

# DONJON5/CLASS coupled simulations of MOX/UO<sub>2</sub> heterogeneous PWR core

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**Abstract.** Most fuel cycle simulation tools are based either on fixed recipes or assembly calculations for reactor modeling. Due to the high number of calculations and extensive computational power requirements, full-core computations are often seen as not viable for this purpose. However, this leads to additional hypotheses and modeling biases, thus limiting the realism of the resulting fuel cycle. For several applications, the current modeling method is sufficient, but precise calculations of discharged fuel composition may require further refinements. CLASS (Core Library for Advanced Simulation Scenarios) is a dynamic fuel cycle simulation code developed since 2012 with reactor models based on neural networks to produce nuclear data and physical quantities. Past work has shown a first coupling between CLASS and DONJON5 to quantify neural networks approach biases. This work assesses the applicability of 3D full-core diffusion calculations using the DONJON5 code coupled with nuclear scenario simulations involving a realistic PWR core at equilibrium cycle conditions. DONJON5 interpolates burnup dependent diffusion coefficients and cross sections generated beforehand by DRAGON5, a deterministic lattice calculation tool. Whereas previous studies considered only homogeneous reactors (i.e. homogeneous assembly in terms of composition and enrichment as well as homogeneous core), the present contribution focuses on the integration of full-core calculations in CLASS for fuel cycles involving a MOX/UO<sub>2</sub> PWR core (i.e. 1/3 MOx–2/3 UOx). The DONJON5 model considered in this work describes a core with critical boron concentration at each time step partially loaded with MOx heterogeneous assemblies composed of three enrichments. In fuel cycle calculations, the main issue is to adapt, in the fabrication stage, the fresh fuel composition for the reactor with regards to the isotopic composition of the available stocks. This work presents a fuel loading model based on power peaking factors minimization that respects irradiation cycle length, <sup>235</sup>U enrichment as well as Pu concentration and fissile quality, hence, ensuring a more uniform power distribution in the core.

## 1 Introduction

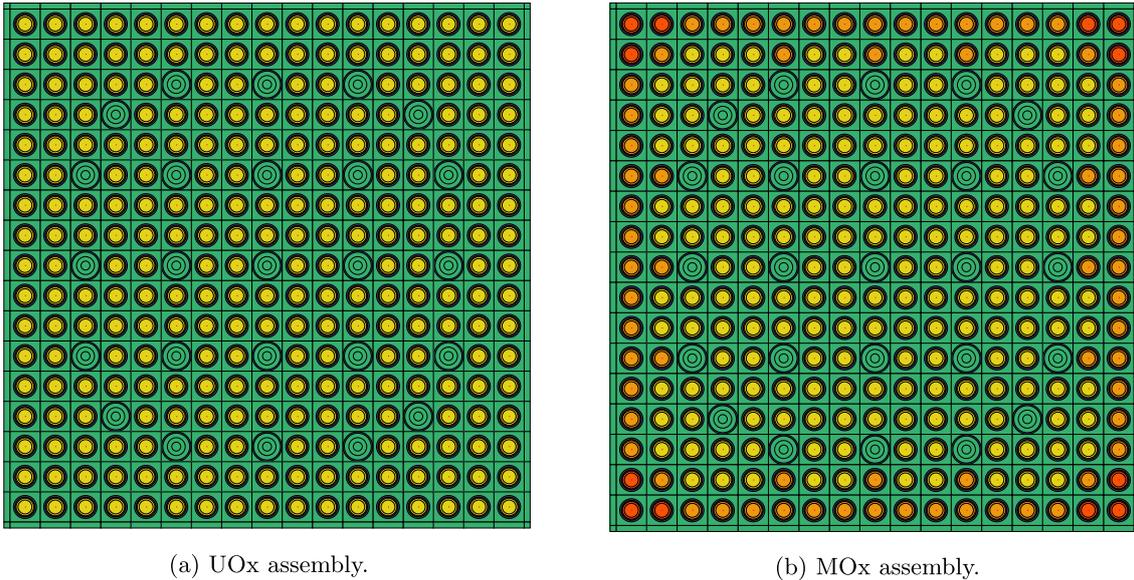
In fuel cycle simulators, reactor models are usually based on infinite assembly calculations both for the depletion simulation and for the fuel loading model that calculate each fresh fuel composition in fuel cycle simulations [1]. In the CLASS package, reactor models rely mostly on ANN (Artificial Neural Networks) to predict infinite neutron multiplication coefficients and average cross-sections ( $(n, f)$ ,  $(n, \gamma)$  and  $(n, 2n)$ ) to solve Bateman equations. Those neural networks are trained on a dedicated 1-group cross-sections database built with any fuel depletion software. Although these models are pretty convenient since they are easy to build and very effective in terms of

computational costs, they do not consider core scale physics and, thus, lead to modeling biases.

In order to increase the reliability of fuel cycle simulations, reference [2] proposed a first coupling between DONJON5 [3] and CLASS [4] allowing full-core calculations for PWRs (Pressurized Water Reactors) in a fuel cycle simulator. This work quantified biases induced by the use of infinite calculations in a full-scale scenario exploring MOx fuels deployment in PWRs after two decades of UOx irradiation. The scenario studied involved homogeneous UOx and MOx reactors (i.e. homogeneous assembly in terms of fresh composition as well as homogeneous core) whereas it is well known that PWRs are loaded with only 30% of MOx for safety reasons.

This work offers a coupling between CLASS and DONJON5 for heterogeneous reactors: PWR loaded with

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**Fig. 1.** UOx (a) and MOx (b) assembly geometries. Materials are identified as follows: moderator in green and fuel clad in purple. For the UOx assembly, fuel pellets are in yellow. For the MOx assembly, yellow, orange and red fuel pellets are characterized by high (9.77%<sub>HM</sub>), medium (6.49%<sub>HM</sub>) and low (3.66%<sub>HM</sub>) Pu contents.

both MOx and UOx fuels. The impact of full-core physics is then investigated on both the fresh fuel loading model and the irradiation model.

The purpose of loading models is to calculate simultaneously the enrichment of the UOx assemblies with the plutonium content (as a function of its isotopic quality) in the MOx assemblies in order to match two reactor criteria, namely the targeted burnup and the power peaking factor. For reactor operations, MOx assemblies are supposed to release as much energy as UOx assemblies. A minimal power peaking factor will then ensure an acceptable power distribution in the core but also an equivalence between MOx and UOx fuels in terms of energy production.

The irradiation model relies on full-core calculations, with critical boron concentration at all time steps. All lattice calculations have been performed with DRAGON5 [5]. These are used to build the reactor database used by DONJON5 for full-core simulations and to build artificial neural networks for models based on assembly considerations.

The contents of this paper is as follows. First, in Section 2, DRAGON5 lattice calculations are detailed. Section 3 describes how diffusion and ANN databases are built from lattice calculations while Section 4 describes calculation options for full-core calculations with DONJON5. The fuel loading model (also referred to as the equivalence model) that estimates the Pu content as a function of the uranium enrichment in the UOx fuels and the plutonium isotopic quality are presented in Section 5 followed respectively, in Sections 6 and 7, by CLASS analyses of an elementary scenario involving a single MOx/UO<sub>2</sub> fuelled PWR and complex scenario that involves both UOx and MOx/UO<sub>2</sub> heterogeneously fuelled PWRs.

## 2 Assembly calculations

The computer code DRAGON5 is a lattice code developed at École Polytechnique de Montréal that enables the resolution of the neutron transport equation [5]. Specifically, this code allows the characterization of the internal reactor lattice, namely unit cells or fuel assemblies, via physics models articulated to achieve the following processes: interpolation of microscopic cross-sections supplied by means of standard libraries; resonance self-shielding calculation; multigroup and multidimensional neutron flux calculation; transport-transport or transport-diffusion equivalence calculation; editing of condensed and homogenized nuclear properties for reactor calculations; and finally isotopic depletion calculations.

