope, elements or groups of elements (*i.e.*: fission products, minor actinides, heavy metal) and other results such as radiotoxicity, decay heat and separative work units. The main differences between TR_EVOL and ANICCA codes were outlined in Table 2.2.

4.4.2 Scenario description

The chosen scenario is inspired by the one currently under study in the *Benchmark Study on TRU management Scenario* driven by the NEA/EG-AFCS (see Section 2.3.1 on page 20). This group has defined a set of scenarios for a further comparison of the codes and models, as well as for the evaluation of the amount of the materials in the SNF can be burnt with different burner fleets, raising the possibility of going to an equilibrium state after the reduction of the TRU stocks, *i.e.* a state where the inventories does not increase nor decrease along the years.

Particularly, in the scenario presented in this study, the electricity production is fixed at 49.05 GW_e or 430 TWh_e (see Fig. 4.8 and Table 4.15), and three different phases are

4.4. Effect of the simulator

Table 4.15: Energy share input ratios of the different technologies (and by fuel type) in the scenario energy production.

Technology	Phase 1	Phase 2	Phase 3
PWR(UOX ₁)	100.0	—	—
PWR(UOX ₂)	—	59.5	66.7
PWR(MOX)	—	34.5	25.5
ADS	—	6.0	7.8

set as follows:

1. Initial phase (0–80)

All electricity is produced by a PWR fleet using UOX fuel. No other technologies coexist in the park.

2. Burning phase (80–190)

After year 80 and during the next 30 years, new PWR and ADS reactors replace the entire PWR(UOX) original fleet. The PWR systems now use both UOX and MOX-IMR (Increased Moderation Ratio) fuels, being the latter an special concept which allows for Pu multirecycling. In this concept the Pu degradation is compensated via higher uranium enrichment in fuel assemblies that substitutes water holes for fuel rods to soften the neutron spectrum [8]. At this phase a large amount of SNF and TRU are accumulated. After the first transition, the new fleets are focused on burning as much TRU elements as possible. The only constraint is to have sufficient fuel to keep the fleets running for the period of the study.

3. Stabilization phase (190–300)

Between years 190 and 220, the energy share of the burning fleets is adjusted in order to achieve a sustainable state beyond year 220 and until year 300. This means a TRU stabilization (or in other words, both Pu and MA total inventories in the cycle reach an equilibrium).

The main facilities are depicted in Fig. 4.9, while their main parameters are described in the following sections.

Reactor technologies

As depicted in Fig. 4.9 and noted in Table 4.16, there are four different reactor technologies taking part in the cycle. Fulfilling the scenario objectives, the initial PWR(UOX₁) fleet that is used during Phase 1 is replaced during Phases 2 and 3 consisting of PWR(UOX₂), PWR(MOX-IMR) [8] and ADS (based on the EFIT design [114]) reactors. Please note that even though the same design has been used in both scenarios, the parameters of

Figure 4.8: Energy share input by fuel type. The dashed areas represent the transition between the different phases.

Table 4.16: Reactor features.

Reactor	Power (GW _e)	Thermal eff. (%)	Load factor (%)	Core mass (t _{HM})	Burn-Up (GW d t _{HM} ⁻¹)
PWR(UOX ₁)	1.600	34.0	85.0	128.9	60.0
PWR(UOX ₂)	1.530	35.6	85.0	109.6	60.0
PWR(MOX)	1.530	35.6	85.0	109.6	49.2
ADS	0.154	38.5	85.0	5.39	78.0

Figure 4.9: Fuel cycle scheme for the different phases. Circles represent reactor fleets (grouped by fuel type), rectangles facilities, and diamonds show the different stocks of materials. The reprocessing stage (one per kind of fuel) separates Pu and MA stocks for new fuel fabrication.

Table 4.17: Fuel specifications.

Parameter	Value
UOX enrichment	4.95%
²³⁵ U enrichment tails	0.25%
Pu in MOX fuel (max.)	12.00%
Pu/MA in ADS fuel	45/55%

the ADS are slightly different than those provided in Section 4.2.1 on page 42 because the initial scenario specifications have been iteratively readapted in order to reduce the discrepancies that could emerge from different interpretations.

Also, although PWR(UOX₂) and PWR(MOX-IMR) are represented (and will be simulated) separately in order to have a better understanding of the fuel and the resources behaviour, both fuels can be used jointly in the same reactor as the connection between them in Fig. 4.9 indicates. This is in line with the fact the PWR(UOX₂) and PWR(MOX) reactor parameters described on Table 4.16 are the same (both fuels are irradiated in practise in the same reactor).

Fuel specification

Three types of fuels are used in the simulation: for the first, second and third phases, UOX for PWR(UOX) reactors, and for the second and third phases MOX-IMR and ADS fuels for the PWR(MOX) and ADS reactors, respectively. The main parameters of these fuels are shown in Table 4.17, where the fabrication time was set to two years.

Regarding the fuel fabrication, the UOX is made from U_{nat}. The MOX-IMR fuel, on the other hand, is mixed using an equivalence formula, limiting the Pu content up to 12% [102]:

$$^{235}\text{U} = -0.00107Q_{\text{Pu}}^2 - 0.13113Q_{\text{Pu}} + 10.77298, \quad (4.4)$$

where Q_{Pu} , the Pu quality, is the ratio between the fissile content and the total mass. The target amount of ²³⁵U could be obtained through enrichment, mixing between U_{nat} and U_{dep} or, on the other hand, if the Pu quality is too high that even the desired content of ²³⁵U becomes below the depleted uranium tails (during the first cycles), the Pu weight can be reduced according to $\text{Pu}(\text{wt}\%) = 12 \cdot Q_{\text{F}}/Q_{\text{Pu}}$, where Q_{F} is obtained solving Eq. (4.4) for Q_{Pu} with ²³⁵U the content in U_{dep} [102]. Finally, the ADS fuel is made with a mixture of Pu and MA with a U-free inert matrix [5].

Reprocessing

The FIFO strategy was applied for the reprocessing of every type of spent fuel after 5 years of cooling. The main parameters can be found in Table 4.18. The reprocessing

Table 4.18: Main parameters of the reprocessing plants.

Spent Fuel	Max. amount (t_{HM})	First year
UOX	850	35
MOX	∞	—
ADS	∞	—

losses are fixed at 0.1% for every type of SNF. Note that no specifications have been done for MOX-IMR and ADS fuels since it is assumed that all the material is reprocessed as soon as possible. This is a reasonable assumption since, for this reference scenario, the maximum MOX-IMR and ADS discharged masses are about 600 t and 50 t, respectively. The recovered Pu and MA are mixed in two different stocks that will be used for feeding the new fuel requirements (see Fig. 4.9).

4.4.3 Methodology

First of all, the different reactors were modeled in detail with ALEPH2 in order to obtain the specific average cross-sections and fission yields, using the JEFF-3.1.1 nuclear data library [128]. Since the purpose of this work is the comparison between fuel cycle tools, instead of carrying out a separated simulation by means of the EVOLCODE system, the above mentioned nuclear data obtained with ALEPH2 was format-converted and used by TR_EVOL so no discrepancies can be caused by different core modeling or collapsing processes. After that, the same scenario was simulated with both ANICCA and TR_EVOL. This has required the continuous update of the scenario in an iterative way since the largest source of discrepancies were initially due to different interpretations of the specifications, as it was typically found in other studies [37] comparing the fuel cycle codes. Finally, an uncertainty quantification process for the input parameters has been done in TR_EVOL in order to compare the differences between both codes and other uncertainty sources.

All the parameters collected from Tables 4.15 to 4.18, plus the starting/ending years of the first and second transitions were considered for the uncertainty analysis. The detailed list of all of them has been recapped on Table 4.19. They include all the numerical values required by the simulation (making a total of 30 variables), apart from the total park energy that was fixed at 49.05 GW_{y_e} as in the reference case. With this constraint, all the simulated scenarios have the same energy output so the results can be coherently compared with the ones of the reference case. In order to model the uncertainty, random sampling was performed on all of them; the uncertainty has been estimated with Eq. (3.2). A symmetric uniform distribution with variation of $\pm 5\%$ over the reference value was chosen for the continuous variables while for the discrete ones (the years) ± 5 years were used as in the previous scenario in Section 4.2.2. The support

of each variable is shown in the table too. Also, sensitivity coefficients were computed for measuring (in a first order approximation) the contribution of each input variable to the total uncertainty (more details can be found in Section 3.1.2).

4.4.4 Results

In the following, the results obtained will be discussed in four different subsections. In a first place, the simulation scenarios are compared with a simple case in order to check that no different interpretations have been made. Then, the full scenario described in Section 4.4.2 is discussed. Finally, the differences due to the codes are shown, and in the last subsection, they are compared against other sources of uncertainties in the fuel cycle.

Simulation set-up with PWR only

Given the complexity of the simulated scenario, it must be ensured that both codes introduce no differences that could be explained by different assumptions interpretation. Also, since the scenario includes multi-recycling of the spent fuel inventories, these possible differences will propagate through the multiple irradiations making it more difficult to identify the true nature of the discrepancies. In order to overcome this issue, in a first approximation only the PWR reactors fed by UOX are considered (the total energy produced for this case will be the sum of the blue and green areas from Fig. 4.8), using in both codes the same isotopic content at the end of the irradiation with the purpose of removing the discrepancies produced by the irradiation process. The total Pu and MA inventories in the cycle (considering the masses in the fabrication plants, in the reactors, in cooling stage and reprocessed) are represented in Fig. 4.10, both in blue and red colors, respectively. Note that ANICCA (dashed line) and TR_EVOL (continuous line) overlap, so no significant differences are found between both simulations: at EOS (End of Simulation), the relative error was computed as $\varepsilon = 0.5|m_A - m_T|(1/m_A + 1/m_T)$ where $m_{A/T}$ refers to the ANICCA/TR_EVOL mass is around 0.1%. As expected, the figure shows inventories increasing along the years with different slopes in each phase since the PWR energy in the park changes, and no reuse of separated materials are considered in this partial scenario.

With this simple scenario, the UOX fuel fabrication as well as its irradiation, reprocessing and decay process of the separated materials stocks that will be used for the MOX and ADS fuels have been tested. There are two additional processes that have not been included here aside the irradiation process of the multirecycled materials: the ADS and MOX-IMR fuel fabrication. The first one uses fixed fractions of nuclear materials, so no differences are expected. For the latter, multiple tests have been done in order to ensure that no differences appear in this part of the simulation.

Table 4.19: Design of Experiment used for the uncertainty propagation. The sampling was performed drawing from a continuous uniform distribution probability $\mathcal{U} \sim (a, b)$ or discrete one $\mathcal{U} \sim \{a, b\}$ if the variable depends on the years. Note that PWR(UOX₂) and PWR(MOX) reactor parameters are taken as a single variable since both fuels are used in the same reactor as explained in Section 4.4.2.

Variable	Units	a	b
Ph. 2 energy share PWR(MOX)	%	34.867	38.537
Ph. 3 energy share PWR(MOX)	%	26.316	29.086
Ph. 2 energy share ADS	%	5.704	6.304
Ph. 3 energy share ADS	%	7.415	8.196
Power PWR(UOX ₁)	GW _e	1.520	1.680
Power PWR(UOX ₂ +MOX)	GW _e	1.454	1.607
Power ADS	GW _e	0.146	0.162
Thermal eff. PWR(UOX ₁)		0.323	0.357
Thermal eff. PWR(UOX ₂ +MOX)		0.338	0.374
Thermal eff. ADS		0.366	0.404
Load factor PWR(UOX ₁)		0.808	0.893
Load factor PWR(UOX ₂ +MOX)		0.808	0.893
Load factor ADS		0.808	0.893
Core mass PWR(UOX ₁)	t _{HM}	122.455	135.345
Core mass PWR(UOX ₂ +MOX)	t _{HM}	104.120	115.080
Core mass ADS	t _{HM}	5.121	5.660
Burn-up UOX ₁	GW d t _{HM} ⁻¹	57.000	63.000
Burn-up UOX ₂	GW d t _{HM} ⁻¹	57.000	63.000
Burn-up MOX	GW d t _{HM} ⁻¹	46.740	51.660
Burn-up ADS	GW d t _{HM} ⁻¹	74.100	81.900
UOX enrichment	%	4.703	5.198
²³⁵ U enrichment tails	%	0.238	0.263
Pu in MOX fuel (max.)	%	11.400	12.600
Pu in ADS fuel	%	42.750	47.250
Reprocessing capacity UOX	t _{HM}	807.500	892.500
Reprocessing beginning UOX	y	30	40
Transition Ph. 2 beginning	y	76	86
Transition Ph. 2 ending	y	105	115
Transition Ph. 3 beginning	y	186	196
Transition Ph. 3 ending	y	215	225

Figure 4.10: Pu and MA inventories in the cycle for the case where only PWR(UOX) reactors are considered. As explained in Section 4.4.4, no irradiation was performed with TR_EVOL for this case. The dashed lines correspond to ANICCA while the continuous lines come from TR_EVOL. The hatched areas represent the transition between the different phases. The same drawing style will be used in the following graphs.

Full scenario

The results for the full scenario are shown in Fig. 4.11. For each color, the dashed line represents the ANICCA value while the continuous one is the TR_EVOL calculation. The shadowed area, as it will be explained in the following section, refers to the uncertainty propagated from the input parameters with TR_EVOL.

Figure 4.11a shows the total TRU inventories in the cycle apart from the final disposal. As the initial reactors are replaced by the second-generation ones, the TRU are consumed (minimization phase) until the arrival of the final phase where the ratios are readapted for maintaining a sustainable or equilibrium state. The amount of TRU reduction will depend on the number of burner reactors and thus, the available mass for fuel fabrication will be the limiting factor, as explained in the following. Note that for this particular case, no MA burning is produced: only a reduction in the production rate was achievable.

The available mass for fuel fabrication is shown in Fig. 4.11b, where the highest demand occurs while the deployment of new reactors takes place in the first transition. This is because of two reasons. The first one is that the entire new cores have to be fabricated. The second reason is that there is not an equilibrium between the SNF mass generated and the needs for reloading since the demand of new fuel corresponds to a larger number of reactors (because the power increases). The figure also shows that

the MA inventories reach their minimum just after the burning phase transition and, therefore, the number of ADS units that can be constructed given the limitation on the available fuel is limited. The inventories start rising from year 35 when the reprocessing plants begin their operation, and continuously increase until the year ~ 80 , when the separated stock is demanded both in the MOX and ADS fuel fabrication plants, as previously mentioned. After the thirty year transition period, the inventories accumulate steadily. Finally, in the year 170, matching the exhaustion of the material produced by the UOX reactors (see Fig. 4.11c), a change in the trend is observed. During the transition to the stabilization phase, multiple effects happen. On one side, more ADS's are being installed, thereby increasing the TRU consumption. On the other side, as some PWR(MOX-IMR) are decommissioned, an accumulation of TRU is observed.

In the case of the interim spent fuel storages plotted in Fig. 4.11c, (*i.e.* after cooling at the reactor sites), the inventories increase during the first years until the commissioning of the UOX reprocessing plant. As the PWR(UOX) are replaced with other technologies in the first transition, on the one hand the total reprocessing capacity increases (since other fuels are considered) while on the other hand, an extra cooled mass is available due to the final cores of the reactors that are being decommissioned). The combination of both effects explains the shape of the curve during the years ~ 90 – 120 . Later, at year 170 all the UOX is exhausted as it was abovementioned, which results in a change in the trend of Fig. 4.11b at the same time. The peak produced at year ~ 195 comes from the PWR(MOX-IMR) cores that are discharged in the second phase in order to accommodate the new energy shares. Finally, the TRU inventories after this date should be zero, given that the reprocessing capacity is larger than the mass to reprocess each year. However, this process has to last one year in the ANICCA code, causing the accumulation of a certain amount of material as TRU inventory during that year.

In Fig. 4.11d the TRU inventories in the reactor cores are shown. The lines are constant during each phase because the energies of the fleets are fixed and therefore no changes in the production/consumption are produced. During the first phase, these inventories come from nuclear reactions in the UOX fuel. When the PWR(MOX) and ADS technologies are implemented in the park, the values increase due to the presence of Pu and MA in the fresh fuel.

Finally, Fig. 4.11e shows the Pu and MA total masses that are sent to the final disposal. Since all the spent fuel is multi-recycled, the TRU flows that must be managed as waste come from the reprocessing losses (fixed at 0.1% of the incoming mass). However, since this process is repeated along the simulation, no stabilization can be reached for this facility.

(a) Total

(b) Available

(c) Interim storage

(d) Reactor cores

(e) Final disposal

Figure 4.11: TRU inventories in different stages for ANICCA (dashed line) and TR_EVOL (continuous line) and its associated uncertainty.

