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Impact of Fuel Loading Models on Fuel Cycle Dynamic Simulations

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This paper shows how important fuel loading models are in nuclear scenario simulations as soon as material recycling, such as plutonium in MOX fuels, are involved. These models aim to identify the fresh fuel composition at each reactor loading in a scenario describing the nuclear fleet evolution. The paper focuses on plutonium recycling in PWRs on a simple academic study and considers several criteria for identifying the right amount of plutonium to be loaded in a given reactor at a given time. These criteria depend on the level of precision and complexity of the reactor modeling, which, historically, was based on infinite assembly depletion calculations. However, in recent years, improved reactor models based on 3D full-core simulations have been developed. This study shows the compromise between the accuracy of the reactor modeling, its numerical costs and the biases implied in a fuel cycle simulation.

KEYWORDS: *fuel cycle simulator, scenario simulations, fuel loading models, plutonium recycling, PWR MOX fuels*

I. Introduction

Nuclear scenarios aim to study the evolution of an entire nuclear fleet to quantify the impact of any change in the fleet such as the deployment of new reactors or the implementation of a new fuel management. They rely on fuel cycle simulators that model all units needed for the fuel fabrication and reprocessing and the reactors where this fuel is irradiated. In case of material recycling, such as plutonium in PWR MOX fuels studied in this paper, the fresh fuel fabrication modeling is of prime importance because it determines, for each reactor loading, the amount of fissile material that should be recovered from spent fuel and inserted in the fresh fuel assembly to be loaded. In these fuel loading models, it is important to take into account the plutonium isotopic vector as a fixed content may bring important biases in fuel cycle simulations.¹⁾ However, the criterion that links the plutonium content in fresh fuel assemblies to the plutonium isotopic composition should also be of prime importance. Usually, the criterion is the reactor average burn-up and the plutonium content is determined by 2D assembly calculations (infinite lattice). Recently, new fuel loading models have been developed based on 3D full-core calculations. Using 3D full-core calculations, the plutonium content in MOX fresh fuel in a PWR heterogeneous reactor can also be determined in such a way as to minimize the radial power factor knowing the UOX fresh fuel composition.²⁾

This work focuses on the impact in nuclear scenarios of different fuel loading models based on the same reactor simulations. It considers two scales for the depletion simulations - infinite lattice or 3D full-core calculations - and

three criteria – maximum achievable burn-up or 2D and 3D power distributions. Finally, some models involving both criteria with an optimization process are investigated.

The paper is organized as follows: a first section details the different fuel loading models that were built for this work, a second section presents the different biases of the plutonium content regarding different models, and the last section illustrates the possible propagation of these biases in an academic scenario study involving only one PWR loaded with MOX fuels.

II. Fuel Loading Model Presentation

1. General Overview

In fuel cycle simulators, the principle of fuel loading models is to determine the fuel initial composition that has to be loaded. Considering plutonium recycling in PWR MOX fuels, the fuel loading model evaluates the plutonium content in the fresh fuel, depending on the available plutonium isotopic vector and on other physical quantities associated to the core parameters.

The fuel loading model commonly relies on databases built from 2D infinite lattice calculations and the Pu content is determined such that the reactor can remain critical up to a given burnup. However, assembly calculations do not take into account the physical phenomena that happen at core scale and that are due to the fuel management, the core geometry or the position or neighborhood of assemblies. Recent works have shown that, first, compared with models using core calculations, models based on assembly calculations can lead to significant discrepancies in some plutonium inventories in fuel cycle simulations,^{2,3)} second, models using core calculations with different loading patterns can also introduce

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biases on the Pu content determination.⁴⁾ Moreover, since core modeling makes it possible to consider new physical quantities, in these same works, the Pu content is estimated in such a way that the power distribution is as flat as possible in the core.²⁾ Thus, various criteria can be used to link the Pu isotopic composition to the Pu content in MOX fresh fuels.

