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Coupled CLASS and DONJON5 3D full-core calculations and comparison with the neural network approach for fuel cycles involving MOX fueled PWRs

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ABSTRACT

The scenario code CLASS relies on infinite assembly simulation to predict fuel actinide inventories at exit burnup. In the current work, we replace these assembly calculations by full-core simulations and evaluate the impact on actinide inventories predicted by CLASS. To achieve this goal, we generate neural network training databanks for CLASS using the lattice code DRAGON5. For UOX fuels, the databanks are sampled stochastically for exit burnup, moderator boron concentration and uranium 235 enrichment while for MOX fuels an eight-dimensional grid is sampled that also accounts for plutonium and americium-241 initial contents. DRAGON5 is used to generate the databases for DONJON5 3D full-core diffusion calculations in CLASS. Results obtained using neural networks CLASS and DONJON5/CLASS calculations are then compared to assess the different assumptions used in classical scenario simulations and determine the major source of errors. A simple UOX scenario involving long-term fuel storage and a more complex scenario involving reprocessed UOX spent fuel and MOX fabrication are then studied. They show that inventories of uranium 235 and minor actinides are sensitive to full-core simulations. Moreover, the neural networks CLASS simulations can be improved using an adapted $k_{\text{threshold}}$ that depends on the initial fuel composition.

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1. Introduction

CLASS (Mouginot et al., 2014) (Core Library for Advanced Scenario Simulation) is an open source package of C++ libraries. It performs simulations of entire fuel cycles based on several facilities: reactors, cooling pools, fabrication plants, storage and separation plants. It contains a fuel loading model that is used to fabricate fresh fuel from a priori unknown fissile materials. An irradiation model is then used to perform in core fuel burnup based on a fourth-order Runge–Kutta solution of the Bateman equations. Thus, reactors are simulated through two independent steps: fuel loading followed by irradiation. These two models are based on MLP (Multi Layer Perceptrons) neutronic predictors (Rosenblatt, 1961; Hoecker et al., 2007) trained on databanks generated by infinite assembly simulations (Leniau et al., 2015). Both UOX and MOX PWRs (Courtin et al., 2017) can be treated and elementary (one reactor type) as well as complex (coupled UOX-MOX reactor) scenarios analyzed.

The models currently used in CLASS for fuel cycle studies lead to several calculation biases. Among them, reactors are simulated with fresh fuel at refueling with the total reactor content being discharged after completion of its irradiation cycles (generally three or four cycles). Moreover, when neutronic predictors are used, additional approximations are considered due to the absence of full-core computations. Since no clear assembly reactivity condition is imposed, the core reactivity margin to criticality at discharge is approximated by the average k_∞ over the whole core assemblies at the end of an irradiation cycle. This value can only be calculated assuming certain burnup values for each fuel batch. Usually, a uniform irradiation rate is considered (Leniau et al., 2015). For these neural networks based approaches, no environment nor neutron leakage (radial, axial, or due to specific assembly positioning or neighbourhood) is taken into account.

Here, we propose to couple CLASS with the deterministic full-core code DONJON5 (Hébert et al., 2019). Since computation time is a key parameter using the diffusion approximation is unescap-

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able. This implies a two-step procedure where DONJON5 reactor databases (cross sections and diffusion coefficients) are generated using burnup dependent infinite assembly transport simulations.

In order to make unbiased comparisons between neural networks based models and full-core calculations, both the neutronic predictors training databanks and the diffusion calculation databases are built in this work using DRAGON5 (Marleau et al., 2018). This lattice code solves the multigroup transport equation for infinite assemblies. Physics considerations imply to build a three-dimensional DONJON5 database for the UOX fuels (exit burnup, moderator boron concentration and uranium 235 enrichment) and an eighth-dimensional database for the MOX fuels (exit burnup, moderator boron concentration as well as plutonium and americium-241 contents). To appropriately sample such hyperspaces hundreds of assembly calculations are necessary for diffusion databases and thousands for neural networks databanks. This leads to a real challenge in terms of computing time. An analysis of the impact on each parameter as well as a global validation of the calculation sequence was performed in (Guillet, 2019). Fast lattice calculations schemes were designed to build consistent neural networks databanks and diffusion databases at a reasonable time cost.

The aim of this paper is to assess the different simplifying assumptions of the neural networks approach in CLASS using DONJON5/CLASS calculations as a reference. To achieve this goal, we will start with a preliminary study of the performances for different fuel types of the individual neural networks models. Then, a simple UOX scenario involving long-term fuel storage and a more complex scenario involving reprocessed UOX spent fuel and MOX fabrication are studied.

The contents of this paper is as follows. In Section 2, DRAGON5 assembly calculations are detailed. Section 3 describes how the diffusion databases are built while Section 4 describes the calculations options used for DONJON5. The performances of the neural networks models are analyzed in Section 5 followed by a discussion of their relevance for CLASS. In Sections 6 and 7 respectively, an elementary scenario for a single UOX fueled PWR and a complex scenario that involves both UOX and MOX fueled PWR are analyzed and discussed. Finally, we conclude in Section 8.

2. DRAGON5 lattice calculations

2.1. Infinite assembly

The geometry of the infinite PWR assembly simulated with DRAGON5 is displayed in Fig. 1. To simplify this study, no control device or structure element is simulated except for guide tubes. Reactivity control, if required, is ensured by adding boron in the moderator. Given its symmetry, computations are performed for one eighth of the assembly using adequate boundary conditions.

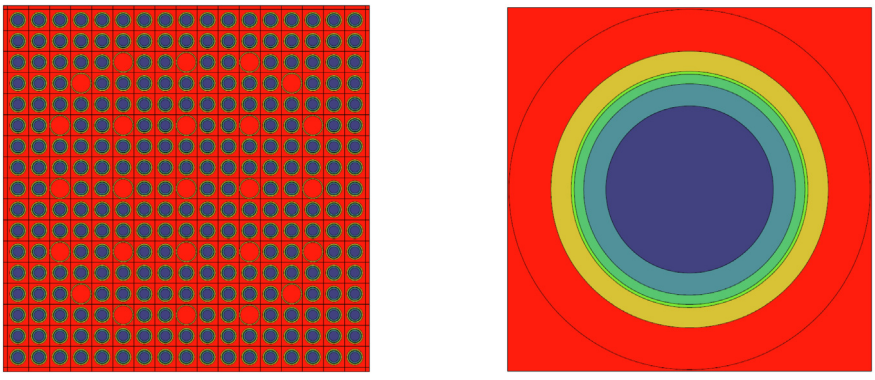
Each fuel pin cell in the assembly (see Fig. 1(b)) is a square region that contains six annular subregions with six different mixtures. The first four rings (inner to outer annular regions) are filled with fuel and contain respectively 50, 30, 15 and 5 % of the fuel pellet volume. This is sufficient to ensure good accuracy for the collision probability (CP) flux solver of DRAGON5 as well as the spatial buildup of ^{239}Pu with irradiation (Santamarina et al., 2004). The next ring represents the fuel clad. The moderator is divided into two zones to account for neutron slowing down in light water and ensure convergence of the flux solution (an annular region followed by a region with outer Cartesian boundaries). For the same reason, the water holes inside the guide tube cells are also subdivided into three concentric rings. Key geometry data for the assembly are listed in Table 1.

The average value for thermal power densities, the fuel density as well as the fuel, clad and moderator temperatures considered for infinite assembly calculations are presented in Table 2 where the subscript HM represents the initial contents of heavy metals (actinides) in the fuel.