### 2.1 Fuel assembly

The heterogeneous PWR core studied here is composed of different assembly designs for UOx and MOx fuels (cf. Fig. 1). The MOx assembly is divided in three zones characterized by different Pu contents to attenuate power variations at the MOx-UOx interface. Pu contents in the three zones were chosen to agree with the loading patterns introduced by the French operator EdF [6].

While guide tube cells are simulated, control rods are not considered in this fuel assembly modeling. Hence, core reactivity management is entirely ensured via boron diluted in the moderator.

To simplify the present study, all DRAGON5 infinite assembly calculations were performed for thermal power densities as well as fuel, clad and moderator temperatures fixed to a specific and theoretical mean value. A 4-rings discretization was used in fuel rods in order to reduce

**Table 1.** Assembly geometrical data [9].

Parameters	Dimension
Cell dimension	1.26 cm
External pellet radius	0.41 cm
External clad radius	0.48 cm
External guide tubes radius	0.56 cm
Guide tubes thickness	0.06 cm
Water strip dimension	0.25 cm
Assembly dimension	21.92 cm
Number of fuel rods	264
Number of guide tubes	25

calculation costs while keeping sufficient precision in flux simulation [7]. Finally, a brief study of the guide tube cell discretization pointed out that 3-rings in the internal moderator suffice to properly take into account neutron moderation in water holes [8]. Table 1 summarize the dimension of geometrical elements previously discussed and Table 2 gives additional information on assembly material properties. Note that the dimension of geometrical elements are considered at cold state (20 °C), and thus, no thermal expansion was considered.

The tracking of the fuel assembly geometry is generated via the NXT: module (this tracking is being used to compute collision probabilities required for solving the transport equation) with white boundary conditions due to greater efficiency in terms of computational costs, when compared to mirror-like boundary conditions. Note that B1 homogeneous models are used here [10].

It is considered preferable to use a simplified tracking for self-shielding calculations which can lead to substantial computing costs. The approach adopted here involves tracking individual cells in the assembly coupled by interface current coupling (SYBILT: module). The USS: module is then used to create physical probability tables required by the subgroup self-shielding approach.

We considered a SHEM multigroup library composed of 295 energy groups detailed in [11]. Simply, the SHEM-295 defers from SHEM-361 in its coarser meshing of the energetic domain from 4.0 to 22.5 eV [12]. This library accuracy was evaluated by measuring discrepancies generated on unloaded isotopic inventories resulting from deterministic calculations via DRAGON5 when compared to a continuous energy calculation performed via SERPENT (i.e. Monte Carlo code [13]). It was shown that the 295-groups library induced negligible discrepancies (< 1% on  $^{235}\text{U}$  and < 0.5% on  $^{239}\text{Pu}$  inventories) for reasonable computing time scale [8].

It should be noted that, although MOx assembly calculations should be carried out in a UOx environment to properly characterize neutronic behaviors expected at UOx/MOx interfaces [14], we considered infinite lattice calculations for UOx and MOx fuels. Previous work showed that this simplification can lead to discrepancies reaching 6.5% on  $\text{Pu}^{239}$  inventories at EOC for a typical MOx assembly [15]. However, this work focuses on the quantification of bias generated by the current ANN approach used in CLASS and, thus, it was considered

**Table 2.** Other assembly properties.

Parameters	Dimension
Fuel density	10.4 g·cm <sup>-3</sup>
Fuel temperature	900 K
Thermal power density	36.0 W/g <sub>HM</sub>
Water density	0.733 g·cm <sup>-3</sup>
Water temperature	569.55 K
Clad material	Zircaloy 4
Clad temperature	633 K

preferable to use ANN and diffusion databases built from identical lattice calculation schemes.

## 2.2 Reflector

Cross-section calculations for the core reflector require a more complex geometry due to the following modeling challenges:

1. the distance between peripheral fuel assemblies and the radial reflector is not constant around the core.
2. In the absence of fissile material in the reflector, a fissile environment must be simulated, namely surrounding fuel assemblies, in order to induce a neutron flux in the reflector itself.
3. The combined thickness of all elements composing the reflector amounts to a much larger geometry than the original assembly defined for full-core calculations.

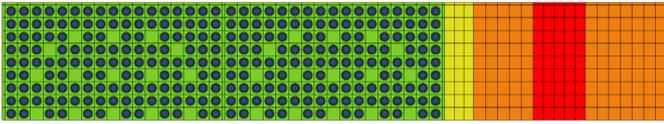
Taking into consideration the whole reflector would tend toward very costly lattice calculations. As for the varying distance between the baffle and core skin, it would lead to an important database dedicated to the reflector material in addition to the database summarizing the fuel cross-sections ultimately entailing costly interpolations in full-core calculations. Thus, the reflector characterization justifies the development of a judicious cross-sections calculation scheme based on diverse approximations. The approach adopted in the previous coupling of CLASS and DONJON5 [16] and inspired by [17] goes as follows:

1. reflector material calculation is performed only at BOC (i.e.  $t = 0$  s). Indeed, while the neutron flux varies in regards to the burnup, the neutron spectrum variation observed in the simulated fuel assembly has a limited impact on the reflector composition itself.
2. Reflector geometry is simplified in two ways: the reflector elements simulated are limited to elements included in the volume of a fuel assembly (cf. Tab. 3); the fuel assembly simulated to account for fissile environment is loaded with UOx (cf. Fig. 2).

Note that two fuel assemblies are simulated. Giving the symmetric conditions imposed at the upper and lower limit of the geometry shown in Figure 2, simulated assemblies can be reduced to their halves. It should also be noted that reflective conditions are used on the left of the

**Table 3.** Reflector geometrical data [16].

Parameters	Dimension (cm)
Baffle (iron)	2.86
Moderator (light water)	5.86
Skin (iron)	5.15
Moderator (light water)	8.05

**Fig. 2.** Reflector geometry. Materials are identified as follows: moderator (fuel assembly) in green, UOx fuel pellet in purple, iron (baffle) in yellow, iron (skin) in red and moderator (reflector) in orange.

fuel assemblies, while void conditions are defined beyond the reflective material.

### 3 Database characteristics

Considering that the isotopic composition of the MOx introduced in PWRs is *a priori* unknown in fuel cycle calculations, the multi-parameter databank built via lattice calculations and used for the interpolation of neutron characteristics requires a large sampling of significant parameters. The databank created in the present study, denoted MULTICOMPO in the following, includes 8 dimensions : boron concentration,  $^{235}\text{U}$  enrichment of UOx fuels and isotopic composition (which amount to 5 dimensions) as well as Pu content of MOx fuels. It should be noted that, while the Pu content and the isotopic composition are varied here, the Pu content ratios between the three enrichment zones of MOx assembly designs are fixed.

#### 3.1 Diffusion database

The sampling space must include all possible configurations that one may encounter in fuel cycle simulations. Consequently, minimal and maximal  $^{235}\text{U}$  enrichments are chosen equal to 3.0 and 5.0% $_{\text{HM}}$ , respectively. It was shown *a posteriori* that those limits enable fuel irradiation between 260 EFPD and 390 EFPD thereby embedding scenarios of interest studied via CLASS. An analog approach was performed to also ensure that the Pu content limits (i.e. 4.5 and 13.5% $_{\text{HM}}$ ) allowed a critical operation of the heterogeneous core with either very good or very bad isotopic compositions.

The sampling for  $^{235}\text{U}$  enrichment, Pu contents and boron concentration are summarized in Table 4. Cubic interpolation method was shown to be satisfactory [16].