In this work, several criteria and core configurations are considered as core parameters. The fuel fabrication model is based on full core calculations and it is seen as the function of three variables given in Eq. (1).

$$\%Pu = f(\overrightarrow{Pu}, Core\ configuration, Criterion) \quad (1)$$

2. Description of the Studied Core Parameters

The purpose of this section is to detail the core parameters that are used to build various fuel loading models in this work. The PWRs studied are EPRs and two elements referring to their core configuration are studied: the MOX core fraction and the core loading pattern. Then, different approaches to link the Pu isotopic vector to the Pu content in the MOX fresh fuel are proposed.

(1) MOX Core Fraction

In order to analyze the biases introduced by a difference of MOX core fraction in the fuel loading models, two EPR cores loaded with 30% and 40% of MOX fuel are considered.

The 30% MOX core is the MOX version at equilibrium of the UK EPR design presented in the Pre-Construction Safety Report (PCSR).⁵⁾ It contains three types of UOX assemblies and one type of MOX assemblies, the loading pattern is given in **Fig. 1**.

The 40% MOX core is an original core built for this work. It originates from the 30% MOX core where MOX assemblies replace 32 UOX assemblies (UOX with 16 gadolinium pins). This 40% MOX core is named *40% (1)* in the rest of this work.

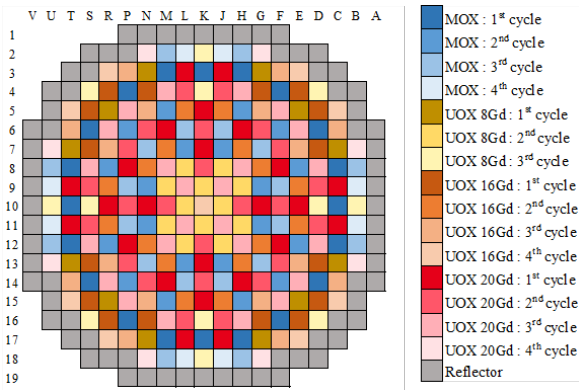


Fig. 1 Core loading pattern of the UK EPR 30% MOX core

(2) Core Loading Pattern

The second core configuration studied is the core loading pattern. Thus, three EPR cores loaded with 40% of MOX fuel are compared, they were all built for this work.

The first 40% MOX core is the core *40% (1)* presented in the previous section.

The second core is named *40% (2)* and originates from an optimization of the *40% (1)* MOX core. Between these two

cores, the position of some assemblies is swapped to flatten the power distribution.

The third core, named *40% (3)*, is derived from the 30% MOX core with MOX assemblies replacing 32 UOX assemblies (UOX with 20 gadolinium pins). The loading pattern of the *40% (3)* core is then optimized from scratch to flatten the power distribution.

(3) Fuel Fabrication Criterion

To estimate the Pu content in the MOX fresh fuel given a Pu isotopic vector, the criteria studied in this work are quoted:

- “LnatTarget”: this is the conventional criterion. The Pu content is determined to reach a cycle length target, which is 16 GWd/t in this paper. This target may be estimated thanks to infinite assembly calculations or full core calculations.^{3,6)}
- “min(F_{2D})”: the Pu content is chosen to minimize the 2D power peak per assembly (F_{2D}) in the core, given a fresh UOX fuel composition. This criterion only relies on full-core simulations;
- “min(F_{3D})”: similarly to the previous criterion, the Pu content is chosen to minimize the 3D power peak (F_{3D}). This criterion also only relies on full core calculations.

Concerning the LnatTarget criterion, given a Pu vector, if the cycle length cannot be reached for any Pu content in the range considered (which is here between 5% and 12%), the Pu content is set to 12.1%. These Pu vectors are then impossible to use for fresh fuel fabrication. 2D and 3D power peaks are also not constraints for the determination of the Pu content. For the min(F_{2D}) and min(F_{3D}) criteria, there is no composition exclusion, but the cycle length is not a constraint and there is no evidence that the reactor will reach the targeted cycle length.

3. 3D Full Core Models Construction

An efficient calculation scheme can be used to simulate a large number of core-scale evolutions, generating a database of different observables depending on the initial MOX composition. All the simulations have been performed with the deterministic codes APOLLO2 and CRONOS2.^{7,8)} This database enables the construction of surrogate models, artificial neural networks in this work, that will be used for the reactor fuel models in dynamic fuel cycle simulations.