In DRAGON5, the global tracking is generated with the `NXT:` (Marleau, 2006) module ensuring very precise flux evaluations with the CP method. For resonance self-shielding calculations, a simplified tracking (module `SYBILT:`) is considered to evaluate CP based on the interface current technique. The `USS:` module is then used to create self-shielded cross sections based on physical probability tables (Hébert and Coste, 2002). An ENDF/B-VII.r1 (Chadwick and Herman, 2011) 172-group nuclear data library in the DRAGR format is selected for our calculations (Hébert et al., 2007). The multigroup transport equation is solved with a B1 homogeneous leakage model (Petrovic et al., 1996). Finally, burnup dependent two groups condensed and homogenized macroscopic cross sections as well as diffusion coefficients are stored in a data-

Table 1
Assembly geometry data.

Number of fuel rods	264
Number of guide tubes	25
Pin pitch	1.2598 cm
Fuel pellet outer radius	0.4096 cm
External clad radius	0.4798 cm
Guide tube inner radius	0.56 cm
Guide tube outer radius	0.62 cm
Water strip	0.2500 cm



(a) Assembly. (b) Pin cell with four ring fuel discretization.

Fig. 1. Assembly (a) and pin cell (b) geometries. Materials are identified as follows: moderator in red, fuel clad in yellow and four rings in fuel pellets ranging from blue to green.

Table 2
Other assembly properties.

Thermal power density	36.0 W/g_{HM}
UO_2 Fuel density	10.4 g/cm^3
Fuel temperature	900 K
Water moderator temperature	569.55 K
Zircaloy 4 clad temperature	633 K

Table 3
Geometry for reflector simulation.

Baffle (steel)	2.86 cm
Moderator (light water)	5.86 cm
Skin (steel)	5.15 cm
Moderator (light water)	8.05 cm

base that will be used by the code DONJON5 to evaluate core discharge burnup. A second database is also created containing 2-group condensed and homogenized microscopic cross sections for 22 relevant nuclides: ^{234}U, ^{235}U, ^{236}U, ^{237}U, ^{238}U, ^{237}Np, ^{238}Np, ^{239}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{242}Am, ^{242m}Am, ^{243}Am, ^{242}Cm, ^{243}Cm, ^{244}Cm, ^{245}Cm, ^{246}Cm. This last database is required to compute discharged fuel isotopic inventories in full core calculations.

2.2. Reflector materials

For full core calculations in DONJON5, two-group homogenized cross sections have to be provided for all materials. In order to get consistent nuclear data for the materials used as reflectors, DRAGON5 simulations were conducted on the geometry displayed in Fig. 2. In this figure, two half-fuel assemblies provide the neutron sources required to solve for the flux distribution inside the baffle (yellow), reactor skin (red) and two moderator layers (orange).

The dimensions of the four simulated reflector regions are listed in Table 3 (Bejaoui, 2012). Given the high number of spatial zones to consider in this simulation, the method of characteristics (MoC) was used for this assembly calculation. Homogenization is performed over the four reflector regions and the cross sections are condensed to two energy groups.

3. Databases construction

3.1. Multiparameter diffusion databases

The calculation sequence detailed in Section 2 generates a burnup dependent diffusion database for fixed reactor operation conditions (temperatures, boron concentration, etc.). However, in order to ensure that the reactor remains critical at each simulation step, moderator boron concentration must be adjusted in time. In CLASS simulations, the isotopic contents of the fuel loaded may also vary at each cycle. Thus, reactor core simulations using DONJON5 require multiparameter cross-section database, or MULTICOMPO, created by DRAGON5 that can be easily interpolated. These MULTICOMPO are sets of burnup dependent diffusion database characterized by local or global parameters selected in such a way that cubic interpolations provide reliable cross sections even with few sampling points (Guillet, 2019). The burnup discretization we used for these MULTICOMPO consists of 25 non-regular depletion steps (first fine, then coarse) going up to 79.2 GWd/t_{HM} (2200 full power days at reference power) (Leroyer, 2009). For moderator boron, three levels were considered, namely 0, 1375 and 2750 ppm.

For UOX fuel, the sampling just consists in selecting 3 ^{235}U enrichment (3, 4 and 5%). For MOX fuel composed of 0.25% depleted uranium and plutonium, the fraction of Pu + Am in the fuel is first selected. Then, ^{238}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu and ^{241}Am relative concentrations with respect to total Pu + Am are considered. ^{239}Pu concentration is used here as a buffer for normalization. provides the fuel parameters sampling values used in this study. One can note that some plutonium composition vectors created by this sampling are highly improbable. However these points are required in the database because our interpolation method assumes that the parameter grid is completely filled. For MOX fuels, the resulting eight-dimensional interpolation process is very costly and cubic interpolation is used for every parameter for which three sampling points or more are required, otherwise a linear interpolation is considered.

3.2. Neural networks databanks

In order to make unbiased comparisons between neural network predictors and full-core diffusion results in CLASS, a DRAGON5 based set of neural predictors was built. The same calculation options and the same multigroup cross-section library are used to compute the neural networks training databank and the diffusion database. The main differences lie in the number of lattice calculations and the sampling method. While regular sampling and 225 (i.e. 3 ^{235}U enrichments $\times$ 3 boron concentrations $\times$ 25 burnup steps) lattice calculations are satisfactory for the DONJON5 UOX database, neural networks require a random sampling of several hundreds of calculations to avoid significant training biases. Estimating the neural network precision with respect to the number of single depletion calculation is not easy. Hence, a conservative sampling process considering more calculations than strictly necessary was chosen. As described in Section 1, MLP (Rosenblatt, 1961) are used to generate both a fuel loading and an irradiation model. One neural predictor is designed to predict the assembly reactivity with irradiation for a priori unknown initial isotopic compositions. Sixty-six additional predictors (by reactor type) are used to generate one group cross sections for the (n,2n), (n,γ), (n,f) reactions simulated in CLASS and for each of the twenty-two relevant nuclides listed in Section 2.1. The number of assembly burnup calculations and neutronic predictors used for our simulations are listed in Table 5. Note that a previous study has shown that discharge isotopic inventories for zero boron assembly calculations are very close to step-by-step critical full-core compu-

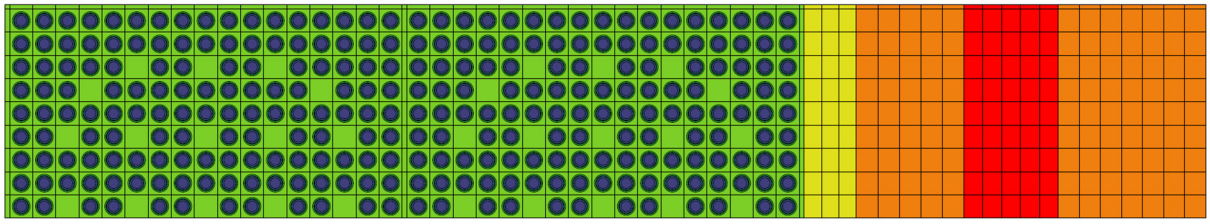


Fig. 2. Calculation geometry for reflector material modeling.