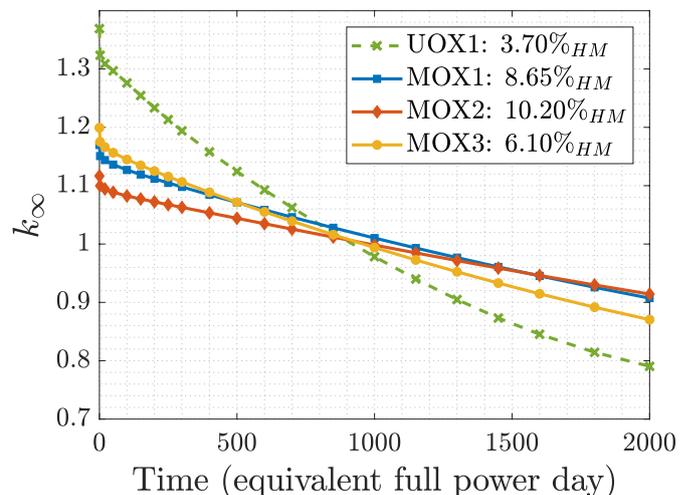
It is worth mentioning that cross-sections saved in this hyperspace are burnup dependent. That is to say they are calculated at 25 non-regular depletion steps (first fine then coarse) as detailed in Table 5. This burnup sampling enables a precise transcription of the significant neutron

**Table 4.** Diffusion database fuel perturbations.

Parameter	Sampling
$^{235}\text{U}$ enrichment(% $_{\text{HM}}$ )	3.00, 4.00 and 5.00
Pu content (% $_{\text{HM}}$ )	4.50, 6.00, 7.50, 9.00, 10.50, 12.00 and 13.50
Boron concentration (ppm)	0, 1375 and 2750

**Table 5.** Diffusion database time sampling.

Time interval (EFPD)	Time step (EFPD)	Burnup step (MWd.t $^{-1}_{\text{HM}}$ )	Number of step
$0 \leq t \leq 5$	2.5	90	3
$5 < t \leq 10$	5.0	180	1
$10 < t \leq 50$	10.0	360	4
$50 < t \leq 300$	50.0	1800	5
$300 < t \leq 700$	100.0	3600	4
$700 < t \leq 1600$	150.0	5400	6
$1600 < t \leq 2000$	200.0	7200	2

**Fig. 3.** Infinite multiplication factor evolution resulting from lattice calculations performed for UOx (green line) and MOx (other lines) fuel assemblies. Isotopic compositions for UOX1 as well as MOX1, MOX2 and MOX3 are presented in Table 6.

spectrum evolution expected in the early stage of irradiation for thermal nuclear reactors (i.e. xenon and samarium effect) and coarse representation of the long time behavior of the irradiation. This ensures a reasonable database size while providing adequate interpolation of macroscopic cross-sections in DONJON5 calculations [8]. As an example, Figure 3 presents  $k_{\infty}$  evolution obtained for different fuel compositions.

Table 7 presents the plutonium and americium 241 sampling points considered for the diffusion database. The  $^{239}\text{Pu}$  concentration acts here as a buffer for the plutonium isotopic vector. It is worth noting that, while only six isotopes are perturbed, the cross-sections for 22 isotopes selected either for their preponderant impact or because of their relatively high concentration are saved in the diffusion database. Reliable isotopic inventories may be obtained with only a few isotopic perturbations. Adding

**Table 6.** Isotopic compositions studied for UOx and MOx assemblies characterization.

Fuel	UOx (%)		PuOx (%)						
	<sup>235</sup> U	<sup>238</sup> U	<sup>238</sup> Pu	<sup>239</sup> Pu	<sup>240</sup> Pu	<sup>241</sup> Pu	<sup>242</sup> Pu	<sup>241</sup> Am	Pu <sub>fissile</sub>
%X <sub>UOX1</sub>	3.70	96.30	–	–	–	–	–	–	–
%X <sub>MOX1</sub>	0.25	99.75	2.50	54.50	25.20	8.60	7.90	1.30	63.10
%X <sub>MOX2</sub>	0.25	99.75	5.00	50.45	28.00	5.00	10.00	1.55	55.45
%X <sub>MOX3</sub>	0.25	99.75	2.00	62.25	22.50	8.00	5.00	0.25	70.25

**Table 7.** Diffusion database isotopic perturbations.

Isotope	Sampling
<sup>238</sup> Pu (%)	0.5 and 5.5
<sup>240</sup> Pu (%)	21.5, 26.5 and 31.5
<sup>241</sup> Pu (%)	1.5, 10.5 and 19.5
<sup>242</sup> Pu (%)	3.5, 8.0 and 12.5
<sup>241</sup> Am (%)	0.01 and 1.75

sampling points (for instance additional <sup>238</sup>Pu or <sup>241</sup>Am perturbations) leads to far greater computational costs (i.e. 150% increase when compared to samplings presented in Tab. 7) for each cross-section interpolation in module NCR: in full-core calculation. *A contrario*, reducing the <sup>242</sup>Pu sampling leads to discrepancies of approximately 1.2% on this isotope and 0.2% on <sup>235</sup>U after only one irradiation cycle of 280 days (equivalent full power).

Finally, note that cross-sections resulting from the lattice calculation are 2-groups condensed and homogenized spatially on the whole assembly before they are stored on the diffusion database.

### 3.2 Neural network database

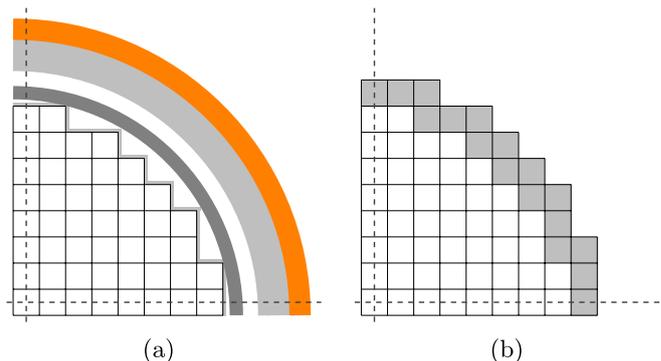
For the sake of clean comparisons, an independent database was built via DRAGON5 calculations in order to train ANNs employed in usual reactor models for CLASS. This enables us to eliminate sources of errors in fuel cycle calculations that are not induced by neural networks or physic models (i.e. different depletion calculation software, nuclear data or different geometrical descriptions).

For ANNs, it is well known that regular sampling of input parameters may lead to significant training biases. Hence, fresh fuel compositions were considered as parameters yielding 600 initial compositions for UOx fuels and 2000 for MOX fuels sampled with the LHS technique (Latin Hyper Square). Furthermore, it has been suggested to set boron concentration to zero at all computed burnup steps to yield correct evaluation of plutonium evolution [16]. All the other parameters remained identical.

## 4 Full-core calculations

### 4.1 Geometry description

In fuel cycle studies, dozens of core calculations are performed for each reactor. Considering the resulting computational requirements, it appears necessary to simplify



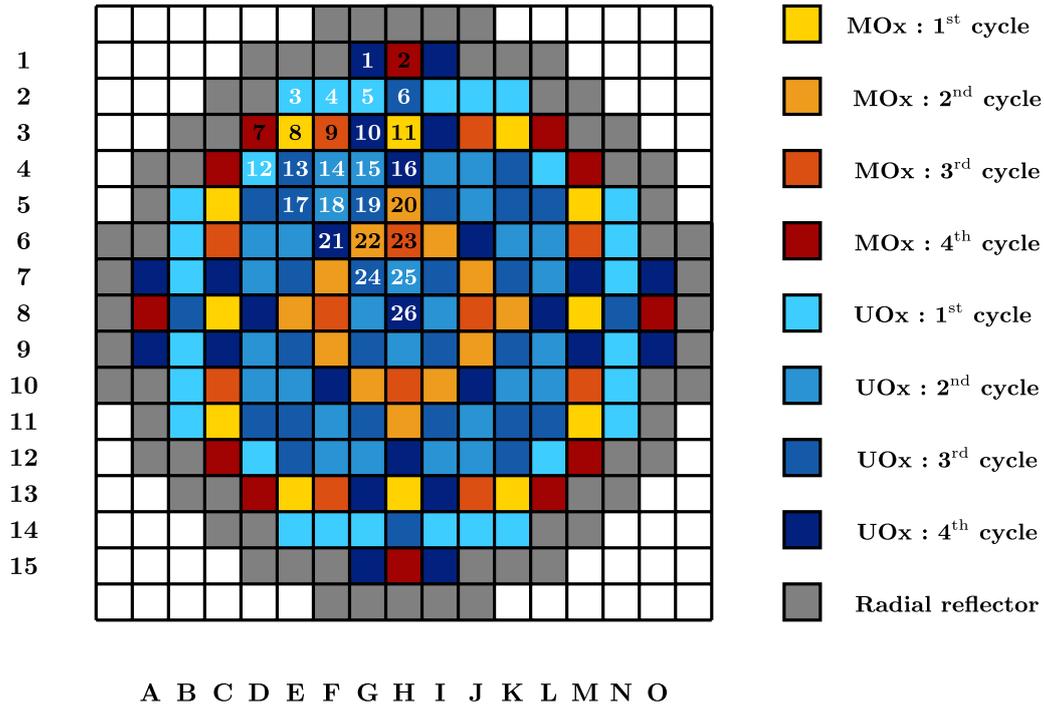
**Fig. 4.** Real (a) and simulated (b) PWR quarter core layout. Assemblies are displayed in white, whereas baffle (light gray), barrel (dark gray), vessel (gray) and thermal insulator (orange) are replaced by reflector elements (gray).