(1) Full Core Depletion Simulation Databases

A sample of 500 MOX fresh fuel compositions was determined using the Latin Hypercube Sampling. The LHS method generates random samples in a multidimensional space, avoiding correlations. The sampling limits, presented in **Table 1**, were determined relatively roughly by identifying the limits of each isotope from the evolution of UOX and MOX fuels at different burn-up and cooling times. Some of the randomly selected compositions therefore appear unrealistic, but the simulation results obtained for these configurations help to consolidate the surrogate models. Similarly, the maximum Pu content is the authorized upper limit to comply with fabrication constraints. The database also can be analyzed to visualize the trends in the simulations

results, depending on the fresh MOX fuel composition.⁹⁾

Table 1 MOX fresh fuel composition phase space definition. The proportion of plutonium 240 is defined as the buffer to reach 100 % in the plutonium vector definition

	Pu content	²³⁸ Pu	²³⁹ Pu	²⁴¹ Pu	²⁴² Pu	²⁴¹ Am
Min	5.3 %	0.7 %	40 %	2 %	4 %	0 %
Max	12 %	5.0 %	65 %	14 %	12 %	3 %

(2) Artificial Neural Networks Construction

Of these 500 evolutions, two subsets were built. The first enables neural networks to be trained for each observable, and the second enables the accuracy of these networks to be tested, to ensure that there is no over-training effect. The impact of the networks architecture was tested empirically, and the configurations obtained, presented in **Table 2**, were chosen because they presented a sufficiently low bias to be acceptable.

Table 2 Artificial Neural Networks (ANN) architecture and precision estimated on a testing data set to compute standard deviations

Observable	ANN architecture	Standard deviation
$Cycle\ length = f(\%Pu, \overline{Pu})$	(4,4)	<0.1 %
$F_{2D}(t) = f(\%Pu, \overline{Pu}, t)$	(16,16) *	<1.25 %
$F_{3D}(t) = f(\%Pu, \overline{Pu}, t)$	(16,16,16)	<0.25 %

*For the 30% MOX core, ANN architecture (8,8) for the F_{2D}

It is important to note that a single neural network was built for each observable and for each core configuration presented in the previous section. The following section presents the use of these different neural networks in fuel loading models in order to estimate the importance of the optimization criterion on the one hand, and the importance of fuel management on the other hand.

III. Pu content Biases Estimations

In this section, the importance of a change in each of the three core parameters presented in the previous section is analyzed. For this purpose, 5 000 Pu isotopic compositions were sampled using the LHS method and the limits presented in Table 1. Then, depending on the fuel fabrication criterion or the fuel management, some neural networks are used to estimate the Pu content in the fresh MOX fuel for each isotopic composition. In the following subsections, Pu contents are compared, considering the options of one core parameter at a time, in order to evaluate the Pu content biases induced by each option. This means that only one core configuration is considered in section III.1 and only one criterion is considered in sections III.2 and III.3.

1. Impact of the Criterion

A first comparison is made on the three fuel fabrication criteria introduced in section II.2(3): cycle length target and minimization of the 2D or the 3D power peaks.

From the neural network that determines the cycle length

as a function of the MOX fuel initial composition, the Pu content needed in the fresh MOX fuel to meet the LnatTarget criterion is estimated by dichotomy for each of the 5 000 Pu isotopic compositions. For the min(F_{2D}) and min(F_{3D}) criteria, the neural networks that compute the 2D and 3D power peaks as a function of the time and the MOX initial composition are used. For each Pu isotopic composition, the Pu content in the definition range of the neural networks that minimizes the 2D or 3D power peaks over time is selected.

Figure 2 shows the Pu content estimations for the min(F_{2D}) criterion (upper scatter plot) and the min(F_{3D}) criterion (lower plot) as a function of the LnatTarget criterion. Scatter plots are colored according to the Pu quality and the black straight lines correspond to the $x=y$ lines.