Table 4
MOX fuel parameters considered for the MULTICOMPO databases

Parameter	Sampling (weight %)
Pu + Am	4.50, 6.00, 7.50, 9.00, 10.50, 12.00 and 13.50
^{238}Pu in Pu + Am	0.50 and 5.50
^{240}Pu in Pu + Am	21.50, 26.50 and 31.50
^{241}Pu in Pu + Am	1.50, 10.50 and 19.50
^{242}Pu in Pu + Am	3.50, 8.00 and 12.50
^{241}Am in Pu + Am	0.01 and 1.75
^{239}Pu in Pu + Am	$100 - (\sum_{j \neq 239}^{j} \text{Pu} + ^{241}\text{Am})$

Table 5
Neural networks key parameters.

Number of random UOX compositions	800
Number of random MOX compositions	3000
Reactivity predictor (by reactor type)	1
Cross section predictors (by reactor type)	66

tations leading to very low biases (Guillet, 2019). This was compared to time averaged boron concentration (calculated with step-by-step critical diffusion computations) that led to important biases on discharge isotopic inventories. Therefore, neural networks training databanks are built with no moderator boron.

4. DONJON5 full-core calculations

Our 3D full-core reactor calculations are performed with DONJON5 for a 2700 MW_{th} reference PWR core. Assembly homogenization is used for the fuel and the four reflector regions (see Fig. 2) are homogenized to form a single reflector material. A 2D axial plane of the real core is displayed in Fig. 3. It is simulated in DONJON5 using the geometry presented in Fig. 4. No reactivity control device nor structural element are considered. No further 2D geometry discretization is necessary to ensure 0.01% precision on fuel enrichment and 50 ppm precision on boron critical concentration

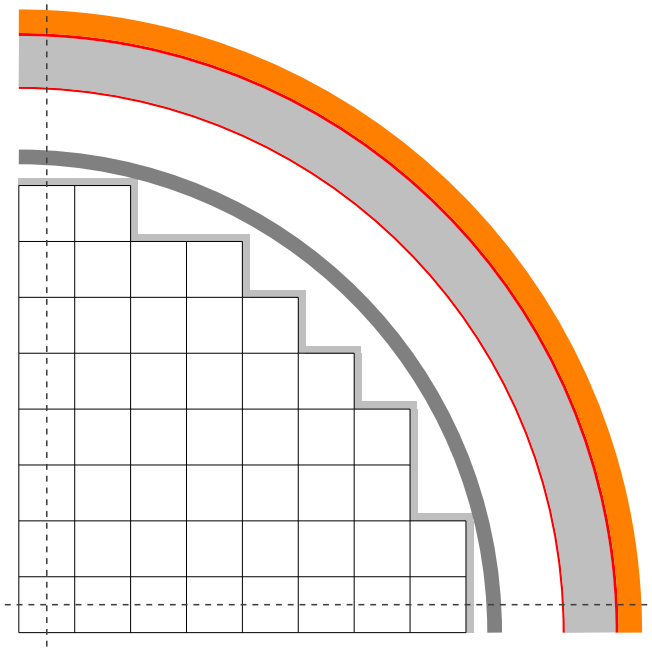


Fig. 3. Real quarter core layout (2D plane). Fuel assemblies (white), steel baffle (light gray), barrel (dark gray), steel vessel (gray) and thermal insulator (red and orange) are displayed.

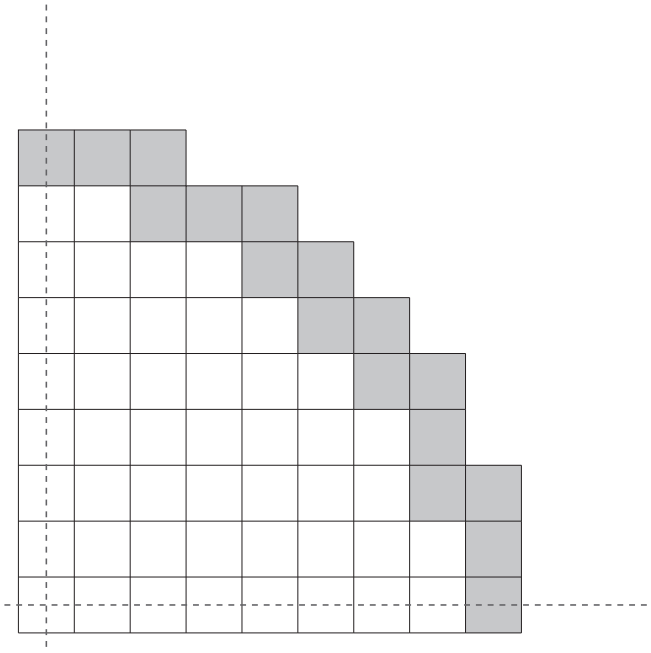


Fig. 4. Simulated quarter core layout (2D plane). Fuel assemblies (white) and reflector elements (gray) are displayed.

in the core. For 3D flux computations, 17 equal thickness fuel planes as well as two reflector planes (lower and upper) are considered. Key core geometry data are listed in Table 6. In the full-core computations, the burnup is different in the mixtures characterizing each of the 2669 fuel subassemblies (157 per plane).

4.1. Fuel loading patterns

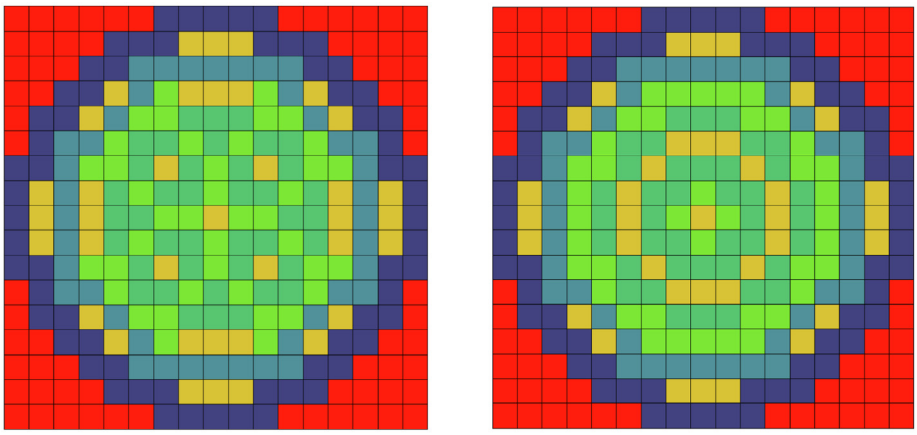
Performing full-core calculations allows one to simulate realistically in-core burnup of assemblies for a specific fuel loading pattern with neighbourhood effects properly taken into account (Trellue, 2006). Since optimizing the fuel loading patterns at each reactor refuelling is not possible in CLASS, reference patterns are pre-defined for UOX and MOX fuels. This leads to acceptable, yet non-optimal, power distributions in the core. Because these power distributions depend on the fuel type (Worrall, 2000), two different 4 cycles fuel loading patterns were considered respectively for the UOX and MOX fuels (see Fig. 5). These loading patterns lead to power form factors that are satisfactory for both fuels. In this work, the module `SIM:` (Salino and Hébert, 2016) is used in DONJON5 to perform in-core fuel management.

4.2. Fuel burnups at reloading

While the contents of the new fuels inserted in the reactor at the time of reloading is known, the isotopic composition and burnup of the fuels having spent 1, 2 and 3 cycles in the core is generally unknown. In CLASS, one generally assumes that the old fuels had the same initial isotopic contents as the new fuel and uniform

Table 6
Reactor core geometry data.

Number of assemblies	157
Core height	416.48 cm
Assembly height	372.64 cm
Assembly HM inventory	475.30 kg



(a) UOX. (b) MOX.