the full-core geometry illustrated in Figure 4. The elementary cell for the core is a homogenized assembly corresponding to a cubic element with height equal to the fuel assembly side. Note that no additional spatial discretization is considered.

As one can see, fuel assemblies are radially surrounded by cubic elements corresponding to the reflector introduced in Section 2. Furthermore, the core geometry proposed here includes additional upper and lower planes representing the reflective mixture (i.e. axial reflectors). To simplify full-core geometry tracking, these two planes have the same height as the core cells. It is also worth mentioning that the core height is split in 9 non-regular planes. This coarse discretization led to reasonable calculation costs and was shown to be adequate given the constant moderator and fuel temperatures within the core [8]. The core dimension and geometrical elements are summarized in Table 8.

### 4.2 Heterogeneous modeling for CLASS

We considered a fixed cyclic fuel reloading scheme consisting of 40 new fuel assemblies (i.e. 28 identical UOx and 12 identical MOx). Note that the number of UOx assembly decreases from 28 to 25 after the third irradiation cycle to maintain a total of 157 assemblies. The proportion of MOx assemblies in the core and the four cycles reloading scheme are defined in accordance with the present industrial practice (i.e. PARITÉ MOX introduced by EdF [18]) as well as the previous coupling considering UOx and MOx homogeneous cores [16].



**Fig. 5.** Loading pattern used in 3D full-core modeling of heterogeneous PWR core. The 26 fuel assemblies indicated correspond to combustion zones composing one eighth of the core.

**Table 8.** Core geometrical data.

Parameters	Dimension
Assembly size (cm)	21.92
Assembly height (cm)	372.64
Number of UOx assembly	109
Number of MOx assembly	48
Radial reflector dimension (cm)	21.92
Axial reflector dimension (cm)	21.92
Core height (cm)	416.48

The heterogeneous reactor models developed are divided in two successive steps involving 3D full-core calculations.

The first calculation step involves a core fully fuelled with UOx in order to determine the minimal  $^{235}\text{U}$  enrichment required to maintain criticality for a given output burnup objective. In detail, two UOx core calculations characterized respectively by enrichment equal to 3.0 and 5.0 % $_{\text{HM}}$  are first performed. Then, the enrichment is adjusted in subsequent UOx full-core calculations (i.e. dichotomic search) until the targeted burnup is reached. The loading pattern used in those core calculations is identical to the heterogeneous pattern displayed on [Figure 5](#). MOx assemblies are then simply substituted by their UOx counterpart.

A second calculation step is then performed to characterize the irradiation of a heterogeneous core composed of UOx assemblies defined in the previous homogeneous DONJON5 calculations as well as energy-equivalent MOx

**Table 9.** Time discretization for full-core calculations.

Time interval (EFPD)	Time step (EFPD)	Burnup step (MWd·t $_{\text{HM}}^{-1}$ )	Number of step
$0 \leq t \leq 10$	2.5	90	5
$10 < t \leq 100$	90.0	3240	1
$100 < t \leq 300$	100.0	3600	2
$t > 300$	$l_{\text{cycle}} - 300.0$	$\text{BU}_{\text{target}} - 10890$	1

assemblies. This equivalence between UOx and MOx is discussed in [Section 5](#).

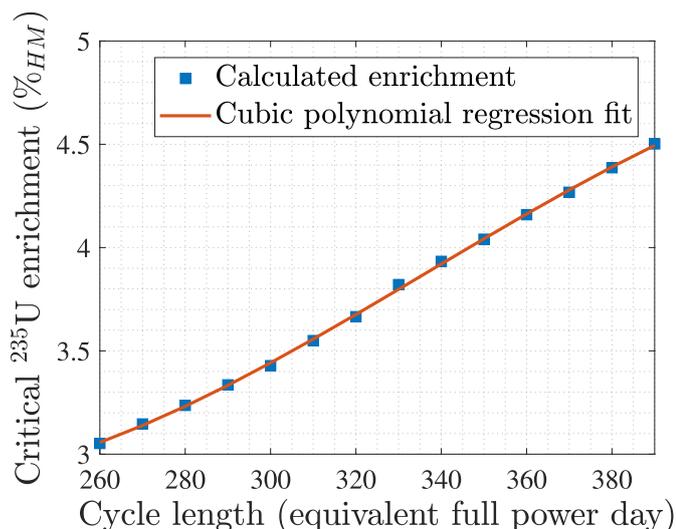
Both UOx and heterogeneous full-core calculations include 9 computed burnup steps as detailed in [Table 9](#).

### 4.3 Acceleration of calculations

As full-core calculations lead to computational costs far greater than ANNs typically used in CLASS, several ways to improve calculation speed have been studied.

#### 4.3.1 Critical $^{235}\text{U}$ enrichment predictions

Considering that UOx full-core calculations are essentially performed to obtain critical fissile contents, we propose a direct relation between  $^{235}\text{U}$  enrichment and cycle length, allowing us to dismiss entirely UOx calculations in CLASS. 14 UOx full-core calculations were performed *a priori* with burnup targets covering evenly irradiation cycles between 260 and 390 days (equivalent full power). Note that these cycles were defined in such a way as to incorporate a multitude of fuel management schemes put forward in the literature [[18–20](#)]. Critical



**Fig. 6.** Critical <sup>235</sup>U enrichment evaluation for UOx full-core calculations performed with DRAGON5-DONJON5.

**Table 10.** Details of the critical enrichment prediction fit.

A	B	C	D
(% <sub>HM</sub> )	(% <sub>HM</sub> )	(% <sub>HM</sub> )	(% <sub>HM</sub> )
$-2.6381 \times 10^{-7}$	$2.6641 \times 10^{-4}$	$-7.7394 \times 10^{-2}$	9.8066

uranium enrichments were then extracted and used to generate a cubic polynomial regression fit as displayed in Figure 6.

One can see that it is possible to correctly predict (for this loading pattern) the critical <sup>235</sup>U enrichment evolution in relation of the cycle length with this relation:

$$\epsilon_{\text{crit.}}(l_{\text{cycle}}) = A \cdot l_{\text{cycle}}^3 + B \cdot l_{\text{cycle}}^2 + C \cdot l_{\text{cycle}} + D, \quad (1)$$

where  $\epsilon_{\text{crit.}}$  and  $l_{\text{cycle}}$  correspond to the critical <sup>235</sup>U enrichment (%<sub>HM</sub>) and the cycle length (equivalent full power days), respectively. Moreover, constants  $A$  to  $D$  are determined empirically and are presented in Table 10. Figure 6 shows negligible discrepancies between predicted and calculated enrichments resulting from DONJON5. The biases induced by this accelerated approach are in the range  $-0.023\%_{\text{HM}}$  ;  $0.014\%_{\text{HM}}$ .