Differences due to the fuel cycle simulators

At EOS, the relative difference between both calculations for the TRU mass in the cycle is about 7.3%, as it can be inferred from Fig. 4.11a. As the scenario specifications were readapted in order to dismiss the discrepancies originating from different interpretations and taking into account the results from the first section of Section 4.4.4, they must be caused by the irradiation models. In order to identify the contribution of each technology, several scenarios were simulated iteratively considering first the open cycle and then each time one additional technology, and measuring for each one of them the amount of TRU at EOS by subtracting the result of the previous scenario. In this way, there are three different scenarios, namely PWR(UOX), PWR(UOX+MOX) and the complete scenario PWR(UOX+MOX)+ADS. Note that this approach is an approximation in the sense that it assumes that for instance, the differences accumulated due to the PWR(MOX) will be the same whatever ADS are considered in the scenario, although the isotopic composition of the initial Pu vector may change. The results are collected in Table 4.20. For the PWR(UOX), the ANICCA code produces slightly more TRU, while for the MOX and ADS there is an underestimation when compared to TR_EVOL results. Since the MOX-IMR grade of enrichment will depend on the Pu quality (Eq. (4.4)), it is reasonable that small changes in the isotopic composition will lead to different fabrications, and thus to different TRU burning, propagated to the ADS fleet as well. However, since the

4.4. Effect of the simulator

Table 4.20: Difference in TRU inventories in all the cycle (considering final disposal) between both codes and per reactor type, defined as $\Delta\text{TRU} = \text{TRU}_{\text{ANICCA}} - \text{TRU}_{\text{TR_EVOL}}$.

	ΔTRU (t)	$\Delta\text{TRU}/E$ (t/GW _{y_e})
PWR(UOX)	4.44	4.00×10^{-4}
PWR(MOX)	-49.29	-1.64×10^{-2}
ADS	-41.01	-5.91×10^{-2}

burn-up of these reactors is fixed, no difference should be induced in the total amount of heavy metals (U + TRU). In the third column of the table, the differences are weighted by the total energy produced by each fuel, indicating that the largest contributor to the discrepancy, per energy produced, is the irradiation in the ADS. As a check of coherence, it has been confirmed that the sum of the values in the second column in this table equals to the combined differences shown in Fig. 4.11a and Fig. 4.11e. In any case, as Fig. 4.11d shows, the effect of the irradiation is purely accumulative, year by year small discrepancies are observed in the reactor inventories.

The effect of the irradiation can not be hence disregarded in practise, although state-of-art reactor depletion codes are used. These codes do not produce the same result (see for example [96, 99]), and even more, EVOLCODE and ALEPH2, which have been validated against experimental data, show an average agreement of about 5% for the major actinides [2, 148]. Consequently this effect will be intrinsic of the fuel cycle simulators.

Uncertainty propagation from the input parameters

As it was mentioned in Section 4.4.3, a global uncertainty propagation based on MC sampling was performed over the input parameter space. In total, 100 000 different scenarios were run with TR_EVOL in order to have enough statistics for the estimation of the different indicators (as an example, for the TRU inventories in the cycle, the calculated standard deviation relative error is close to 0.2%). Since in the reference scenario the minimization of the TRU inventories is pursued, perturbations around this solution could lead to broken scenarios, *i.e.* scenarios that cannot be completed since the demand of TRU for fuel fabrication exceeds the available amount in storage. This issue has been overcome adding artificially the required mass (without changes in the isotopic composition), but this extra inventory has been removed in the presented graphs. This approach is equivalent to allowing negative masses in the separated inventories as is the case in Fig. 4.11b for the Pu inventories during the year ~ 190 , and it can be understood as borrowing from an external supplier.

The results of the uncertainty analysis were shown in Fig. 4.11 on the facing page, where the shadowed area represents the uncertainty in the output parameter associated

with the TR_EVOL simulation when the uncertainties in the input parameters are considered, which is calculated as 1σ deviation from the average value*. This is shown more clearly in Fig. 4.12, where the standard score ($z = (x - \mu_x)/\sigma_x$ with x the observable and μ_x and σ_x his mean value and standard deviation, respectively) is represented for the total inventories in cycle. As a criterion, we considered that the effects of the fuel cycle simulators are relevant when $|z| > |1|$, which means that the discrepancies due to the simulation tools are above the uncertainty propagated from the inputs. Note that for these observables, while both Pu and MA values are constrained in 1σ intervals along the simulations, the total TRU inventories come out of this range during the stabilization phase, becoming more significant along the years which is expected since the stabilization is lost. In this way, when performing long-term studies, the results must be taken carefully into account when comparing different codes.

On another note, one can observe in particular the large uncertainty that appears on the spent fuel in storage (Fig. 4.11c), whereas it is not reflected in the total inventories in the cycle (Fig. 4.11a). This is caused by the way the different observables are constructed and that may create a compensation effect: the total inventories are calculated as the addition of material in multiple stages in the cycle. For example, if the effect of the uncertainties leads to an increase/decrease of the reprocessing capacity, there will be more/less mass available for fabrication, although the inventories in storage will follow the opposite trend. In this way, when both inventories are considered as a single observable, the uncertainties will cancel each other.

The previous criterion established that the difference between codes is relevant when it falls out of the 1σ interval. However, the opposite does not necessary imply that the difference is small or acceptable: the uncertainty was propagated from a large input parameter space, and hence, the obtained value could be caused either by the large contribution of a small group of variables, or by the overall effect of all of them. In the first case, if the difference between codes is below the contribution of such reduced group, the final effect is that it does not play any role in the simulation result. On the contrary, for the second case, although contained in 1σ interval, the discrepancy between simulation tools will dominate the other uncertainties. This is illustrated in Fig. 4.13, where the standard score of the total Pu in cycle is compared against the successive k -largest contributors to the variance H_k (definition in Eq. (3.7)). The figure shows that after the first transition, the difference due to the codes (red line) exceeds the contribution to the uncertainty of the most relevant variables, indicating thus that the use of the fuel cycle simulator is the most important source of uncertainty. This is in fact in agreement with the aforementioned results discussed in Section 4.4.4: the discrepancies between fuel cycle simulators are caused by the irradiations and, in particular, when

*It must be noted that in general, the probability density function could not be assumed to be normally distributed, so the $68 - 95 - 99.7$ rule might not apply for these cases.

Figure 4.12: Number of standard deviations that the ANICCA results differ from the average value of the observable distribution.

the materials are reused (in the PWR(MOX) and ADS reactors). Thus, it can be said that as different isotopic compositions are iteratively used for new fuel fabrication, the differences will accumulate and the results will differ even more. Finally, at the year 300, the red line (difference due to the codes) reaches approximately 0.8, meaning that it is as large as the added contribution of the six other most contributing variables. On the other hand, during the first phase, there are less variables that could contribute to the total uncertainty (for example, all the uncertainty related with MOX and ADS reactors does not come into play until year ~ 80), so it is to be expected that a single variable (or a very small group) causes most of it. When the other technologies are considered, the relative contribution of each parameter will reduce and H_1 will diminish as the black lines in Fig. 4.13 show.

Finally, Table 4.21 collects the normalized sensitivity coefficients for the seven most relevant variables in the case of both the MA and Pu total inventories in the cycle observables. The seven variables have been chosen in accordance with the results of the PATEROS scenario discussed in Section 4.2.1. In this manner, the results of Table 4.7 and Table 4.21 can be put side-by-side for analyzing the effect of the uncertainties in both scenarios. Note that only the general trend of both tables can be compared and not their particular values. For the PATEROS scenario the relative contribution of each coefficient was recalculated for those seven parameters (and thus their sum equals one), while the results of this section are not. Furthermore, as the scenario are different the variables will differ too. However, despite these differences some similarities can be identified. In

Figure 4.13: Standard score (in absolute value, red line) and the $H_1, H_2, \dots, H_{30}$ coefficients ordered from bottom to top for the total Pu inventories in the cycle. A gradient color scheme has been used to help visualization.

the case of the MA inventories in the cycle, the Pu fraction loaded in the ADS shows to be one of the most dominant variables in both scenarios, followed by the thermal efficiency of the reactors. In the case of the Pu, now the maximum amount loaded in the MOX(IMR) systems dominates as well as the energy shares of these technologies. In the PATEROS scenario, the most relevant parameter for the Pu was ε_{UOX} , followed by the MOX energy ratio.

These results shows that, very generally, the effect of the uncertainties in the MA inventories in the cycle are more similar between scenarios than for the Pu. This behaviour is reasonable since for the PATEROS scenario only the MA inventories were stabilized (the Pu was assumed to be a resource for the future deployment of FR), while in this case, both Pu and MA reach the equilibrium. This illustrates the limited scope the uncertainty analyses have, being only extrapolated to similar scenarios having comparable goals.

4.4.5 Conclusions

In order to evaluate the key aspects of the nuclear fuel cycle, multiple institutions have developed their own tools during the last years. However, the wide range of physics they have to cover leads to a different choice of approximations and solving techniques by their developers, which is ultimately translated into discrepancies in the results as several benchmarking exercises have shown in the recent years. In this work, these

4.4. Effect of the simulator

Table 4.21: Normalized sensitivity indices and their signs for the selected parameters. The variables are ordered according to their contribution to the variance.

Label	Variable	MA cycle			Pu cycle		
		Var.	Sign	η_i	Var.	Sign	η_i
r_{IMR_2}	Ph. 2 energy share PWR(MOX)	Pu_{ADS}	+	0.30	Pu_{IMR}	−	0.32
r_{IMR_3}	Ph. 3 energy share PWR(MOX)	ε_{PWR}	−	0.24	r_{IMR_2}	−	0.16
ε_{UOX}	Thermal eff. PWR(UOX ₁)	ε_{ADS}	+	0.14	r_{IMR_3}	−	0.12
ε_{PWR}	Thermal eff. PWR(UOX ₂ +MOX)	Pu_{IMR}	+	0.06	Pu_{ADS}	−	0.09
ε_{ADS}	Thermal eff. ADS	ε_{UOX}	−	0.05	ε_{UOX}	−	0.08
Pu_{IMR}	Pu in MOX fuel (max.)	r_{IMR_2}	+	0.02	ε_{PWR}	+	0.01
Pu_{ADS}	Pu in ADS fuel	r_{IMR_3}	+	0.02	ε_{ADS}		0.00

discrepancies have been quantified with the help of the sensitivity analysis for two different fuel cycle simulators, namely ANICCA and TR_EVOL for an advanced nuclear fuel cycle. Additionally, the uncertainty in the input parameters has been propagated using a MC approach for the observable's variance estimation, while the contribution of each individual variable has been calculated through the sensitivity coefficients, in order to assess the relevance of the discrepancies between the fuel codes simulators.

After a first approach where it was found that the largest source of discrepancy was due to different scenario interpretations, a verification has been then done between both codes using a complex transition scenario. This process has required the iterative update of the scenario specifications until no differences could be found due to different hypotheses. After that, results have shown in general that both codes behave in a similar way, producing the same trends and therefore leading to the same conclusions. This demonstrates that they are reliable tools and thus any of them can be used in the analysis of advanced nuclear fuel cycles. However, when looking closely, certain differences between them appeared. It was shown that the simulator codes behave like any other source of uncertainty: they depend on the observable and become larger as the scenario extends over time due to their cumulative nature. Also, when compared with other sources of uncertainty in the fuel cycle, the simulator codes are the major source of uncertainty, even dominating. Consequently, the fuel cycle simulator introduces a non-negligible effect in the simulations that cannot be avoided while dealing with studies of uncertainty quantification. The results demonstrate that the dominant effect may be mainly produced by the irradiation for certain observables (other scenarios might lead to different conclusions). Indeed, even if the irradiation part of the simulators are replaced with high accuracy depletion codes, as they are not exact, discrepancies will still exist at the end of the irradiation when the same isotopic composition is used as fresh fuel. Therefore, it is expected that this effect gains extra relevance in advanced nuclear fuel cycle scenarios where the reuse of the materials is pursued. Additionally, although only

two codes have been considered in this study, for the reasons exposed in the previous lines, it is reasonable to expect similar results in other tools. This should be investigated in future works.

Chapter 5

Optimization of electronuclear scenarios

Until now, the simulations have been performed in a forward approach in which the scenarios are parametrized in a series of inputs and when the simulation is completed, several outputs were obtained. However, the inverse problem which implies an optimization problem is usually more interesting in scenario studies. This is essential in advanced electronuclear transition scenarios in which multiple parameters have to be fine-tuned in order to achieve a set of predefined objectives chosen by experts or policy makers. Consequently, nuclear fuel cycle simulators have been upgraded in the recent years in order to solve these kind of problems. However, in the presence of uncertainties the solutions obtained in this way may not be stable since small perturbations could break the delicate balance between different parts of the scenario.

The purpose of this chapter is to illustrate how the uncertainties can affect the robustness of the optimized solutions. To this end, a global multiobjective transition scenario aimed to reduce the inventory masses while keeping fuel cycle cost low has been chosen for its study with TR_EVOL code. The methodology used can be easily adopted by any fuel cycle simulator, although the high computational demand may make it unaffordable for slow tools or institutions with limited computational capabilities.

5.1 Introduction: why uncertainty matters

As it has been already mentioned and proven in the previous chapters, nuclear fuel cycle simulators have become crucial for predicting and evaluating the performance and viability of a particular electronuclear scenario in the mid and long term. This approach implies that the desired scenario is firstly parametrized in terms of a set of particular input parameters, obtaining different metrics measuring the quality of the solution when the simulation is completed. Nonetheless, in scenario analyses for planning or decision

Table 5.1: Objective and metrics for nuclear fuel cycle optimization proposed by [72].

Objective	Criteria
Electricity production	Fuel cycle cost
Energetic independence	Importation cost of natural uranium
Commercial balance	Importation costs of fuel and services
National technological level	Skilled labour in nuclear industry
Impact on environment	Volumes of wastes in final disposal
Proliferation risk	Compound risk utility function for each stage of the fuel cycle

making the inverse problem is presented. Now the desired outcomes of the scenario are firstly defined, and given a relaxed set of initial conditions, the best case fulfilling the requirements has to be found. Taking into account the large design space that can be explored, it becomes clear that this is not a trivial work. For that reason, in the recent years nuclear fuel cycle simulators have been upgraded for performing optimization analyses in an automatized way without user interaction (see for example [41, 159]).

Despite the technique used for the optimization, the first step of these analyses is to define the problem in a realistic and useful manner. This implies that the objectives of the scenarios and their particular metrics have to be precisely determined. These metrics can include, among others, the mass of TRU inventories, the radiotoxicity of the waste, the natural uranium requirements or the fuel cycle cost. Note that objective refers to the generic goals of the scenario while a metric is the particular mathematical function that can be evaluated in order to measure the goodness of the solution.

The metrics enumerated in the previous lines represents the most obvious choices in the case of advanced nuclear fuel cycles since they are directly linked with the P&T goals, but other not so-trivial objectives can be used too. For example, in Table 5.1 several objectives and their associated metrics that have been proposed by Kunsch and Teghen for their use in nuclear fuel cycle optimization problems are collected [72]. Additional metrics based on the economic, environmental impact, resource utilization and proliferation risk objectives has been more recently proposed in [105]. They include the construction of SNF recycling plants, the amount of U_{dep} tails and the U_{nat} or separative work unit requirements, among others. Nevertheless, it should be noted that these lists are not exhaustive and may not collect some crucial aspects that may be decisive for certain experts or policy makers. The impact of an electronuclear scenario covers a wide range of aspects and consequently the specific goals of a particular implementation should emerge from the collaboration between the multiple agents involved and their specific objectives.

Besides, uncertainty analyses in fuel cycle simulations are recently gaining attention as it was discussed in Chapter 4. As general remark, these studies show that the

uncertainties can impact on the robustness of the scenarios since perturbations can break the equilibrium balance between different facilities or processes. This aspect is crucial in optimization studies since during the minimization/maximization process certain materials stocks can be pushed to the limit beyond which the scenario is no longer viable due to a lack of material, producing a broken scenario (see Section 2.2.3). Therefore, if the scenario has been optimized without uncertainties (replacing for example the random variables by their expectation or reference values), there is no guarantee that when input parameters are selected from random sampling, the scenario will remain stable/viable.

Some studies have been conducted by the nuclear fuel cycle community under this topic. For example, Kunsch [72] uses a multiobjective stochastic linear programming for evaluating the best policy for the LWR SNF. In another work, Lee [73] performs sensitivity analysis in a case aimed to find the best growth pattern in a scenario consisting of LWR and SFR, employing linear programming too. In Hays [53], a transition scenario from LWR to fast breeder reactors is optimized with the simulated annealing algorithm, showing also the effect of varying the uranium conversion ratio or the costs. Nevertheless, linear programming techniques assume that the objective function and constraints can be expressed in linear form. This cannot be assumed in general, as Passerini [105] shows by comparing the results of a multiobjective transition nuclear scenario solved with linear programming and a genetic algorithm. Hence, global optimization techniques should be chosen, although according to the results discussed in Section 4.2, the election of linear tools can be justified if the range of the input parameters is not too wide. In addition, given that changes in the input parameters have the ability to transform the results of the optimization as the mentioned works have shown, it is clear that the uncertainties must be part of the optimization problem.

5.2 Optimization under uncertainty

Based on the discussed ideas, this section is devoted to study the effect of the uncertainties in optimization problems. To that end, the techniques discussed in Section 3.2 that were implemented in TR_EVOL has been applied to a multiobjective advanced European transition scenario in which Generation IV technologies are added to a LWR park with the objective of reaching a sustainable state and pursues both TRU and nuclear fuel cycle cost minimization.

