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Sensitivity studies of PWR MOX fuel management to the plutonium initial vector using Artificial Neural Networks

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Abstract. This paper presents new metamodels based on artificial neural networks trained on full core 3D depletion simulations performed with APOLLO2 and CRONOS2. They are used to estimate the irradiation cycle length, discharge burn-up of each fuel assembly type and radial power factor of a PWR loaded with 30% of MOX fuels, as a function of the initial plutonium composition. They allow to explore the impact of the plutonium isotopic vector on the reactor characteristics and can be used for scenarios studied for future fuel cycle. Some exclusion domains in the plutonium isotopic vector phase space are identified as a function of the cycle length. As an example, the potentialities of such fuel management for plutonium recycling from MOX spent fuel are studied.

1 Introduction

Nuclear scenario studies aim to provide an overview of the influence of strategies (deployment of a new type of reactor/fuel, evolution of installed power, etc.) on a nuclear fleet and the associated fuel cycle. Based on hypotheses on the initial state of the nuclear fleet and its evolution, they also aim to quantify the impact of a change in strategy, according to different evaluation criteria formulated on the observables of the cycle: evolution of isotope flows of materials, resource use, plant capacities, waste production, etc. These studies rely on nuclear fuel cycle simulations produced with a nuclear scenario simulation tool, modelling evolving reactor fleets and all operations carried out on nuclear fuel from the mine to final storage (extraction, enrichment, manufacturing, reactor irradiation, cooling, reprocessing, etc.).

The dynamic scenario code developed and used at CEA is the code COSI [1]. The one developed at CNRS is the code CLASS [2]. They both model complex nuclear fleets whose composition can change over time and calculate the isotopic evolution of inventories and material flows at each moment in each unit of the cycle (fabrication and enrichment plants, reactors, cooling pools, reprocessing plants, etc.). Different physical processes have to be

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taken into account to model the evolution of the material inventory (fresh fuel building, fuel irradiation, radioactive decay, etc.) as well as the different material flows passing through the units (fresh fuel, spent fuel, recoverable materials, waste, etc.). COSI and CLASS are based on physical models allowing to build fresh fuels (fuel loading model) and to calculate their evolution under irradiation (irradiation model). The fuel loading model determines the content of fissile material to be integrated into the fresh fuel based on the isotopic composition of the available material and the targeted cycle length [3] [4]. This model is usually based on a fuel fissile content estimator, such as an artificial neural network, built before the scenario simulation.

The construction of the estimators (for the fuel loading and irradiation models) is based on the elaboration of a database bringing together the results of hundreds of neutronic calculations carried out for each reactor and fuel management. In the case of Pressurized Water Reactors (PWR), neutronic calculations are usually performed at the fuel assembly scale to allow a database building within acceptable calculation times. These calculations represent an average homogeneous fuel assembly, and do not take into account the heterogeneities in the actual loading of the assemblies. In particular, these models do not consider the impact of the core loading plan, as well as neighbouring assemblies. Issues associated to this simplifying assumption particularly arise in the case of heterogeneous fuel management, where different types of assemblies coexist in the core, such as 30% MOX fuel management in PWR (i.e. 30% of MOX assemblies and 70% of UOX assemblies). Recent studies have shown that this approximate representation can lead to significant biases in scenario calculations [5].

The work presented in this paper focuses on the development of a PWR 30% MOX full core calculation scheme in order to produce physical models for scenario simulations. After presenting the full core calculation scheme optimization process, this paper endeavours to detail the calculation database construction. Then, artificial neural networks calculating the maximum fuel cycle length and power factors as a function of the plutonium isotopy and content in fresh MOX fuel are built. Finally, these estimators are used to explore the phase space of plutonium isotopic vector and identify exclusion domains that do not reach a viable solution. Indeed, in plutonium recycling strategies, the isotopic vector quality can vary regarding the plutonium origin. For instance, plutonium coming from low burn-up UOX spent fuel is quite different from plutonium coming from high burn-up MOX spent fuel. The aim of this work is then to identify all the isotopic vectors that cannot be loaded in a PWR 30% MOX core due to different constraints such as maximum plutonium content and maximum power factor. Finally, the models are used to study the possibilities of plutonium from spent UOX and spent MOX mixing for fresh MOX fuel fabrication, that would be loaded in a PWR 30% MOX core.