In the interest of quantifying errors generated on heterogeneous full-core calculations by critical enrichment predictions, we compare unloaded inventories resulting from two heterogeneous PWR cores : one fuelled with the predicted enrichment characterized by the largest deviation noted in Figure 6 and another one fuelled with the corresponding calculated enrichment. We obtained relative errors smaller than 1.5% on all Pu and U isotopes with significant concentration. It should be noted that the largest mass deviation, that is to say 1.5%, is observed on <sup>235</sup>U inventory and is larger than the initial bias on the predicted enrichment. Considering that it yields calculations cost 12.5% less important, this accelerated approach is adopted albeit the minor bias on initial fissile inventory.

### 4.3.2 Reloading burnup predictions

Due to the *a priori* unknown used assemblies burnup at each reloading step, the usual practice relies on an initial calculation with fuel assemblies reloaded with burnups in direct proportion to the mean irradiation rhythm. In order to calculate real in-core burnups for all assemblies composing the heterogeneous core at equilibrium, preliminary irradiation cycles are performed until convergence is reached in all combustion zones. To avoid these preliminary cycles altogether (from 4 to 8 cycles in our case) and greatly accelerate 3D full-core calculations, we propose to predict reloading burnup values using ANNs. Based on the core symmetry visible on Figure 5, we limit burnup predictions to 26 combustion zones (i.e. 20 used assemblies and 6 new assemblies) located in one eighth of the core.

To generate these neural networks, a multidimensional training databank covering campaign length included between 260 and 390 irradiation days (equivalent full power) was constructed. This hyperspace also take into consideration the <sup>235</sup>U enrichment in UOx assemblies and the Pu content as well as the isotopic composition in MOx assemblies. Again, an LHS method was used to randomly generate core characteristics within the hyperspace of interest. A total of 3000 full-core calculations were performed and resulting unloaded burnups were extracted for all 20 used assemblies and saved in 20 distinct training databases.

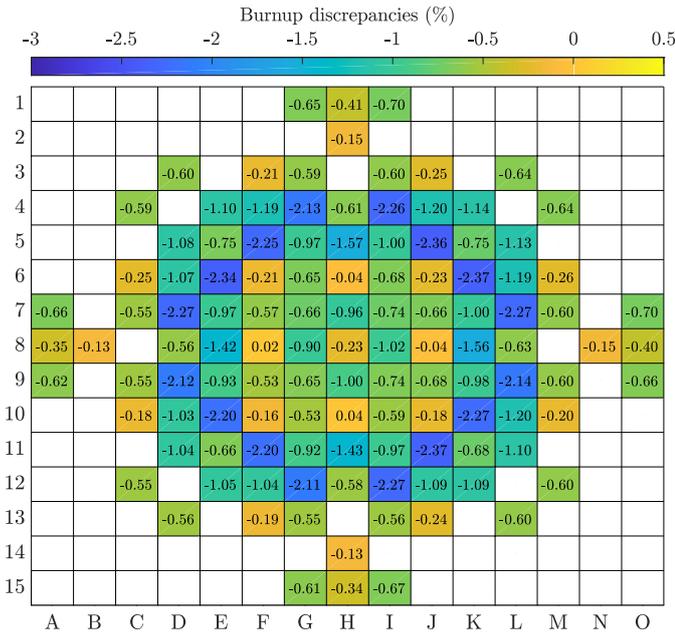
For accuracy validation, 300 additional and independent full-core calculations were performed in order to validate the 20 trained neural networks. Overall, 95.52% of burnups predicted via the 20 ANNs tested in this experiment are characterized by a discrepancy under 2%, when compared to the correspondent calculated burnup value.

Furthermore, relative discrepancies between calculated and predicted burnups obtained for a UOX1-MOX1 heterogeneous core (cf. Tab. 6) are indicated in Figure 7. In this figure, fresh fuels are not represented as they have a zero initial burnup.

It is worth recalling that, although calculated burnups are determined for all 157 assemblies, predicted values are obtained only for one eighth of the core and redistributed by symmetry. Power asymmetries generated in preliminary cycles, which in itself leads to varying burnups within symmetric combustion zones, are not reproduced by the accelerated approach proposed here. Consequently, slight deviations will be observed in symmetric combustion zones (p. ex. combustion zones A8, H1, O8, and H15). However, these variations are less than 0.2% and can be decreased significantly by reducing the convergence criteria imposed to the diffusion equation solutions obtained with the FLUD: module in full-core calculations [8].

### 4.3.3 Critical boron calculations

3D full-core calculations are carried out with critical boron concentration at every computed burnup steps. Critical boron is determined in an iterative process similar to critical enrichment calculations as introduced in Section 4.3.1. Based on the stationary irradiation (i.e. the reloading



**Fig. 7.** Burnup discrepancies between predicted and calculated values at reloading.

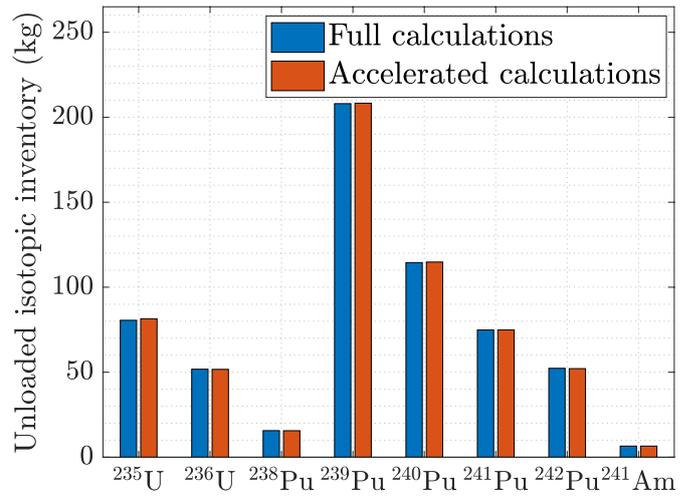
scheme is cyclic and uniform), the core's reactivity evolution can be assumed identical for every cycle. Thus, the critical boron concentration is calculated only for the first cycle and is reproduced in the subsequent ones. Previous works have shown that this approach yields negligible boron concentration discrepancies while decreasing substantially computational costs [8,16].

#### 4.3.4 Resulting accelerated calculations

In order to estimate errors generated by the three simplifications ( $^{235}\text{U}$  enrichment fit, burnup neural networks and boron simplified calculation), we examined unloaded isotopic inventories resulting from one irradiation cycle of the UOX1-MOX1 heterogeneous core. Figure 8 compares isotopic inventories obtained with typical and accelerated full-core calculations. As one can see, deviations between isotopic inventories resulting from these approaches are very small. This is also the case for  $^{238}\text{U}$  which is not introduced in this figure in order to simplify presentation. On the other hand, these two approaches are characterized by costs amounting to 4014 seconds (i.e. 480 seconds for the preliminary UOx full-core calculation and 3534 seconds for the heterogeneous full-core calculation) and 1185 seconds, respectively, leading to almost four times less computational costs for each core calculation.

## 5 Fuel fabrication: matching MOx composition to UO<sub>2</sub> enrichment

Previous sections were dedicated to the elaboration of an optimized full-core calculation scheme that may be integrated in the CLASS package for fuel cycle simulations.



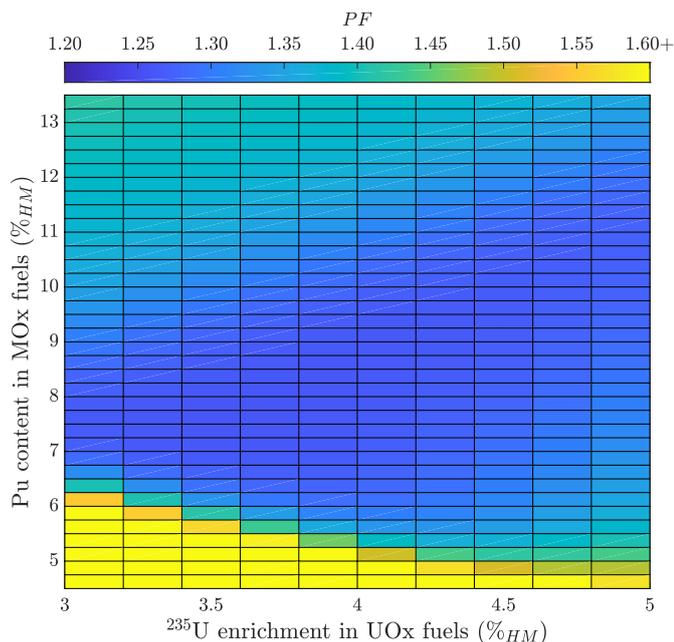
**Fig. 8.** Unloaded actinides inventories obtained with full and accelerated calculations.