5.2.1 Scenario description

The scenario chosen for this study is based on the one investigated under the CP-ESFR project [44]. Framed in a European collaborative strategy, the scenario defined in this project considers an initial fleet of Generation II LWR that is replaced by a fleet consisting

Figure 5.1: Main facilities in the scenario. The circles corresponds to the different reactor technologies, the diamonds to the stocks of materials and the boxes represents the facilities.

of only SFR systems with a middle phase where EPR (European Pressurized Reactor) and SFR coexist in order to produce enough Pu for feeding the SFRs. In this work, we have redefined this scenario with the objective of pursuing both minimization of the TRU inventories and minimization of costs. For this reason, the SFR design has been adapted to act as a burner instead of as a breeder reactor. Furthermore, ADS have been introduced for burning the MA inventories, in particular Am, Np and Cm. In this new scenario, which starts in year 2010 and ends in 2300, three different phases (which are depicted on Fig. 5.1), can be differentiated:

1. Initial phase (2010–2040)

The fleet consists entirely of PWR using either UOX or MOX fuel (denoted respectively as PWR(UOX) and PWR(MOX)). There also exists a legacy inventory of SNF which accounts for the current European legacy (see Table 5.2*).

*As the CP-ESFR scenario was inspired in the PATEROS project, the initial legacy inventories

Table 5.2: Initial SNF stock per year of inclusion in the scenario and fuel type.

Year	UOX fuel (t)		MOX fuel (t)	
	2010	2022	2010	2022
^{234}U	5.40	0.25	0.20	0.15
^{235}U	207.50	78.50	2.00	2.70
^{236}U	148.50	40.20	0.40	0.50
^{238}U	27 384.00	8247.30	1308.40	920.00
^{237}Np	19.10	5.70	0.30	0.30
^{238}Pu	8.00	2.00	2.30	1.00
^{239}Pu	170.90	49.30	29.90	19.20
^{240}Pu	75.20	21.00	20.40	14.60
^{241}Pu	39.30	6.70	9.80	3.00
^{242}Pu	23.30	5.50	7.50	4.50
^{241}Am	12.30	6.70	4.10	5.20
^{243}Am	5.90	1.40	2.00	0.90
^{242}Cm	0.20	0.00	0.00	0.00
^{244}Cm	1.80	0.40	0.90	0.20
^{245}Cm	0.10	0.04	0.10	0.06
FP	1327.60	363.00	57.10	40.00
Total	29 429.10	8827.99	1445.40	1012.31

2. Burning phase (2040–2100)

The initial fleet gradually transitions during 20 years (2040–2060) to a new one consisting of EPR, SFR and ADS systems, with the objective of burning as much TRUs as possible. After this replacement, the composition of the fleet remains stable between 2060 and 2100.

3. Stabilization phase (2100–2300)

Starting in year 2100 the burner fleet composition is readapted in order to reach a sustainable level in which the TRU inventories do not increase nor decrease. This transition also has a duration of 20 years (from 2100 to 2120) after which no further modifications are made to the fleet.

During the whole scenario, the electricity production is fixed at 800 TWh_e per year. In the first phase, 43.83 TWh_e y⁻¹ are produced by the PWR(MOX) systems while the rest comes from the PWR(UOX). The power share of PWR, EPR, SFR and ADS reactors in the forthcoming phases are the free parameters which are going to be optimized in order to fulfill the scenario objectives (minimization of TRU inventories and costs). They will be precisely defined at the end of this section. In the following, the fuel cycle parameters are specified.

values were equal in both cases. In this way, Table 5.2 is the same as Table 4.1 but with the isotopes disaggregated now by fuel type instead of by producing country.

Table 5.3: Reactor features.

Reactor	Power (GW _e)	Thermal eff. (%)	Load factor (%)	Core mass (t _{HM})	Burn-Up (GW d t _{HM} ⁻¹)
PWR(UOX)	1.008	34.0	80.84	79.462	50.0
PWR(MOX)	1.008	34.0	80.84	79.067	45.0
EPR	1.652	36.0	90.00	123.513	55.0
SFR	1.440	40.0	90.00	78.120	100.0
ADS	0.154	40.0	87.00	5.325	78.3

Reactor technologies

Main reactor parameters are shown on Table 5.3. In the case of the PWR(UOX), PWR(MOX) and EPR reactors, these specifications were taken from the CP-ESFR project. On the other hand, the SFR is based on the ESFR-SMART design [115] while for the ADS, the EFIT concept [4] was selected as in the previous studies of Chapter 4. The operating life of the units has been assumed to be 60 years in all cases.

Fuel specification

The fuel specifications can be found on Table 5.4. The UOX and EPR fuels are made from U_{nat}. The Pu recovered from the reprocessed UOX SNF is mixed with depleted uranium and is monorecycled in MOX fuels by the PWR systems until their complete decommission at the ending of the first transition between the initial and the burning phase. During the burning and stabilization phases, all the Pu and MA are multirecycled and reused as part of the SFR (using Pu and U_{dep}) and ADS (Pu, Np, Am and Cm) systems fuels. If there is not enough multirecycled Pu for these systems, the monorecycled stock will be used, as depicted with the dashed line on Fig. 5.1. The Pu content of the SFR fuel, calculated according to the Baker&Ross equivalent method [7], has been increased compared to the original design in order to have a Pu burner reactor. Note that this modification will surely impact on the safety coefficients of the reactor. However, as this issue is beyond the scope of this work in the following we will assume that the reactor design remains unchanged with no safety concerns. Finally, the fabrication time is two years, and the cooling period is set to 5 years.

Reprocessing

Homogeneous reprocessing has been considered in this study. UOX SNF reprocessing starts with the scenario (in year 2010) while MOX SNF reprocessing starts in year 2035. Both the initial SNF legacy and the SNF produced by the PWR during the scenario are reprocessed in these plants. For the SFR and ADS fuels, it has been assumed that

Table 5.4: Fuel specifications.

Parameter	Value
^{235}U enrichment for UOX	4.20%
^{235}U enrichment for EPR	4.50%
^{235}U enrichment tails	0.25%
Pu content for MOX	8.65%
Pu equivalent content for SFR	17.79%
Pu/MA content for ADS	45/55%

Table 5.5: Main parameters of the reprocessing plants.

Spent Fuel	Max. amount (t_{HM})	First year
UOX	2000	2010
MOX	850	2035
SFR	∞	—
ADS	∞	—

all the material is reprocessed after the 5-years cooling period. Main parameters of the reprocessing plants can be found in Table 5.5. The reprocessing losses for all fuels are set to 0.1%

Introducing the uncertainty

Given the unclear position the nuclear energy will play in the European electricity mix, two major assumptions of this scenario have been considered affected by uncertainties. The first one is that the energy production of the nuclear fleet will remain constant at $800 \text{ TWh}_e \text{ y}^{-1}$ during the burning and stabilization phases. The other is that the reprocessing capacity is set at $2000 + 850 t_{\text{HM}}$ in addition to the ability of reprocessing all the SFR and ADS SNFs. These figures may seem too optimistic nowadays. However, they may be achievable if these new technologies are developed by those countries sharing an interest in the objectives of this work. The lack of knowledge in the nuclear energy future will be parametrized with an (arbitrary) variation of $\pm 10\%$ of the values described in the previous lines in order to show the impact uncertainties have in the optimization problem.

Defining the objective function

As stated above, the objective of this study is to obtain the optimum sustainable scenario. However, this statement must be precisely defined since the optimum scenario could be determined depending on multiple criteria. For this study, the TRU inventory masses and the fuel cycle cost at the end of scenario in year 2300 will be considered. The TRU

Table 5.6: Cost of each technology from the bibliography and fleet values considering 60 years of operating life. No EPR information was available in [31], so for this particular work, LWR costs are assumed also for EPR since according to [120] both are quite similar.

Tech.	Reference [120]			Reference [31]			Average
	Capital (€/kW _e)	O&M (€/kW _e /y)	Fleet/ Fleet _{EPR}	Capital (\$/kW _e)	O&M (\$/kW _e /y)	Fleet/ Fleet _{EPR}	Fleet/ Fleet _{EPR}
EPR	3002	75	1	4300	72	1	1
SFR	3902	86	1.21	4700	78	1.09	1.15
ADS	14 760	223	3.75	13 900	319	3.83	3.80

inventory masses will be measured as the total Pu and MA masses present at all the stages of the cycle depicted in Fig. 5.1 (fabrication and reprocessing plants, reactor cores and storage facilities). Reprocessing losses are not included in the inventories.

Regarding the nuclear fuel cycle cost, it will be measured as the relative cost of the proposed scenario with respect to a LWR fleet in an open fuel cycle with the same installed power. In order to estimate this relative cost, only investment capital and O&M have been considered, since in similar scenario studies they have been shown to account for 80% of the nuclear electricity costs [120]. Thus, as a first approximation fuel and decommission, dismantling & disposal costs will not be considered in this study. Table 5.6 outlines the capital and O&M costs, obtained from [120, 31]. In this way, the cost of each fleet has been estimated from the sum of the capital costs plus O&M costs during 60 years of reactor operational life. Relative costs calculated as the average of the two provided references in this way with respect to a fleet consisting only of LWRs are given in the last column of the table. Finally, the figures provided for the scenario cost are obtained by integrating this relative cost from the beginning of the burning phase to the end of the scenario.

Besides, there are two implicit constraints in this scenario. The first one, related with the lack of materials during the simulation (scenario breaking), demands that the TRU mass needed for new fuel fabrication cannot exceed the available mass which is represented in Fig. 5.1 as the Pu_{mono/multi} and MA stocks. The second one is a consequence of the sustainability goal: the inventories have to be stabilized and thus they can neither increase nor decrease along the years. The first case can be mathematically described with an equality constraint which reflects that no additional mass should be added to the scenario in order for it to be implementable. For the stabilization, the condition will be described with an inequality constraint demanding that the change in the TRU mass inventories must be less than certain value per year or period of time. It has been assumed, to limit the computational cost of the constraint, that this change must be less than a ton for the last ten years of the simulation. Hence, given that the simulation ends in year 2300,

this constraint will be defined as $\Delta m_{\text{TRU}}(\mathbf{x}) := \sum_i |m_i(\mathbf{x}, t = 2300) - m_i(\mathbf{x}, t = 2290)|$ with $i \in \{\text{Pu}, \text{MA}\}$. This expression has been broken down into its components to avoid solutions in which Pu and MA change in opposite directions in such a way their sum fulfills the condition. In this manner, the optimization problem can be mathematically expressed as

$$\min_{\mathbf{x} \in \mathbb{R}^d} (m_{\text{TRU}}(\mathbf{x}), \text{Cost}(\mathbf{x})) \quad \text{subject to} \quad \begin{cases} m_{\text{add}}(\mathbf{x}) = 0, \\ \Delta m_{\text{TRU}}(\mathbf{x}) < 1 \text{ ton}, \end{cases} \quad (5.1)$$

in which $\mathbf{x}$ are the energy shares of each technology during the burning and stabilization phases.

5.2.2 Methodology

In order to solve the optimization problem, the approach described in Section 3.2.2 has been followed: the problem has been solved with the DEMO algorithm introducing the ε level comparison for the constrained part of the problem and with the use of the SAA approximation. In this way, the penalty function of the problem of Eq. (5.1) constructed as Eq. (3.27) takes the following form

$$\phi(\mathbf{x}) := \max(0, \Delta m_{\text{TRU}}(\mathbf{x}) - 1 \text{ ton})^2 + m_{\text{add}}(\mathbf{x})^2, \quad (5.2)$$

In general it is not possible to know in advance if there exist any feasible solution. However, with the methodology presented in the previous lines, if it does not exist, it can be easily identified since the problem will eventually converge towards the minimum (but not zero) value of $\phi(\mathbf{x})$ given that the ε level comparison always selects the solutions with the minimum penalty.

Furthermore, as the SAA has to be computed for every candidate solutions, to reduce the computational effort instead of taking multiple samples only parametric variations will be evaluated. As in this case only two variables are considered to have uncertainty, the expected value of the random functions will be approximated by

$$\mathbb{E}[f(\mathbf{x}, \xi_1, \xi_2)] \approx \frac{1}{5} \left(f(\mathbf{x}, \xi_1^0, \xi_2^0) + \sum_{i,j \in \{m, M\}} f(\mathbf{x}, \xi_1^i, \xi_2^j) \right), \quad (5.3)$$

being $f(\mathbf{x})$ the objective and penalty functions to be optimized, $\mathbf{x}$ the set of input parameters that have to be found and $\xi_i^{0/m/M}$ the stochastic variables i at the parametric variations which are reference, minimum and maximum values respectively.

5.2.3 Results

In this section the results of the optimization problem are presented. The discussion has been divided in three different parts. In a first approximation, the scenario has been optimized without considering uncertainties. These solutions will be identified as the reference solutions, and once obtained, their robustness will be analyzed in the second part. Finally, in the last part the scenario has been optimized again but introducing this time the uncertainties in the energy production and the reprocessing capacity.

It is important to note that due to the metaheuristic nature of the optimization algorithm, there is no guarantee that all the possible solutions are found. In order to overcome this issue, the problem has been solved several times and the multiple solutions have been combined. In particular, more than a million simulations have been run for this study requiring less than five days of calculations[†]. Nonetheless it should be mentioned that this number strongly depends on the desired precision of the final solution.

Without uncertainty

The results of the optimization problem (*i.e.* fuel cycle cost and TRU masses at the end of the scenario), are plotted in Fig. 5.2. Grey points corresponds to each feasible solution obtained with the DEMO optimization algorithm while the coloured curve (the meaning of the different colors will be explained in the next part) represents the Pareto front formed by the dominant solutions. An L-shaped dependence between the scenario cost and the TRU inventory masses can be observed. This has an easy explanation: in order to reduce the TRU inventory more transmutation technologies (SFRs and ADSs) have to be included in the scenario increasing thus the cost. It can also be observed that below ~ 2200 t the cost of further reducing the TRU mass rises sharply; from the slopes of the Pareto front it can be concluded that in this region burning an extra ton is nearly 20 times more expensive. The reason for this behaviour will be explained below. Finally note that the cost axis has been normalized to the cost of an open cycle in which the initial fleet is replaced by only EPR systems as explained at the end of Section 5.2.1. For this EPR-only scenario, ~ 8100 tons of TRU will be accumulated by year 300 in all stages of the scenario including the SNF legacy of Table 5.2. Hence, with an increase of 15% to 20% in the electricity cost, the TRU stocks can be reduced by a factor that ranges between 60 and 75% respectively when compared with an open fuel cycle strategy.

Pareto optimal front solutions in the input parametric space can be found in Fig. 5.3.

[†]It now becomes clear how important was the development of a faster version of TR_EVOL code as described in Section 2.2.2: the computation of a tenth of cases for estimating Sobol indices in Section 4.2 required almost two weeks of calculations with a previous version of the code. Although these figures cannot be directly compared since they were performed on a different HPC (see Section 2.4) and also the scenarios differ, they can serve for illustrating the relevance of having a fast tool that allows for making more complex studies.

Figure 5.2: Pareto front of the optimization problem. The two colors which are separated by the vertical line, correspond to the different penalty violations of the reference case when uncertainties are considered (more details can be found in the following part). In grey, the set of solutions obtained with DEMO.

This scatter matrix plot represents all the pairwise relationships between the two objectives (TRU and cost minimization) and the input parameters that are being optimized (energy share of each fleet by technology, with the subscript indicating the phase, *e.g.* ADS₂ means the fraction of ADS during the burning phase and SFR₃ means the SFR fraction during the stabilization phase). The first column plots the values against the TRU inventories, while last row does it against the cost; the other elements corresponds to the correlations between the input parameters. With this representation the Pareto front, shown in Fig. 5.2, is placed in the bottom-left corner (Subfig. (5,1)). In this way, when one of the represented variables is fixed, the values on the others can be determined by finding the points where the vertical/horizontal projection from the axes cuts the multiple correlation plots.

In all subfigures, two well differentiated branches can be observed, indicating that the solutions can be classified in two different groups for which the correlations decompose into more simple dependencies. This is illustrated in the figure with the different colors, each one corresponding to a group of solutions defined as a function of the TRU inventory masses: Orange < 2205 t < Blue. This can be interpreted as those solutions minimizing the TRU inventories (orange) or the cost (blue). Note that with this clustering, the correlations for each group are almost linear and each branch can be clearly identified (with the exception of Subfig. (4,4) in which an overlying region in the zero energy region is observed). For example, in order to maximize the reduction of TRU inventories, during the burning phase the energy share of the SFR has to be between ~ 34 and 42%

(Subfigure (1,1)), while for the ADS this number ranges between 0 and 4% (Subfig. (3,1)), existing a negative correlation between both variables (Subfig. (3,2)). On the other hand, the cheapest scenarios are obtained when no ADS are installed in the burning phase (Subfig. (5,4)) and the number of SFR is kept as low as possible (Subfig. (5,2)). Additionally, now the reason for the sharp cost increase observed below ~ 2200 t of TRU in the Pareto front which was described in the first paragraph of this section becomes clear: it is produced by the introduction of ADS during the burning phase as the orange points in Subfig. (5,4) show.