2 Full core depletion calculation scheme optimization

2.1 Core definition and simulation parameters

The PWR core studied here corresponds to the UK European Pressurized Reactor (EPR) design that is described in the Pre-Construction Safety Report given in reference [6]. The core considered here is the MOX version at equilibrium, loaded with UOX and MOX fuels (with approximately 30% of MOX assemblies). It is composed of 3 types of UOX assemblies (differing in their number of gadolinium poisoned rods) and one type of MOX assemblies, each assembly being unloaded after 3 or 4 irradiation cycles. The configuration of each assembly is given in Figure 1 and the loading pattern in Figure 2. This loading pattern is not considered as a variable for this work, neither the UOX fuels configurations. The ^{235}U

enrichment of the UOX fuel rods is equal to 5.0% in each UOX pins while it is equal to 3.0% in the gadolinium rods. The MOX assembly is divided into three zones, depending on their plutonium content, to reduce the power peaks at the UOX/MOX interfaces and the Pu content cannot exceed 12% (in one fuel rod) due to fabrication constraints and void reactivity feedback [6]. This limit leads to a maximum of 11.3% for the average plutonium content in MOX fuel assemblies.

The core modelling is performed using two-step deterministic calculations. The first step is the resolution of the neutron transport equation on 2D infinite lattices using the APOLLO2 code [7]. Fuel pins and guide thimbles are precisely described and the SHEM 281-group energy mesh is considered. Two numerical methods for the transport equation resolution are compared: the interface current probability method (Pij) computed with 281 energy groups on a coarse spatial mesh, and the REL2005 scheme [8] (the interface current collision probability method provides 26-group cross sections that are used in a calculation with the method of characteristics on a refined spatial mesh).

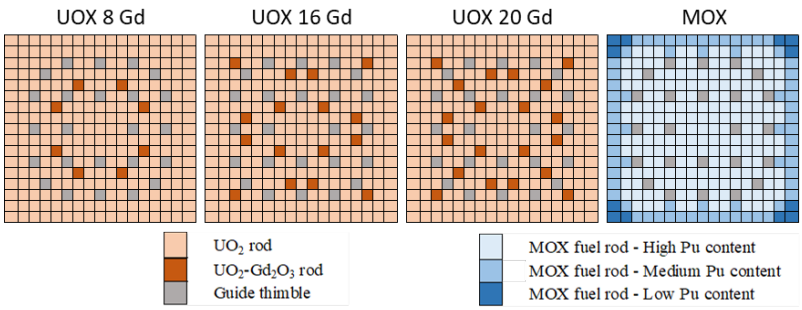

Fig. 1. Lattice definition of the different fuel assemblies loaded in the core

At the end of the lattice calculations, the cross-sections are condensed in 2 energy groups and homogenized over the whole assembly (option called HOM in the following) or on pin cells (option called HET) and stored in multi-parameters cross-section libraries. The HET option allows a 3D core calculation with a geometrical discretization at the pin-cell level.