For most of the Pu isotopic compositions, the min(F_{2D}) criterion overestimates the Pu content (up to 2.73% in absolute) compared to the cycle length target criterion whereas the min(F_{3D}) criterion underestimates it (up to 3.36% in absolute). This shows that, compared to the MOX fuel compositions that reaches the cycle length target, higher Pu contents tend to minimize the 2D power peaks and lower Pu contents minimize the 3D power peaks most of the time.

Moreover, as introduced in the previous section, these observations show that an optimization of the 2D or 3D power distributions moves the initial MOX fuel composition away from the one that reaches the cycle length target.

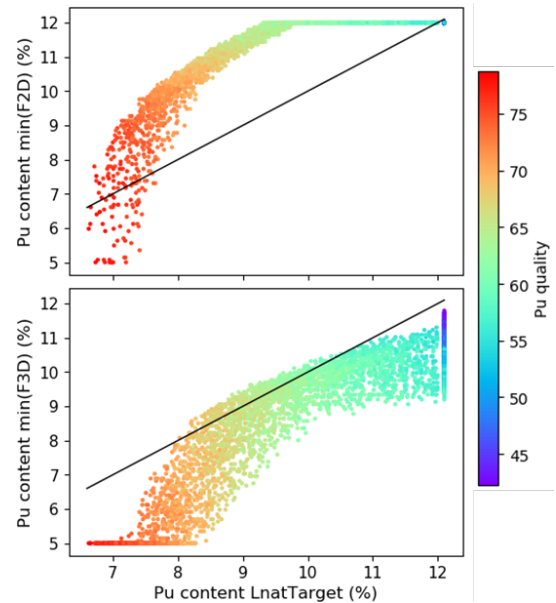


Fig. 2 Pu content estimations for the min(F_{2D}) et min(F_{3D}) criteria as a function of the Pu contents estimated with the LnatTarget criterion, for the 5 000 Pu isotopic compositions

2. Impact of the MOX Core Fraction

As mentioned in section II, two types of fuel management are studied for this work: a first core configuration containing around 30% MOX assemblies, and a second one raising its proportion of MOX assemblies to 40% in the core (core configuration 40% (I)).

For each core, the neural network that calculates the cycle length as a function of the initial plutonium composition in

the fresh MOX fuel assemblies is then used to identify the content required to achieve the target irradiation time for each of the 5 000 isotopic compositions used in the previous section. **Figure 3** shows the calculated Pu content for the core containing 40% of MOX assemblies as a function of the Pu content obtained for the 30% MOX core.

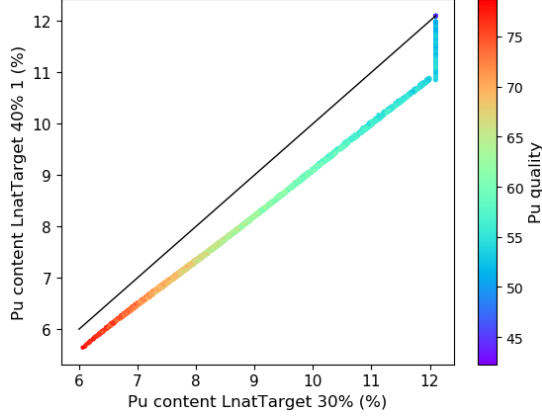


Fig. 3 Pu content estimations for the 40% (1) MOX core as a function of the Pu content estimations for the 30% MOX core, for the 5 000 Pu isotopic compositions

The deviation between the scatter plot (colored as a function of the Pu quality) and the black line, corresponding to the $x=y$ curve, shows a deviation between the two Pu contents that can reach 1.15% in absolute. It is worth noticing that the lower the Pu quality, the greater the deviation between the two calculated Pu content. The figure also shows, for the considered loading pattern, that the 40% MOX core seems to be more tolerant to degraded plutonium than the 30% MOX core. Indeed, some isotopic compositions reach a content higher than 12% (the hard limit considered here) in the x-axis where the Pu content is lower than 12% in the y-axis.

