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Impact of fresh fuel loading management in fuel cycle simulators: A functionality isolation test

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ABSTRACT

Fuel cycle simulator development started many years ago by several research and engineering institutions or consulting firms for a wide range of applications. To improve confidence in the results, institutions may be tempted to increase the complexity of their software even if this complexity might not be necessary. On the other hand, some simulators may be used outside their range of validity when used in very specific applications. The FIT (Functionality Isolation Test) project is an international effort devoted to improve the confidence in the data produced by fuel cycle simulation tools. The scientific goal is to determine the optimum level of detail a fuel cycle simulator needs according to the type of study and the required confidence level. The project relies on a wide variety of fuel cycle simulators with a large range of complexity levels. The FIT project consists of isolating the impact of one targeted functionality on fuel cycle simulations. The impact of the functionality is assessed using a set of simple basic exercises specifically designed for this purpose, called "functionality isolation." The present work focuses on the impact on simulation results of using a fuel loading model (a relation that links the stock isotopic composition with the fresh fuel fabrication according to the reactor requirements) or a fixed fraction approach (the fresh fuel fissile fraction is fixed and does not depend on the stock isotopic composition). The paper first presents the FIT project. The exercise design is described and results show that using a fuel loading model approach has an important impact on fuel cycle outputs under certain conditions that are described. This result is reinforced by the fact that all fuel cycle simulators used in this exercise provide similar conclusions.

1. Introduction

Since the 1990s, many different nuclear fuel cycle simulators have been developed by several institutions. A fuel cycle simulator aims to model an entire fleet of nuclear facilities such as nuclear reactors, fuel fabrication plants, reprocessing plants, cooling pools, and waste repositories. These tools help to identify drivers and interactions between parameters in the fuel cycle. They implement physics models for key points in the cycle such as fuel enrichment, fabrication, and depletion, with various levels of complexity.

Fuel cycle simulators are used worldwide for a wide range of applications: optimizing the industrial operation of an existing nuclear fleet, assessing the future of nuclear energy, providing valuable information to political decision makers, and evaluating/verifying the operation of an

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existing nuclear fleet by national or international safety authorities. Moreover, these tools are used for Research and Development and teaching as an access point to key data related to the fuel cycle.

The myriad institutions that develop and use fuel cycle simulators pursue myriad goals. Consequently, software development decisions (e.g., fidelity) are often made in agreement with the institution's simulation goals. To improve confidence in the results, institutions may be tempted to increase the complexity of their software even if this complexity might not be necessary.

As an example, neutron and gamma dose calculations require the precise knowledge of each material isotopic composition in each facility as well as a description of the spatial configuration of these isotopes whereas uranium consumption calculation does not require the same level of detail. As a consequence, some functionalities may not be needed depending on the technical question the code assesses, which is here, solving a given technical question associated with a targeted precision will require a limited set of functionality. Knowing the importance of each will help users choose an appropriate software tool or may guide future code development to solve a specific question. Also, some technical issues are assessed by numerous studies performed with different software and it is often difficult to compare them. Knowing the impact of functionalities on different simulation outputs helps to estimate the level of confidence of the different fuel cycle studies.

The Functionality Isolation Test (FIT) Project has been conceived to understand the circumstances under which the choice of algorithms and/or model influences the conclusions that one might draw from a fuel cycle simulation. The project aims to characterize the relationship between model fidelity and the desired confidence level in the context of many different research questions. Among functionalities of interest, this first FIT focuses on the ability of fuel cycle software to adapt the fresh fuel to the qualities of the available material and the associated reactor requirements.

Section 2 describes the FIT project, its philosophy, the participants, and their associated simulators. It explains how the FIT project is not a traditional benchmark. That is, FIT project does not aim to make inter-simulator comparison, but focuses on intra-simulator comparison, evaluating differences between simulation results produced by the same simulator, enabling and disabling isolated features. To build confidence in the conclusion, such comparisons will be performed across multiple simulators. Section 2 ends with the description of the particular feature tested in this work, the fuel loading management model. Section 3 then presents the numerical experiment used to test this particular feature, including simulation input parameter descriptions and other technical specifics necessary to perform the test. Additionally, this section details output metrics that quantify the impact of the use of fuel loading management in fuel cycle studies. Section 4 presents characteristics of reactors and models used in the exercise. Next, Sections 5 and 6 are dedicated to the presentation and discussion of results achieved by each software tool involved in this first exercise, for Pressurized Water Reactor (PWR) and c application. Finally, in Section 7 some conclusions are drawn.

2. Framework and Description Of The FIT Project

The FIT (Functionality Isolation Test) Project is an international effort devoted to improve confidence in fuel cycle tools. This section aims to precisely describe and to present the framework of the project.

2.1. Nuclear fuel cycle dynamic simulation tool

Fuel cycle simulators (McCarthy et al., 2012) development started many years ago by several research and engineering institutions or consulting firms for a wide range of applications. For research and engineering institutions in charge of supporting the operated nuclear installations, fuel cycle simulators are used to facilitate and optimize the industrial operations. For research and engineering institutions studying energetic transition, fuel cycle simulators are used to study and analyze future trajectories for prospective reflections on the electric component of the transition. Also, for institutions in charge of educational and training purposes in the nuclear field, such tools help understand the physics mechanisms that drive a nuclear fleet and can be used as an educational support. Consulting firms develop and use those tools to provide enlightened advice to politics. For those reasons, a fuel cycle simulator can be seen as a decision-making tool since results and analyses are directly or indirectly used by industrial and political worlds.

A fuel cycle simulator is based on a computer software used to model and to compute the evolution of isotopes of interest in nuclear facilities, strategic stocks and waste disposal. A large effort in tool development concerns physics driven modeling that aims to describe complex physics or industrial processes. A nuclear fuel cycle is then simulated as a very complex system in which isotopes evolution can be impacted by various parameters such as reactor technology deployment, fuel reprocessing strategies, etc. A fuel cycle simulator computes radionuclides and elements evolution in all the nuclear facilities from the defined nuclear fleet. The material evolution is estimated during the irradiation process in reactors and during cooling phases in other facilities. Taking into account all the physics phenomena and industrial practices would require a large effort in software development and would lead to codes consuming large amounts of calculation power and create outputs consuming large storage space. For these reasons, fuel cycle simulators include many modeling simplifications.

Bias or uncertainties in fuel cycle simulators outputs are difficult to quantify due to the multiple levels of simplifications imposed by the complexity of the simulated system. There are many sources of uncertainties. Nuclear data uncertainty has an impact on reactor calculation output used to tune fuel cycle codes (Krivtchik, 2014). Moreover, reactor models rely on simplified reactor descriptions, implying the use of biased neutronic data in such simulators (Somaini, 2017). At the fuel cycle scale, simplifications are also required.

While comparisons with operated nuclear fleets are possible, they are complex and often require the use of sensitive industrial data, which makes them really difficult. For prospective simulations involving innovative reactors, it is completely impossible. Evaluation of these biases and uncertainties must therefore rely almost entirely on comparison between codes and models.

Some international efforts (McCarthy et al., 2012) focus on benchmarking fuel cycle simulators comparing output metrics at the scale of an operated nuclear fleet. Results produced in the framework of those works are decisive to test the ability of multiple simulators to be in agreement. Nevertheless, such comparisons are focused on aggregated data and deviations between simulators may be hard to interpret. The FIT project is designed in complementarity with those international benchmarks and aims to provide information allowing greater trust in the data produced by fuel cycle simulators.

2.2. Goals and intended impact of the FIT project

The FIT Project was initiated in 2017. It aims to improve the confidence in the data produced by fuel cycle simulation tools. The first goal is to gather the community of fuel cycle specialists around the question of the confidence in simulation outputs. The second goal is to determine the optimum level of detail a fuel cycle simulator needs relative to the type of study and the required confidence level. The project relies on the wide variety of fuel cycle simulators with a large range of complexity levels.

Improving the ability to reproduce an operated nuclear fleet involves increasing the complexity of the simulation tool by developing new functionalities. A fuel cycle functionality is the translation of a physical or technical process, related to nuclear facilities, into computer software language. Table 1 lists a set of functionalities that could be implemented in addition/replacement of the default model of the simulator.

The FIT project consists in isolating the impact of a functionality on

Table 1
Examples of simplified/complex functionality couples.

Simplified	Complex
Fix fresh fuel composition for each fuel batch loading	Update fresh fuel composition with regards of the available material composition
Averaged thermal power over the cycles	Dynamic thermal power followup
Use of fixed/averaged macroscopic cross section for fuel depletion	Time/Burn-Up -dependent cross sections
Steady state reactor start (no starting batches)	Fuel starting batches modeling

fuel cycle simulations. The impact of each functionality is assessed using a set of simple basic exercises specifically designed for this purpose, called "functionality isolation." Each exercise of a functionality isolation will be focused on a subset of output metrics related to a category of problems covered by the fuel cycle study.

For example, the total mass of plutonium is used as an output of interest for fuel cycle studies dealing with recycled nuclear fuels. Minor actinides production could be added to the analyses to take into account fuel cycle studies concerned by radio-protection. Once the choice of the output of interest is made, the effect of the functionality is quantified by specific estimators computed with the functionality enabled and with the reference case. Each participant submits a resolution for the exercise and conclusions can be drawn according to the level of agreement of participants.

With this methodology, the FIT project provides information about which functionalities are required to answer specific questions with an associated precision or confidence. When starting a new fuel cycle study, the fuel cycle simulator user starts from a technical question. One example can be: "In a PWR fleet, considering spent Uranium OXide (UOX) fuel plutonium reprocessing into Mixed OXide (MOX) fuel, what is the optimum PWR UOX-MOX ratio that allows no/low plutonium accumulation?" The user then identifies the set of output metrics required to answer the technical question and the precision needed for each of them. In the example above, the user needs to assess the plutonium inventory contained in facilities between the UOX spent fuel and the PWR MOX fuel. The user may then refer to the FIT project results to decide what are the required functionalities to produce a reliable result.