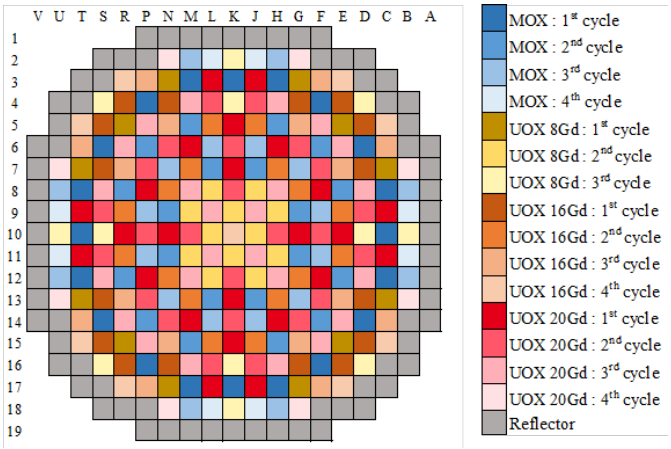

Fig. 2. Core loading pattern definition

The second step is the resolution of the diffusion equation with 3D full core calculations using the CRONOS2 code [9]. It computes the neutron flux and the criticality for different time steps during the depletion simulation. CRONOS2 offers several possibilities such as neutronic/thermal hydraulics coupled calculation (to consider the impact of the fuel

temperature and coolant density distribution in the core on the power deposit distribution) or a critical boron concentration monitoring for instance.

Eventually, four different options defining the calculation schemes have been considered for this work: Pij or REL2005 for the lattice calculation, HET or HOM for the spatial discretization of the core, to perform coupled or isothermal calculations, with or without reactivity monitoring by critical boron concentration adjustment (equal to 0 in the last case).

2.2 Comparison results

Considering the possible combinations of those options, 16 different calculation schemes have been defined. Each of them has been used for depletion simulations and cycle length estimations. Moreover, 3 different isotopic vectors and plutonium contents were considered to ensure, that numerical biases do not depend on the initial MOX fuel composition. The definition of these 3 initial compositions is given in Table 1.

The computed cycle lengths have been compared for the 4 sets of hypotheses. The results are presented in Table 2 and show that the biases on the cycle length estimation are limited (under 2%).

Table 1. 3 Different MOX fresh fuel composition for testing the computational scheme for complete 3D core depletion simulation

	Plutonium content	^{238}Pu	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu	^{241}Am
Compo 1	7 %	4.0 %	50.0 %	23.0 %	12.0 %	9.5 %	1.5 %
Compo 2	7 %	1.89 %	60.95 %	23.22 %	8.0 %	5.13 %	0.81 %
Compo 3	11.29%	2.55 %	57.86 %	28.45 %	1.09 %	9.61 %	0.44 %

Considering the reduction of the computational time by over a factor 25 when considering the set of parameters {Pij, HOM, Isothermal, No boron} compared with {REL2005, HET, Coupled simulation, Critical boron monitoring} (which should be considered as the reference set of parameters), the first set of parameters is then considered for this work.

Table 2. Cycle length differences regarding different calculation scheme options.

	Compo 1	Compo 2	Compo 3
Pij vs REL 2005	Min : 0.31 % Max : 0.69 %	Min : 0.37% Max : 0.77%	Min : 0.63% Max : 0.90%.
HOM vs HET	Min : 1.3% Max : 2.1%	Min : 1.23% Max : 2.00%	Min : 1.40% Max : 1.74%.
Isothermal vs coupled simulation	Min : 0.01% Max : 0.08%	Min : -0.02% Max : 0.06%	Min : -0.05% Max : -0.09%
Boron follow up vs non boron	Min : -0.05% Max : 0.11%	Min : -0.01% Max : 0.14%	Min : 0.23% Max : 0.28%

3 Artificial neural network on core depletion simulations

Once the two-level calculation scheme optimized, a numerical database has been built in order to explore the core characteristics as a function of the MOX initial composition. This database is then used for artificial neural networks training.

3.1 Database construction

3.1.1 Phase space sampling

The sampling of MOX fresh fuel compositions should be chosen carefully, as it will define the validity domain of the metamodels and their use. As the goal is to use them to explore possibilities to load EPR MOX with degraded plutonium, the phase space should cover all possible plutonium isotopic composition coming from UOX and MOX spent fuels with various cooling times.

Plutonium isotopic compositions from spent UOX and MOX fuels can be found in [4] and Table 3 presents the limits chosen in this work. The ^{240}Pu proportion is considered as a buffer (the sum of all the isotopes should be equal to 100%) and is not an independent random variable. Plutonium content in the MOX fresh fuel is also sampled.