3. Impact of the Loading Pattern

In order to investigate the importance of the loading pattern in fuel loading models, several neural networks corresponding to different loading patterns have been built. The three different loading patterns are the configurations (1), (2) and (3) of the 40% MOX core. As previously, the neural networks are used to identify the Pu content required to reach the irradiation time for the 5 000 considered isotopic compositions for each loading pattern.

Figure 4 shows the scatter plot of those plutonium contents (colored as a function of the Pu quality). A few conclusions can be drawn from the comparison of the results with the $x=y$ curve (in black). Firstly, the loading patterns (1) and (2) are rather similar (only three assembly permutations) and show very limited deviation on the plutonium content ($\sim 0.5\%$). Loading pattern (3) is very different from loading pattern (1) which explains much higher deviations (up to 1.6%) and also a larger dispersion with the $x=y$ line. Second, it seems that loading patterns (1) and (2) are more suitable for high quality plutonium whereas loading pattern (3) is more suitable for low quality plutonium. Indeed, this latest leads to smaller values and is more tolerant to very degraded plutonium.

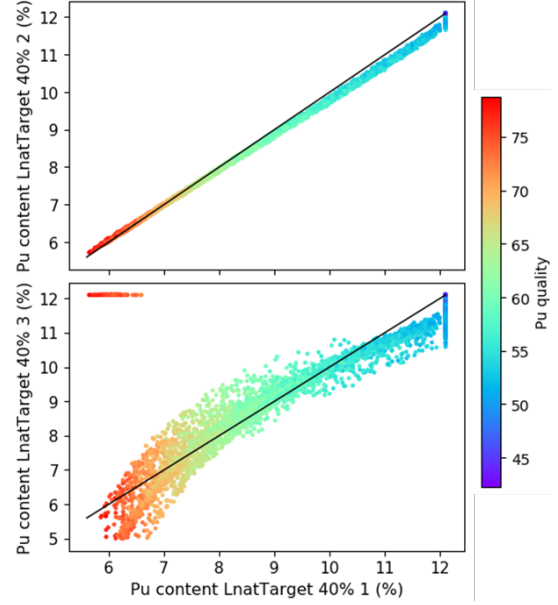


Fig. 4 Pu content estimations for the loading patterns 40% (2) and (3) as a function of the Pu content estimations for the core configuration 40% (1), for the 5 000 Pu isotopic compositions

Finally, for the same irradiation time criterion, the plutonium content in MOX fresh fuel is rather sensitive to the fraction of MOX fuel in the core and the loading pattern. The impact of the MOX fraction seems to be quite independent of the plutonium quality whereas the loading pattern effect is very dependent on it. Pu content biases due to the core configuration remain lower than those estimated for the same core configuration but with different fuel fabrication criteria. This highlights the importance of the criterion selection when building fuel loading models based on full core calculations.

IV. Impact of the Fuel Loading Model in a Scenario Simulation

Several PWR MOX fuel loading models have been built in this work depending on the fuel management MOX ratio (30% and 40%), the fuel loading pattern (40% (1), (2) and (3)) and the fuel fabrication criterion (LnatTarget, $\min(F_{2D})$, $\min(F_{3D})$). The impacts of these different modeling choices on MOX fuel manufacturing are illustrated, in this section, on an academic MOX recycling scenario frame.

1. Fuel Cycle Simulation Definition

The strategies of material multi-recycling in PWR currently evaluated focus especially on the resorption of the historical MOX spent fuel stock, usually by mixing UOX and MOX spent fuels at reprocessing. In fact, plutonium recovered from MOX spent fuels cannot be loaded directly because of its low fissile grade. Pursuing the mono-recycling strategy in the current French fleet, the historical UOX and MOX spent fuels could amount to 10 kt and 5,5 kt respectively by 2050.¹⁰⁾ Considering these spent fuel amounts, a minimum fraction of MOX spent fuel in the mixture at reprocessing of 35% is required to fully absorb the historical

MOX spent fuel stock before ending the historical UOX spent fuel stock.

A simple UOX/MOX mono-recycling fuel cycle simulation performed with the scenario code CLASS⁽¹⁾ allows us to estimate averaged Pu isotopic compositions in UOX and MOX spent fuels by 2050, presented in **Table 3**.