Fig. 5. Core loading patterns for UOX (a) and MOX (b) fuels. Red stands for void regions, dark blue for radial reflector material, light blue for new assemblies, and dark green, light green and yellow respectively for assemblies burned for one, two and three cycles.

batch burnups $B_{i,\mathrm{U}}$ of 13, 26 and 39 GWd/t_{HM} for a cycle length of T_{Ref}=350 days.

We studied several ways to improve this choice, both for UOX and MOX fuels. First, instead of taking a uniform burnup, zone dependent burnups are considered. These are obtained at equilibrium refueling conditions for a reference fuel of enrichment ϵ_{Ref}. For UOX cores, the burnups after a time T_{Ref} are nearly independent of the ^{235}U enrichment and a single set of values $B_i(\epsilon)$ all evaluated at the same reference enrichment ϵ_{Ref} can be used. For MOX fuels, the problem is more complex since the fuel is characterized both by the total Pu and Am contents of the fuel and by the concentrations of individual fissile and fertile heavy isotopes. Defining the initial enrichment ϵ of the MOX fuels as

$$\epsilon = \left(\sum_{j\in\text{fissiles}} N_j\right) \Big/ \left(\sum_{j\in\text{HM}-\text{U238}} N_j\right), \tag{1}$$

where HM-U238 represents all heavy metal excluding ^{238}U, and assuming that $\epsilon_{\mathrm{Ref}} = 0.63$ is the value at which reference zone burnups are calculated, then we will approximate $B_i(\epsilon)$ as follows

$$B_i(\epsilon) = B_i(\epsilon_{\mathrm{Ref}}) + \frac{\epsilon - \epsilon_{\mathrm{Ref}}}{0.125}\Delta B_i \tag{2}$$

where ΔB_i is determined numerically. As a result, for a fixed total plutonium contents, B_i varies linearly with the total fissile isotope concentration in the fuel.

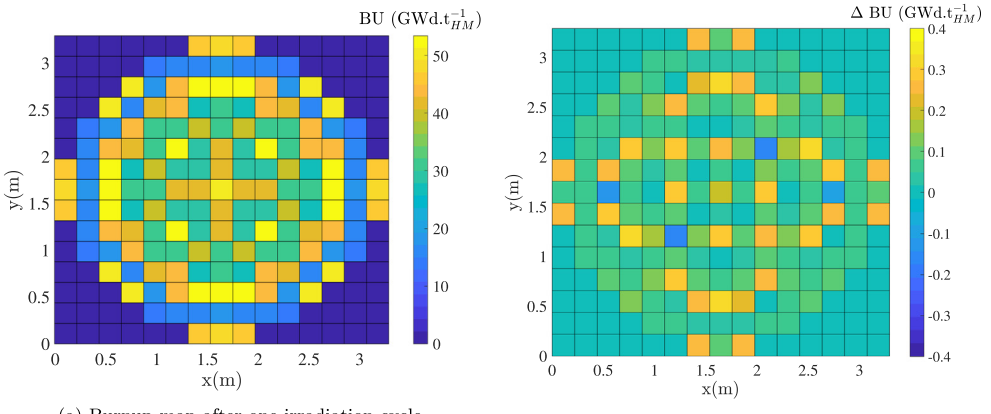
Finally, it is also important to take into account the cycle length on assembly burnups. Assuming the reference cycle is T_{Ref}=350 days long, then for a cycle length T between 320 and 390 days, we can use a linear correction of the form

$$B_i(\epsilon, T) = B_i(\epsilon)\frac{T}{T_{Ref}}. \tag{3}$$

One can see respectively in Figs. 6 and 7 UOX and MOX (MOX1 composition in Table 7) burnup predictions after one irradiation cycle as well as end-of-cycle burnup differences between one and four irradiation cycles (350 EFPD). For UOX, maximum absolute burnup differences lower than 0.2 GWd/t_{HM} are observed (to be compared with a discharge value of 50 GWd/t_{HM}). For MOX fuels, similar results are displayed. However, the maximum end of cycle burnup differences are now larger and reaches 1.0 GWd/t_{HM}. These two examples show that the linear corrections we proposed leads to accurate predictions with an impact lower than 1% on the average discharge burnup. This error may seem pretty large with respect to the standard performances of industrial codes, but considering the need for reasonable computational costs, it is more than acceptable for scenario studies.

4.3. Critical boron concentration

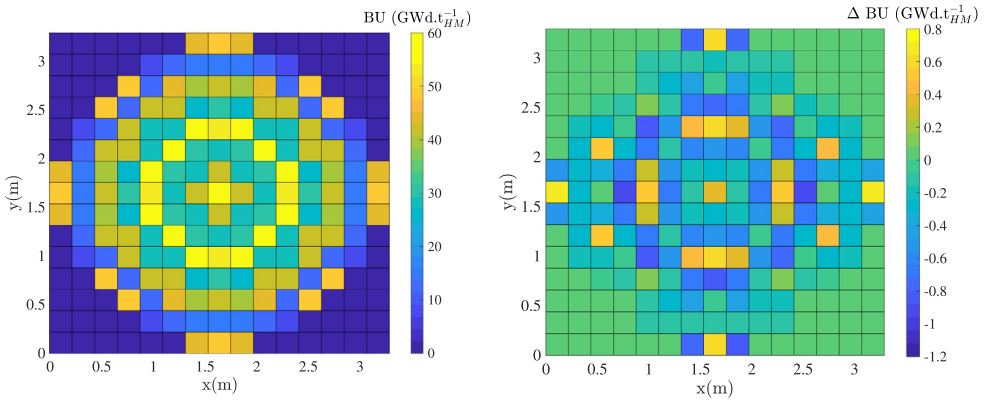
Critical conditions are necessary at each burnup step in DONJON5 to compute realistic in-core flux distributions, burnups and



(a) Burnup map after one irradiation cycle.

(b) Burnup differences between first and fourth cycle.

Fig. 6. UOX burnup predictions.



(a) Burnup map after one irradiation cycle.

(b) Burnup differences between first and fourth cycle.

Fig. 7. MOX burnup predictions.

Table 7
MOX fuel compositions in weight % of total plutonium and ^{241}Am.

Fuel	^{238}Pu	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu	^{241}Am
MOX0	3.12	51.84	24.32	11.75	8.04	1.18
MOX1	1.98	62.25	22.50	8.00	5.00	0.27
MOX2	2.87	49.99	30.91	4.54	10.92	0.77

ultimately isotopic compositions under irradiation. For the first irradiation cycle, an iterative process is used at each burnup step to evaluate the moderator boron concentration that ensures the whole core is critical. The convergence of this process to 5 ppm accuracy in DONJON5 relies on the Brent algorithm programmed in the `FINDO:` module (Press et al., 1994). The corresponding deviation in reactivity is 20 to 50 pcm depending on fuel composition since boron efficiency is a function of plutonium contents (Trellue, 2006).