290 random initial compositions have been identified with a Latin Hyper Square sampling, leading to 290 different depletion simulations. For this paper, cycle length (or the average core burn-up within one irradiation cycle), the discharge burn-up of all different types of fuel assembly and the radial assembly power factor are calculated as a function of the initial MOX composition. The different assembly batches are named after the fuel type (UOX or MOX) and the number of irradiation cycles they went through before discharge (3 or 4). For example, UOX3 is a UOX fuel that is discharged after 3 irradiation campaigns. The radial power factor (named F_{xy}), is calculated as the ratio of the maximal power delivered by one assembly over the average assembly power. It varies along the irradiation time but only its maximal value is studied.

Table 3. 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.

	Plutonium content	^{238}Pu	^{239}Pu	^{241}Pu	^{242}Pu	^{241}Am
Min	5.3 %	0.7 %	40.0 %	2.0 %	4 %	0.0 %
Max	12.0 %	5.0 %	65.0 %	14 %	12 %	3 %

3.1.2 Database exploration

The results of the 290 depletion simulations are presented in Figure 3 that represents the cycle length, and the discharge burn-up of each batch as a function of the initial MOX composition. It can be noted that, among all possibilities of the phase space determined by Table 3, the cycle length varies from 13.3 GWd/t to more than 18 GWd/t. The discharge burn-up of MOX3 and MOX4 are always rather close (with a difference of a few GWd/t) and the discharge burn-up of UOX3 is the less dependant to the initial MOX composition whereas the burn-up of batch UOX4 is quite dependant to it.

Another visualisation of the results is presented in Figure 4, that shows a scatter plot of the initial plutonium content, its fissile quality (defined as the proportion of fissile nucleus), the cycle length and discharge burn-up of each assembly type. From this figure, it is clear that all the different burn-up of each assembly type are strongly correlated.

3.2 Artificial neural networks training and precision estimation

From this database, one neural network has been trained for each of the different observables considered. In order to quantify the precision of the metamodels, the database has been split

in two different ones: 230 random simulations make the first set of data needed to build the neural networks with the TMVA library [10], the 60 others are used to compare the values obtained from these numerical models with calculated reference values. The standard deviations of the biases of the neural networks are computed and are presented in Table 4.

4 Use of neural networks for phase space exploration under constraints

The purpose of this work is to identify sensitivities of the EPR MOX fuel management to the initial MOX fuel composition. This core is defined by a loading pattern (that is not considered as a variable here), the fresh composition of the UOX assemblies (that are also kept constant) and the initial fresh composition of MOX fuel.

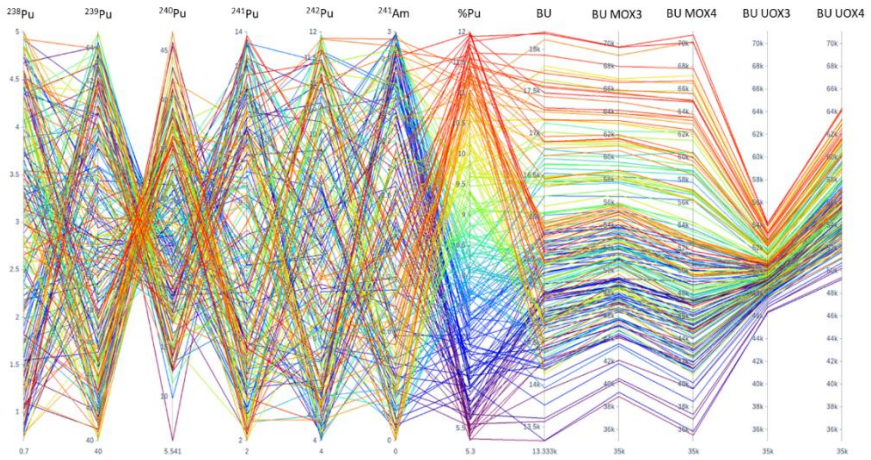

Fig. 3. Representation of different core observables as a function of the plutonium isotopic vector and the plutonium content in fresh MOX fuels. The colorization is function of the plutonium content.