Although the resulting calculation scheme enables us to reliably simulate fuel irradiation in the PWR considered here, further development is required to insure adequate fuel loading in regards to the isotopic composition of the available stocks.

Whereas previous works (either based on infinite calculations [1] or on full-core calculation [16]) depended entirely on core criticality as a criterion to calculate optimal Pu content, we propose an alternative approach based essentially on power peaking factor minimization for fresh MOx fabrication.

### 5.1 Power equivalence for fresh fuel determination

The approach consists of adjusting the plutonium content in fresh MOx fuels according to its isotopic composition and critical  $^{235}\text{U}$  enrichment to obtain similar unloaded burnups for UOx and MOx assemblies. Considering that similar power measured on UOx and MOx assemblies lead to small burnup differences in unloaded assemblies for uniform UOx and MOx irradiation lengths (i.e. four cycles reloading scheme), we adopted the peaking factor at EOC (**End Of Cycle**) as a measure of equivalence between these two fuels [8]. Literature usually defines the peaking factor as the maximum ratio between a fuel pin power over pin mean power. Given that the elementary cell defined for 3D full-core calculations is the assembly, the peaking factor definition is measured on fuel assemblies. As an example, Figure 9 recapitulates peaking factors resulting from DONJON5 calculations carried out with a fixed standard Pu quality (i.e. MOX1 in Tab. 6) and for a wide array of  $^{235}\text{U}$  enrichment in UOx fuels and Pu content in MOx fuels. One can clearly see that for a given isotopic composition and  $^{235}\text{U}$  enrichment, there is one Pu content that leads to a minimal peaking factor and thus, according to the relation previously mentioned, a small burnup differences in unloaded assemblies.



**Fig. 9.** Power peaking factors ( $PF$ ) calculated for different Pu content and  $^{235}\text{U}$  enrichment combinations with a fixed standard isotopic composition.

## 5.2 ANN calculations for peaking factor estimation

The layout of the peaking factor surface displayed in Figure 9, which can be reproduced for any isotopic composition, gave rise to the methodology adopted for fuel loading: predicting peaking factors via an ANN and identifying which Pu content leads to the minimal factor. Consequently, another ANN is built to calculate peaking factors with respect to  $^{235}\text{U}$  enrichment in UOx fuel and Pu content as well as isotopic composition in MOx fuel. Pseudo-random core characteristics were defined via an LHS method and lead to a training database built on 3000 full-core calculations. To validate the neural network precision, predicted peaking factors were compared to calculated factors resulting from thousands of independent heterogeneous full-core calculations. From this comparison, we found that 94.26% of predicted factors are characterized by relative deviations under 5%. On the other hand, it should be mentioned that 1.28% of predictions display absolute discrepancies over 0.2. Albeit their small proportion, large negative discrepancies significantly affect equivalent Pu content determination and thus limit the precision of this equivalence. Let us recall that the approach adopted here consists of predicting peaking factors at a fixed enrichment and for a fine and regular Pu content vector, and thus enables us to identify which content leads to the minimal factor.

## 5.3 Fresh fuel loading model for heterogeneous reactors

Finally, our reactor modeling with DONJON5 for dynamic fuel cycle calculations relies on three steps:

1. a calculation step involving a homogeneous core fuelled entirely with UOx in order to determine the critical  $^{235}\text{U}$  enrichment.
2. An estimation of the Pu content according to isotopic compositions available in stocks and the critical enrichment resulting from the previous step. This content leads to a minimal peaking factor at EOC and ensures that the discharged burnups of MOx and UOx assemblies are similar.
3. A calculation step characterizing heterogeneous core depletion is finally performed for UOx and MOx assemblies as defined in previous steps and with critical boron concentrations follow up.

It is worth noting that the loading pattern of this reactor modeling is supposed to be constant. Hence, artificial neural networks and uranium enrichment calculations developed here are specific to this loading pattern. Further developments could include a loading pattern selection with respect to UOx and MOx fuel composition. Reference [8] shows that this methodology could be used with other typical loading patterns if required.

## 6 Elementary scenarios

Previous sections explained how fuel loading and fuel depletion modeling with DONJON5 were designed and implemented in a dynamic fuel cycle simulation within the CLASS package. Let us recall that this new calculation scheme differs from reactors modeling based on ANN [1] and commonly used approaches by taking into account neutrons phenomena at core level. Before investigating model biases in a full scenario calculation over several years, it appears necessary to highlight differences between the DONJON5 and ANN approach on basic park configurations involving a single fresh fuel loading followed by one irradiation cycle.

### 6.1 Reactor modeling with artificial neural networks

Usual CLASS reactor models rely on artificial neural networks to estimate the core criticality evolution and average cross-sections of main reactions [1]. Note that these models perform heterogeneous PWRs simulation via independent UOx and MOx modeling. Mass and power of UOx and MOx fuel assemblies are then proportionally adjusted to represent reactor mass.

Specifically, each fresh composition is elaborated according to the estimation of the maximal achievable burnup for each assembly considered independently (i.e. based on their respective infinite calculations). Maximal achievable burnup is defined here as the burnup for which the average value of  $k_{\infty}$  over the different batches does not compensate for neutron losses induced by structural material capture and neutron leakage. This criticality margin is represented by a single parameter denoted  $k_{\text{threshold}}$  in the following. As MOx fuels and UOx fuels have different neutron spectrum, different neutron leakage rates and neutron capture rates on structural materials are expected. While this margin depends on the fuel type

**Table 11.** Reactor modeling description and denomination.

Denomination	Fuel loading model		Irradiation model		$k_{\text{threshold}}$	
	Heterogeneous		Heterogeneous		Heterogeneous	
CLASS-DONJON5	DONJON5		DONJON5		-	
	UOx	MOx	UOx	MOx	UOx	MOx
CLASS-MLP	MLP	MLP	MLP	MLP	1.045	1.025

in the present study, it does not depend on the fuel composition yet. Finally, the fuel loading model calculate the fresh fuel composition regarding its isotopic vector in such a way as to fulfill equation (2) during the whole fuel evolution. In other words, EOC burnups are achieved when the equality is no longer verified.

$$k_{\text{threshold}} \leq \langle k_{\infty} \rangle = \frac{1}{N} \sum_{n=1}^N k_n(\text{BU}_{\text{unload}}). \quad (2)$$

UOx and MOx depletion are also calculated independently via ANNs that predict 1-group cross-sections of three reactions:  $(n, f)$ ,  $(n, \gamma)$  and  $(n, 2n)$  for significant isotopes. Bateman equations are then solved with a Runge-Kutta fourth-order method, ultimately yielding an estimation of discharged compositions.

Artificial neural networks considered in this work are MLP (**M**ulti **L**ayer **P**erceptrons) trained on a dedicated database built on neutron characteristics resulting from DRAGON5 calculations with the exact same simulation options used for the diffusion database (cf. Sect. 2). This modeling is denoted CLASS-MLP in the following, whereas the notation CLASS-DONJON5 refers to heterogeneous full-core calculations.

## 6.2 Scenario analysis

Scenario calculations studied here (defined with the specific concerns to be as simple as possible) consider sufficient fissile materials to properly load one heterogeneous reactor. Three initial isotopic compositions have been considered for the comparison of DONJON5 and MLP approaches (cf. Tab. 6). The fuel fabrication process is set to two years. This is done to simulate chemical separation to extract plutonium and uranium inventories required for UOx and MOx fuel assemblies fabrication. Moreover, unloaded fuel assemblies are cooled for two years in order to account for radioactive decays expected in cooling pools. Further modeling options selected for this comparison are summarized in Table 11.