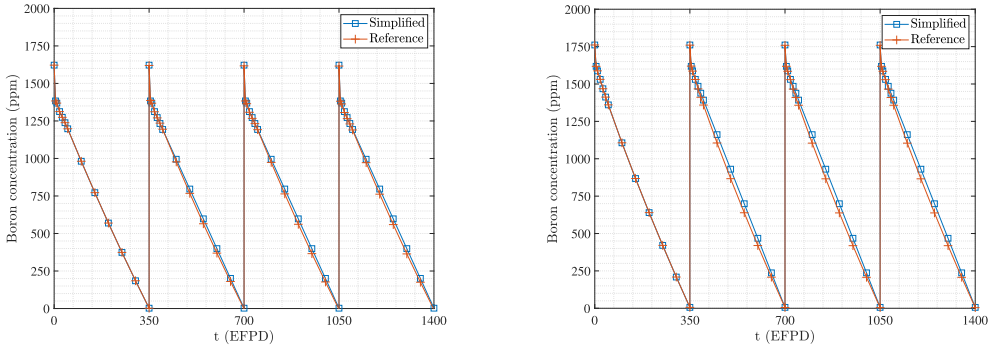
Even if each core calculation is relatively fast, the number of such simulation required by the iterative process leads to significant computation costs. Considering the boron concentration profile with irradiation (see Fig. 8) for 4 burnup cycle, we see that the boron concentrations in cycles 2 to 4 are nearly identical to those obtained in cycle 1 since the fuel loading sequences are all identical. Consequently, it is only necessary to determine boron concentration for the first cycle. Moreover, observing that the boron profile is mostly linear after the ^{135}Xe initial drop off, a simplified linear interpolation for boron concentration is used until the next fuel loading. This leads to the simplified boron concentration profiles displayed on Fig. 8 where reference values are also presented.

5. Neural networks analysis

To identify the main sources of error in neural networks models based on infinite assembly simulations, preliminary studies were conducted on the neural networks themselves. Hence, the results produced by CLASS reactor physics models (i.e. fuel loading and irradiation models) based on neural networks are compared with CLASS-DONJON5 simulation results.

5.1. $k_{\text{threshold}}$ and the fuel loading model

CLASS scripts were first produced to control the fuel composition for loading from the isotopic contents of stockpiles. These scripts enabled us to call both fuel loading models (assembly or core based) with the same isotopic composition. Thus, the accuracy of the reactivity predictors can be evaluated by comparing the required enrichments for the same discharge burnup. CLASS reac-



(a) UOX.

(b) MOX.

Fig. 8. In-core boron concentration for UOX (a) and MOX (b) fuels.

tivity predictors are based on the parameter $k_{\text{threshold}}$ that is calculated according to

$$k_{\text{threshold}} = \frac{1}{N}\sum_{n=1}^{N} k_{\infty}(B_{n,\text{discharge}}) \tag{4}$$

Here, $k_{\text{threshold}}$ is the average of k_{∞} for the N assemblies at discharge burnup $B_{n,\text{discharge}}$. It is an infinite assembly estimation of the reactivity margin needed at end-of-cycle to maintain the core critical.

Usually, because the burnup is a priori unknown, an arbitrary value $k_{0,\text{threshold}}$ is selected but never justified precisely (Nuttin et al., 2012). It is used to evaluate the maximal burnup achievable at discharge. One alternative approach consists in averaging the k_{∞} obtained from assembly calculations assuming the irradiation rate is constant for all assemblies (Nuttin et al., 2012). Although this approximation is relatively coarse, the threshold value $k_{a,\text{threshold}}$ obtained should improve the predicted value of the fuel enrichment required to achieve a specific burnup target.

The reference approach we used for comparison consists in calculating the threshold k by taking the average over the N assemblies in the core at the discharge burnup $B_{n,\text{discharge}}$ calculated using DONJON5 core simulations. Thus, chained DONJON5 diffusion and DRAGON5 transport calculations are used for different fuels. Fuel enrichment is determined by DONJON5 (for a specific isotopic vector) as well as batch discharge burnups. Then, an assembly with this enrichment is simulated with DRAGON5 generating a k_{∞} burnup curves from which the reference value $k_{r,\text{threshold}}$ can be determined. In Fig. 9, k_{∞} curves are displayed for one UOX and two different MOX fuels (MOX1 and MOX2) with compositions listed in Table 7. For each fuel type, the symbols (blue, yellow and green) represent the average of assembly k_{∞} for all the fuels burned for one, two, three or four cycle of 350 days in the core at local DONJON5 powers. The red dots represents assembly k_{∞} after one, two, three and four cycles at constant power.

During the first, second and third cycles, the UOX assemblies are burning significantly faster in a reactor environment than when a constant irradiation rate is considered. For the fourth cycle they are burning slower. For MOX fuels, these observations remain valid for the second, third and fourth cycles. On the other hand, the behaviour of the first cycle depends strongly on the exact fuel composition and the first cycle burnup can be larger or smaller than the constant irradiation rate value.

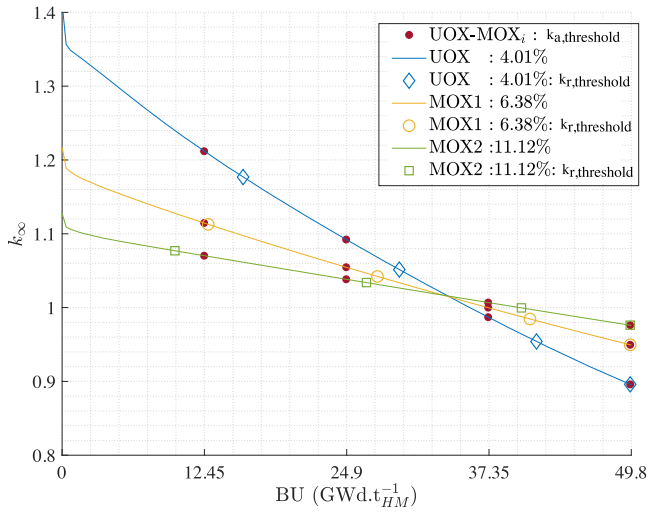


Fig. 9. Assembly reactivity evolution and reactivity at each refueling time evaluated with chained DONJON5-DRAGON5 calculations.

Reactivity changes induced by irradiation are flatter for MOX fuels than for UOX. These different observations combined with Table 8 results show that UOX $k_{\text{threshold}}$ is more sensitive to the constant irradiation rate approximation, meaning that the difference between calculated $k_{a,threshold}$ and $k_{r,threshold}$ are larger for UOX than for MOX fuels. In Table 8, $k_{a,threshold}$ ($k_{r,thershold}$) for a given fuel composition is the batch volume weighted average of the k_{∞} associated with the red dots (other symbols). It is also worth mentioning that $k_{r,\text{threshold}}$ is nearly independent of the fuel composition. This is expected because this $k_{\text{threshold}}$ is evaluated using assembly end-of-cycle burnups from reactor core simulations and the equivalent enrichments of the fuels were selected in such a way that their average discharge burnups after 350 days are identical.

Finally, the fuel loading model accuracy is measured by comparing fuel enrichments computed by neural networks based reactivity predictors and DONJON5 for the same isotopic vectors (for MOX fuels) with the same burnup target. Table 9 lists the maximum relative differences in MLP predicted enrichment between the reference DONJON5 value and that obtained using neural networks trained using $k_{a,\text{threshold}}$. We can then see that for the UOX, MOX0 and MOX1 fuels, neural networks predict a very precise enrichment when the $k_{\text{threshold}}$ parameter is averaged over the assemblies assuming constant irradiation rates. For the more extreme MOX2 fuel with a highly non-fissile composition (^{240}Pu and ^{242}Pu) and a large effective enrichment ϵ_{eq}=11.12% (Youinou et al., 1999), $k_{a,\text{threshold}}$ still leads to a difference of 7.1% in the fuel enrichment required to achieve a specific discharge burnup. This indicates that the neural networks intrinsic precision is indeed very good for relatively standard fuels with appropriate $k_{\text{threshold}}$, but this model has more difficulties with fuels that have concentrations closer to the limits of the sampling ranges (see Table 4). To measure the general impact of $k_{\text{threshold}}$ on enrichments, the process is repeated with neural networks trained using values for $k_{0,\text{threshold}}$ covering the whole range of variation of this parameter, namely from 1.040 to 1.050 and from 1.020 to 1.030 respectively for UOX and MOX fuels. These results are also listed in Table 9. From these results, it is quite clear that the fuel loading model prediction accuracy relies strongly on $k_{\text{threshold}}$ precision.