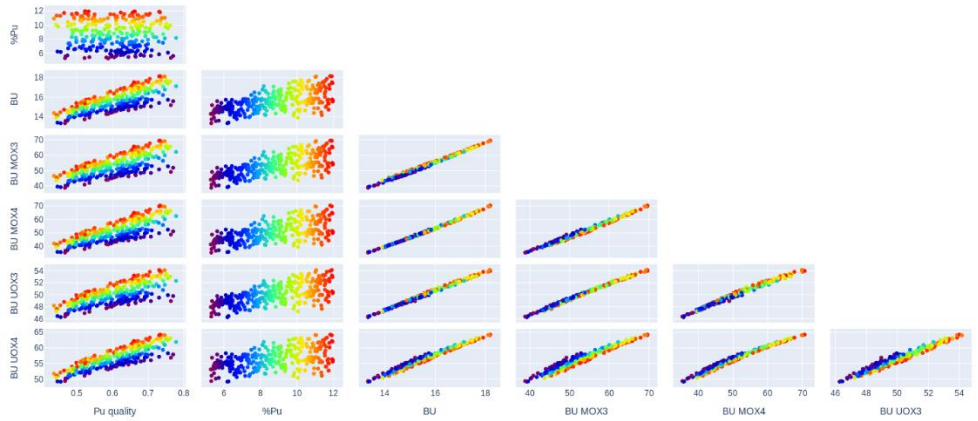

Fig. 4. Correlation between discharge burn-up (GWd/t) of different fuel assemblies with plutonium quality and plutonium content of fresh MOX fuels. The colorization is function of the plutonium content.

The use of neural networks allows a phase space exploration under constraints in order to identify possible limits for the fresh MOX fuel composition. The first constraint considered

is the cycle length that should reach a given target. This constraint links the plutonium content to its isotopic vector. Two additional constraints have been also considered: first, this plutonium content should be less than 11.3% (so as not to have a plutonium content higher than 12% in all MOX fuel pins), and second, the radial power factor should be less than 1.7 (limit chosen arbitrarily that should be discussed further on thermal-hydraulics considerations but allows the methodological development of this work).

Table 4. Artificial Neural Network precision estimated on an additional data set to compute standard deviations

Observable	Neural network architecture	Input Variable	Standard deviation
Cycle length	2 hidden layers of 4 neurons each	MOX fuel composition	0.07%
Average burn-up of UOX3			0.05%
Average burn-up of UOX4			0.07%
Average burn-up of MOX3			0.11%
Average burn-up of MOX4			0.16%
F_{xy}	2 hidden layers of 8 neurons each	MOX fuel composition + Irradiation Time	1.23 %

4.1 Global phase space exploration

The phase space defined in Table 3 is sampled to identify 5000 different initial plutonium isotopic vectors. For each of them, the plutonium content that allows to reach a targeted cycle length is calculated. Two different values are considered for this paper: 15 GWd/t and 16.5 GWd/t (reference value for the optimized calculation scheme considered here). Then, all the different observables defined in the previous section are calculated. The results are presented in Figure 5. It shows scatter plots of the plutonium quality, the initial MOX composition and the radial power factor. The acceptable solutions are represented respectively in pink and in red. Blue dots represent plutonium isotopic vectors that are rejected by the F_{xy} constraint (<1.7), and black dots are the ones rejected by the plutonium content constraint (<11.3%).

It should be noted that the excluded phase space is much bigger for the lower cycle length target due to the high power factor in this case. Indeed, UOX fuel assemblies may be very powerful due to a low plutonium content in MOX assemblies.

Figure 6 shows the difference between discharge burn-up of each fuel type assembly batch with the average values for isotopic composition that leads to a plutonium content lower than 11.3%. It shows that a minimal radial power factor leads to minimal differences for discharge burn-up, and then to an energy equivalence between different fuel assembly types.