2.3. Fuel cycle Simulators and institutions

The originality and the efficiency of the FIT project lie in the large amount of fuel cycle simulators participating in a set of exercises of a specific functionality isolation. It is the guarantee that the impact calculated is the impact of the functionality and not an artifact from hidden code options. Table 2 presents the participating institutions with used fuel cycle code.

The aim of the FIT project is to assemble set of exercises, each testing a specific functionality isolation. If each set of exercises aims to have the highest number of participating simulators as possible, some simulators and or institutions might not be participating in some exercises, or might only participate partially. The participation in an exercise also depends on the availability of participants and on the ability of each simulator to activate and deactivate the tested functionality.

Table 2
List of institutions and fuel cycle codes involved in FIT project.

Fuel cycle code	Institution
ANICCA (Rodriguez et al., 2020)	TRACTEBEL (BEL) Catholic Univ. of the Maule (CHL)
CLASS (Thiollière et al., 2018)	CNRS/ IN2P3 (FRA)
COSI6 (Coquelet-Pascal et al., 2015)	CEA Cadarache
CYCLUS (Huff et al., 2016)	Univ. of Wisconsin Madison (USA) Univ. of Illinois (USA)
JOSSETE (Halász, 2018)	BME (HUN)
TR_EVOL (Merino-Rodríguez et al., 2016)	CIEMAT (ESP)

3. Exercise design

3.1. Description of the tested functionality

The present work focuses on the impact of using an Fuel Loading Model (FLM) or an Fixed Fraction (FF) approach to build fresh fuel in fuel cycle studies.

An FLM adapts the fresh fuel composition according to the reactor requirements and the isotopic compositions of available materials. For example, it adjusts the fissile fraction depending on the fissile stock quality in order to reach specific criteria, such as the required Burn-Up (BU) of the reactor for instance. An FLM uses a model that can be of varying complexity. It could be based on neural networks Leniau et al. (2015), plutonium equivalence model Baker and Ross (1963), analytic functions Mouginot et al. (2015), built-in depletion, etc. an FLM is usually built from physics constraints and reactor physics calculations.

An FF model uses the same constant fissile fraction at each fresh fuel loading regardless of the isotopic composition of the available fissile materials. Using a PWR MOX which is always loaded with a fresh fuel that contains 7% of plutonium regardless the ^{239}Pu content.

The present work aims to quantify the impact of using FLM versus FF approach. The FLM is considered to be the better approach since it takes into account more physics. The FF approach is the cheapest method to deal with fresh reprocessed fuel fabrication, both in development and calculation time. Testing the impact of using an FLM rather than an FF aims to identify the studies that require dedicating time and effort in an FLM and the one solvable with FF.

The choice of testing FLM and FF approach prevent us from doing inter-code comparisons.

Indeed, comparisons between FLM used in fuel cycle simulators are laborious because comparison steps finish at the scale of the neutron transport code and the Bateman solver. Differences between models mainly depends on the interpretation of the scenario specifications made by participants (Skarbeli et al., 2020) but also on neutronic codes assumptions and bias (geometry, materials, temperatures, nuclear data, etc.). For those reasons, even comparisons between two codes may be highly complex.

Besides this last remark, some fuel cycle simulator developers don't want to share precise methodology related to physics models, due to industrial concerns.

The second problem we face when trying to compare FLM from different codes is to decide which approach better describe the physics since we don't have access to experimental precise data, especially for MOX fuel. The FIT project philosophy has been built to avoid those issues. There is no inter-code comparisons in this work. A fuel cycle simulator user can use FIT results provided in this paper to decide whether to use an FF or a FLM approach.

3.2. Outputs of interest

Fuel fabrication models can influence fuel cycle simulation in several ways. This exercise aims to understand some of their impacts on an overall fuel cycle calculation. Change in the plutonium content in a MOX fuel could play a role in the fuel cycle outputs in two majors ways:

- Total amount of plutonium: a variation in the plutonium content in the MOX fuel might lead to an increase of the amount of plutonium burnt in the PWR reactor and/or a change in the breeding/burning ratio in a Sodium Fast Reactor (SFR) reactor, impacting over time the overall amount of plutonium in the simulation.
- Location of the plutonium: the amount of plutonium in the MOX fuel will shift the location of the plutonium from the front-end to the

back-end of the cycle, which could change its availability for other uses (deployment of new reactors, fabrication of other fuels, …).

Those two effects also produce an effect on the amount of plutonium at the reactor discharge. This is not an exhaustive list of fuel fabrication model impacts on fuel cycle studies, but this work will only focus on them and will not consider potential consequences on the fuel composition change after depletion due to over/under-estimate the amount of plutonium in the MOX fuel.

In order to investigate those impacts across multiple fuel cycle simulation tools and associated models, the following experience has been designed.

3.3. Exercise specifications

The exercise is divided in two independent parts related to the reactor involved. PWR and SFR will be considered in this work.

The schematic representation of the fuel cycle is shown on Fig. 1. The simulation includes infinite streams of materials (large enough to build all the fuels in all options): one plutonium stream and one depleted uranium stream. Both streams feed a fuel fabrication plant, which builds the MOX fuel for the reactor (PWR or SFR) according to its technical requirements. The reactor spent fuel is sent away to a storage facility or to the waste.

The simulation lasts one single reactor cycle. At $t = 0$, the fabrication plant produces the fresh fuel according to reactor requirements. To avoid radioactive decay, the fabrication process and the reactor fuel loading are simultaneous and instantaneous. The MOX-fuel stays in the reactor for a full cycle (it reaches its designed BU) and is then sent to the back-end storage. It is expected that, for a set of reactors, the MOX-fuel plutonium content needed to achieve a given BU depends on the plutonium isotopic composition. To highlight the difference between FLM and FF modeling, a large range of plutonium isotopic compositions have been considered.

Moreover the defined isotopic space has been designed to cover a wide range of fuel history: a CANDU fuel with low discharge BU (high fissile fraction (Guillemin, 2010)), PWR multi-recycled MOX fuel (high even isotopes fraction in the plutonium Courtin et al., 2017), long cooling time (low ^{241}Pu fraction).

The performance of the models is expected to depend widely on the plutonium used to build the fresh fuel. Therefore, the conclusion of this work cannot be transposed to a study where an only narrow plutonium isotopic space is encountered, in this case difference between an FF model and an FLM would probably be far smaller and an FF could be sufficient. Table 3 presents plutonium isotopic space covered in this work. Each plutonium vectors sampled in the framework of this study will be contained inside those isotopic ranges.

3.4. Problem-solving methodology

In order to investigate the impact of using an FLM rather than an FF model on fuel cycle simulations, the following experiment has been designed. For each simulator, the two fuel fabrication models will be compared within the same simulator and the same user, allowing the evaluation of the difference between two almost identical simulations: same simulator, reactor description, depletion algorithm, etc. The only difference being the method used to build the fresh fuel.

Table 3
Minimum and maximum mass fraction in weight % for plutonium vector at reactor beginning of cycle used in the framework of this work.

Isotope	Min. Mass Fr.	Max. Mass Fr.
Pu-238	0	10
Pu-239	25	90
Pu-240	0	40
Pu-241	0	25
Pu-242	0	30
Am-241	0	10

The experiment consists in running numerous small fuel cycle calculations according to specifications laid down above. We use a method that we call ”Wide Parametric Sweep” method. The principle is to randomly populate the predefined isotopic space (see in Table 3). For each random plutonium composition the simulation will be run twice, once using the FF model, i.e., the fraction of plutonium in the fuel is fixed regardless to its isotopic composition, and once with the FLM model adapting plutonium fraction in the fuel to its isotopic composition.

3.5. Global and local effects on the fuel cycle

Effects of using an FLM or an FF approach can be divided into two families: global effect and local effect. Fig. 2 illustrates those differences. On this figure, a simple fuel cycle example is used and is composed of the following facilities:

- a stock that feeds the reactor called ”upstream stock”
- a reactor that starts a unique cycle at $t = 6$ years up to $t = 10$ years
- a stock fed by the reactor spent fuel called ”downstream stock”

The case A (left plot) represents one cycle of a reactor in which the plutonium inventory time variations are the same, but the plutonium fractions at Beginning of Cycle (BoC) are different. In this case, we see that there is no global effect since the total inventory is similar. There are local effects since inventories in upstream and downstream stocks are different for the two examples. The case B (right plot) represents a case in which the plutonium fraction at BoC is similar to the two examples, but the plutonium time variations are different. For this specific case, there is a global effect that can be seen on the total inventory evolution. There are also local effects in the reactor and the downstream stock located after the reactor. Nevertheless, there is no effect on the upstream stock that feeds the reactor.

To sum up, the global effect impacts the overall simulation, such as the total amount of some elements in the simulations (plutonium, minor actinides, …). The local effect may correspond to the amount of those

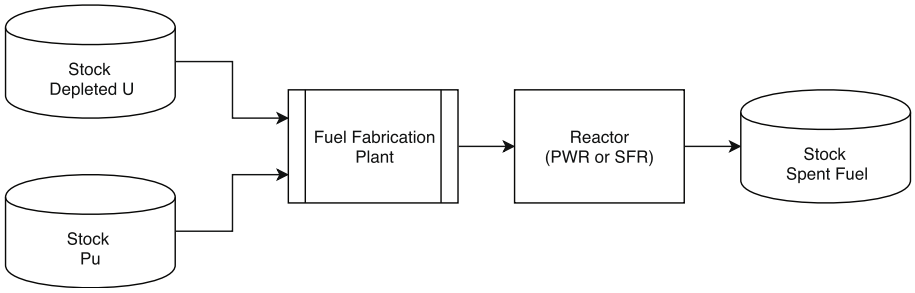

Fig. 1. Schematic representation of the simulated fuel cycle facilities.