5.2. The irradiation model

The irradiation model of CLASS is used to determine in-core and discharge fuel isotopic inventories. Its input is the fresh fuel isotopics coming from the fuel loading model and the fabrication plant, and its output is the discharge fuel isotopics that goes to the reactor pool. In order to simulate in-core isotopes depletion, the irradiation model relies on cross-section predictors from which averaged microscopic cross sections are generated and used to solve the Bateman equations with a fourth order Runge–Kutta method. Sixty-six one group cross Sections (3 reactions for each of the twenty-two isotopes treated) are predicted at each time step. To compare the irradiation model based on neural networks with results obtained using DONJON5 without other biases, another adapted CLASS script was developed. It consists in fueling reactors with fixed fuel compositions (avoiding the fabrication

Table 8
Comparison of $k_{r,\text{threshold}}$ and $k_{a,\text{threshold}}$ for different fuels to reach the same discharged burnup of 49.8 GWd/t$_{\text{HM}}$.

Fuel (ϵ_{eq})	$k_{r,\text{threshold}}$	$k_{a,\text{threshold}}$
UOX (4.01%)	1.022	1.047
MOX0 (7.68%)	1.024	1.027
MOX1 (6.38%)	1.024	1.030
MOX2 (11.12%)	1.023	1.023

Table 9
Maximum differences in enrichment for $k_{\alpha,\text{threshold}}$ and $k_{0,\text{threshold}}$ MLP models.

Fuel type	$k_{\alpha,\text{threshold}}$	$k_{0,\text{threshold}}$
UOX	0.3%	4.6%
MOX0	1.3%	8.2%
MOX1	1.4%	7.8%
MOX2	7.1%	7.8%

plant and the fuel loading model) both for neural networks and DONJON5 based irradiation calculations. Differences in discharge inventories of selected isotopes for 4.01% enriched UOX, MOX0 with 7.68% plutonium, MOX1 (6.38% plutonium) and MOX2 (11.12% plutonium) fuels are listed in Table 10.

Relatively large errors (>5%) are observed for the minor actinides in UOX and MOX fuels in spite of the dilution effect due to ^{241}Pu decay occurring more significantly in MOX. Total differences on plutonium inventories are much lower in both cases remaining at less than 5%. The higher biaises for uranium than plutonium isotopes come from the different simulation hypothesis considered when creating the neural networks training databanks. Indeed, the simulations are carried out with zero moderator boron to minimize errors in plutonium for PWR fuel recycling studies. These results provide an estimation of the typical calculation biases of the irradiation model in fuel cycle simulations. The consequences on integral quantities relevant for scenario studies like natural uranium ore consumption, waste production or plutonium recycling capabilities are not straightforward. Propagation of those biases on complex and industrial scenarios should be studied in order to calculate operational margins on different relevant quantities.

6. Elementary scenario

An example of an elementary scenario is presented in Fig. 10. It considers a single reactor and includes a fuel fabrication plant as well as disposal of spent fuel to storage after a cooling down period in a pool. This is the simplest fuel cycle that can be simulated with CLASS but this study can be generalized to more reactors given a constant set of operational parameters. To simplify the present study, the following time scales are considered: 2-year fabrication time for one batch of fuel for one reactor loading irradiated during 4×350 days and finally a cooling period of 5 years starting after reactor discharge. Moreover, the $k_{0,\text{threshold}}$ values selected for the CLASS fuel loading model are 1.045 and 1.025 respectively for UOX and MOX fuels. These values should be close enough to the exact values to induce respectively 3% maximum deviation in the UOX fuel enrichment loading and 2% maximum deviation in the MOX total plutonium loading.

If one only looks at the fuel composition on a chemical element level, the CLASS-MLP to CLASS-DONJON5 relative mass differences are relatively small, not exceeding 1% for uranium, 5% for plutonium and 10% for the minor actinides. However, from the point of view of UOX fuels reprocessing or long-term storage of irradiated fuels, the large differences in contents for individual isotope are important. Thus, absolute (kg) and relative differences (%) between MLP and DONJON5 in the isotopic contents of discharged UOX and MOX (see MOX0 in Table 7) assemblies are presented in



Fig. 10. Elementary scenario architecture.

Fig. 11 for isotopes of interest. Here, it is clear that the fuel loading model (leading to different core load enrichment for UOX and plutonium total contents for MOX) is the main source of error. Differences in core mass discharge are a result of both the fuel loading model and the irradiation model discrepancies.

For some isotopes, pool discharge mass differences are larger than core discharge mass differences in absolute value. For UOX fuels, the higher difference in ^{240}Pu inventory at pool discharge than at core discharge is due mainly to the α decay of the excessive amount of ^{244}Cm present in the fuel at core discharge. Similarly, the β decay of ^{241}Pu to ^{241}Am means that an overestimation of the ^{241}Pu contents in the discharge UOX fuel (conversely, an under estimation for MOX) will lead to a large over prediction (under production) of ^{241}Am. For example, in MOX reactors, neural networks are underestimating ^{241}Pu core discharge concentration by approximately 20 kg. Roughly 20 % of ^{241}Pu decays during cooling, this leads to a 4 kg reduction in ^{241}Am inventory after cooling.

7. Complex scenario with UOX and MOX reactors

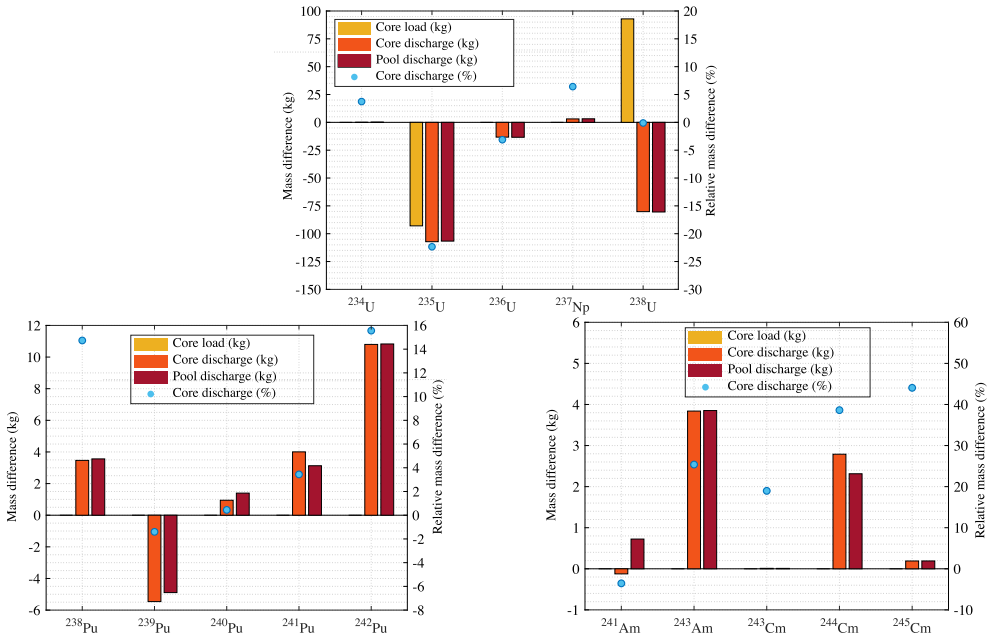
In complex scenarios involving both UOX and MOX fueled reactors, all the effects mentioned previously are combined. Moreover, additional error compensations can take place. This leads to results that are strongly dependent on the scenario selected (i.e. reactor lifetimes, load factors, fuel management strategies, etc.). Here, we will consider a fleet composed of 9 UOX reactors (fueled with enriched uranium produced from natural ore) and 1 MOX reactor (fueled with reprocessed UOX spent fuel). This ratio between the two types of reactor ensures that discharged fuel from UOX reactors will provide enough plutonium to fabricate the MOX. Reactor interactions in such a scenario are represented in Fig. 12. The life spans of the UOX and MOX reactors are respectively 60 and 40 years.