4.2 Potentialities of spent MOX dilution in spent UOX for plutonium recycling

Our methodology allows to study the potentialities of the EPR MOX fuel management defined in this paper to recycle plutonium from spent MOX fuels. It is well known that plutonium recovered from spent MOX fuel reprocessing cannot be loaded directly, but this plutonium may be mixed with plutonium coming from spent UOX fuel reprocessing.

Our artificial neural networks are used in this section to identify a limit of the proportion of plutonium from MOX spent fuel that can be introduced in plutonium coming from UOX spent fuel for new fresh fuel assembly fabrication. This plutonium mixing would allow a partial plutonium multi-recycling.

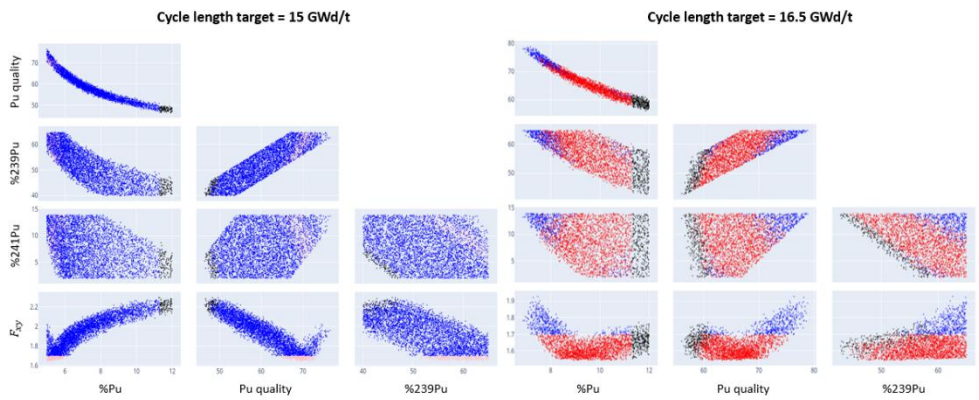

Fig. 5. Identification of the phase space that allows acceptable solutions for a cycle length of 15 GWd/t (on the left) and 16.5 GWd/t (on the right). Pink and red dots represent viable solutions (with a plutonium content lower than 11.3% and a radial assembly power factor lower than 1.7). Blue dots represent the excluded phase space due to the power factor constraint and black dots are excluded due to the plutonium content limits.

4.2.1 Plutonium vector definition

A specific calculation has been performed with the initial MOX fuel composition described in [6]. From it, plutonium isotopic compositions are extracted from UOX and MOX spent fuels at discharge and the obtained isotopic vectors are presented in Table 5. It should also be pointed out that the spent fuels have to be cooled between 5 and 30 years before reprocessing and that the fabrication process is supposed to last 2 years and leads to americium 241 production.

Table 5. Plutonium isotopic vector for average UOX and MOX spent fuel extracted from the APOLLO2/CRONOS2 simulation of the reference composition

	^{238}Pu	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu
Spent UOX	2.23 %	50.5 %	24.0 %	14.5 %	7.73 %
Spent MOX	5.33 %	36.7 %	28.2 %	15.6 %	14.1 %

4.2.2 Results

The plutonium content and the maximal radial assembly power factor (F_{xy}) have been computed with neural networks as a function of the mixing proportion. Again, two cycle length targets have been considered: 15GWd/t and 16.5 GWd/t. The results are presented in Figure 7 and shows the mixing limitation between the different sources of plutonium for different cooling time. With the reference cycle length of 16.5 GWd/t, it is not possible to build fresh MOX fuel with more than 40% of plutonium coming from MOX spent fuel reprocessing. This limit drops to 30% when the MOX spent fuel is cooled 30 years before reprocessing.

With a lower cycle length, the proportion of plutonium recovered from MOX spent fuel reprocessing can be much higher due to the lower plutonium content in the new MOX fresh fuel. The drawback is a much higher radial power factor that exceed the 1.7 limits defined in the previous section.