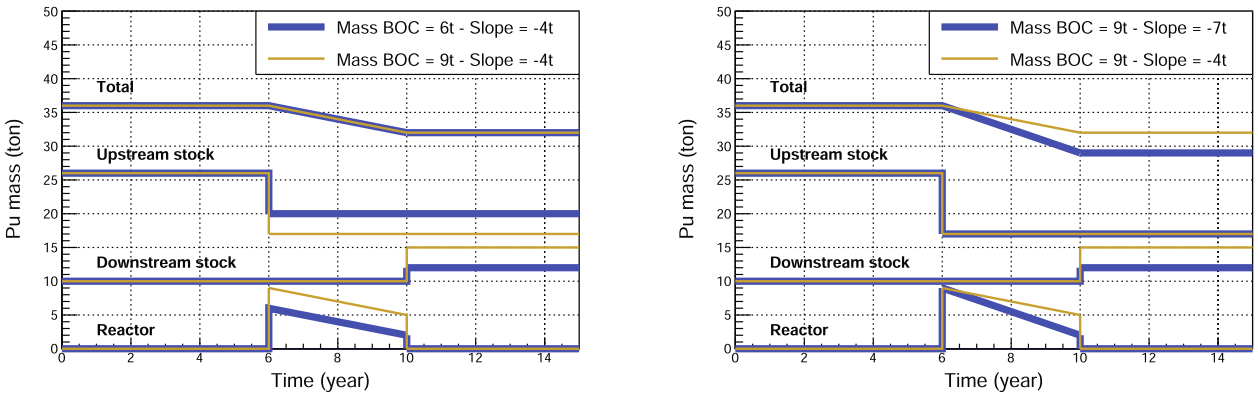

Fig. 2. Schematic view of the local and global effects on plutonium inventory. Two cases are represented. The plot on the left considers two cycles based on reactors loaded with 9 tons and 6 tons of plutonium with similar mass slopes during the irradiation. The plot on the right is based on two cycles with reactors loaded with 9 tons but with different mass slopes.

elements in specific facilities or storage. While global effects are associated with one or multiple local effects, local effects do not necessarily have a global impact, as another local effect can compensate their impacts.

3.6. Raw outputs

Each code produces for each reactor, PWR and SFR, two sets of output data representing FLM and FF runs. We call $M_{Pu}(BoC)$ and $M_{Pu}(EoC)$ the plutonium mass at BoC and End of Cycle EoC. Since there is ^{241}Am in the plutonium vector at BoC, this isotope is included in $M_{Pu}(BoC)$. At the end of the cycle, only plutonium isotopes are considered to calculate $M_{Pu}(EoC)$. M_{fuel} is the total mass of the fuel. For each case, outputs of interest are listed below:

- Plutonium fraction in the fuel at BoC:

$$F_{Pu}(BoC) = \frac{M_{Pu}(BoC)}{M_{fuel}}$$

- Plutonium fraction in the fuel at EoC:

$$F_{Pu}(EoC) = \frac{M_{Pu}(EoC)}{M_{fuel}}$$

- Plutonium isotopic fraction at BoC:

$$F_{Pu-i}(BoC) = \frac{M_{Pu-i}(BoC)}{M_{Pu}(BoC)}$$

- Plutonium fissile fraction in the fuel at BoC:

$$F_{Pu-fis}(BoC) = F_{Pu-239}(BoC) + F_{Pu-241}(BoC)$$

Pu −i represents the isotope i of the plutonium vector.

In order to measure the influence of using an FF versus an FLM in outputs, several estimators have been defined. Those estimators aim to highlight local and global effects and are defined in the following sections.

3.7. Estimators construction

From output data produced by the different simulators, estimators have been designed to measure the impact of using an FF model over an FLM.

The first estimator aims to measure the difference on the plutonium enrichment in the MOX fuel between the FLM and the FF. This estimator is a local estimator that measures local effects at each reactor loading that directly impacts the amount of plutonium present in the back-end part of the fuel cycle. This estimator is then proportional to the standard deviation of the plutonium fraction ($F_{Pu}(BoC)$) distribution at BoC. Indeed, this standard deviation shows the discrepancy of using an FLM approach compared to an FF approach when the fixed plutonium content is chosen as the plutonium fraction average of the FLM approach.

Estimator 1 has been defined as:

$$E_1 = \frac{\sigma(F_{Pu}^{FLM}(BoC))}{\mathbb{E}(F_{Pu}^{FLM}(BoC))} \quad (1)$$

$\sigma(F_{Pu}^{FLM}(BoC))$ represents the standard deviation of the distribution $F_{Pu}^{FLM}(BoC)$ built from all simulations run for each code. $\mathbb{E}(F_{Pu}^{FLM}(BoC))$ represents the average of the distribution $F_{Pu}^{FLM}(BoC)$. The higher the estimator 1 is, the higher the deviation between the plutonium fraction at BoC for FLM and FF approaches is. This estimator is used for both PWR and SFR analysis.

The second estimator aims to estimate the relative speed of plutonium consumption in the reactor between the FLM and the FF approach. One defines for one simulation the relative slope of plutonium consumption as follow:

$$\delta F_2^{mod} = \frac{F_{Pu}^{mod}(BoC) - F_{Pu}^{mod}(EoC)}{F_{Pu}^{mod}(BoC)} \quad (2)$$

Where mod can be FLM or FF. This equation can be written from plutonium fraction or mass. This parameter represents the relative plutonium consumption during one reactor cycle. For example, $\delta F_2^{FLM} = 0.30$ means that the plutonium fraction at EoC represents 70% of the fraction at BoC for the FLM data sample. The ratio between those two outputs is the calculated as:

$$R_2 = \frac{\delta F_2^{FLM}}{\delta F_2^{FF}} \quad (3)$$

With all simulations set for each code, it is then possible to plot the distribution for R_2. The second estimator E_2 is computed like a doublet composed by the mean value and the standard deviation of R_2 :

$$E_2 = \{\mathbb{E}(R_2), \sigma(R_2)\} \quad (4)$$

Estimator 2 measures a global effect since the plutonium consumption speed is calculated from evolution of the total plutonium mass. This estimator is suitable for reactor simulations characterized by plutonium decrease and is then used for PWR analysis.

In the SFR case, the estimator 2 can tend toward infinity if the reactor

is break-even for the FF approach. To avoid such behavior, a parameter inspired by the Fissile Inventory Ratio (FIR) (Perry and Weinberg, 1972; Guillemin et al., 2014) is created as:

$$\delta F_{2b}^{mod} = \frac{F_{Pu}(EoC)}{F_{Pu}(BoC)} \quad (5)$$

The relative deviation from the parameter defined in Eq. 5 for FLM compared to FF approach is defined as following:

$$R_{2b} = 100 \cdot \frac{\delta F_{2b}^{FLM} - \delta F_{2b}^{FF}}{\delta F_{2b}^{FF}} \quad (6)$$

From this distribution that can be defined for each simulator, the estimator E_{2b} is defined as the doublet composed by the mean value and the standard deviation of R_{2b} :

$$E_{2b} = \{\mathbb{E}(R_{2b}), \sigma(R_{2b})\} \quad (7)$$

Estimator 2b measures a global effect and will be used for SFR results.

The third estimator measures the absolute speed of plutonium consumption in the reactor between the FLM and the FF approach. First, we define for one simulation the relative slope of plutonium consumption as:

$$\delta F_{3}^{mod} = 100 \cdot \frac{F_{Pu}^{mod}(BoC) - F_{Pu}^{mod}(EoC)}{T_C} \quad (8)$$

Where mod can be FLM or FF. T_C is the reactor cycle time, connected to the reactor BU and the specific thermal power. This parameter represents the absolute plutonium balance during one reactor cycle. For example, $\delta F_3^{FLM} = 0.5\% \cdot y^{-1}$ means that the plutonium content in the fuel decreases at a rate of 0.5% each year on average for the FLM data sample. The ratio between FLM and FF factor is the calculated as:

$$R_3 = \frac{\delta F_3^{FLM}}{\delta F_3^{FF}} \quad (9)$$

Statistical parameters can be calculated from the distribution of R_3 for all simulations performed with one fuel cycle tool. The third estimator E_3 is computed like a doublet composed by the mean value and the standard deviation of R_3:

$$E_3 = \{\mathbb{E}(R_3), \sigma(R_3)\} \quad (10)$$

Estimator 3 measures a global effect since the plutonium consumption speed is calculated from evolution of the total plutonium mass. This estimator will be used for PWR analysis.

The estimator 3 can also tend toward infinity if the reactor is break-even for the FF approach. The SFR estimator 2 is then considered precise enough to estimate FLM effect for SFR calculation.

4. Reactors characteristics

This section aims to present briefly reactor models used by each simulator to describe PWR and SFR. In the proposed exercise, each participant is free to choose reactor technical parameters.

4.1. PWR simulations description

4.1.1. ANICCA

The PWR used by the code ANICCA target a BU of 41GW·d/t. The load factor is 85% and the thermal power is $3GW_{th}$. The fuel heavy mass represents 22.291t/y. The cycle time is then 1390 EFPD. Finally, the FLM is based on Baker and Ross approach (Baker and Ross, 1963).