Finally, it can be noticed that for all solutions, the ADS energy share in the stabilization phase increases when compared to the burning one. This implies that the MA consumption in the stabilization phase (in which by definition inventories do not increase nor decrease) is higher than in the burning one, during which the inventories must therefore accumulate. This can be explained by a shortage in the stock of the materials used for the fabrication of the ADS fuels: as there is not enough TRU mass during the deployment of the ADS fleet (when the TRU demand is higher), the number of units that can be installed in this phase is limited. Consequently, the MA reduction of the scenario is constrained. This effect will become clearer with the discussion of the results in the forthcoming section.

Robustness of the solutions

Once the solutions have been obtained, their robustness is studied by introducing the uncertainties in the total energy production and the reprocessing capacity. To this end, for each solution obtained in the previous section, the parametric average described in Eq. (5.3) is calculated and the constraint violation is analyzed as a measurement of their robustness. In this work, it was obtained that none of the solutions of the Pareto front was stable. All of them violate the stabilization constraint, while a small subset (depicted in red in Fig. 5.2) also required an additional mass in order to avoid scenario breaking, hence violating both constraints. The solutions that only violate the stabilization constraint are represented in blue. It should be clear that the vertical line in Fig. 5.2 only separates solutions located in the Pareto front. The reference non-dominant feasible solutions (*i.e.* grey points) that will violate the additional mass constraint in the presence of uncertainties could be located either to the left or to the right of this vertical line. Anyway, the red subset corresponds to the solutions minimizing the TRU inventories, since they push the stocks to the limits in order to achieve the higher TRU reduction it is understandable and expectable that they violate this constraint. This evidences the complexity of dealing with uncertainties: the process may lead to a suboptimal solution and, worse than that, there is no guarantee that this solution will be stable. Nonetheless, it should be pointed out that there exist solutions more stable

Figure 5.3: Pairwise plot of the two objectives and the input optimization parameters. The different colors group the solutions by the values of the objective functions.

Figure 5.4: Stabilization violation for the reference solutions in the presence of uncertainties.

than others in the sense that they only violate one of the two constraints. Therefore, if the inequality constraint were relaxed no penalty will occur for the blue solutions of the figure.

Whereas the additional mass constraint can be easily identified with an underlying physical effect (the minimization of TRU inventories), this is not the case of the stabilization condition. This is represented with more detail in Fig. 5.4, in which the stabilization constraint violation of all the solutions is represented with different colors. The stabilization violation can be produced in both the Pu and MA inventories (orange), only in the Pu or MA ones (blue and red, respectively) or that the constraint is not violated (green). In particular, if the additional mass constraint is fulfilled too, the latter will correspond to the desirable solutions. The figure indicates the existence of some kind of correlation since different regions show up. However, the results should be carefully interpreted since some of the points may overlap in the space. Unfortunately, it has not been possible to further extend the analyses of the solutions for searching the origin of this effect due to a limitation in the computational resources. This graph has required almost 300000 simulations, each one of them leading to an output file of around 2 MB. Hence, in order to manage the massive amount of data that will be produced, the results are analyzed on-the-fly and only the values of the objective functions and the constraints are stored. In this manner, it is not possible to search in the raw data for the source of this correlation.

Figure 5.5 shows an example of two unstable reference scenarios of the Pareto front. In Fig. 5.5a, the Pu stock mass used for fuel fabrication (see Fig. 5.1) is represented for one of the solutions minimizing the cost and that will violate the stabilization constraint

(a) Pu

(b) Burning energy share

Figure 5.5: Plutonium stock and burning energy share for two of the scenarios in the Pareto front of Fig. 5.2. The shaded areas represents the transition between the different phases.

when uncertainties are considered (blue line, corresponding to one of the solutions in the blue region of Fig. 5.2), and another solution that minimizes the TRU inventories (red) and that will violate both the stabilization and the need of additional mass. Figure 5.5b shows the energy share of the burning technologies (ADS and SFR) for the same cases.

Concerning the red scenario, it can be observed that the Pu stocks begins to accumulate when the UOX reprocessing plant starts its operation in year 2010, and then the slope increases when the MOX plant starts in 2035. All the initial SNF UOX and MOX inventories are completely reprocessed by years ~ 2040 and 2085 respectively, which explains the change in the trend observed in the curve: as less material is recovered, for the same TRU consumption the Pu stock decreases. In addition, during the two transitions between phases, the Pu stock is reduced due to the large consumption the deployment of new reactors (the new cores need to be fabricated and since the number of units is increasing, the demand of new fuel corresponds to a larger number of reactors than the ones from which the SNF can be recycled). As the increase in the fraction of burning technologies (SFR and ADS) is larger in the transition from the initial phase to the burning phase (2040–2060) than in the transition from the burning to the stabilization phases (2100–2120) as Fig. 5.5b indicates, this reduction is more important during the first transition. Note that, as the Pu stock is completely exhausted at around year 2062, small perturbations may produce a lack of material breaking the scenario. Aside from this effect occurring at transitions, for this case, the Pu during the rest of the burning phase cannot be consumed (on the contrary, it is accumulated) due to a limitation in the burning technologies (ADS/SFR) that can be installed in the park to avoid a shortage of material. This can be observed again in the bottom graph noticing that the ADS and SFR energy share is higher during the last phase.

For the blue case neither ADS nor SFR reactors are deployed during the burning phase so the Pu inventories increase steadily during this phase. Hence, no scenario breaking can occur for this case although the stabilization of the inventories could be compromised in the presence of uncertainties. Obviously, as there are no burner reactors in the burning phase, the Pu inventories at the end of the scenario are much larger than for the previous case.

Including the uncertainties

In this section the optimization problem is solved taking into account the uncertainties in the energy production and the reprocessing capacity, minimizing the expected values of the objectives functions approximated with Eq. (5.3) and averaging the penalty function too. The solutions are shown in Figs. 5.6 and 5.7. Figure 5.6, compares the new Pareto front obtained with uncertainties (in red) with the Pareto front in Fig. 5.2. For this particular scenario, the blue solutions are almost coincident in the objective space with

Figure 5.6: Comparison of the Pareto front with and without uncertainties.

Figure 5.7: Scatter plots between cost and input parameters plus TRU inventories for the uncertainty case (in color). In grey, the results of the reference case discussed in the first part of Section 5.2.3.

a region of the reference front, (although the case without uncertainties is always below), being the case with uncertainties a small region of the reference calculation. The area between both fronts were feasible solutions in the reference case for which the constraints cannot be fulfilled in the presence of uncertainties. As the blue part of the Pareto front is very close to the reference one, the elbow of the L-shaped new front is located approximately at the frontier that was defined in the previous section which divided the solutions based on the penalty violation (the vertical line is the same in both Figs. 5.2 and 5.6).

The solutions in the input parameter space are shown in Fig. 5.7 with the colored points in blue and orange, and the grey dots being results of the reference case (last row in Fig. 5.3). For the shake of clarity, only the scatter plot between the cost and the other variables is represented; note that as in the previous case Fig. 5.6 corresponds

to Subfig. (1). Focusing on the blue and orange results, again two major clusters can be observed: Orange < 2440 t < Blue. Following the interpretation introduced in the previous section this can be identified again with TRU minimization (orange) and cost minimization (blue). For this particular case, the uncertainty solutions exhibit the same shape that was obtained in the previous section but extending over a smaller region of the input parameters and objective spaces, so similar conclusions can be derived.

In general, the effect of the uncertainties is to shrink the solutions space. From the comparison between the Pareto fronts, it can be observed that for both the TRU and cost minimization, there are solutions that are now lost when compared to the reference case. As it was explained in the previous section, those solutions minimizing the TRU inventories violate the additional mass constraint in the presence of perturbations. Consequently, as the TRU reduction is limited when compared to the reference case, the maximum energy share of the ADS+SFR technologies during the burning phase must be lower when compared to that case, as the obtained results show. In the case of the lost solutions minimizing the costs, this effect is produced by the stabilization constraint. However, no further reason was found to explain this behaviour.

Finally, despite the fact that the results in both the reference and the uncertainty cases exhibit the same shape, some differences can be identified. Although in Subfigs. (2–4) the blue dots are very close to the dots of the reference calculation, in the case of the ADS share during the stabilization phase (Subfig. (5)) the solution lies in a region that is not accessible from the reference case. This agrees with the results of the previous section in which none of the reference solutions were found to be robust against perturbations. However, an important remark is the existence of an overlapping region between all input parameters but the installed power fraction of ADS during the stabilization phase. This indicates that the scenario can be corrected: if the reference input parameters were chosen in this zone, it would be possible to readapt the scenario in the presence of uncertainties towards an optimum sustainable state by changing the number of ADS during the stabilization phase. In this way, from a decision making point of view, there exist solutions more interesting than others given the ability of readaptation.

5.2.4 Conclusions

The complexity of nuclear fuel cycle scenarios has driven in the recent years the development of automatic optimization tools that are able to obtain the best scenario or set of scenarios when precise objectives are pursued, a key task in decision making. Nonetheless, these analyses cannot be decoupled from the uncertainty ones since perturbations can break scenario equilibriums between different facilities as several studies have shown. In this work, a methodology for optimizing electronuclear scenarios in the presence of uncertainties has been presented. To this end, the TR_EVOL fuel cycle code has

been upgraded with the DEMO evolutionary multiobjective algorithm which was further extended for handling constraints and uncertainties. This methodology has been applied to an advanced and sustainable nuclear scenario consisting of EPR, ADS and SFR systems and LWR in the initial phase. The optimization problem aims to find the fleet shares of each technology that minimize both the TRU inventories and the cost after 300 years. Additionally, the energy production and the reprocessing capacity of the plants were assumed to be variables affected by uncertainty.

In a first approach, the two-objective optimization problem has been solved without considering uncertainties. The Pareto front obtained indicates that the TRU inventories can be reduced by a factor that ranges between 60 and 75% implying a cost increase of 15–20% respectively when compared to an open fuel cycle strategy. However, a posterior analysis shows that these solutions were unstable, and thus the imposed scenario constraints will not be longer fulfilled in the presence of uncertainties. In this way, the uncertainties not only lead to a non-optimum solution but also compromise the robustness of the scenarios.

Secondly, the problem has been solved considering this time the effect of the uncertainties. Results have shown that their effect is to shrink the Pareto front when compared to the previous case as a consequence of constraint violation. Additionally, the power shares of the different technologies in the optimum solutions in the case with uncertainties are different than in the case without, although in some cases an overlapping region exists. Consequently, if these input parameters were firstly chosen in these regions, it would be possible to correct the scenario.

The obtained results evidence the fact that uncertainties play a major role in scenario optimization and must therefore be taken into account beforehand to ensure the reliability of the obtained solutions. Besides, the methodology presented can be implemented by any fuel cycle simulator able to perform a large number of simulations in a feasible amount of time. Although this approach is automatic, future works should focus on the massive data analysis required for identifying the physical process that constraints the solutions.

Chapter 6

Conclusions & Future work

The sustainable future of nuclear energy necessarily involves the study of electronuclear scenarios, which are ultimately analyzed with nuclear fuel cycle simulators. This thesis has been focused on improving the confidence of the results provided by these tools when advanced scenarios with Generation IV reactors are studied. For this purpose, different uncertainty propagation and quantification as well as optimization state-of-the-art techniques and methodologies have been implemented in TR_EVOL code.

The work was divided in two major parts. In the first one, the uncertainties surrounding fuel cycle simulations were studied. Based on their nature, these uncertainties have been categorized in three major groups. The first one corresponds to the uncertainties in the input parameters used for describing the scenario. In the second category nuclear data is included, and the latter one is dedicated to the modelling effects introduced by the fuel cycle simulator. As the first group of uncertainties is the most straightforward to calculate, it has been used as reference estimation against which the other groups will be compared in order to quantify their relevance. The second part of the thesis was dedicated to the study of how these uncertainties can impact the optimization of electronuclear scenarios. In the following, the main conclusions and findings of this thesis are discussed, and after that, future lines of research are proposed.

TR_EVOL simulator

The necessary improvement of the capabilities existing in the TR_EVOL code has finally represented an important part of this work. The studies performed in this thesis required a large number of simulations, especially in the case of the optimization problem analyzed in the previous chapter. Thanks to the multiple updates performed along nearly four years of continuous development, the execution of TR_EVOL has been speeded up by more than 200 times. Hence, it would not have been possible to perform these works in a feasible amount of time with the old version of the code. Chapter 2 outlines the most

relevant modifications introduced in the code. If prior to this thesis TR_EVOL was among of the world reference fuel cycle simulators, these improvements have positioned it as one of the leading tools for performing uncertainty and optimization studies. Although these modifications are very specific to the particular implementation of TR_EVOL and the computational environment used at CIEMAT and thus, they cannot be easily extrapolated, it is hoped that some of them can serve as inspiration to other institutions for improving their codes too. Additionally, since most of the simulations are executed using massive parallelization, multiple tools were developed for the automatic on-the-fly data processing required for reducing the huge amount of results that are produced when multiple instances are launched simultaneously. Finally, this works presented several methodologies for dealing with uncertainties and optimization in the nuclear fuel cycle, as well as their possible implementation by any other code. This was mainly discussed in Chapter 3.

Scenario uncertainties

In Section 4.2, Sobol indices of the input parameters of one of the PATEROS scenarios have been estimated. In order to overcome the excessive computational demand of these techniques, in a first approach a hybrid methodology has been employed for reducing the input parameter space dimension. Sensitivity coefficients for all input parameters were estimated, and those with the largest contribution to the variance were retained for their Sobol indices estimation. These indices were estimated via direct integration and with the Polynomial Chaos expansion, sampling in both cases with quasi-random sequences which have proven to outperform Monte Carlo. Both methodologies provide the same results, reducing the latter in more than a thousand times the computational effort. Regarding the results obtained, no interactions nor higher order effects were found for this particular scenario, although the uncertainties can produce a lack of materials that prevents the simulation from being completed. Additionally, the results were quite different depending on the observable. For the MA inventories, the PWR park energy and the Pu fraction loaded into the ADS produce most of the uncertainty. In the case of the Pu stocks, the thermal efficiency of the UOX reactors was the dominant parameter.

Nuclear data uncertainties

Section 4.3 was dedicated to study how the uncertainties in the nuclear data affect the fuel cycle simulations. The uncertainties of the major isotopes involved in thermal systems were propagated with a Monte Carlo methodology in which multiple perturbed libraries were generated with SANDY using the information available in covariance matrices. This methodology was in a first step verified with GODIVA integral experiment, and then, it was extended to the irradiation of a simplified PWR pin cell which can be identified

with an open fuel cycle strategy. In this way, the uncertainties in the actinides at the end of the irradiation were estimated. Note that this simple case does not require the use of a complete fuel cycle simulation; as it does not involve movement of materials between different facilities, the calculation was directly performed with EVOLCODE. Following this, the uncertainties due to the input parameters of this open fuel cycle were calculated too in a very conservative approach with parametric variations. In this manner, the effect of both sources of uncertainties (nuclear data and fuel cycle parameters) can be compared, and hence it is possible to determine the relevance of the nuclear data uncertainties in fuel cycle studies. Results have shown that for certain isotopes, nuclear data uncertainties dominate fuel cycle parameters uncertainties, despite these input parameters uncertainties were upper-bounded in a very conservative way. In particular, this was the case of ^{239}Pu and ^{241}Pu , being especially remarkable the ^{239}Pu result for which the nuclear data effect even dominates. These isotopes, apart of constituting more than 2/3 of the produced Pu in thermal reactors, are fissile and will therefore play a fundamental role in the behaviour of the nuclear fuel during the forthcoming irradiations if Pu recycling is implemented. Hence if in this simple case the nuclear data produce a significant effect, in advanced scenarios using fast systems for which the reactions will have larger uncertainties and in which multiple recycling will be performed, their contribution to the uncertainty will be magnified.

Simulator uncertainties

Finally, the last group of uncertainties has been analyzed in Section 4.4. This work was devoted to the quantification of the discrepancies produced when different fuel cycle simulators are used. Since modelling effects are inherent to the fuel cycle simulator and in general there is no analytical solution to which the results can be compared, their impact cannot be directly addressed. Therefore, it is only possible to infer their effects through verification, that is, comparison with other tools. In this manner, this case has required the collaboration with SCK·CEN in order to compare ANICCA and TR_EVOL fuel cycle codes. The same advanced transition scenario was studied with both tools, and additionally, the same reactors libraries were used to reduce discrepancies that might have appeared by different core modelling or collapsing methodology. As in the previous case, in a second step the uncertainties in the input parameters of the fuel cycle were propagated in order to have a reference uncertainty to which discrepancies can be compared in order to determine their relevance. After isolating all the effects, it was found that the simulation of the irradiation was the source of the discrepancies. These discrepancies grow with the recycling of the materials until becoming the most important source of uncertainty when compared with other sources of uncertainties.