Figures 10(a) and 10(b) display uranium and plutonium evolution resulting from the simulated reactor, respectively. From these figures, we denote that plutonium inventories required for the reactor loading is higher for the DONJON5 approach, when compared to inventories predicted with MLP. Considering that initial heavy metals mass is fixed for all reactors in CLASS, plutonium underestimation necessarily lead to an overestimated proportion of depleted uranium in MOx fuels fabricated with MLP models. Therefore, less fissile materials are introduced in MLP cores and, given that the power is constant for all simulations, predicted  $^{235}\text{U}$  fission rates should necessarily

be higher in MLP models, when compared to DONJON5 calculations. Ultimately, this observation translates to a greater use of uranium via the CLASS-MLP approach.

Regarding the plutonium inventories, note that discrepancies between CLASS-DONJON5 and CLASS-MLP are similar at BOC (**B**eginning **O**f **C**ycle) and EOC. Although some deviations may be seen for HET2, the general observation is that plutonium production from heterogeneous irradiation is reliably simulated with both approaches.

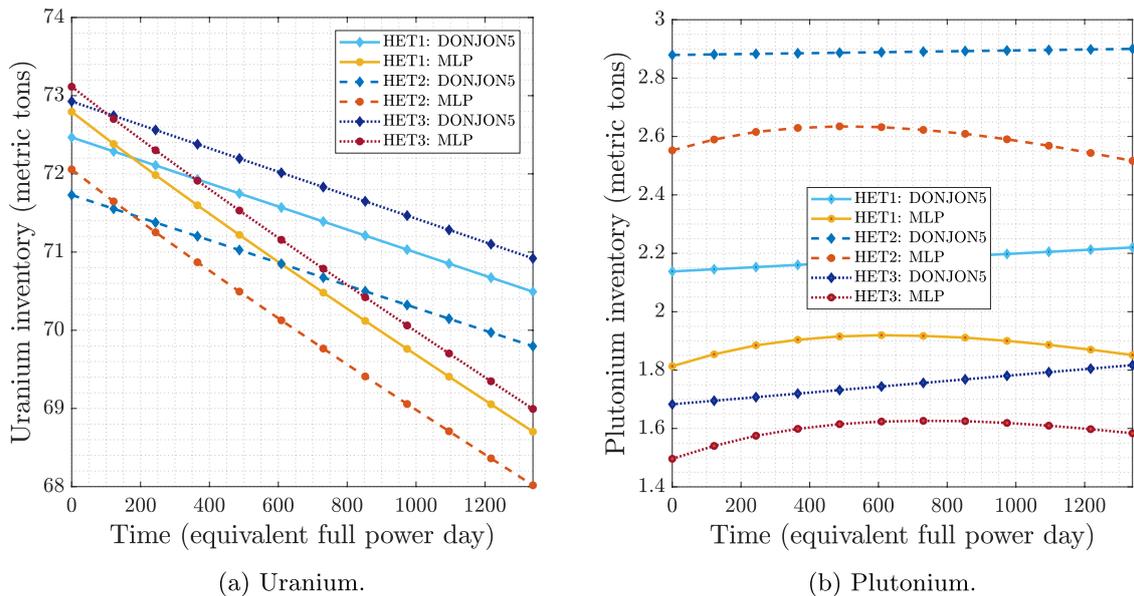
Thus, we conclude from this comparison that the main source of bias lies in the loading model. Let us recall that MLP and DONJON5 core reloading are based on distinct modeling philosophy : whereas the MLP model relies entirely on a criticality search, the DONJON5 model is based on peaking factor minimization. DONJON5 model leads to a higher plutonium inventory for fresh fuel fabrication that impacts uranium evolution and, eventually, discharged inventories. Overall these observations do not necessarily refute MLP models applicability for heterogeneous reactors, but highlight and challenge their limitations.

## 7 Complex scenarios involving UOx and heterogeneous reactors

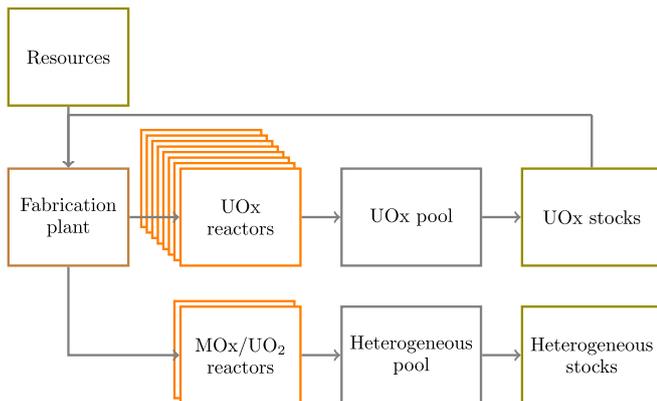
Finally, CLASS-DONJON5 coupling was evaluated on full scenarios involving MOx fuels loading in a reactor fleet composed of PWRs initially loaded with UOx assemblies. The purpose of this section is once again to quantify discrepancies between discharged isotopic inventories resulting from reactor models considering the core scale (i.e. CLASS-DONJON5) and simplified models (i.e. CLASS-MLP).

### 7.1 Scenario characteristics

As will be apparent shortly, studied scenarios were kept rather simple, yet realistic, due to their academic nature. Consequently, the reactor fleet considered here includes only 10 identical 900 MWe PWRs. Note that these PWRs are entirely loaded with UOx fuels and operated for 20 cycles. This is done in order to accumulate sufficient irradiated UOx stockpiles to constantly fabricate MOx fuels. Two UOx reactors are then partially loaded with MOx fuels. Those ten reactors (8 UOx and 2 UOx/MOx) are operated for an additional 30 cycles, amounting to approximately 50 years (standard reactor life time), before shutting down. A simplified illustration of this scenario is presented in Figure 11. Through the variation of stock management options, three different scenarios have been



**Fig. 10.** Uranium (a) and plutonium (b) inventories simulated with CLASS-DONJON5 and CLASS-MLP approach for three different compositions denoted HET1, HET2 and HET3 (i.e. based on MOX1, MOX2 and MOX3, respectively).



**Fig. 11.** Representative schematization of the reactor fleet simulated in scenarios.

studied : a first scenario representing stationary fuel management as well as two scenarios describing dynamic operations characterized by distinct UOx and MOx/UO<sub>2</sub> discharged burnups. For all scenarios, UOx and MOx fuel fabrications are started at year 2.0 and year 24.5, respectively. Scenario descriptions are further detailed in Table 12.

## 7.2 Results and physical analysis of scenario A

Figure 12 presents the global evolution of plutonium inventories in UOx spent fuels and in MOx spent fuels for scenario A. Essentially, conclusions reached here conform to findings in Section 6. Pu content resulting from DONJON5 modeling is higher, when compared to the MLP fuel loading model, allowing for greater procurement from UOx stockpiles for MOx loading or, stated another way, less UOx spent fuel accumulation with DONJON5. It is worth clarifying that this overestimated Pu content

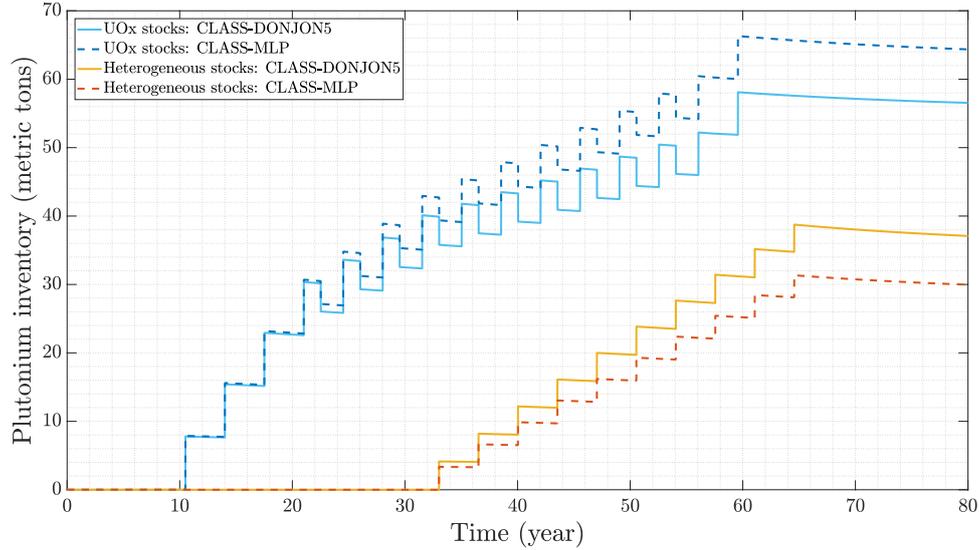
**Table 12.** Scenario denomination and reactors descriptions. Cycle lengths ( $l_{\text{cycle}}$ ) are in full power equivalent days and discharged burnups (BU) are in  $\text{GWd}\cdot\text{t}_{\text{HM}}$ .