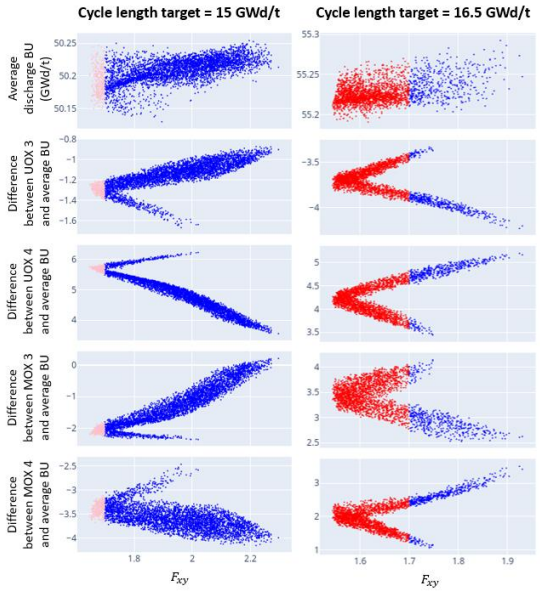

Fig. 6. Representation of different discharge burn-up as a function of the radial assembly power factor of the different 5000 sampled fresh composition (under the cycle length constraints and the plutonium content limit of 11.3%).

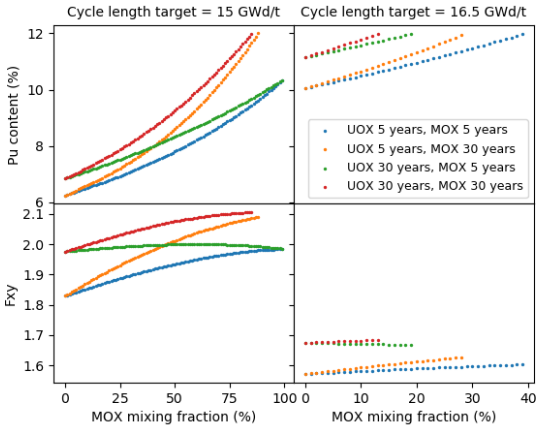

Fig. 7. Plutonium content and radial power factor as a function of the mixing fraction of plutonium coming from MOX spent fuel in plutonium from UOX spent fuel.

5 Conclusions

This paper presents new metamodels for PWR 30% MOX core depletion simulations based on the use of artificial neural networks. They characterize the core behaviour in terms of cycle length, discharge burn-up of different fuel assembly batches and radial assembly power factor as a function of the fresh MOX fuel composition. The purpose of these metamodels is to be used in scenario simulations for plutonium recycling studies.

To build the depletion simulation database, a calculation scheme has been optimized with APOLLO2 and CRONOS2 to perform hundreds of calculations within a reasonable computational time and with minimal biases (under 2%). APOLLO2 lattice simulations are

performed with the collision probability method (Pij) and the assemblies are fully homogenized. Core simulations with CRONOS2 were performed without any multiphysics models (isothermal hypothesis) nor boron concentration calculation in order to monitor the criticality.

290 fresh fuel compositions have been sampled to build a numerical database and Artificial Neural Network that estimates the cycle length, the discharge burn-up of each fuel assembly type and the radial power factor.

Those neural networks have been then used to explore the phase space of plutonium isotopic vector under reactor constraints. The plutonium content is adjusted to reach a given cycle length target and the radial power factor and discharge burn-up are then calculated. 5000 new random isotopic compositions have been tested and the results show that the exclusion space (isotopic compositions without any viable solution) is strongly dependant on the cycle length target. Finally, the neural networks have been used for studying the potential recycling of plutonium coming from MOX spent fuel by diluting it with UOX spent fuel plutonium. The results show that the mixing limit can be extended by reducing the core cycle length, leading to high radial power factors and differences in the discharge burn-up of different types of assembly. In that case, the deterioration of the fuel management (lower cycle length and non-equivalence between UOX and MOX) allows some fuel cycle flexibility by possible loads of more degraded plutonium.

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