4.1.2. CLASS

The PWR used by the code CLASS is based on infinite assembly reactor model for which reactivity time dependency is predicted by neural network (Leniau et al., 2015). The fuel cycle simulation considers a heavy mass of 72 tons in the PWR. The thermal power and load factor are respectively $3GW_{th}$ and 75%. The BU is 34GW·d/t.

4.1.3. COSI

The reactor simulated in COSI is a $3GW_{th}$ PWR. The BU is 45GW·d/t. The FLM used in the framework of this exercise is a data-driven approach based on neutronic evaluations to calculate plutonium content at BoC.

4.1.4. CYCLUS

The reactor simulated in CYCLUS is a $2.7GW_{th}$ PWR, loaded with 72 tons of heavy nuclides. The BU is around 41.1GW·d/t. The FLM used in the framework of this exercise is using a Baker and Ross approach to calculate plutonium content at BoC.

4.1.5. TR_EVOL

The reactor simulated in TR_EVOL code has a $1.13GW_{th}$ thermal power and a load factor of 0.9%. The targeted BU is 40GW·d/t and the irradiation cycle time is around 1470 days. The FLM used in the framework of this exercise is using a Baker and Ross approach to calculate plutonium content at BoC.

4.2. SFR simulations description

4.2.1. CLASS

The SFR used by the code CLASS for this exercise has a $3GW_{th}$ loaded with approximately 72 tons of heavy nuclei with a load factor of 0.75 leading to a BU close to 105GW·d/t. The FLM is based on the prediction of the reactivity coefficient at beginning of the cycle according to the plutonium isotopic composition thanks to an artificial neural network, trained on thousands of previous full-core criticality calculations.

4.2.2. TR_EVOL

The reactor simulated in TR_EVOL is a $3.6GW_{th}$ SFR, loaded with 45 tons of heavy nuclides. The load factor is 90%. The BU is around 136GW·d/t. The FLM used in the framework of this exercise is using a Baker and Ross approach to calculate plutonium content at BoC. The SFR concept is based on the benchmark described in (McCarthy et al., 2012).

4.2.3. JOSSETE

The reference SFR core used in JOSSETE for the exercise is the $3.6GW_{th}$ ESFR (European Sodium-cooled Fast Reactor) core with oxide fuel, developed in the framework of the CP-ESFR project (Fiorini et al., 2011). The core contains 225 hexagonal inner fuel assemblies and 228 outer fuel assemblies with different plutonium content. The actinide mass of the core is 71.4 tons, and the average discharge BU of the fuel is 103GW·d/t (5 cycles of 410 EFPD). The FLM used in the exercise applies iteration of the plutonium fraction with secant method, based on second-order polynomial fitting of the k_{eff} as a function of the fuel composition (16 actinides and total FP mass) obtained from two thousand full-core calculations.

5. Results for Pressurized Water Reactor

This section presents the different calculation results from the different simulators and the estimator distributions defined in the previous section. This section focuses on PWR results.

5.1. Plutonium input vectors at beginning of cycle

Plutonium vectors used by each code are represented on Fig. 3. A box plot representation has been chosen. It shows the median and quartile (q1, q3) for plutonium isotopes fraction for each code. The figure shows that the different designs of experiments are roughly similar. Nevertheless, the COSI6 sampling shows a more focused range, especially for ^{239}Pu.

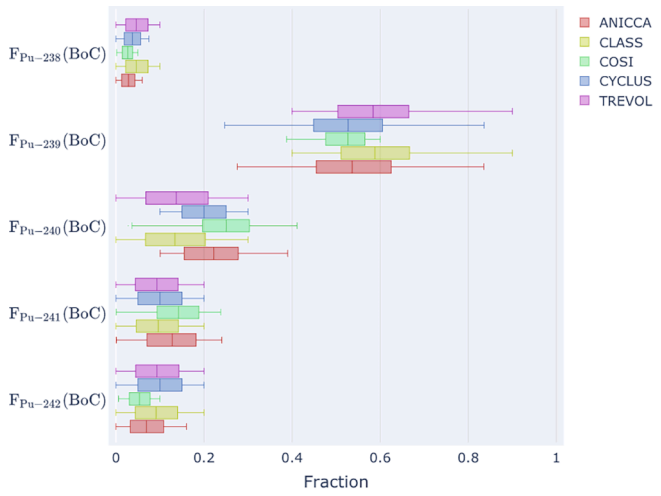

Fig. 3. Plutonium vectors represented as a box plot for all simulators. ANICCA code is in red. CLASS code is in yellow. COSI6 is in green. CYCLUS in blue and TR_EVOL in violet.

5.2. *Plutonium fraction analyses*

Fig. 4 left column presents the plutonium fraction at BoC predicted by each FLM and the plutonium fraction at EoC deduced by each software. As each FLM as the sampling for each simulator is different, the BoC plutonium fractions differ between simulators. The widest prediction is given by the CLASS code that predicts plutonium fraction from 4% up to 15%. This range is a direct consequence of the plutonium sampling used for this work. A 15% plutonium content is outside typical industrial range but some plutonium isotopic composition sampled are also unrealistic with their low fraction of fissile isotopes (^{239}Pu and ^{241}Pu). This simply reflects the algorithm result without any control. These extreme values that FLMs may reach may be problematic. However, this is a question for each FLM developer to answer and is not within the scope of the FIT project.

The EoC plutonium fractions have collectively lower values than the BoC fractions, showing plutonium net consumption during the irradiation like it should be in PWRs.

Fig. 4 also shows (right column) the plutonium fraction at BoC and EoC according to the fissile plutonium fraction. For BoC data, a negative correlation is observed for all simulators. That illustrates the fact that a high fissile content of the plutonium vector is associated with a small plutonium content in the fresh fuel: at a constant burn-up, the plutonium content in the fresh fuel increases to compensate the fissile content

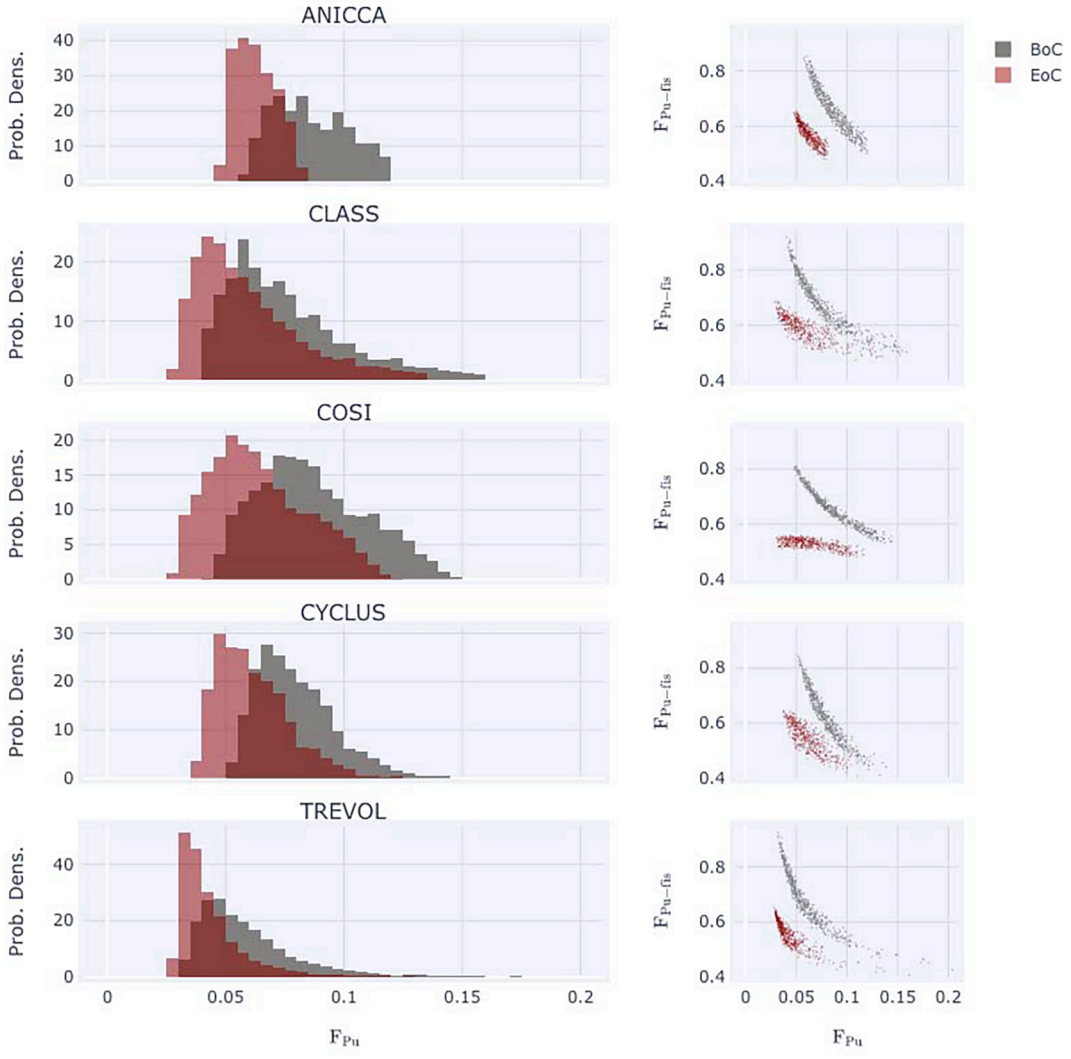

Fig. 4. Plutonium fraction at BoC (gray distribution) and EoC (red distribution) for all the codes (left column). The right column represents the plutonium fraction dependency according tho the fissile content of the fuel at BoC and EoC.

decrease. Similar behaviors are observed at EoC except for COSI6 that shows a smaller fissile content in the spent fuel for small plutonium content at BoC. This tends to show that COSI6 burns more fissile plutonium than other simulators.