Special attention has to be paid to these last two studies. Since the nuclear data

uncertainties enters in the fuel cycle simulation mainly through the irradiation (the other part in which they are used is during the decay), and this is precisely the process that was found to originate the discrepancies when two fuel cycle simulators were compared, it is clear that both uncertainty sources are closely linked. In fact, whatever the depletion code or method is used, its accuracy will be constrained by the nuclear data uncertainties. This implies that when two different fuel cycle simulators will be compared, in the best case, differences compatible with the nuclear data uncertainties will be obtained. These differences, no matter how small, will grow with the simulation gaining special relevance in advanced scenarios in which the materials are continuously recycled since the discrepancies will accumulate in the successive irradiations along the years. This effect has proven to be comparable to uncertainties in the parameters used for the scenario modeling and hence, it cannot be disregarded in fuel cycle uncertainty analyses.

Optimization and uncertainties

Optimization studies are crucial since, given a precise set of scenario outcomes, the set of input parameters that lead to the desired solutions can be determined. However, as it has been pointed out by the previous studies, the uncertainties can introduce large effects in the solutions. Under these ideas, Chapter 5 was dedicated to study how uncertainties affect the optimization results. The optimization was performed with and without uncertainties using an evolutionary algorithm, and both results were compared. The problem considered an advanced sustainable transition scenario aimed to reduce the TRU inventories while keeping low the fuel cycle cost. The energy shares of the advanced technologies (ADS and SFR) were the free parameters to be optimized. Results without considering uncertainties showed that all TRU inventories in the cycle can be reduced by a factor ranging between 2.8 and 3.4 with an increase in the cost of 15% to 20% when compared with an open fuel cycle strategy after 300 years. Additionally, this multiobjective solutions produces two well differentiated branches in the input parameter space, which were identified with those solutions minimizing each one of the objectives separately. However, the solutions achieved in this way were unstable. In the presence of uncertainties, it was not possible for any of them to fulfill the sustainability conditions imposed to the scenario, and furthermore, some of them presented a lack of material in a certain stage of the cycle too. When the problem was resolved again but considering the uncertainties during the optimization process this second time, similar conclusions were found in the objective space, although the Pareto front was highly reduced. Nevertheless, the configurations of energy shares producing these Pareto optimal solutions were different, although some overlapping regions exists when compared to the case without uncertainties. In this manner, if the uncertainties were not taken into account in the optimization problem, in their presence the solution would be suboptimal

without any reliability on the scenario viability.

Relevant scenario studies

For each particular study (with the exception of the nuclear data uncertainties for which a simple open fuel cycle was chosen), a different advanced transition scenario has been analyzed. These scenarios have been chosen/inspired on realistic scenarios defined under the PATEROS and CP-ESFR projects as well as on scenarios that are currently being investigated under the NEA EG-AFCS activities. Although they make use of different assumptions and technologies, it is possible however to derive some general conclusions from all of them. First of all, with the use of advanced reactors, it is possible to fix the energy share of the reactors in such a way the TRU inventories are stabilized achieving thus a sustainable state that can be perpetuated in time. Additionally, the reduction of TRU inventories can be achieved in those scenarios playing only with these energy shares, without introducing any additional change in the design of the reactors. Hence, it is possible to perform a two-step transition from the current LWR fleet to advanced fleets in which the first one is intended to reduce the inventories as much as possible while the latter stabilizes for achieving the sustainability. In this manner it is possible to reduce the TRU inventories by a considerable factor without increasing too much the scenario cost when compared with an open scheme. Nevertheless, this TRU reduction will be constrained by the availability of materials for fuel fabrication and core deployment both during the transition as well as the speed this transition occurs.

Future Work

In the following, possible continuations of this thesis are proposed.

Code improvement

The profiling of the latest version of TR_EVOL shows that the bottleneck of the simulations occurs during the internal ORIGEN calls. It would be interesting to consider the replacement of ORIGEN by another depletion tool in order to check if the performance of TR_EVOL can be improved. Additionally, instead of using one-group cross sections for solving the Bateman equations, it may be useful to replace this approximation with other methods such as artificial neural networks which have been shown to provide reliable results too [74]. Note that under these ideas, the FIT collaboration described in Section 2.3.2 is perfect since as different approaches are tested, it will serve for identifying alternative techniques used by other institutions that may perform better than the current strategies implemented in TR_EVOL.

Uncertainty and optimization studies

The execution speed gain of TR_EVOL will allow for the inclusion of more variables and observables in these studies. In particular, detailed costs estimations can be considered with the economic module of TR_EVOL. Additionally, nuclear data uncertainties have proven to be relevant even in open fuel cycles. This evaluation should be further extended to advanced closed cycles, coupling the results with the uncertainties in the input parameters simultaneously. Also, the quality of the result obtained will be improved if better probability distributions for modeling input parameters uncertainties are used. Besides, the results of the uncertainty problems seem to be very observable and scenario dependent. A further exploration in which multiple scenarios are evaluated and unsupervised learning techniques are used over the results will be insightful to check if general rather than scenario-dependent conclusions can be obtained. These techniques could also be useful for finding patterns in the huge raw data that is obtained during optimization studies. Note that all of these analyses will require too a new outlook on how the massive amount of data that will be produced should be efficiently stored.

New capabilities

The impossibility of completing the simulation when there is not enough material has been present along all the studies performed in this thesis. One alternative to overcome this situation will be the implementation of predictive techniques that, in face of these issues, can change the input specification recursively in such a way the simulation can be completed. This problem will be closely related with the optimization studies since each time this effect occurs, the best input modification has to be found. Another possible use of these techniques will be the analysis of the scenario self-adaptation ability in the presence of random and unpredicted events in the middle of the simulations, such as for example, the unscheduled shutdown of a certain nuclear power plant. Besides, the introduction of new reactors such as the MSR which does not use a batch-wise fuel management but a continuous one, will require a new modeling approach in TR_EVOL.

Scenario analyses

The study of advanced nuclear fuel cycles will be continued in the future. In particular, the first Work Package of the Horizon 2020 PUMMA project of which CIEMAT is task leader, will address the study of plutonium management in connection with the fuel cycle through scenario evaluations. Note that the impact of any newer technology should be investigated too and hence, as new designs and fuels appear, their performance in the scenario should be addressed. Examples of such new technology can be the Small Modular Reactors, which are nowadays gaining attention, or Accident Tolerant Fuels,

consisting of new fuels or claddings made of different materials that can lead to the creation of different waste streams (activation products), also yet to be implemented in the code. Additionally, with the new capabilities of TR_EVOL, it will be possible to study also the impact of load following in scenarios with a high share of renewable energies, which seems to be the future trend given the goals established for emission reduction.

Appendix A

Quasi-Monte Carlo methods

QMC (Quasi-Monte Carlo) methods refers to numerical techniques that rely on quasi-random sequences to obtain results. These sequences are deterministic sequences with the property of having low discrepancy, as described in the following. For this reason they are also known as low-discrepancy sequences. Roughly speaking, the discrepancy is a measurement of how uniformly the numbers of the sequence are distributed. In this manner, they provide better space filling than random or pseudo-random sampling and consequently, they can be used for more efficient numerical integration [90]. Several quasi-random sequences can be found in the literature, such as Faure, Halton, Niederreiter or Sobol sequences; Fig. A.1 shows a comparison between pseudo-random sampling with the $2d$ -Sobol sequence.

Amongst their applications, QMC methods can be used for numerical integration in the same way than MC (Monte Carlo) methods

$$\int_{[0,1]^d} d\mathbf{x} f(\mathbf{x}) \approx \frac{1}{n} \sum_{i=1}^n f(\mathbf{x}^{(i)}), \quad (\text{A.1})$$

being the difference that now the points $\mathbf{x}^{(i)}$ are chosen deterministically instead of pseudo-randomly. In general, there are two different types of QMC methods: open and closed. The open uses the first n points of an infinite sequence, while the closed uses a finite point set which depends on n . The clear advantage of the open type is that increasing n only requires the evaluation of the new points that are added; for the latter the entire new set has to be evaluated.

The integration error of both MC and QMC methods can be defined as

$$\varepsilon_f := \left| \int_{[0,1]^d} d\mathbf{x} f(\mathbf{x}) - \frac{1}{n} \sum_{i=1}^n f(\mathbf{x}^{(i)}) \right|. \quad (\text{A.2})$$

In the case of MC, if $f(\mathbf{x})$ is an squared-integrable function the root mean squared

Figure A.1: Distribution of the sampling points over the unit $2d$ -hypercube by pseudo-random and quasi-random methods for 2048 points.

error will be

$$\text{RMSE} = \mathbb{E}[\varepsilon_f^2]^{1/2} = \frac{\sigma_f}{\sqrt{n}} \sim \mathcal{O}(n^{-1/2}), \quad (\text{A.3})$$

which shows that the integral has a convergence rate inversely proportional to the square root of the number of points and that does not depend on the dimension of the problem. Note that due to the random nature of the solution this is a probabilistic error.

For QMC methods, as the sampling points are deterministic, the integral value will be deterministic too and hence it is only possible to provide an upper bound of the integration error. In this manner, according to the Koksma-Hlawka inequality, the integration error of these methods will be bounded by [19]

$$\varepsilon_f \leq \frac{c \text{Var}_{\text{HK}}[f] \log^d(n)}{n} \sim \mathcal{O}(\log^d(n) n^{-1}), \quad (\text{A.4})$$

where $\text{Var}_{\text{HK}}[f]$ is the variation of the function in the Hardy-Krause sense (a measure connected with differentiability properties; more details can be found in the previous reference) and c is a constant independent of n but that could depend on the dimension d . Although the upper limit of Eq. (A.4) has now a strong dependence with d , for certain classes of functions (smooth ones or with an effective dimension lower than real dimension) quasi-random sequences outperform random numbers even in high dimensions [29, 18].

Appendix B

Scientific production

Peer-reviewed publications

1. Skarbeli, A. V. and Álvarez-Velarde, F. “Sparse Polynomial Chaos expansion for advanced nuclear fuel cycle sensitivity analysis”. In: *Annals of Nuclear Energy* 142 (July 2020), p. 107430. DOI: [10.1016/j.anucene.2020.107430](https://doi.org/10.1016/j.anucene.2020.107430).
2. Skarbeli, A. V. et al. “Quantification of the differences introduced by nuclear fuel cycle simulators in advanced scenario studies”. In: *Annals of Nuclear Energy* 137 (Mar. 2020), p. 107160. DOI: [10.1016/j.anucene.2019.107160](https://doi.org/10.1016/j.anucene.2019.107160).
3. Skarbeli, A. V. and Álvarez-Velarde, F. “Uncertainty quantification on advanced fuel cycle scenario simulations applying local and global methods”. In: *Annals of Nuclear Energy* 124 (Feb. 2019), pp. 349–356. DOI: [10.1016/j.anucene.2018.10.018](https://doi.org/10.1016/j.anucene.2018.10.018).
4. Merino-Rodríguez, I. et al. “Economics and Resources Analysis of the Potential Use of Reprocessing Options by a Medium Sized Nuclear Reactor Fleet”. In: *Energies* 10.12 (May 2017), p. 690. DOI: [10.3390/en10050690](https://doi.org/10.3390/en10050690).

Other publications

1. Álvarez-Velarde, F. and Skarbeli, A. V. *Dose rate calculations involving irradiated PWR fuel assemblies: Verification and validation benchmark*. Informe interno CIEMAT DFN/IN-01/II-19. 2019.
2. Álvarez-Velarde, F., Romojaro, P., and Skarbeli, A. V. *Application of a coupled MCNP-SUBCHANFLOW code for MYRRHA transients*. Deliverable D3.26 MYRTE EU project, Grant Agreement 662186. 2019.

3. Álvarez-Velarde, F., Romojaro, P., and Skarbeli, A. V. *Application of a coupled MCNP-SUBCHANFLOW code for MYRRHA transients*. Informe interno CIEMAT DFN/IN-03/II-19. 2019.

Ongoing publications

1. Skarbeli, A. V. et al. “Impact of the uncertainties in nuclear data on nuclear fuel cycle parameters”. To be submitted.
2. Skarbeli, A. V., Álvarez-Velarde, F., and Bécares, V. “Optimization under uncertainty for robust fuel cycle analyses”. Submitted.
3. Thiollière, N. et al. “Impact of Fresh Fuel Loading Management in Fuel Cycle Simulators: A Functionality Isolation Test”. Under elaboration.
4. OECD/NEA. *Benchmark on TRU management*. Under elaboration.

Proceedings & Congresses

1. Skarbeli, A. V. et al. “Exploration and quantification of the main differences on nuclear fuel cycle simulators applied to ADS scenarios”. In: *Fourth International Workshop on Technology and Components of Accelerator-Driven Systems* (Oct. 14–17, 2019). Antwerp, Belgium, 2019.
2. Skarbeli, A. V. et al. “Quantification of the modelling effect on nuclear fuel cycle scenarios”. In: *45^a Reunión Anual SNE* (Sept. 23–28, 2019). Vigo, Spain, 2019.
3. Álvarez-Velarde, F., Romojaro, P., and Skarbeli, A. V. “Asymmetrical transient simulation for MYRRHA reactor with the COUNTER code”. In: *45^a Reunión Anual SNE* (Sept. 23–28, 2019). Vigo, Spain, 2019.
4. Romojaro, P. et al. “Nuclear data assimilation for MYRRHA”. in: *45^a Reunión Anual SNE* (Sept. 23–28, 2019). Vigo, Spain, 2019.
5. Thiollière, N. et al. “The FIT Project: Improving confidence in fuel cycle model”. In: *4th Technical Workshop on Fuel Cycle Simulation* (June 26–28, 2019). Urbana-Champaign, USA, 2019.
6. Mendoza, E. et al. “Study of photon strength functions of ^{241}Pu and ^{245}Cm from neutron capture measurements”. In: *ND2019: International conference on nuclear data for science and technology* (May 19–24, 2019). Beijing, China, 2019.

-
7. Álvarez-Velarde, F., Skarbeli, A. V., and Romojaro, P. “TR_EVOL: a fuel cycle scenario code for energy policy planning”. In: *Technical Meeting on Nuclear-Renewable Hybrid Energy Systems for decarbonized Energy Production and Cogeneration* (Oct. 22–25, 2018). Viena, Austria, 2018.
 8. Skarbeli, A. V. *Optimización de ciclos de combustible avanzados para la toma de decisiones estratégicas*. 2018.
 9. Skarbeli, A. V. and Álvarez-Velarde, F. “Optimization of advanced nuclear fuel cycles for decision making strategies”. In: *15th International Exchange Meeting on P&T and advanced fuel cycles* (Sept. 30–Oct. 3, 2018). Manchester, UK, 2018.
 10. Skarbeli, A. V. and Álvarez-Velarde, F. “Uncertainty Propagation in Advanced Nuclear Fuel Cycle Scenarios”. In: *15th International Exchange Meeting on P&T and advanced fuel cycles* (Sept. 30–Oct. 3, 2018). Manchester, UK, 2018.
 11. Skarbeli, A. V. and Álvarez-Velarde, F. “Hybrid Uncertainty Propagation on Advanced Nuclear Fuel Cycles”. In: *44^a Reunión Anual de la SNE* (Sept. 26–28, 2018). Ávila, Spain, 2018.
 12. Skarbeli, A. V. and Álvarez-Velarde, F. “Strategies for the Uncertainty Quantification of Fuel Cycle Scenarios”. In: *3rd Technical Workshop on Fuel Cycle Simulation* (July 9–11, 2018). Paris, France, 2018.
 13. Skarbeli, A. V. *Metodologías para la propagación de las incertidumbres en ciclos de combustible avanzados*. 2018.
 14. Álvarez-Velarde, F. et al. “Analysis of Reprocessing Options for Medium Sized Nuclear Fleets”. In: *2nd Technical Workshop on Fuel Cycle Simulation* (June 19–21, 2017). Columbia, USA, 2017.
 15. Skarbeli, A. V., Álvarez-Velarde, F., and López, D. “Preliminary analysis of the uncertainty propagation using a Monte Carlo method in PATEROS fuel cycle scenarios”. In: *14th Information Exchange Meeting on Actinide and Fission Product Partitioning and Transmutation* (Oct. 17–20, 2016). San Diego, USA, 2016.
 16. Álvarez-Velarde, F., López, D., and Skarbeli, A. V. “Residual Dose Rate Calculations Involving Irradiated LWR Fuel Assemblies”. In: *42^a Reunión Anual de la SNE* (Sept. 28–30, 2016). Santander, Spain, 2016.