Table 3 Averaged Pu isotopic compositions in UOX and MOX spent fuels

	Pu content	²³⁸ Pu	²³⁹ Pu	²⁴⁰ Pu	²⁴¹ Pu	²⁴² Pu
UOX	1.1 %	2.5 %	58.5 %	23 %	9.5 %	6.5 %
MOX	5.5 %	3 %	48 %	33 %	5 %	11 %

To assess the impacts of the different MOX fuel fabrication models, several PWR MOX loading simulations are performed with CLASS. Each simulation differs from another by the implemented fuel loading model among the 7 models available (an infinite MOX assembly model based on APOLLO2 calculations has also been produced for comparison purpose):

- Core 30%, Lnat target
- Core 30%, Min(F_{2D})
- Core 30%, Min(F_{3D})
- Core 40%, (1), Lnat target
- Core 40%, (2), Lnat target
- Core 40%, (3), Lnat target
- Infinite MOX assembly, Lnat target

For each of the 7 PWR MOX simulations, several MOX fuel loading calculations are performed. Each calculation is characterized by an input isotopic composition of the Pu used to build the fresh MOX depending on x_{MOX} , the fraction of spent MOX fuel in the mixture at reprocessing (0 to 100%), as presented in **Fig. 5**. A fabrication time of 2 years has been set in these simulations. The fissile quality of the input Pu varies between 52 % and 67 %. As a result, the tested fuel loading model calculates the Pu content required to satisfy its criterion depending on the input Pu isotopic composition.

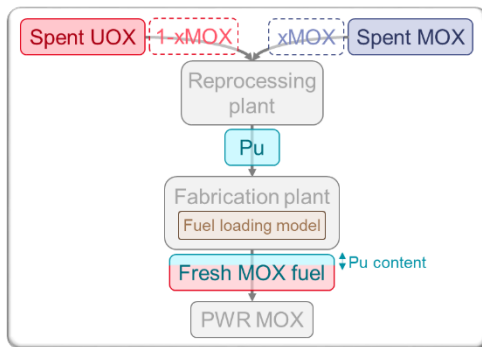


Fig. 5 Description of a PWR MOX fuel loading calculation for a fraction x_{MOX} of spent MOX fuel at reprocessing

2. Results of the Scenario Simulations

Figures 6 and 7 present the Pu content in fresh MOX fuel calculated by each fuel loading model as a function of x_{MOX} . The historical infinite assembly model is the most limiting as

it reaches the upper limit of 12% Pu content for 20% of MOX spent fuel in the mixture at reprocessing. This spent MOX fuel resorption rate leads to end the historical UOX spent fuel stockpile before the MOX one. Fuel loading models based on full core calculations allow to satisfy the minimum x_{MOX} value of 35%.

The variations on Pu content observed in section III between the full core loading models are confirmed with these MOX recycling scenario simulations. For the 30% MOX fuel management and a given x_{MOX} , min(F_{2D}) criterion overestimates Pu contents compared to LnatTarget criterion whereas min(F_{3D}) criterion underestimates Pu contents compared to LnatTarget criterion. A higher Pu content in MOX fresh fuel is required for the 30% MOX fuel management than for 40% MOX fuel managements to reach the same cycle length. x_{MOX} up to 100% are reached with two fuel loading patterns of the 40% MOX fuel management.

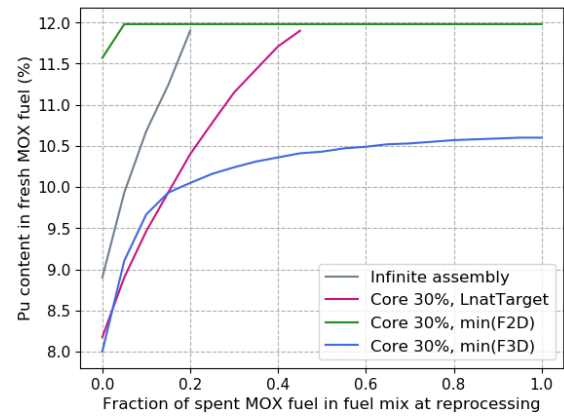


Fig. 6 Pu content in fresh MOX fuel as a function of x_{MOX} for core based fuel loading models involving the 30% MOX core and for the infinite MOX assembly model