5.3. Estimators calculations

5.3.1. Estimator 1

Estimator 1 quantifies biases created by the use of an FF model on the plutonium enrichment calculation for the fresh fuel construction. It measures the amount of plutonium used for MOX fuel fabrication.

Table 4 shows statistic parameters calculated from plutonium distributions at BoC and EoC. The first estimator (E_1) has been calculated according to the definition provided by the Eq. 1.

Order of magnitude for estimator E_1 is similar among fuel cycle simulators and spreads from 19% up to 40%. This highlights the importance of the FLM by showing that between 20% and 40% of average local deviation could be observed by using an FF approach.

5.3.2. Estimator 2

Estimator 2 is based on the variations of the amount of plutonium consumption divided by the plutonium mass at BoC. It depends on the proportion of plutonium burnt during irradiation for FF and FLM approaches. Estimator 2 distribution gives an evaluation of the precision of total inventory estimation, regardless of the location of the plutonium.

The plots on the right column of the Fig. 5 represent scatter plots of δF_2^{FF} versus δF_2^{FLM} superimposed with the function $\delta F_2^{FF} = \delta F_2^{FLM}$. Points on the line mean that relative plutonium mass consumption is similar between FLM and FF. CLASS, COSI6 and CYCLUS show similar trends with a positive correlation between δF_2^{FF} and δF_2^{FLM}. TR_EVOL and ANICCA differ since a negative correlation is observed between δF_2^{FF} and δF_2^{FLM}.

First, it is observed that the plutonium net consumption for FF approach (quantified by δF_2^{FF}) weakly depends on the plutonium isotopic fraction. This behavior is common to all simulation codes.

The positive trend (CLASS, COSI6 and Cyclus) is explained as follows. For the FLM approach, a high quality plutonium is characterized by a high fissile content (marker color tends to be blue). This corresponds to a small plutonium content at BoC (See Fig. 4) which means that the plutonium net consumption is low compared to other simulations. Indeed, the smaller the plutonium fraction in the fresh fuel is, the smaller the plutonium mass decrease during the evolution is. Nevertheless, the factor δF_2^{FLM} represents the plutonium consumption divided by the initial plutonium fraction, which is also small in this case. This last effect is the most important and blue markers are then characterized by a high value of δF_2^{FLM}.

A good quality plutonium loaded from an FF approach is also characterized by a small conversion rate in the reactor: fission reactions are mainly generated by the fissile materials in the core. As a consequence, the plutonium net consumption is high and blue markers correspond to a high value of δF_2^{FF}.

If plutonium quality decreases (markers color tends to be orange and yellow), the denominator effect of the parameter δF_2^{FLM} leads to a decrease for this factor since plutonium content at BoC increases.

For the FF approach, the plutonium content at BoC is unchanged. As the fissile content of the plutonium is smaller, there is a higher uranium to plutonium conversion and the net plutonium consumption is smaller, therefore so is the δF_2^{FF} parameter.

On the other hand, a negative trend for δF_2^{FF} and δF_2^{FLM} relation (ANICCA and TR_EVOL) is explained the same way for the FF approach. The difference is coming from the FLM approach. In this case, the effect of the plutonium consumption slope is dominant compared to the effect of the denominator.

It is worth pointing out that for all codes, the smaller difference between FF and FLM approaches is reached for plutonium fissile fraction in fuel close to 65%. This can be verified by checking regions for which the distributions correspond with the line $\delta F_2^{FF} = \delta F_2^{FLM}$. This plutonium fissile fraction corresponds to a standard MOX fuel and this highlights the fact that the FF approach deviation increases with the exotic level of plutonium composition.

Plots on the left column of the Fig. 5 represent distribution of R_2 for all simulation codes. Two trends are visible in those distributions: CLASS, COSI6 and CYCLUS show limited bias whereas TR_EVOL and ANICCA calculates larger biases. From those distributions, it is possible to calculate the estimator E_2, which is summarized in Table 5.

According to standard deviations calculated, effect of using an FLM produces a difference on the plutonium relative consumption between 9% up to 19%. This impact will be propagated in fuel cycle calculation at each reactor fuel loading.

5.4. Estimator 3 for PWR

By definition, the estimator 3 is quite similar to the estimator 2. The difference is coming from the denominator in the calculation of the parameter δF_3^{mod} (See Eq. 8). This estimator is based on the variations of the amount of plutonium consumption divided by the reactor cycle time. Associated distributions also provide an assessment of the effect of the fuel loading methods on the total plutonium inventory. Fig. 6 shows the distribution of R_3 variable for all the simulators. The scatter plots representing δF_3^{FF} versus δF_3^{FLM} are also represented in order to add information related to R_3 distributions.

Two types of tendencies appear for the scatter plots analyses (right column). CLASS, COSI6 and CYCLUS show constrained values for δF_3^{FLM} and δF_3^{FF} since wider values are observed for ANICCA and TREVOL. Unlike the case presented for estimator 2 in the previous paragraph, the scatter plot analysis is here similar for all codes and is interpreted as follows. For the FLM approach, a high quality plutonium (blue points) corresponds to a small plutonium content at BoC. The absolute net plutonium balance during the irradiation cycle is then limited and the value of δF_3^{FLM} is small. Decreasing the plutonium quality induces an increase of the plutonium content at BoC and then, a higher absolute net plutonium balance during the reactor cycle. The value of δF_3^{FLM} increases then.

For the FF approach, a high quality plutonium is loaded at a constant plutonium content at BoC. In those conditions, neutron flux in the fuel is relatively low by power normalization. With a rather low neutron flux, the ^{238}U capture rate leads to a small plutonium production. As a consequence, the value of δF_3^{FF} is high. For a smaller plutonium quality, as fissile content decreases, the neutron flux increases to reach the reactor required thermal power. As a consequence, uranium to plutonium conversion increases and plutonium absolute mass decrease during the reactor cycle is smaller.

The distribution of R_3 variable for all simulators (left column) allows calculating estimator 3 values, summarized in Table 6.

For the estimator 3, similar conclusions can be drawn than in the previous section. CYCLUS and COSI6 show limited deviation, respectively 11% and 13%. CLASS has a 22% bias on the total plutonium net

Table 4
Statistic parameters calculated from plutonium fraction distribution at BoC. The mean plutonium fraction and the standard deviation are computed for BoC and EoC distributions. The estimator E_1 is also represented.

Code	$\mathbb{E}(F_{Pu}^{FLM}(BoC))$	$\sigma(F_{Pu}^{FLM}(BoC))$	E_1
ANICCA	0.086	0.016	0.19
CLASS	0.076	0.025	0.33
COSI6	0.087	0.023	0.26
CYCLUS	0.079	0.016	0.20
TR_EVOL	0.060	0.024	0.40

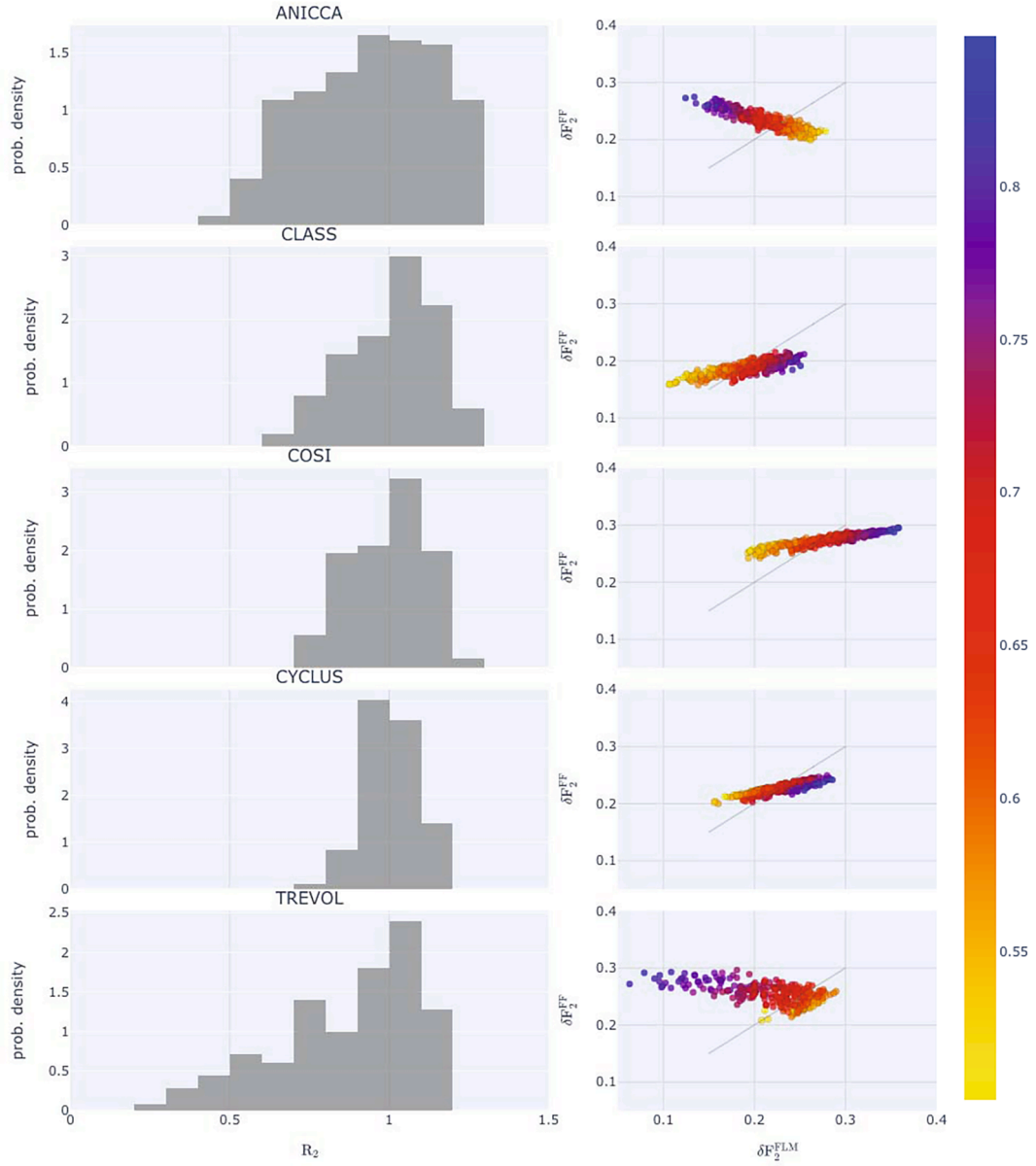

Fig. 5. Distribution of R_2 variable for all the fuel cycle simulators (left column). Scatter plot of δF_2^{FF} versus δF_2^{FLM} for all the codes (right column). The color scale on the right represents the plutonium fissile fraction of the plutonium vector at BoC. The function $\delta F_2^{FF} = \delta F_2^{FLM}$ is represented in gray.