Acronyms

A

ADS Accelerator Driven Subcritical System [2](#), [9](#), [13](#), [18](#), [21](#), [42](#), [44–48](#), [51–54](#), [56](#), [58](#), [71](#), [72](#), [74–77](#), [79](#), [82](#), [83](#), [85–87](#), [92–96](#), [98–100](#), [104](#), [106](#), [107](#), [110](#), [112](#)
ANL Argonne National Laboratory [10](#)

B

BME *Budapesti Műszaki és Gazdaságtudományi Egyetem* [10](#)
BNL Brookhaven National Laboratory [10](#)

C

CEA *Commissariat à l'Énergie Atomique et aux Énergies Alternatives* [10](#)
CIEMAT *Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas* [7](#), [10](#), [11](#), [15](#), [20–22](#), [33](#), [54](#), [110](#), [114](#)
CNRS *Centre National de la Recherche Scientifique* [10](#), [21](#)
CV Cross-Validation [30](#), [31](#), [54](#), [55](#)

D

DE Differential Evolution [34–37](#)
DEMO Differential Evolution for Multiobjective Optimization [37](#), [97–99](#), [107](#)

E

EDF *Électricité de France* [10](#)
EFIT European Facility for Industrial Transmutation [45](#), [71](#), [94](#)
EG-AFCS Expert Group on Advanced Fuel Cycle Scenarios [20](#), [70](#), [113](#)
ENDF Evaluated Nuclear Data File [61](#), [62](#)
EOS End of Simulation [76](#), [82](#)
EPR European Pressurized Reactor [92–96](#), [98](#), [107](#)
ESNII European Sustainable Nuclear Industrial Initiative [2](#)

F**FIFO** First In First Out [12](#), [18](#), [19](#), [74](#)**FIT** Functionality Isolation Test [21](#), [113](#)**FP** Fission Product [12](#), [43](#), [93](#)**FR** Fast Reactor [8](#), [9](#), [13](#), [42](#), [50–52](#), [58](#), [86](#)**G****GFR** Gas Fast Reactor [2](#)**H****HM** Heavy Metal [46–48](#), [72](#), [75](#), [77](#), [94](#), [95](#)**HPC** High Performance Cluster [21](#), [22](#), [98](#)**I****IAEA** International Atomic Energy Agency [10](#), [20](#)**IMR** Increased Moderation Ratio [71](#), [74–76](#), [79](#), [82](#), [86](#), [87](#)**IN2P3** *Institut National de Physique Nucléaire et de Physique des Particules* [21](#)**INL** Idaho National Laboratory [10](#)**IPPE** Institute of Physics and Power Engineering [10](#)**IRSN** *Institut National de la Recherche Scientifique* [10](#)**J****JAEA** Japan Atomic Energy Agency [10](#)**JEFF** Joint Evaluated Fission and Fusion [19](#), [61](#), [75](#)**K****KAERI** Korea Atomic Energy Research Institute [10](#)**KTH** *Kungliga Tekniska Högskolan* [10](#)**L****LANL** Los Alamos National Laboratory [10](#)**LASSO** Least Absolute Shrinkage and Selection Operator [29–31](#), [55](#), [58](#)**LFR** Lead Fast Reactor [2](#)**LHS** Latin Hypercube Sampling [24](#)**LIFO** Last In First Out [12](#), [18](#)**LWR** Light Water Reactor [8](#), [9](#), [13](#), [21](#), [42](#), [59](#), [64](#), [91](#), [96](#), [107](#), [113](#)

M

MA Minor Actinides [9](#), [12](#), [42](#), [46–48](#), [50–60](#), [71](#), [73–76](#), [78](#), [79](#), [84–87](#), [92](#), [94–97](#), [100](#), [102](#), [110](#)

MC Monte Carlo [24](#), [26](#), [33](#), [49](#), [83](#), [87](#), [117](#)

MIT Massachusetts Institute of Technology [10](#)

MO Multiobjective Optimization [37](#)

MOX Mixed Oxides [8](#), [13](#), [18](#), [21](#), [42–48](#), [51–54](#), [56](#), [57](#), [71](#), [72](#), [74–77](#), [79](#), [82](#), [83](#), [85–87](#), [92–95](#), [104](#)

MSR Molten Salt Reactor [2](#), [114](#)

N

NEA Nuclear Energy Agency [11](#), [12](#), [20](#), [70](#), [113](#)

NNL National Nuclear Laboratory [10](#)

NWTRB Nuclear Waste Technical Review Board [10](#)

O

O&M Operation & Maintenance [14](#), [96](#)

OECD Organisation for Economic Co-operation and Development [20](#)

OLS Ordinary Least Squares [29–31](#), [58](#)

P

P&T Partitioning and Transmutation [2](#), [3](#), [9](#), [90](#)

PATEROS Partitioning and Transmutation European Roadmap for Sustainable Nuclear Energy [42](#), [85](#), [86](#), [110](#), [113](#)

PUMMA Plutonium Management for More Agility [20](#), [114](#)

PWR Pressurized Water Reactor [8](#), [18](#), [21](#), [42](#), [43](#), [45](#), [46](#), [48](#), [51–54](#), [56–62](#), [69](#), [71](#), [72](#), [74](#), [76–79](#), [82](#), [83](#), [85](#), [87](#), [92–94](#), [110](#)

Q

QMC Quasi-Monte Carlo [24](#), [49](#), [54](#), [117](#), [118](#)

S

SAA Sample Average Approximation [33](#), [97](#)

SCK·CEN *Studiecentrum voor Kernenergie · Centre d'Étude de l'Énergie Nucléaire* [10](#), [70](#), [111](#)

SCWR Super Critical Water Reactor [2](#)

SFR Sodium Fast Reactor [2](#), [91–96](#), [98–100](#), [104](#), [106](#), [107](#), [112](#)

SNETP Sustainable Nuclear Energy Technology Platform [2](#)

SNF Spent Nuclear Fuel [42–47](#), [51](#), [70](#), [71](#), [75](#), [78](#), [90–95](#), [98](#), [104](#)

T

TR__EVOL Transition Evolution code [4](#), [7](#), [10–12](#), [14–20](#), [22](#), [23](#), [31](#), [33](#), [39](#), [45](#), [70](#), [75](#), [76](#), [78](#), [82–84](#), [87](#), [89](#), [91](#), [98](#), [106](#), [109–111](#), [113–115](#)

TRU Transuranic [2](#), [8](#), [9](#), [21](#), [47](#), [51](#), [52](#), [58](#), [70](#), [71](#), [78](#), [79](#), [82–84](#), [90–93](#), [95–100](#), [102](#), [104–107](#), [112](#), [113](#)

U

UOX Uranium Oxide [13](#), [18](#), [42–44](#), [46–48](#), [51–56](#), [58](#), [71](#), [72](#), [74–79](#), [82](#), [83](#), [86](#), [87](#), [92–95](#), [104](#), [110](#)

UW University of Wisconsin [10](#)

V

VHTR Very High Temperature Reactor [2](#)

Bibliography

- [1] Álvarez-Velarde, F. and González-Romero, E. M. “TR_EVOL, upgrading of EVOLCODE2 for transition scenario studies”. In: *First Workshop on Technology and Components of the ADS (TCADS-1)*. Karlsruhe, Germany: OECD/NEA, 2010.
- [2] Álvarez-Velarde, F., González-Romero, E. M., and Rodríguez, I. M. “Validation of the burn-up code EVOLCODE 2.0 with PWR experimental data and with a Sensitivity/Uncertainty analysis”. In: *Annals of Nuclear Energy* 73 (Nov. 2014), pp. 175–188. DOI: [10.1016/j.anucene.2014.06.049](https://doi.org/10.1016/j.anucene.2014.06.049).
- [3] Álvarez-Velarde, F., León, P. T., and González-Romero, E. “EVOLCODE2, a combined neutronics and burn-up evolution simulation code”. In: *Actinide and Fission Product Partitioning and Transmutation*. 6282. Nîmes, France: OECD/NEA, 2007, pp. 443–450. ISBN: 978-92-64-99030-2. URL: <https://www.oecd-neo.org/science/pubs/2007/nea6282-iempt9.pdf>.
- [4] Artioli, C., Glinatsis, G., and Petrovich, C. *EFIT Core Reference Cycle Analysis and Reactivity Coefficients*. Tech. rep. Version FPN-P9EH-015 Rev. 0. ENEA, 2008.
- [5] Artioli, C. et al. “Optimization of the Minor Actinides transmutation in ADS: The European Facility for Industrial Transmutation EFIT-Pb Concept”. In: *Eighth International Topical Meeting on Nuclear Applications and Utilization of Accelerators*. 2007. URL: <https://www.tib.eu/en/search/id/TIBKAT%3A562259376/Eighth-International-Topical-Meeting-on-Nuclear/>.
- [6] Bae, J. W., Peterson-Droogh, J. L., and Huff, K. D. “Standardized verification of the Cyclus fuel cycle simulator”. In: *Annals of Nuclear Energy* 128 (June 2019), pp. 288–291. DOI: [10.1016/j.anucene.2019.01.014](https://doi.org/10.1016/j.anucene.2019.01.014).
- [7] Baker, A. and Ross, R. “Comparison of the value of plutonium and uranium isotopes in fast reactors”. In: *USAEC, Breeding, Economics, and Safety in Large Fast Breeder Reactors (Argonne National Laboratory, Illinois, 1963)* (1963), pp. 329–365.

-
- [8] Barbrault, P. and Larderet, P. *Plutonium multi-recycling in increased moderating ratio reactors (IMR)*. Tech. rep. EDF-98-NB-00028. EDF, 1998. URL: https://inis.iaea.org/search/search.aspx?orig_q=RN:30001874.
- [9] Basheer, I. A. and Hajmeer, M. “Artificial neural networks: fundamentals, computing, design, and application”. In: *Journal of Microbiological Methods* 43.1 (Dec. 2000), pp. 3–31. DOI: [10.1016/S0167-7012\(00\)00201-3](https://doi.org/10.1016/S0167-7012(00)00201-3).
- [10] Blatman, G. and Sudret, B. “Adaptive sparse polynomial chaos expansion based on least angle regression”. In: *Journal of Computational Physics* 230.6 (Mar. 2011), pp. 2345–2367. DOI: [10.1016/j.jcp.2010.12.021](https://doi.org/10.1016/j.jcp.2010.12.021).
- [11] Boor, C. de. *A Practical Guide to Splines*. Springer, Nov. 29, 2001. ISBN: 978-0-387-95366-3.
- [12] Broeders, C. H. M. “Entwicklungarbeiten fuer die neutronenphysikalische Auslegung von Fortschrittlichen Druckwasserreaktoren (FDWR) mit kompakten Dreiecksgittern in hexagonalen Brennelementen.” PhD thesis. Institut für Neutronenphysik und Reaktortechnik, 1992. URL: <http://inrwww.webarchiv.kit.edu/pdfs/KFK5072.pdf>.
- [13] Brolly, Á. et al. “Physical model of the nuclear fuel cycle simulation code SITON”. In: *Annals of Nuclear Energy* 99 (Jan. 2017), pp. 471–483. DOI: [10.1016/j.anucene.2016.10.001](https://doi.org/10.1016/j.anucene.2016.10.001).
- [14] Brun, R. and Rademakers, F. “ROOT — An object oriented data analysis framework”. In: *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 389.1-2 (Apr. 1997), pp. 81–86. DOI: [10.1016/S0168-9002\(97\)00048-X](https://doi.org/10.1016/S0168-9002(97)00048-X).
- [15] Busquim e Silva, R., Kazimi, M. S., and Hejzlar, P. *A system dynamics study of the nuclear fuel cycle with recycling: options and outcomes for the US and Brazil*. Tech. rep. MIT-NFC-101-TR. Massachusetts Institute of Technology. Center for Advanced Nuclear Energy, 2008. URL: <http://hdl.handle.net/1721.1/75238>.
- [16] Buss, O., Hoefer, A., and Neuber, J. “NUDUNA - Nuclear Data Uncertainty Analysis in Criticality Safety”. In: *Proc. International Conference on Nuclear Criticality (ICNC)*. Edinburgh, Scotland, Jan. 2011.
- [17] Cacuci, D. G. *Sensitivity & Uncertainty Analysis, Volume 1*. Vol. I. Taylor & Francis Inc, May 28, 2003. 304 pp. ISBN: 978-1-58488-115-5. URL: <https://www.crcpress.com/Sensitivity--Uncertainty-Analysis-Volume-1-Theory/Cacuci/p/book/9781584881155>.

-
- [18] Caflisch, R., Morokoff, W., and Owen, A. “Valuation of mortgage-backed securities using Brownian bridges to reduce effective dimension”. In: *The Journal of Computational Finance* 1.1 (1997), pp. 27–46. DOI: [10.21314/jcf.1997.005](https://doi.org/10.21314/jcf.1997.005).
 - [19] Caflisch, R. E. “Monte Carlo and quasi-Monte Carlo methods”. In: *Acta Numerica* 7 (Jan. 1998), p. 1. DOI: [10.1017/s0962492900002804](https://doi.org/10.1017/s0962492900002804).
 - [20] Carlier, B. *COSAC: a computational code dedicated to fuel cycle back-end simulations in AREVA*. Tech. rep. PTDN-2013-037. France: AREVA, 2013.
 - [21] Carlson, A. D. et al. *Nuclear Data Standards*. Ed. by OCDE/NEA. Vol. NEA/WPEC-7. Nuclear Series. OECD Publishing, 2006. ISBN: 978-92-64-02313-0. URL: <https://www.oecd-neo.org/science/wpec/volume7/volume7.pdf>.
 - [22] Chmielarz, B. “FANCSEE - Development of a fuel cycle code with Graphical User Interface”. MA thesis. KTH - Nuclear Reactor Physics, 2016.
 - [23] Clarke, S. M., Griebisch, J. H., and Simpson, T. W. “Analysis of Support Vector Regression for Approximation of Complex Engineering Analyses”. In: *Journal of Mechanical Design* 127.6 (Aug. 2004), pp. 1077–1087. DOI: [10.1115/1.1897403](https://doi.org/10.1115/1.1897403).
 - [24] Coquelet-Pascal, C. et al. “COSI6: A Tool for Nuclear Transition Scenario Studies and Application to SFR Deployment Scenarios with Minor Actinide Transmutation”. In: *Nuclear Technology* 192.2 (Nov. 2015), pp. 91–110. DOI: [10.13182/nt15-20](https://doi.org/10.13182/nt15-20).
 - [25] Croff, A. G. “ORIGEN2: A Versatile Computer Code for Calculating the Nuclide Compositions and Characteristics of Nuclear Materials”. In: *Nuclear Technology* 62 (3 Sept. 1983). DOI: [10.13182/nt83-1](https://doi.org/10.13182/nt83-1).
 - [26] Das, S., Konar, A., and Chakraborty, U. K. “Two improved differential evolution schemes for faster global search”. In: *Proceedings of the 2005 conference on Genetic and evolutionary computation - GECCO '05*. ACM Press, 2005. DOI: [10.1145/1068009.1068177](https://doi.org/10.1145/1068009.1068177).
 - [27] Das, S. and Suganthan, P. N. “Differential Evolution: A Survey of the State-of-the-Art”. In: *IEEE Transactions on Evolutionary Computation* 15.1 (Feb. 2011), pp. 4–31. DOI: [10.1109/tevc.2010.2059031](https://doi.org/10.1109/tevc.2010.2059031).
 - [28] Deb, K. et al. “A fast and elitist multiobjective genetic algorithm: NSGA-II”. In: *IEEE Transactions on Evolutionary Computation* 6.2 (Apr. 2002), pp. 182–197. DOI: [10.1109/4235.996017](https://doi.org/10.1109/4235.996017).
 - [29] Dick, J., Kuo, F. Y., and Sloan, I. H. “High-dimensional integration: The quasi-Monte Carlo way”. In: *Acta Numerica* 22 (Apr. 2013), pp. 133–288. DOI: [10.1017/s0962492913000044](https://doi.org/10.1017/s0962492913000044).

-
- [30] Díez, C. J. et al. “Comparison of nuclear data uncertainty propagation methodologies for PWR burn-up simulations”. In: *Annals of Nuclear Energy* 77 (Mar. 2015), pp. 101–114. DOI: [10.1016/j.anucene.2014.10.022](https://doi.org/10.1016/j.anucene.2014.10.022).
- [31] Dixon, B. W. et al. *Advanced Fuel Cycle Cost Basis – 2017 Edition*. Tech. rep. Sept. 2017. DOI: [10.2172/1423891](https://doi.org/10.2172/1423891).
- [32] Efron, B. et al. “Least Angle Regression”. In: *The Annals of Statistics* 32.2 (June 23, 2004), pp. 407–499. DOI: [10.1214/009053604000000067](https://doi.org/10.1214/009053604000000067). arXiv: [math/0406456v2](https://arxiv.org/abs/math/0406456v2) [math.ST].
- [33] EG-AFCS. *Working Party On Scientific Issues of the Fuel Cycle*. OECD/NEA. URL: https://www.oecd-neo.org/science/wpfc/index_afcs.html (visited on 09/01/2020).
- [34] European Commission. *A Clean Planet for all: A European strategic long-term vision for a prosperous, modern, competitive and climate neutral economy*. COM(2018) 773. Nov. 2018.
- [35] European Commission. *United in delivering the Energy Union and Climate Action - Setting the foundations for a successful clean energy transition*. COM(2019) 285. June 2019.
- [36] European Parliament. *Resolution on the 2019 UN Climate Change Conference in Madrid, Spain (COP25)*. P9_TA(2019)0079. Nov. 2019.
- [37] Feng, B. et al. “Standardized verification of fuel cycle modeling”. In: *Annals of Nuclear Energy* 94 (Aug. 2016), pp. 300–312. DOI: [10.1016/j.anucene.2016.03.002](https://doi.org/10.1016/j.anucene.2016.03.002).
- [38] Fiorito, L. et al. “Nuclear data uncertainty propagation to integral responses using SANDY”. In: *Annals of Nuclear Energy* 101 (Mar. 2017), pp. 359–366. DOI: [10.1016/j.anucene.2016.11.026](https://doi.org/10.1016/j.anucene.2016.11.026).
- [39] Fishbone, L. G. and Abilock, H. “Markal, a linear-programming model for energy systems analysis: Technical description of the bnl version”. In: *International Journal of Energy Research* 5.4 (1981), pp. 353–375. DOI: [10.1002/er.4440050406](https://doi.org/10.1002/er.4440050406).
- [40] FIT. *Functionalty Isolation Test*. URL: <https://github.com/FuelCycleFIT/FITProject> (visited on 09/01/2020).
- [41] Freynet, D. et al. “Multiobjective optimization for nuclear fleet evolution scenarios using COSI”. In: *EPJ Nuclear Sciences & Technologies* 2 (2016), p. 9. DOI: [10.1051/epjn/e2015-50066-7](https://doi.org/10.1051/epjn/e2015-50066-7).
- [42] Galassi, M. et al. *GNU Scientific Library Reference Manual - Third Edition*. Network Theory Ltd., 2009. ISBN: 978-0-9546120-7-8. URL: <http://www.gnu.org/software/gsl/>.