Fabrication and cooling times are respectively fixed to 2 and 5 years. The starting time of the MOX reactor is chosen in such a way that sufficient spent fuel is available for reprocessing so that initial plutonium shortages are avoided. Two different scenarios, differing only on cycle lengths and burnup targets are simulated. They are called OneBU and TwoBU. Table 11 lists the parameters used in each case. The MOX reactor starting time represent the number of years after the fuel fabrication initially started (two years before UOX reactors started operating). The same $k_{\text{threshold}}$ values as those used for the simple scenario are considered for the OneBU and TwoBU scenarios. Given that targeted burnups are different, $k_{\text{threshold}}$ for TwoBU should also be different. Hence, comparing the results produced in both cases enables us to measure the impact of $k_{\text{threshold}}$ on final isotope inventories.

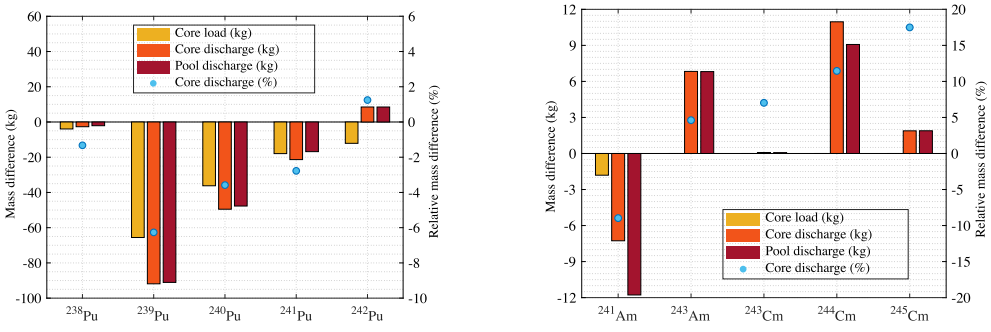
In Fig. 13, we present the variation with time of the plutonium and minor actinides inventories for the two scenarios considered. Fig. 13(a) and 13(b) provides cumulative values including total discharged and current core inventories. For DONJON5 simulations

Table 10
Assembly based irradiation model relative error (%) for isotopes depletion.

Fuel	^{235}U	^{238}Pu	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu	^{241}Am	^{243}Am	^{244}Cm
UOX	−11.0	13.9	0.7	−1.1	4.5	10.5	−2.2	19.0	28.1
MOX0	−5.6	−0.2	−2.0	−1.5	0.3	0.7	−7.0	4.5	12.3
MOX1	−5.7	−0.3	−1.1	−2.4	0.5	1.1	−5.6	5.5	13.3
MOX2	−4.6	−0.2	−1.3	−2.3	1.9	0.8	−3.8	3.9	12.9



(a) UOX one reactor scenario.



(b) MOX one reactor scenario.

Fig. 11. Differences in isotopic inventories between CLASS-MLP and CLASS-DONJON5.

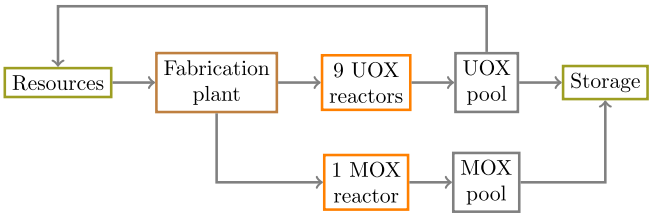


Fig. 12. Complex CLASS scenario with UOX-MOX fueled reactors interacting.

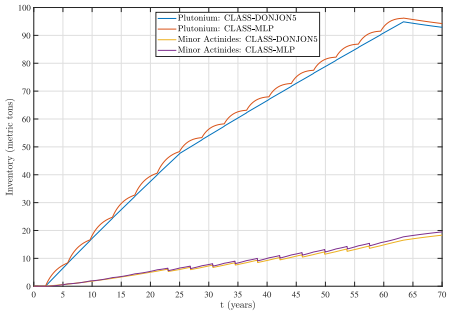
Table 11
Parameters for OneBU and TwoBU scenarios.

	burnup (GWd/t_{HM})		starting time (years)
Scenario	UOX	MOX	MOX
OneBU	49.8	49.8	25.0
TwoBU	45.5	55.4	19.5

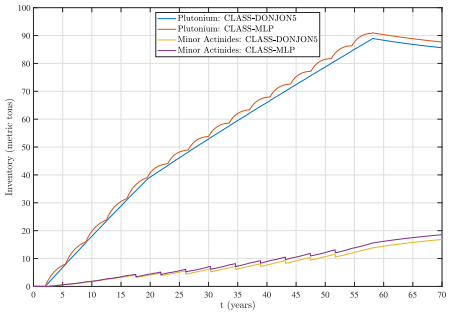
with a given fuel loading, only discharged inventories (not at each burnup step) were explicitly evaluated to reduce calculation costs (nearly 80% reduction). The isotopic concentrations at intermediate time steps when the fuel is still in the core, are interpolated assuming a linear behavior of the inventories between load and discharge times. Although this approximation is relatively coarse, it has no impact on the discharge inventories which is the value of interest. Fig. 13(c) and 13(d) provide plutonium inventories in UOX and MOX storage installations.

In these figures, we see that the differences in cumulative minor actinides and plutonium inventories at the end of the scenarios (70 years) are respectively 1 and 1.5 tonnes for scenario OneBU, and 1.5 and 3 tonnes for scenario TwoBU. These values should be compared to global plutonium inventories of approximately 92 and 87 tonnes respectively for scenario OneBU and twoBU leading to a bias of up to 1.7%. The bias for minor actinides global inventories increases to approximately 16% for the twoBU scenario.