Table 5
Estimator 2 doublet parameters calculated from R_2 distribution.

	E_2	
Code	$\mathbb{E}(R_2)$	$\sigma(R_2)$
ANICCA	0.95	0.18
CLASS	1.01	0.11
COSI6	1.00	0.12
CYCLUS	1.00	0.09
TR_EVOL	0.89	0.19

consumption rate. ANICCA reaches a bias around 34% while TR_EVOL deviation is close to 47%. Those results show that the impact of using a FLM approach rather than a FF approach on plutonium evolution is non-negligible for all codes.

6. Results for Sodium Fast Reactor

This section presents the different calculation results from the different simulators and the estimator distribution for the SFR simulations.

6.1. Plutonium vectors at beginning of cycle

Plutonium vector used by each code is represented on Fig. 7. A box plot representation has been chosen. It shows the median and quartile (q1, q3) for each code and plutonium isotopes. Design of experiments are in this case also very close. CLASS and JOSSETE allow very small ^{239}Pu isotopic fraction in the fresh fuel.

6.2. Plutonium fraction analyses

Fig. 8 left column presents the plutonium fraction at BoC predicted by each FLM and the plutonium fraction at EoC deduced by each

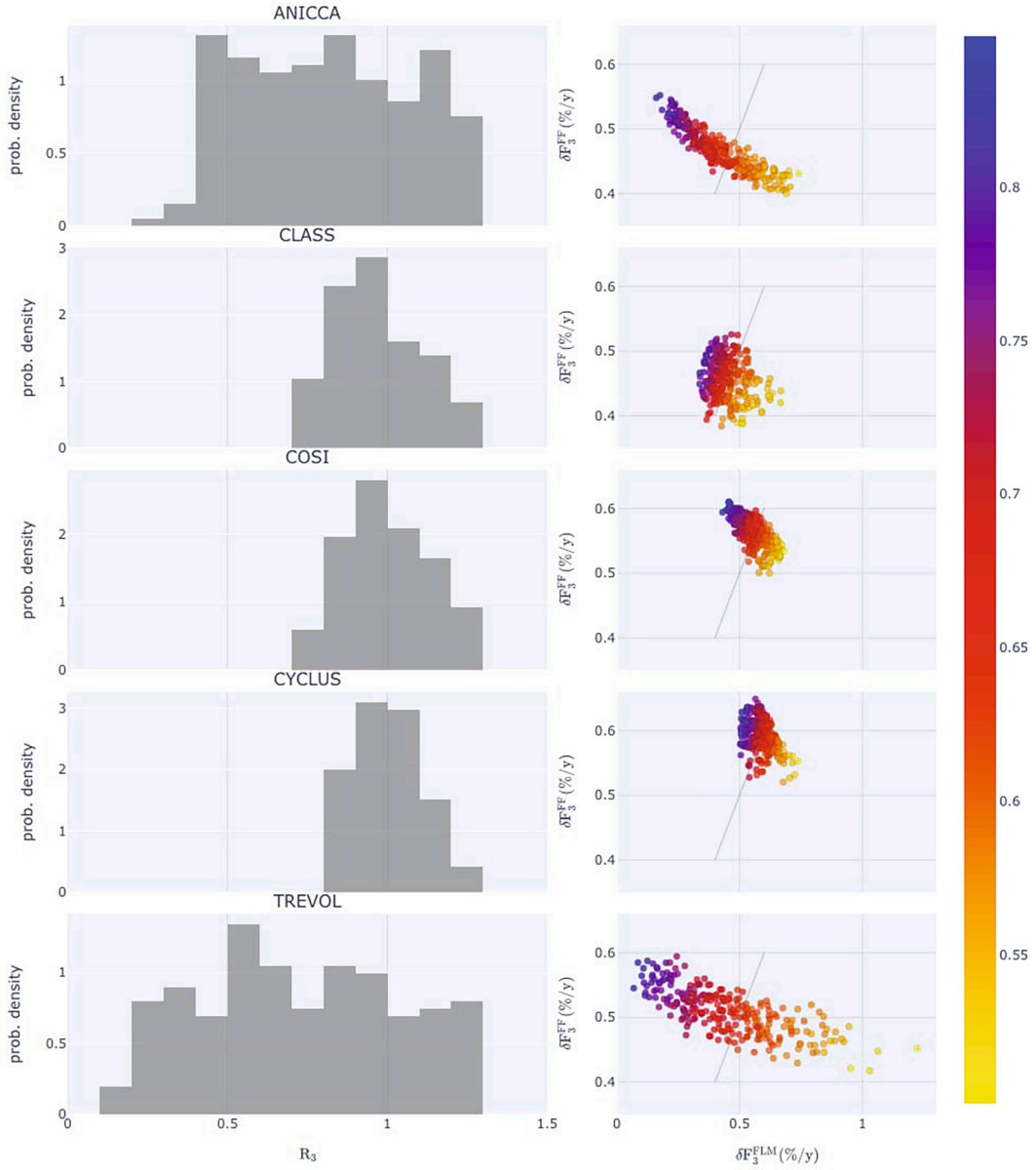

Fig. 6. Distribution of R_3 variable for all the fuel cycle simulators (left column). Scatter plot of δF_3^{FF} versus δF_3^{FLM} for all the codes (right column). The color scale on the right represents the plutonium fissile fraction of the plutonium vector at BoC. The function $\delta F_3^{FF} = \delta F_3^{FLM}$ is represented in gray.

Table 6
Estimator 3 doublet parameters calculated from R_3 distribution.

	E_3	
Code	$\mathbb{E}(R_3)$	$\sigma(R_3)$
ANICCA	0.95	0.34
CLASS	1.01	0.22
COSI6	1.00	0.13
CYCLUS	1.00	0.11
TR_EVOL	0.92	0.47

software for SFR calculations. As each FLM and the sampling for each simulator is different, the BoC plutonium fractions differ between simulators. From left column distributions, it appears that CLASS and JOSSETE have similar plutonium content at reactor BoC since TR_EVOL is characterized by higher values. It is also shown that, on average, CLASS SFR is a breeder reactor, JOSSETE SFR is iso-breeder and TR_EVOL SFR is plutonium incinerator.

The Fig. 8 also shows the plutonium fraction at BoC and EoC according to the fissile plutonium fraction (right column). BoC data are characterized by a negative correlation which means that a good fissile plutonium quality needs less plutonium to reach a given BU. Simulations from JOSSETE code show that the SFR is iso-breeder whatever the plutonium content is.

6.3. Estimators calculations

6.3.1. Estimator 1

This section aims to present estimator 1 calculations that represent bias created by the use of an FF approach for SFR calculations. Table 7 shows statistic parameters calculated from plutonium distributions at BoC and EoC presented in Fig. 8.

The estimator 1 for SFR are similar to the three fuel cycle simulators used in this work. From 10% to 14%, calculated values are smaller than PWR values, which can be explained by the higher mean plutonium content at SFR BoC since similar standard deviation distributions are

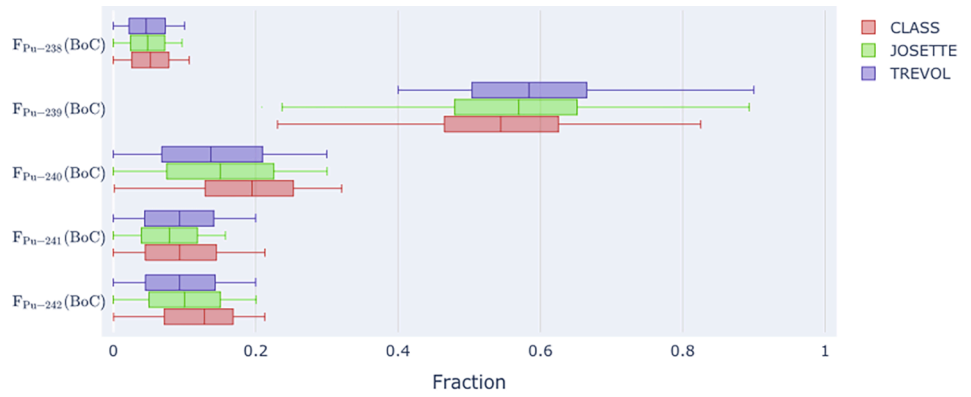

Fig. 7. Plutonium vectors represented as box plots for all simulators. CLASS code is in red. JOSSETE code is in green and TR_EVOL in blue.