-
- [43] García-Herranz, N. et al. “Propagation of statistical and nuclear data uncertainties in Monte Carlo burn-up calculations”. In: *Annals of Nuclear Energy* 35.4 (Apr. 2008), pp. 714–730. DOI: [10.1016/j.anucene.2007.07.022](https://doi.org/10.1016/j.anucene.2007.07.022).
 - [44] Garzenne, C. et al. *Scenarios of ESFR deployment in Europe*. CP–ESFR SP2.1.1 D2 Contract Number 232658. 2011.
 - [45] Ghanem, R. G. and Spanos, P. D. *Stochastic Finite Elements: A Spectral Approach*. Springer New York, 1991. ISBN: 978-1-4612-7795-8. DOI: [10.1007/978-1-4612-3094-6](https://doi.org/10.1007/978-1-4612-3094-6).
 - [46] GIF. *A Technology Roadmap for Generation IV Nuclear Energy Systems*. Tech. rep. GIF-002-00. Generation IV International Forum, Dec. 2002.
 - [47] GIF. *GIF R&D Outlook for Generation IV Nuclear Energy Systems*. Tech. rep. Generation IV International Forum, Aug. 2009.
 - [48] Gilli, L. et al. “Performing uncertainty analysis of a nonlinear Point-Kinetics/Lumped Parameters problem using Polynomial Chaos techniques”. In: *Annals of Nuclear Energy* 40.1 (Feb. 2012), pp. 35–44. DOI: [10.1016/j.anucene.2011.09.016](https://doi.org/10.1016/j.anucene.2011.09.016).
 - [49] Gregg, R. and Grove, C. “Analysis of the UK nuclear fission roadmap using the ORION fuel cycle modeling code”. In: *ICHEME Nuclear Fuel Cycle Conference*. Manchester, United Kingdom, 2012.
 - [50] Halász, M. G. “Development of a fast burn-up method and investigation of transmutation in Generation IV fast reactors”. PhD thesis. Budapesti Műszaki és Gazdaságtudományi Egyetem, 2018. URL: <http://hdl.handle.net/10890/5812>.
 - [51] Hastie, T., Friedman, J., and Tibshirani, R. *The Elements of Statistical Learning*. Springer New York, 2001. ISBN: 978-0-387-21606-5. DOI: [10.1007/978-0-387-21606-5](https://doi.org/10.1007/978-0-387-21606-5).
 - [52] Hastie, T., Tibshirani, R., and Wainwright, M. *Statistical Learning with Sparsity: The Lasso and Generalizations*. Taylor & Francis Inc, May 7, 2015. 367 pp. ISBN: 978-1-4987-1216-3. URL: <https://web.stanford.edu/~hastie/StatLearnSparsity/>.
 - [53] Hays, R. and Turinsky, P. “Stochastic Optimization for Nuclear Facility Deployment Scenarios Using VISION”. In: *Nuclear Technology* 186.1 (Apr. 2014), pp. 76–89. DOI: [10.13182/nt13-68](https://doi.org/10.13182/nt13-68).
 - [54] Herman, M. and Trokv, A. *ENDF-6 Formats Manual*. CSEWG Document ENDF-102 BNL-90365-2009. Rev. 1. Upton, NY 11973-5000: Brookhaven National Laboratory, July 2010.

-
- [55] Homma, T. and Saltelli, A. “Importance measures in global sensitivity analysis of nonlinear models”. In: *Reliability Engineering & System Safety* 52.1 (Apr. 1996), pp. 1–17. DOI: [10.1016/0951-8320\(96\)00002-6](https://doi.org/10.1016/0951-8320(96)00002-6).
- [56] Huff, K. D. et al. “Fundamental concepts in the Cyclus nuclear fuel cycle simulation framework”. In: *Advances in Engineering Software* 94 (Apr. 2016), pp. 46–59. DOI: [10.1016/j.advengsoft.2016.01.014](https://doi.org/10.1016/j.advengsoft.2016.01.014). arXiv: [1509.03604](https://arxiv.org/abs/1509.03604) [cs.SE].
- [57] IAEA. *Nuclear Fuel Cycle Simulation System (VISTA)*. TECDOC Series 1535. Vienna: INTERNATIONAL ATOMIC ENERGY AGENCY, 2007. ISBN: 978-92-0-115806-2. URL: <https://www.iaea.org/publications/7639/nuclear-fuel-cycle-simulation-system-vista>.
- [58] IAEA. *Nuclear Fuel Cycle Information System*. TECDOC Series 1613. Vienna: INTERNATIONAL ATOMIC ENERGY AGENCY, 2009. ISBN: 978-92-0-102109-0. URL: <https://www.iaea.org/publications/8079/nuclear-fuel-cycle-information-system>.
- [59] IAEA. *Use of Reprocessed Uranium: Challenges and Options*. Nuclear Energy Series NF-T-4.4. Vienna: INTERNATIONAL ATOMIC ENERGY AGENCY, 2010. ISBN: 978-92-0-106409-7. URL: <https://www.iaea.org/publications/8010/use-of-reprocessed-uranium-challenges-and-options>.
- [60] IAEA. *Country nuclear power profiles*. Vienna: International Atomic Energy Agency, 2018. ISBN: 978-92-0-157718-4.
- [61] IAEA. *Enhancing Benefits of Nuclear Energy Technology Innovation through Cooperation among Countries: Final Report of the INPRO Collaborative Project SYNERGIES*. Ed. by IAEA. Nuclear Energy Series NF-T-4.9. Vienna: International Atomic Energy Agency, 2018. ISBN: 978-92-0-101118-3. URL: https://www-pub.iaea.org/MTCD/Publications/PDF/PUB1807_web.pdf.
- [62] IAEA. *Nuclear Fuel Cycle Simulation System: Improvements and Applications*. TECDOC Series 1864. Vienna: INTERNATIONAL ATOMIC ENERGY AGENCY, 2019. ISBN: 978-92-0-101219-7. URL: <https://www.iaea.org/publications/13502/nuclear-fuel-cycle-simulation-system-improvements-and-applications>.
- [63] IEA. *Nuclear Power in a Clean Energy System*. Paris, May 2019. URL: <https://www.iea.org/reports/nuclear-power-in-a-clean-energy-system>.
- [64] IEA. *World Energy Outlook 2019*. Paris: IEA Publications, 2019. ISBN: 978-92-64-97300-8. URL: <https://www.iea.org/reports/world-energy-outlook-2019>.

-
- [65] Jacobson, J. J. et al. “Verifiable Fuel Cycle Simulation Model (VISION): A Tool for Analyzing Nuclear Fuel Cycle Futures”. In: *Nuclear Technology* 172.2 (Nov. 2010), pp. 157–178. DOI: [10.13182/nt172-157](https://doi.org/10.13182/nt172-157).
 - [66] Kalashnikov, A. G. et al. “Evolution of the CYCLE code for the system analysis of the nuclear fuel cycle”. In: *Nuclear Energy and Technology* 2.2 (June 2016), pp. 114–118. DOI: [10.1016/j.nucet.2016.05.008](https://doi.org/10.1016/j.nucet.2016.05.008).
 - [67] Kim, S. K., Ko, W. I., and Lee, Y. H. “Development and validation of a nuclear fuel cycle analysis tool: a FUTURE code”. In: *Nuclear Engineering and Technology* 45.5 (2013), pp. 665–674. ISSN: 1738-5733. DOI: [10.5516/NET.06.2012.081](https://doi.org/10.5516/NET.06.2012.081).
 - [68] Koch, L. and Schoof, S. *The isotope correlation experiment, ICE. Final report*. Tech. rep. KfK-3337 EUR 7766 EN ESARDA 2/81. 1981. DOI: [10.5445/IR/270017557](https://doi.org/10.5445/IR/270017557).
 - [69] Kodeli, I. “Sensitivity analysis and uncertainty propagation from basic nuclear data to reactor physics and safety relevant parameters”. In: *Proc. Evaluation of uncertainties in relation to severe accidents and level-2 probabilistic safety analysis*. Aix-en-Provence, France, Nov. 2005.
 - [70] Koning, A. J. and Rochman, D. “Towards sustainable nuclear energy: Putting nuclear physics to work”. In: *Annals of Nuclear Energy* 35.11 (Nov. 2008), pp. 2024–2030. DOI: [10.1016/j.anucene.2008.06.004](https://doi.org/10.1016/j.anucene.2008.06.004).
 - [71] Krivtchik, G. “Analysis of uncertainty propagation in nuclear fuel cycle scenarios”. Theses. Université de Grenoble, Oct. 2014. URL: <https://tel.archives-ouvertes.fr/tel-01131207>.
 - [72] Kunsch, P. L. and Teghem, J. “Nuclear fuel cycle optimization using multi-objective stochastic linear programming”. In: *European Journal of Operational Research* 31.2 (Aug. 1987), pp. 240–249. DOI: [10.1016/0377-2217\(87\)90028-2](https://doi.org/10.1016/0377-2217(87)90028-2).
 - [73] Lee, J.-W. et al. “Linear programming optimization of nuclear energy strategy with sodium-cooled fast reactors”. In: *Nuclear Engineering and Technology* 43 (Aug. 2011). DOI: [10.5516/NET.2011.43.4.383](https://doi.org/10.5516/NET.2011.43.4.383).
 - [74] Leniau, B. et al. “A neural network approach for burn-up calculation and its application to the dynamic fuel cycle code CLASS”. In: *Annals of Nuclear Energy* 81 (July 2015), pp. 125–133. DOI: [10.1016/j.anucene.2015.03.035](https://doi.org/10.1016/j.anucene.2015.03.035).
 - [75] Macfarlane, R. et al. *The NJOY Nuclear Data Processing System, Version 2016*. Tech. rep. LA-UR-17-20093. United States: Los Alamos National Lab., Jan. 2017. DOI: [10.2172/1338791](https://doi.org/10.2172/1338791).

- [76] Marcinkevicius, B., Simakov, S., and Pronyaev, V. *$^{209}\text{Bi}(n,f)$ and $^{nat}\text{Pb}(n,f)$ Cross Sections as a New Reference and Extension of the ^{235}U , ^{238}U and $^{239}\text{Pu}(n,f)$ Standards up to 1 GeV*. Tech. rep. INDC(NDS)–0681. International Atomic Energy Agency, 2015. URL: <https://www-nds.iaea.org/publications/indc/indc-nds-0681.pdf>.
- [77] Martinez-Val, J. *P&T Roadmap proposal for Advanced Fuel Cycles leading to a Sustainable Nuclear Energy*. PATEROS EU 6th FP, D6.2, Contract Number 036418. 2008.
- [78] Massara, S. et al. “Prospective scenarios of nuclear energy evolution on the XXIst century over the world scale”. In: *Nuclear Engineering and Design* 239.9 (Sept. 2009), pp. 1708–1717. DOI: [10.1016/j.nucengdes.2009.04.005](https://doi.org/10.1016/j.nucengdes.2009.04.005).
- [79] Mattoon, C. M., Brown, D., and Elliott, J. B. “Covariance Applications with Kiwi”. In: *EPJ Web of Conferences* 27 (2012), p. 00002. DOI: [10.1051/epjconf/20122700002](https://doi.org/10.1051/epjconf/20122700002).
- [80] McKay, M. D., Beckman, R. J., and Conover, W. J. “Comparison of Three Methods for Selecting Values of Input Variables in the Analysis of Output from a Computer Code”. In: *Technometrics* 21.2 (May 1979), pp. 239–245. DOI: [10.1080/00401706.1979.10489755](https://doi.org/10.1080/00401706.1979.10489755).
- [81] Meinshausen, N. “Relaxed Lasso”. In: *Computational Statistics & Data Analysis* 52.1 (Sept. 2007), pp. 374–393. DOI: [10.1016/j.csda.2006.12.019](https://doi.org/10.1016/j.csda.2006.12.019).
- [82] Merino-Rodríguez, I. “Simulation system for advanced fuel cycle transition scenarios”. PhD thesis. Universidad Politécnica de Madrid, 2012. URL: <http://oa.upm.es/35024/>.
- [83] Merino-Rodríguez, I. et al. “Cross check of the new economic and mass balance features of the fuel cycle scenario code TR_EVOL”. In: *EPJ Nuclear Sciences & Technologies* 2 (2016), p. 33. DOI: [10.1051/epjn/2016029](https://doi.org/10.1051/epjn/2016029).
- [84] Miettinen, K. *Nonlinear Multiobjective Optimization*. Springer US, Oct. 12, 2012. 324 pp. ISBN: 978-1-4613-7544-9.
- [85] Mills, R. W. et al. *Report with transmutation calculations for advanced reactors with new covariance data + updated sensitivity tables*. ANDES EU project, Deliverable 2.5 Grant Agreement No:249671. 2013.
- [86] MINETCO. *7º Plan General de Residuos Radioactivos*. Borrador. Ministerio para la Transición Ecológica y el Reto Demográfico, Mar. 2020.
- [87] Mouginot, B. et al. “Core library for advanced scenario simulation, C.L.A.S.S.: principle & application”. In: Poster. Sept. 2014, 12 p. URL: <http://hal.in2p3.fr/in2p3-01119778>.

-
- [88] Mukaiyama, T. et al. “Review of research and development of accelerator-driven system in Japan for transmutation of long-lived nuclides”. In: *Progress in Nuclear Energy* 38.1-2 (Jan. 2001), pp. 107–134. DOI: [10.1016/S0149-1970\(00\)00098-6](https://doi.org/10.1016/S0149-1970(00)00098-6).
- [89] Myung-Seung, Y. et al. “The status and prospect of DUPIC fuel technology”. In: *Nuclear Engineering and Technology* 38 (Jan. 2006).
- [90] Niederreiter, H. *Random number generation and quasi-Monte Carlo methods*. Philadelphia: Society for Industrial and Applied Mathematics, 1992. ISBN: 978-0-89871-295-7.
- [91] Nishihara, K. et al. “Utilization of rock-like oxide fuel in the phase-out scenario”. In: *Journal of Nuclear Science and Technology* 51.2 (Nov. 2013), pp. 150–165. DOI: [10.1080/00223131.2014.846834](https://doi.org/10.1080/00223131.2014.846834).
- [92] NWTRB. *Nuclear Waste Assessment System for Technical Evaluation (NUWASTE): Status and Initial Results*. Tech. rep. Topical Report #2. U.S. Nuclear Waste Technical Review Board, June 2011. URL: <https://www.nwtrb.gov>.
- [93] OECD/NEA. *Accelerator-driven systems (ADS) and fast reactors (FR) in advanced nuclear fuel cycles*. Tech. rep. NEA/3109-ADS. 2002. URL: <https://www.oecd-nea.org/ndd/reports/2002/nea3109-ads.pdf>.
- [94] OECD/NEA. *Advanced Nuclear Fuel Cycles and Radioactive Waste Management*. 2006, p. 244. DOI: [10.1787/9789264024861-en](https://doi.org/10.1787/9789264024861-en).
- [95] OECD/NEA. *Benchmark Study on Nuclear Fuel Cycle Transition Scenarios Analysis Codes*. Nuclear Science NEA/NSC/WPFC/DOC(2012)16. 2012. URL: <https://www.oecd-nea.org/science/docs/2012/nsc-wpfc-doc2012-16.pdf>.
- [96] OECD/NEA. *International Comparison of a Depletion Calculation Benchmark on Fuel Cycle Issues*. Nuclear Science NEA/NSC/DOC(2013)1. 2013. URL: <https://www.oecd-nea.org/science/docs/2013/nsc-doc2013-1.pdf>.
- [97] OECD/NEA. *Transition Towards a Sustainable Nuclear Fuel Cycle*. Ed. by OECD. Nuclear Science 7133. OECD, Sept. 2013, p. 67. DOI: [10.1787/9789264205093-en](https://doi.org/10.1787/9789264205093-en).
- [98] OECD/NEA. *Minor Actinide Burning in Thermal Reactors*. 6997. 2014, p. 82. ISBN: 978-92-64-20853-7. DOI: [10.1787/9789264208537-en](https://doi.org/10.1787/9789264208537-en).
- [99] OECD/NEA. *MOx Depletion Calculation Benchmark*. Nuclear Science NEA/NSC/R(2016)3. 2016. URL: <https://www.oecd-nea.org/science/docs/2016/nsc-r2016-3.pdf>.
- [100] OECD/NEA. *The Effects and of the Uncertainty of Input Parameters on Nuclear Fuel Cycle Scenario Studies*. Nuclear Science NEA/NSC/R(2016)4. 2017.