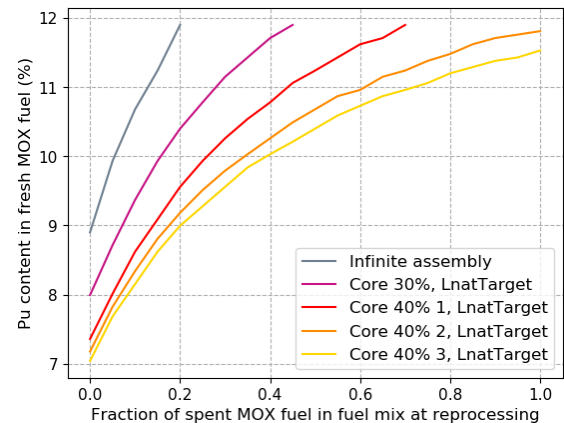


Fig. 7 Pu content in fresh MOX fuel as a function of x_{MOX} for core based fuel loading models involving the LnatTarget criterion and for the infinite MOX assembly model

V. Conclusion

Nuclear scenarios are used to assess different possible futures for a nuclear fleet by simulating a temporal evolution of every material flow that occurs within each fuel cycle facility. Scenario calculations rely on physical models for fuel

fabrication and fuel irradiation. The accuracy and precision of such models are essential as they can be used hundreds of time during one scenario calculation.

This paper focuses specifically on the fabrication model for MOX fuels. Usually, this kind of model is used to provide a fresh fuel initial plutonium content for a given targeted burn-up that accounts for plutonium available isotopy. Recent studies have highlighted that historical models made from 2D assembly calculations can show biases in comparison with 3D full core calculations. Moreover, the use of burn-up as the only objective is questionable as other relevant criteria are available at a core scale (e.g. minimizing power peak factors). In this context, this work proposes to study the impact of different core parameters and criteria for the fuel fabrication model. The core parameters studied are the MOX core fraction and the loading pattern. The observables chosen are the burn-up, the 2D and the 3D peak factors. The related criterion are whether to reach a burn-up of 16 GWd/t or minimizing the 2D or the 3D power peak factors.

The PWRs studied are variations from the UK EPR design presented in the Pre-Construction Safety Report (PCSR).⁵⁾ Two MOX core fractions have been used (30% and 40%) and three different loading patterns have been tested in the case of a 40% MOX core. Neutronic calculations have been done with the determinist codes APOLLO2 and CRONOS2 to produce databases of 500 fresh MOX fuel isotopies for each core configuration. With these calculations, artificial neural networks have been trained for each observable and an algorithm has been created to provide a plutonium content that matches a given criterion for a given isotopy.

The impact of each core parameter and criterion on the plutonium content estimation has been assessed for one loading. On the one hand, sensitivity to the MOX core fraction and the fuel loading pattern has been highlighted. More specifically, the effect of the MOX core fraction seems to be independent from the plutonium quality. It is not the case for the loading pattern. On the other hand, the criterion choice stands out as the most impactful when it comes to plutonium content.

The different fabrication models built have then been tested within a simple scenario application case that involves UOX and MOX fuels recycling in a PWR fleet. The first conclusion is that the historical model (assembly calculation and target burn-up as criterion) appears to be more conservative than the new fabrication models based on core calculations. When it comes to core parameters, both the increase of the MOX core fraction and the optimization of the loading pattern lead to a flexibility gain on the acceptable plutonium isotopy. Regarding criterion choice, the 3D power peak minimization leads to the smallest plutonium content whereas the 2D power peak minimization is more conservative than the assembly model.

It is imperative that the physical models employed in scenario calculations are selected with great care, as they exert a profound influence on the resulting outcomes. A dedicated study on the irradiation models for the scenario will be conducted in the future. Further investigation into more complex cases concerning plutonium recycling may prove beneficial in order to gain a deeper understanding of the impact that reactor models have on the outcomes of scenarios.

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