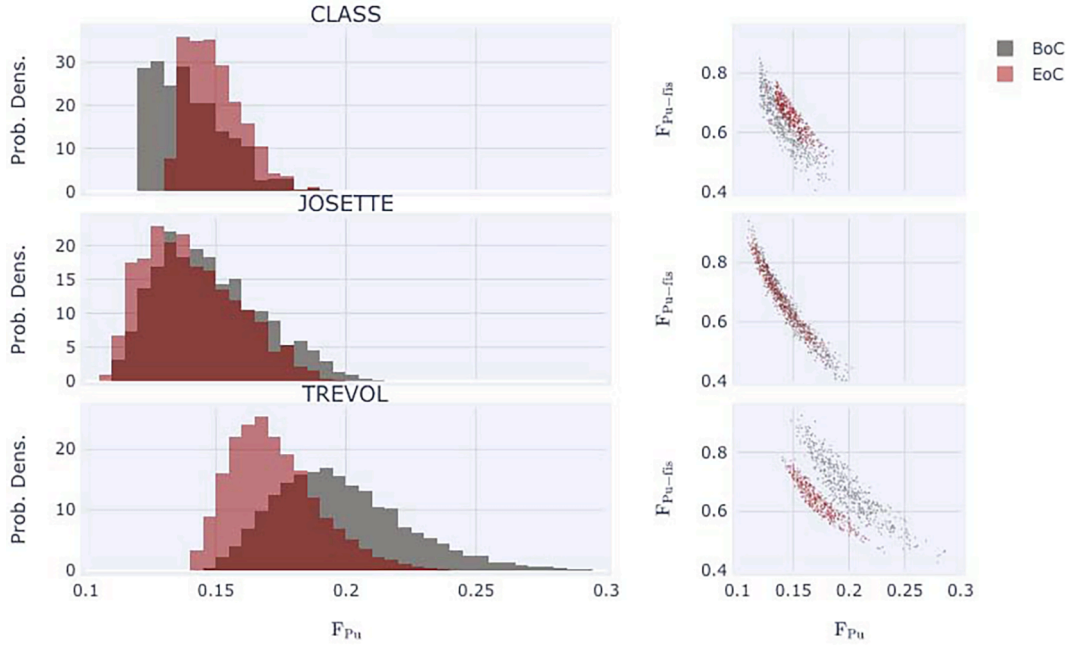

Fig. 8. Plutonium fraction at BoC (gray distribution) and EoC (red distribution) for all the codes (left column). The right column represents the plutonium fraction dependency according to the fissile content of the fuel at BoC and EoC.

Table 7
Statistic parameters calculated from plutonium fraction distribution at BoC and EoC for SFR calculations. The mean plutonium fraction and the standard deviation are computed for BoC and EoC distributions. The estimator E_1 is also represented.

Code	$\mathbb{E}(F_{Pu}^{FLM}(BoC))$	$\sigma(F_{Pu}^{FLM}(BoC))$	E_1
CLASS	0.140	0.014	0.10
JOSSETE	0.148	0.020	0.14
TR_EVOL	0.199	0.026	0.13

observed. This points out the fact that the effect of using an FLM seems to be less important in SFR applications.

6.3.2. *Estimator 2b*

Fig. 9 highlights data used to calculate estimator 2b for SFR.

The plots on the right column of Fig. 9 represent scatter plots of δF_{2b}^{FF} versus δF_{2b}^{FLM} superimposed with the function $\delta F_{2b}^{FF} = \delta F_{2b}^{FLM}$. A value higher (resp. lower) than 1 indicates that the SFR is breeder (resp. incinerator). Scatter plots show that CLASS SFR is breeder for almost all simulations runs from FLM approach, and closed to the break-even for FF approach. For this code, a negative trend is observed. That means that if FLM approach leads to a high plutonium breeding, this will correspond to a small plutonium breeding for the FF approach. TR_EVOL code has a similar trend, but SFR simulations are plutonium incinerator. Finally, JOSSETE results show that the SFR is closed to break-even. Also, for this code, δF_{2b}^{FF} and δF_{2b}^{FLM} approaches lead to similar evolution.

Plots on the left column of Fig. 9 represents distribution of R_{2b} for all simulation codes. Here, the distribution deviation for the JOSSETE code is much smaller compared to CLASS and TR_EVOL. This means the effect of using an FLM in JOSSETE is small compared to other codes. From those distributions, it is possible to calculate the estimator E_{2b}, which is summarized in Table 8.

This table shows that using an FF approach induces a deviation on the reactor cycle inventory evolution. The relative deviation is measured by the standard deviation and close to 2% for JOSSETE, and 6% for TR_EVOL and CLASS. If those deviations are not negligible, the effect is not so important for the design of experiments used in this work, especially when compared to the effects observed for PWR.

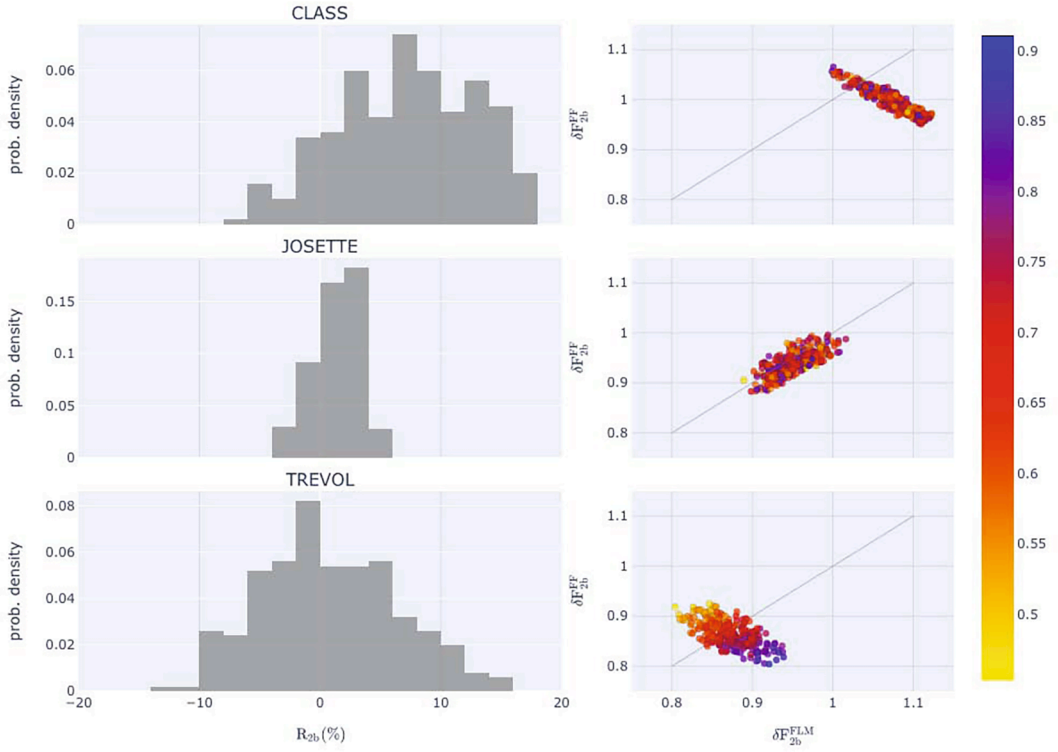

Fig. 9. Distribution of R_{2b} variable for all the fuel cycle simulators (left column). Scatter plot of δF^{FF}_{2b} versus δF^{FLM}_{2b} for all the codes (right column). The color scale on the right represents the plutonium fissile fraction of the plutonium vector at BoC. The function $\delta F^{FF}_{2b} = \delta F^{FLM}_{2b}$ is represented in gray.

Table 8
Estimator 2b doublet parameters calculated from R_{2b} distribution for SFR simulations.

	E_{2b}(%/cycle)	
code	$\mathbb{E}(R_{2b})$	$\sigma(R_{2b})$
CLASS	7.2	5.6
JOSSETE	1.3	1.9
TR_EVOL	0.8	5.7

7. Conclusions and Perspectives

Substantial resources have been invested in a variety of nuclear fuel cycle simulators, whether to serve specific purposes, or as they expanded to more general purposes. However, confidence in each new analysis remains fragile because of a lack of generic methodology to develop confidence in such tools. Fuel cycle simulators can be used to answer different questions that require different levels of precision. To increase the confidence level of those studies, all institutions are willing to increase the level of complexity of the software even if it does not necessarily improve the precision of the calculations.

This paper presents the FIT project that provides a rigorous scientific method allowing researchers, developers and analysts to determine whether a feature, a functionality or a model refinement is required to perform a nuclear fuel cycle study within a certain precision goal.

The FIT project is not a benchmark. The goal is not inter-simulator but intra-simulator comparisons. The impact of each functionality is assessed by comparing the simulator outputs from the same simulator, with and without the functionality to test. Outputs of interest are not physical quantities observable in the fuel cycle, but the deviations between the results with and without the functionality. The strength of this project relies on the diversity of simulators used to solve the different problems that make it possible to reach nearly simulator-agnostic conclusions. Following this principle, the FIT project will provide information about which functionalities are required according to the question that needs to be answered and the precision level to reach.

The work presented here is dedicated to fuel cycle simulators ability to vary fresh fuel compositions according to the available materials. Two treatments have been considered: a fixed enrichment for fresh fuels, regardless of the isotopic composition, or a model to adjust the fresh fuel composition in accordance with the isotopic composition of materials available in spent fuel stocks. For this first exercise, the output estimators focus on availability of the plutonium in the fuel cycle. As a consequence, results are probably more valuable for fuel cycle study involving plutonium recycling.