Scenario	UOx		MOx/UOx		Stocks management
	$l_{\text{cycle}}$	BU	$l_{\text{cycle}}$	BU	
A	320	46.0	320	46.0	LiFo
B	350	50.5	280	40.5	LiFo
C	320	46.0	350	50.5	Mix

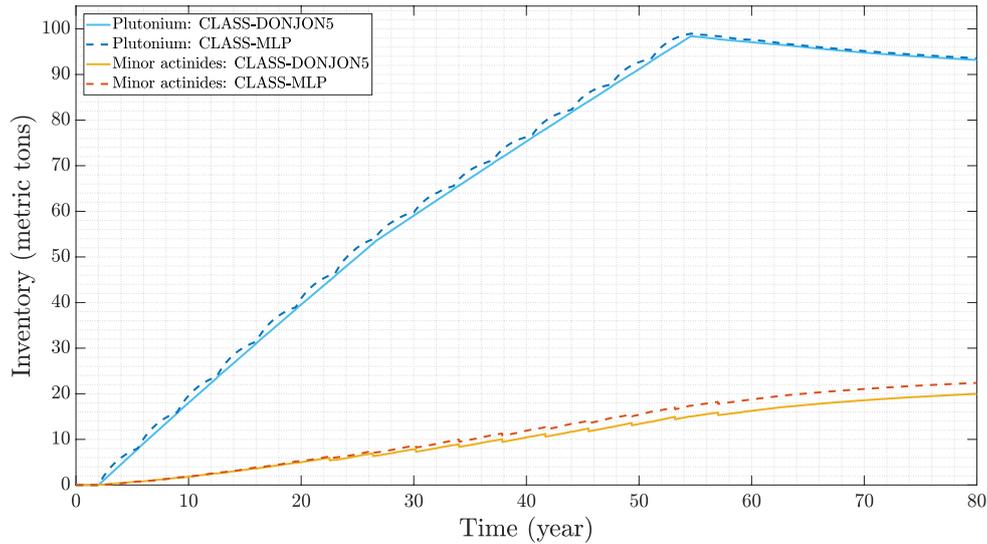
calculated with DONJON5 does not reflect higher plutonium consumption at the fleet scale. Indeed, plutonium inventories in MOx stockpiles are also higher in CLASS-DONJON5 simulations, when compared to CLASS-MLP simulations.

As one can see in Figures 10 and 12, discharged plutonium inventories obtained with MLP models differed greatly from DONJON5 at the reactor scale. It is worth mentioning that these biases may not be as visible at full-cycle scale (i.e. in wastes and all cycle installations). Considering that plutonium discrepancies in MOx spent fuels predicted with MLP are primarily generated by the fuel loading model and assuming that fuel irradiation with MLP is roughly accurate, plutonium leftover is still accounted for in UOx spent fuel.

Figure 13 shows total plutonium and minor actinides inventories in-cycle. From this figure, we can see a remarkable compensation of biases for plutonium as simulations with MLP and DONJON5 give very similar plutonium evolution. Nonetheless, the minor actinides show strong biases, consistent with previous comparison between DONJON5 and MLP [16]. As 8 reactors are entirely fuelled with UOx fuels, differences are mainly driven by UOx behavior.



**Fig. 12.** Plutonium quantity accumulated UOx and heterogeneous stocks.



**Fig. 13.** Global plutonium and minor actinides inventories accumulated in-cycle.

### 7.3 Impact of reactor parameters

Scenario B differs from scenario A by its higher UOx discharged burnup and its smaller MOx discharged burnup. This leads to smaller Pu content for MOx fuels and lower isotopic plutonium quality, when compared to results from scenario A. Scenario C presents a higher MOx burnup. Also note that this scenario considers a different stock management option denoted Mix: MOx fuel fabrication is supplied in an alternating sequence between the last and first UOx spent fuel (i.e. LiFo and FiFo) resulting in a succession of degraded and improved isotopic compositions.

For the sake of brevity, only discrepancies on Pu and MA (Minor Actinides) inventories at the end of the simulation (i.e. 80 years) between CLASS-MLP and CLASS-DONJON5 are displayed for scenarios B and C (cf. Tab. 13). Differences between each scenario are not

**Table 13.** Relative differences (%) for plutonium and minor actinides between simulations performed with DONJON5 and MLP models after 80 years.

Scenario	Plutonium	Minor actinides
A	0.73	10.09
B	2.10	11.11
C	0.40	10.50

discussed here, but the total in-cycle plutonium inventory in scenario B ( $\sim 100$  tons) is higher than in scenarios A and C ( $\sim 95$  tons). Note in addition that differences between MLP and DONJON5 approaches for a given scenario.

We then conclude that, although reactor models based on MLP do not represent accurately reactor physics and thus lead to possible erroneous evaluation of discharged

inventories, they seem suitable for global plutonium evolution in large fuel cycle calculations. Stated another way: while calculations performed with MLP can yield acceptable values for global inventories, MLP models do not predict correctly material availability for fresh fuel fabrications as they induce a significant error on plutonium location in the fuel cycle.

## 8 Conclusion

In this paper, DONJON5 full-core diffusion calculations were effectively coupled to CLASS for dynamic fuel cycle simulations. Some procedures were designed to accelerate full-core computations while keeping the scenario code CLASS capability to dynamically adapt reactor fuel loading to respect available fissile materials specifically taking into account isotopic quality. Great efforts were invested to ensure critical depletion at all time and to adequately simulate fuel environment whilst maintaining reasonable calculation costs. Original methods were also developed to avoid the initial balancing processes and to reduce the number of iterations to determine the boron critical content in the moderator.

The coupling of DONJON5 with CLASS for heterogeneous reactors required the development of a dedicated original fuel loading model. The one proposed here relies on identifying Pu content to ensure a minimal power peaking factor. It differs from previous loading models based on infinite neutron multiplication coefficient considerations.

Full-core calculations were used to analyze some of the parameters considered in the neural networks based approach and their impact on scenario accuracy. It was shown that the main source of discrepancy for plutonium inventory estimations is primarily due to the fuel loading model. The irradiation model was also shown unsatisfactory for  $^{235}\text{U}$  in-core inventory prediction as well as minor actinides production. The above observations are coherent with previous work like [21] and with physics [22] because  $^{235}\text{U}$  and minor actinides are much more sensitive to neutron flux induced effects. The 2-groups diffusion scheme for full-core calculations seems to be a minimum requirement to take these differences into account.

One possible way to improve neural networks models would be to use the full-core database built for this work to calculate fresh fuel compositions based on power peaking factors for heterogeneous reactors. This database also enables a  $k_{\text{threshold}}$  calculations that are adapted for Pu quality. In that case, it was shown that MLP processed results are both good (less than a 1% discrepancy on ore consumption and plutonium production) and very fast (few minutes compared to hours for coupled executions). This raises the question of code flexibility: although  $k_{\text{threshold}}$  models specifically developed for each reactor geometry could lead to more precise fuel fabrication with ANNs in CLASS, this would lead to considerably less flexible physic models. On the other hand, it seems that no intrinsic core effects can be simulated without considering specific core characteristics.

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## Author contribution statement

All the authors have read and approved the final manuscript.

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