-
- [101] OECD/NEA. *International Handbook of Evaluated Criticality Safety Benchmark Experiments*. NEA/NSC/DOC(95)03. Oct. 2019. URL: <https://www.oecd-neo.org/tools/abstract/detail/nea-1486>.
- [102] OECD/NEA. *Benchmark on TRU management*. Under ellaboration.
- [103] Oliver, K. et al. “Studying international fuel cycle robustness with the GENIUSv2 discrete facilities/materials fuel cycle systems analysis tool”. In: *Proceedings of GLOBAL*. 2009.
- [104] Palmiotti, G., Salvatores, M., and Assawaroongruengchot, M. “Impact of the Core Minor Actinide Content on Fast Reactor Reactivity Coefficients”. In: *Journal of Nuclear Science and Technology* 48.4 (Apr. 2011), pp. 628–634. DOI: [10.1080/18811248.2011.9711743](https://doi.org/10.1080/18811248.2011.9711743).
- [105] Passerini, S., Kazimi, M. S., and Shwageraus, E. “A Systematic Approach to Nuclear Fuel Cycle Analysis and Optimization”. In: *Nuclear Science and Engineering* 178.2 (Oct. 2014), pp. 186–201. DOI: [10.13182/nse13-20](https://doi.org/10.13182/nse13-20).
- [106] Pedregosa, F. et al. “Scikit-learn: Machine Learning in Python”. In: *Journal of Machine Learning Research* 12 (2011), pp. 2825–2830. URL: <http://jmlr.csail.mit.edu/papers/v12/pedregosa11a.html>.
- [107] Perkó, Z. et al. “Large scale applicability of a Fully Adaptive Non-Intrusive Spectral Projection technique: Sensitivity and uncertainty analysis of a transient”. In: *Annals of Nuclear Energy* 71 (Sept. 2014), pp. 272–292. DOI: [10.1016/j.anucene.2014.03.035](https://doi.org/10.1016/j.anucene.2014.03.035).
- [108] Plompen, A. J. M. *Announcing JEFF-3.3 release*. Tech. rep. JEFDOC-1864. OCDE/NEA, 2017.
- [109] Price, K. V., Storn, R. M., and Lampinen, J. A. *Differential evolution : a practical approach to global optimization*. Berlin New York: Springer, 2005. ISBN: 978-3-540-31306-9. DOI: [10.1007/3-540-31306-0](https://doi.org/10.1007/3-540-31306-0).
- [110] PRIS. *Power Reactor Information System*. IAEA. URL: <https://pris.iaea.org/PRIS/home.aspx> (visited on 09/01/2020).
- [111] Pusa, M. “Rational Approximations to the Matrix Exponential in Burnup Calculations”. In: *Nuclear Science and Engineering* 169.2 (Oct. 2011), pp. 155–167. DOI: [10.13182/nse10-81](https://doi.org/10.13182/nse10-81).
- [112] Radiation Shielding Information Center, Oak Ridge National Laboratory (United States). *ORIGEN-2.2, Isotope Generation and Depletion Code Matrix Exponential Method*. Tech. rep. Nuclear Energy Agency of the OECD (NEA), Oct. 2002. URL: https://inis.iaea.org/search/search.aspx?orig_q=RN:39098827.

-
- [113] Rearden, B. T. and Jessee, M. A. *SCALE Code System, Version 6.2.3*. Tech. rep. ORNL/TM-2005/39. Tennessee: Oak Ridge National Laboratory, 2018.
- [114] Rimpault, G. et al. *General Synthesis Report of the Different ADS Design Status. Establishment of a Catalogue of the R&D needs*. Contract. EURATOM, Aug. 2010. URL: <https://hal.archives-ouvertes.fr/hal-01084509>.
- [115] Rineiski, A. et al. *Specification of the new core safety measures*. ESFR-SMART D1.1.2. 2018.
- [116] Robič, T. and Filipič, B. “DEMO: Differential Evolution for Multiobjective Optimization”. In: *Lecture Notes in Computer Science*. Springer Berlin Heidelberg, 2005, pp. 520–533. DOI: [10.1007/978-3-540-31880-4_36](https://doi.org/10.1007/978-3-540-31880-4_36).
- [117] Rochman, D. and Sciolla, C. M. *Total Monte Carlo Uncertainty propagation applied to the Phase I-1 burnup calculation*. Tech. rep. 113696. Petten, The Netherlands: Nuclear Research and Consultancy Group, Apr. 2012.
- [118] Rochman, D. and Sciolla, C. M. “Nuclear data uncertainty propagation from a typical PWR fuel assembly with burnup”. In: *Nuclear Engineering and Technology* 46.3 (June 2014), pp. 353–362. DOI: [10.5516/NET.01.2014.712](https://doi.org/10.5516/NET.01.2014.712).
- [119] Rodríguez, I. M. et al. “The nuclear fuel cycle code ANICCA: Verification and a case study for the phase out of Belgian nuclear power with minor actinide transmutation”. In: *Nuclear Engineering and Technology* (Apr. 2020). DOI: [10.1016/j.net.2020.04.004](https://doi.org/10.1016/j.net.2020.04.004).
- [120] Rodríguez, I. M., Álvarez-Velarde, F., and Martín-Fuertes, F. “Analysis of advanced European nuclear fuel cycle scenarios including transmutation and economic estimates”. In: *Annals of Nuclear Energy* 70 (Aug. 2014), pp. 240–247. DOI: [10.1016/j.anucene.2014.03.015](https://doi.org/10.1016/j.anucene.2014.03.015).
- [121] Romojaro, P., Álvarez-Velarde, F., and García-Herranz, N. “SUMMON: A Sensitivity And Uncertainty Methodology For MONte Carlo Codes”. In: *Proceedings of International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering (M&C 2017)*. Jeju, Korea, Apr. 2017.
- [122] Ruszczyński, A. and Shapiro, A. *Stochastic programming*. Amsterdam Boston: Elsevier, 2003. ISBN: 978-0-444-50854-6.
- [123] Saltelli, A. et al. *Global Sensitivity Analysis. The Primer*. John Wiley & Sons, Ltd, Dec. 2007. ISBN: 978-0-470-05997-5. DOI: [10.1002/9780470725184](https://doi.org/10.1002/9780470725184).
- [124] Saltelli, A. et al. “Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index”. In: *Computer Physics Communications* 181.2 (Feb. 2010), pp. 259–270. DOI: [10.1016/j.cpc.2009.09.018](https://doi.org/10.1016/j.cpc.2009.09.018).

-
- [125] Salvatores, M. “Nuclear fuel cycle strategies including Partitioning and Transmutation”. In: *Nuclear Engineering and Design* 235.7 (Mar. 2005), pp. 805–816. DOI: [10.1016/j.nucengdes.2004.10.009](https://doi.org/10.1016/j.nucengdes.2004.10.009).
- [126] Salvatores, M., Slessarev, I., and Uematsu, M. “Physics Characteristics of Nuclear Power Systems with Reduced Long-Term Radioactivity Risk”. In: *Nuclear Science and Engineering* 120.1 (May 1995), pp. 18–39. DOI: [10.13182/nse95-a24103](https://doi.org/10.13182/nse95-a24103).
- [127] Salvatores, M. et al. *Results of the Regional Scenarios Studies*. PATEROS EU 6th FP, D2.2, Contract Number 036418. 2008.
- [128] Santamarina, A. et al. “The JEFF-3.1.1 Nuclear Data Library. Validation Results from JEF-2.2 to JEFF-3.1.1”. In: *OECD 2009 NEA No. 6807, ISBN 978-92-64-99074-6* (Jan. 2009). URL: https://www.oecd-nea.org/dbdata/nds_jefreports/jefreport-22/nea6807-jeff22.pdf.
- [129] Sanz, J., Cabellos, O., and García-Herranz, N. *ACAB Inventory code for nuclear applications: User’s Manual v.2008*. Dec. 2008. URL: <https://rsicc.ornl.gov/codes/ccc/ccc7/ccc-758.html>.
- [130] Schneider, E. A., Bathke, C. G., and James, M. R. “NFCSim: A Dynamic Fuel Burnup and Fuel Cycle Simulation Tool”. In: *Nuclear Technology* 151.1 (July 2005), pp. 35–50. DOI: [10.13182/nt05-4](https://doi.org/10.13182/nt05-4).
- [131] Schneider, E. A. “A physical and economic model of the nuclear fuel cycle”. PhD thesis. Cornell University, Jan. 2002.
- [132] Shwageraus, E., Hejzlar, P., and Kazimi, M. S. “Use of Thorium for Transmutation of Plutonium and Minor Actinides in PWRs”. In: *Nuclear Technology* 147.1 (July 2004), pp. 53–68. DOI: [10.13182/nt04-a3514](https://doi.org/10.13182/nt04-a3514).
- [133] Skarbeli, A. V. et al. “Quantification of the differences introduced by nuclear fuel cycle simulators in advanced scenario studies”. In: *Annals of Nuclear Energy* 137 (Mar. 2020), p. 107160. DOI: [10.1016/j.anucene.2019.107160](https://doi.org/10.1016/j.anucene.2019.107160).
- [134] SNETP. *The Sustainable Nuclear Energy Technology Platform: A vision report*. Tech. rep. EUR 22842. Sustainable Nuclear Energy Technology Platform, 2007. URL: <http://www.snetp.eu/>.
- [135] SNETP. *ESNII The European Sustainable Nuclear Industrial Initiative*. Tech. rep. Sustainable Energy Technology Platform, 2010. URL: <http://www.snetp.eu/>.
- [136] Sobol, I. M. “Sensitivity Estimates for Nonlinear Mathematical Models”. In: *Mathematical Modeling and Computational Experiment* 1.4 (1993), pp. 407–414. ISSN: 1061-7590.

-
- [137] Stankovskiy, A. and Van den Eynde, G. “Advanced Method for Calculations of Core Burn-Up, Activation of Structural Materials, and Spallation Products Accumulation in Accelerator-Driven Systems”. In: *Science and Technology of Nuclear Installations 2012* (2012), pp. 1–12. DOI: [10.1155/2012/545103](https://doi.org/10.1155/2012/545103).
 - [138] Storn, R. and Price, K. *Differential Evolution - A simple and efficient adaptive scheme for global optimization over continuous spaces*. Tech. rep. TR-95-012. Berlekey: International Computer Science Institute, 1995.
 - [139] Storn, R. and Price, K. “Differential Evolution – A Simple and Efficient Heuristic for global Optimization over Continuous Spaces”. In: *Journal of Global Optimization* 11.4 (1997), pp. 341–359. DOI: [10.1023/a:1008202821328](https://doi.org/10.1023/a:1008202821328).
 - [140] Sudret, B. “Global sensitivity analysis using polynomial chaos expansions”. In: *Reliability Engineering & System Safety* 93.7 (July 2008), pp. 964–979. DOI: [10.1016/j.ress.2007.04.002](https://doi.org/10.1016/j.ress.2007.04.002).
 - [141] Sun, W. and Yuan, Y.-X. *Optimization Theory and Methods*. Springer US, May 24, 2006. 700 pp. ISBN: 978-0-387-24975-9. DOI: [10.1007/b106451](https://doi.org/10.1007/b106451).
 - [142] Takahama, T. and Sakai, S. “Constrained Optimization by ε Constrained Particle Swarm Optimizer with ε -level Control”. In: *Advances in Soft Computing*. Springer Berlin Heidelberg, 2005, pp. 1019–1029. DOI: [10.1007/3-540-32391-0_105](https://doi.org/10.1007/3-540-32391-0_105).
 - [143] Thiollière, N. *From neutronics to nuclear scenarios*. Joliot-Curie School. 2019. URL: https://ejc2019.sciencesconf.org/data/pages/PresJC_NT2019.pdf.
 - [144] Thiollière, N. et al. “A methodology for performing sensitivity analysis in dynamic fuel cycle simulation studies applied to a PWR fleet simulated with the CLASS tool”. In: *EPJ Nuclear Sciences & Technologies* 4 (2018), p. 13. DOI: [10.1051/epjn/2018009](https://doi.org/10.1051/epjn/2018009).
 - [145] Tsibulskiy, V. et al. “DESAE (Dynamic Energy System- Atomic Energy): Integrated Computer Model for Perfoming Global Analysis in INPRO Assessment Studies”. In: *14th International Conference on Nuclear Engineering*. Vol. Volume 3: Structural Integrity; Nuclear Engineering Advances; Next Generation Systems; Near Term Deployment and Promotion of Nuclear Energy. ASMEDC, Jan. 2006. DOI: [10.1115/icone14-89865](https://doi.org/10.1115/icone14-89865).
 - [146] United Nations. *Adoption of the Paris Agreement*. FCCC/CP/2015/L.9/Rev.1. Dec. 2015.
 - [147] Van Den Durpel, L., Wade, D. C., and Yacout, A. “DANESS: a system dynamics code for the holistic assessment of nuclear energy system strategies”. In: *Proceedings of the 2006 system dynamics conference*. 2006.

-
- [148] Van den Eynde, G. et al. “ALEPH2 Monte Carlo burn-up code”. In: Jan. 2011, pp. 1–12.
- [149] Vasile, A. et al. “Advanced fuels for plutonium management in pressurized water reactors”. In: *Journal of Nuclear Materials* 319 (June 2003), pp. 173–179. DOI: [10.1016/S0022-3115\(03\)00148-x](https://doi.org/10.1016/S0022-3115(03)00148-X).
- [150] Weise, T. *Global Optimization Algorithms - Theory and Application*. en. Second. Self-Published, June 2009. URL: <http://www.it-weise.de/>.
- [151] Werner, C. J., ed. *MCNP Users’s Manual – Code Version 6.2*. LA-UR-17-29981. Los Alamos National Laboratory, Oct. 2017. URL: https://laws.lanl.gov/vhosts/mcnp.lanl.gov/pdf_files/la-ur-17-29981.pdf.
- [152] Wiener, N. “The Homogeneous Chaos”. In: *American Journal of Mathematics* 60.4 (Oct. 1938), p. 897. DOI: [10.2307/2371268](https://doi.org/10.2307/2371268).
- [153] Williams, M. M. R. “Polynomial chaos functions and stochastic differential equations”. In: *Annals of Nuclear Energy* 33.9 (June 2006), pp. 774–785. DOI: [10.1016/j.anucene.2006.04.005](https://doi.org/10.1016/j.anucene.2006.04.005).
- [154] WNA. World Nuclear Association. URL: <https://www.world-nuclear.org/> (visited on 09/01/2020).
- [155] Wu, X. and Kozlowski, T. “Inverse uncertainty quantification of reactor simulations under the Bayesian framework using surrogate models constructed by polynomial chaos expansion”. In: *Nuclear Engineering and Design* 313 (Mar. 2017), pp. 29–52. DOI: [10.1016/j.nucengdes.2016.11.032](https://doi.org/10.1016/j.nucengdes.2016.11.032).
- [156] Xiu, D. and Karniadakis, G. E. “The Wiener–Askey Polynomial Chaos for Stochastic Differential Equations”. In: *SIAM Journal on Scientific Computing* 24.2 (Jan. 2002), pp. 619–644. DOI: [10.1137/S1064827501387826](https://doi.org/10.1137/S1064827501387826).
- [157] Xiu, D. and Karniadakis, G. E. “Modeling uncertainty in flow simulations via generalized polynomial chaos”. In: *Journal of Computational Physics* 187.1 (May 2003), pp. 137–167. DOI: [10.1016/S0021-9991\(03\)00092-5](https://doi.org/10.1016/S0021-9991(03)00092-5).
- [158] Yacout, A. et al. “Modeling the nuclear fuel cycle”. In: *The 23rd International Conference of the System Dynamics Society, Boston*. INL/CON-05-00162. 2005. URL: <https://inldigitallibrary.inl.gov/sites/sti/sti/3169906.pdf>.
- [159] Yue, Q. et al. “Fuel cycles optimization of nuclear power industry in China”. In: *Annals of Nuclear Energy* 111 (Jan. 2018), pp. 635–643. DOI: [10.1016/j.anucene.2017.09.049](https://doi.org/10.1016/j.anucene.2017.09.049).
- [160] Zhu, T. et al. “NUSS-RF: stochastic sampling-based tool for nuclear data sensitivity and uncertainty quantification”. In: *Journal of Nuclear Science and Technology* 52.7-8 (May 2015), pp. 1000–1007. DOI: [10.1080/00223131.2015.1040864](https://doi.org/10.1080/00223131.2015.1040864).

-
- [161] Zwermann, W. et al. “Influence of nuclear covariance data on reactor core calculations”. In: *Second International Workshop on Nuclear Data Evaluation for Reactor Applications (WONDER 2009), Cadarache, France*. Vol. 29. 2009, pp. 99–104.