In agreement with the FIT project principles, all calculations were performed with a fixed fraction and with the use of a model that calculates fissile enrichment for fresh fuels. Some inter-software comparisons have been performed but each code is tested against itself. FF and FLM have been compared on two different reactors technologies, across many simulators (ANICCA, CLASS, COSI6, TR_EVOL and CYCLUS) for the PWR and (CLASS, TR_EVOL, JOSETTE) for the SFR. The importance of adjusting fresh fuel compositions have been tested around 3 estimators designed to quantify global and local effects on plutonium inventory.

In the analysis related to PWR loaded with MOX fuel, it is shown that using an FLM approach has an important impact on plutonium fractions at BoC. This impact has been quantified as the coefficient of variation of the required plutonium content at BoC and ranges between 19% and 40% depending on fuel cycle simulators. This effect represents a local effect since more or less quantity of plutonium will be taken and pushed from stocks. This can have a strong impact on outputs which are connected to stock data, such as estimated time for deploying a new reactor technology. Global effect for PWR loaded with MOX fuel are also quantified. It is shown that the effect of using an FLM produces a difference on the plutonium relative consumption that ranges from 9% to 22%. In addition, using an FLM introduces between 11% and 18% bias on the total plutonium net consumption rate. In conclusion, we have

shown that using an FLM approach has a significant effect on plutonium local and global inventories. This conclusion can be nevertheless tempered. A large plutonium isotopic space has been used and the calculated effect probably decreases with the size of the isotopic space. For very well-tuned fuel cycle simulations based on standardized plutonium isotopic composition, using an FF approach may be justified.

In the analysis related to SFR, it is shown that using an FLM approach leads to smaller effects. The coefficient of variation of the required plutonium content at BoC has been calculated between 10% and 14%. This local effect is not negligible, but can be put in perspective with simulation uncertainties related to SFR. It is also shown that the effect of using an FLM for SFR calculations produces a deviation on the plutonium inventory ratio between 2% and 6%. If those deviations are not negligible, the effect is not so important for the design of experiments used in this work.

All the results presented here aim to estimate biases induced by an FF for plutonium enrichment for fresh-fuel composition. They do not give any clues about FLM accuracy and relevance. To qualify FLM, benchmarks and comparison with full-core calculations are needed. Those are out of the FIT project scope and is the responsibility of each software developers. The estimators treated here are linked to plutonium inventories for reprocessing studies. Whether FF induces bias on other output of use for other applications should be assessed in the future within other exercises designed on purpose.

CRediT authorship contribution statement

N. Thiollière: Methodology, Investigation, Writing - original draft. **X. Doligez:** Methodology, Investigation. **G. Krivtchik:** Methodology, Investigation. **Ivan Merino:** Investigation, Methodology. **B. Mouginot:** Methodology, Investigation. **Aris Skarbeli:** Investigation, Methodology. **A. Hernandez-Solis:** Investigation, Methodology. **F. Alvarez-Velarde:** Writing - review & editing. **F. Courtin:** Writing - review & editing. **H. Druenne:** Writing - review & editing. **M. Ernoult:** Writing - review & editing. **K. Huff:** Writing - review & editing. **M. Szieberth:** Writing - review & editing. **B. Vermeeren:** Writing - review & editing. **P. Wilson:** Methodology.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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References

A. Baker, R. Ross, Comparison of the value of plutonium and uranium isotopes in fast reactors, Tech. rep., ANL (1963).

C. Coquelet-Pascal, M. Tiphine, G. Krivtchik, D. Freynet, C. Cany, R. Eschbach, C. Chabert, Cosi6: A tool for nuclear transition scenario studies and application to sfr deployment scenarios with minor actinide transmutation, Nuclear Technology 192 (2) (2015) 91–110. arXiv:https://doi.org/10.13182/NT15-20, doi:10.13182/NT15-20. url:https://doi.org/10.13182/NT15-20.

Courtin, F., Leniau, B., Thiollière, N., Mouginot, B., Doligez, X., Somaini, A., Zakari-Issoufou, A.-A., David, S., Bidaud, A., Clavel, J.-B., 2017. Neutronic predictors for pwr fuelled with multi-recycled plutonium and applications with the fuel cycle simulation tool class. Progress Nuclear Energy 100, 33–47. https://doi.org/10.1016/j.pnucene.2017.04.018 url:http://www.sciencedirect.com/science/article/pii/S0149197017300938.

G. Fiorini, A. Vasile, European commission – 7th framework programme: The collaborative project on european sodium fast reactor (cp esfr), Nuclear Engineering and Design 241 (9) (2011) 3461–3469, seventh European Commission conference on Euratom research and training in reactor systems (Fission Safety 2009). doi:10.1016/j.nucengdes.2011.01.052. url:http://www.sciencedirect.com/science/article/pii/S0029549311001737.

P. Guillemin, Recherche de la haute conversion en cycle thorium dans les réacteurs candu et rep - développement des méthodes de simulation associées et étude de scénarios symbiotiques, Ph.D. thesis, Grenoble Institute of Technology, France (2010).

Guillemin, P., Nuttin, A., Bidaud, A., Brizi, J., Capellan, N., David, S., Meplan, O., Wilson, J., 2014. Feasible ways to achieve high conversion in thorium-fueled candu and pwr reactors. Revue Générale Nucléaire 62–72. https://doi.org/10.1051/rgn/20096062.

M.G. Halász, Development of a fast burn-up method and investigation of transmutation in Generation IV fast reactors, Ph.D. thesis, Budapest University of Technology and Economics, Doctoral School of Physical Sciences (2018).

Huff, K.D., Gidden, M.J., Carlsen, R.W., Flanagan, R.R., McGarry, M.B., Opotowsky, A.C., Schneider, E.A., Scopatz, A.M., Wilson, P.P., 2016. Fundamental concepts in the cyclus nuclear fuel cycle simulation framework. Adv. Eng. Software 94, 46–59. https://doi.org/10.1016/j.advengsoft.2016.01.014 url:http://www.sciencedirect.com/science/article/pii/S0965997816300229.

G. Krivtchik, Analysis of uncertainty propagation in nuclear fuel cycle scenarios, Theses, Université de Grenoble (Oct. 2014). url:https://tel.archives-ouvertes.fr/tel-01131207.

Leniau, B., Mouginot, B., Thiollière, N., Doligez, X., Bidaud, A., Courtin, F., Ernoult, M., David, S., 2015. A neural network approach for burn-up calculation and its application to the dynamic fuel cycle code CLASS. Ann. Nuclear Energy 81, 125–133. https://doi.org/10.1016/j.anucene.2015.03.035 url:http://hal.in2p3.fr/in2p3-01158081.

K.A. McCarthy, B. Dixon, Y.-J. Choi, L. Boucher, K. Ono, F. Alvarez-Velarde, E.M. Gonzalez, B. Hyland, Benchmark study on nuclear fuel cycle transition scenarios - analysis codes, Tech. rep., N.E.A., Nuclear Energy Agency of the OECD (NEA) (2012). url:http://inis.iaea.org/search/search.aspx?orig_q=RN:44089401.

Merino-Rodríguez, Iván, García-Martínez, Manuel, Álvarez-Velarde, Francisco, López, Daniel, Cross check of the new economic and mass balance features of the fuel cycle scenario code tr_evol, EPJ Nuclear Sci. Technol. 2 (2016) 33. doi:10.1051/epjn/2016029. url:https://doi.org/10.1051/epjn/2016029.

Mouginot, B., Leniau, B., Thiollière, N., Bidaud, A., Courtin, F., Doligez, X., Ernoult, M., 2015. MOX fuel enrichment prediction in PWR using polynomial models. Ann. Nuclear Energy 85, 812–819. https://doi.org/10.1016/j.anucene.2015.06.038 url:http://hal.in2p3.fr/in2p3-01189018.

A.M. Perry, A.M. Weinberg, Thermal breeder reactors, Annual Review of Nuclear Science 22 (1) (1972) 317–354. arXiv:https://doi.org/10.1146/annurev.ns.22.120172.001533, doi:10.1146/annurev.ns.22.120172.001533. url:https://doi.org/10.1146/annurev.ns.22.120172.001533.

I.M. Rodríguez, A. Hernández-Solís, N. Messaoudi, G.V. den Eynde], The nuclear fuel cycle code anicca: Verification and a case study for the phase out of belgian nuclear power with minor actinide transmutation, Nuclear Engineering and Technology doi:10.1016/j.net.2020.04.004. url:http://www.sciencedirect.com/science/article/pii/S1738573319309271.

A. Skarbeli, I. Merino Rodriguez, F. Alvarez-Velarde, A. Hernandez-Solis, G. Van den Eynde, Quantification of the differences introduced by nuclear fuel cycle simulators in advanced scenario studies, Annals of Nuclear Energy 137 (2020) 107160. doi:10.1016/j.anucene.2019.107160. url:https://www.sciencedirect.com/science/article/pii/S030645491930670X.

A. Somaini, Analysis of Biases Induced by a Simplified Modelisation on PWR Fuel Evolution-Neutron Leakage Impact in the Cell Calculations, Theses, Université Paris-Saclay (Sep. 2017). url:https://tel.archives-ouvertes.fr/tel-01687837.

Thiollière, Nicolas, Clavel, Jean-Baptiste, Courtin, Fanny, Doligez, Xavier, Ernoult, Marc, Issoufou, Zakari, Krivtchik, Guillaume, Leniau, Baptiste, Mouginot, Baptiste, Bidaud, Adrien, David, Sylvain, Lebrin, Victor, Perigois, Carole, Richet, Yann, Somaini, Alice, A methodology for performing sensitivity analysis in dynamic fuel cycle simulation studies applied to a pwr fleet simulated with the class tool, EPJ Nuclear Sci. Technol. 4 (2018) 13. doi:10.1051/epjn/2018009. url:https://doi.org/10.1051/epjn/2018009.