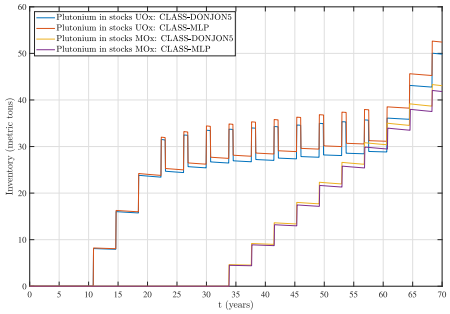
The figures also illustrate the effect of adding a MOX reactor on the plutonium in UOX storage facilities. For scenario OneBU, the MOX reactor leads nearly to an equilibrium state visible on Fig. 13(c). In scenario TwoBU, due to different burnup targets and the consequent different cycle lengths (load factors are equal to 1) no clear equilibrium is reached and significant differences between full-core calculations and neural networks results appear. These observations imply that the relatively good results visible on a scenario scale are partially due to an error compensation phenomenon. This can be easily identified in Fig. 13(d) for which an overestimation of approximately 5 tonnes is measured in MLP results for plutonium in UOX storage installations whereas an



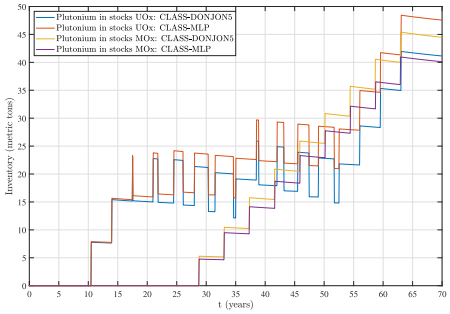
(a) Cumulative plutonium and MA inventories for OneBU scenario.



(b) Cumulative plutonium and MA inventories for TwoBU scenario.



(c) Storage plutonium inventories for OneBU scenario.

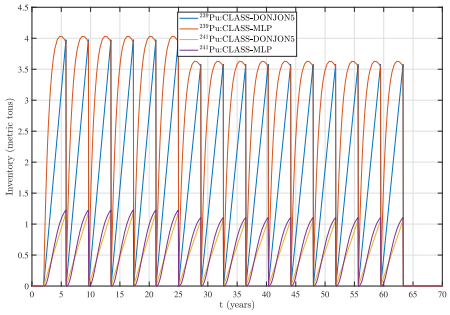


(d) Storage plutonium inventories for TwoBU scenario.

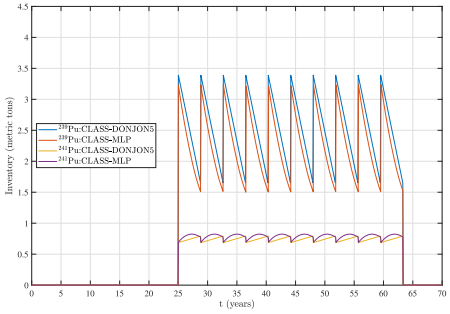
Fig. 13. Cumulative plutonium and minor actinides (MA) inventories from the fuel cycle and plutonium inventories in storage facilities for OneBU and TwoBU scenarios.

underestimation of 2.5 tonnes is observed for plutonium in MOX storage installations.

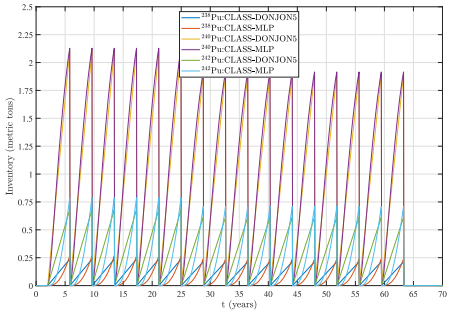
In-core inventories of fertile and fissile plutonium for the OneBU scenario are displayed in Fig. 14. The propagation of irradiation models differences on a scenario can be easily seen on these graphs. However, it only concerns the total amount of plutonium required for MOX reactors loading and the natural ore consumption in UOX reactors. Although small compared with the irradiation model differences previously seen, a small change in the UOX assemblies neutron flux due to a change in uranium enrichment can be observed. For example, Figs. 14(c) and 14(d) show that the differences in MOX spent fuel contents is entirely a consequence of the UOX irradiation model for ^{238}Pu or ^{242}Pu (similar differences between MLP and DONJON5 at MOX reactor loading and



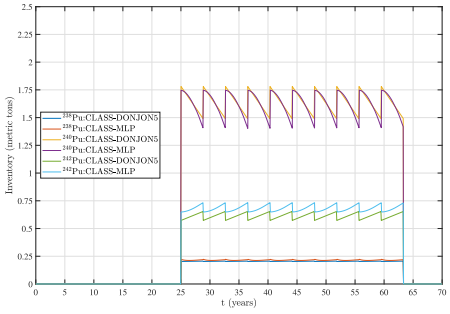
(a) Fissile plutonium isotopes in UOX reactors.



(b) Fissile plutonium isotopes in MOX reactors.



(c) Fertile plutonium isotopes in UOX reactors.



(d) Fertile plutonium isotopes in MOX reactors.

Fig. 14. In-core fertile and fissile plutonium for scenario OneBU.

discharge) whereas very small differences for fissile plutonium isotopes contents are displayed in Figs. 14(a) and 14(b).

8. Conclusion

In this paper, the CLASS scenario code was coupled to DONJON5 for full core diffusion calculations. Some simplified models are designed to accelerate full-core computations in DONJON5 while keeping the capability of CLASS to dynamically adapt reactor fuel loading to available fissile materials. Great efforts were invested to ensure that the core remains critical at all time in DONJON5 while keeping reasonable calculation costs. Original methods were also developed to reduce the number of iterations required in DONJON5 to determine the boron critical content in the moderator.

Full core calculations are used to analyze some of the parameters considered in the neural networks based approach and their impact on scenario accuracy as well as full scenarios both for individual isotopes and aggregated chemical elements. DONJON5 discharge burnup values for each batch allowed us to compute reference $k_{\text{threshold}}$ values for different fuels and cycle lengths and to assess the specific impact of this parameter on scenario studies. This approximation was shown to be the main source of uncertainties for the prediction of plutonium fuel contents. Adapted CLASS scripts were used to quantify the respective impact of fuel loading and irradiation models on the results. The irradiation model was shown to be poor for ^{235}U in-core inventories as well as minor actinides production. Given that no reactivity margins at discharge are considered and that a very low ^{235}U content is observed in spent fuel, we showed that in-core inventories for this isotope is not a problem in the scenarios presented.

The previous observations are coherent with previous work like (Somaini et al., 2016) and with physics (see reference (Reuss, 2012)) because ^{235}U and minor actinides are much more sensitive to neutron flux induced effects. The two-group assembly-homogenized diffusion scheme for full-core calculations seems to be a minimum requirement to take these differences into account. One way to get very good equivalence models in CLASS is to calculate, for neural networks, a $k_{\text{threshold}}$ that is well adapted for the fuel selected. We showed that MLP results are both good (less than a 1% differences on ore consumption and on plutonium production) and very fast (few minutes compared to one day for DONJON5 coupled executions). This raises the question of code flexibility because $k_{\text{threshold}}$ models would need to be developed for each reactor geometry making the code considerably less flexible.

Further work will focus on building improved estimators for $k_{\text{threshold}}$ with neural networks. It will also address the question of the validity of our conclusions for heterogeneous cores loaded with both UOX and MOX assemblies and for MOX assemblies with heterogeneous fuels (3 enrichments) which were not considered here.

CRediT authorship contribution statement

Martin Guillet: Visualization, Investigation, Writing - original draft. **Xavier Doligez:** Conceptualization, Methodology, Software, Investigation. **Guy Marleau:** Supervision, Methodology, Software, Writing - review & editing. **Maxime Paradis:** Investigation. **Marc Ernoult:** Validation. **Nicolas Thiollière:** Validation.

Declaration of Competing Interest

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

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