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1 Intro/specification

This memo presents the modeling results of cases 1.1 to 1.3 of the EG29 scenario, defined by the use of a plutonium equivalent model for the fuel fabrication. Case 1 of the EG29 calculation involves the modeling of a single MOX-PWR at steady-state (see figure 1).

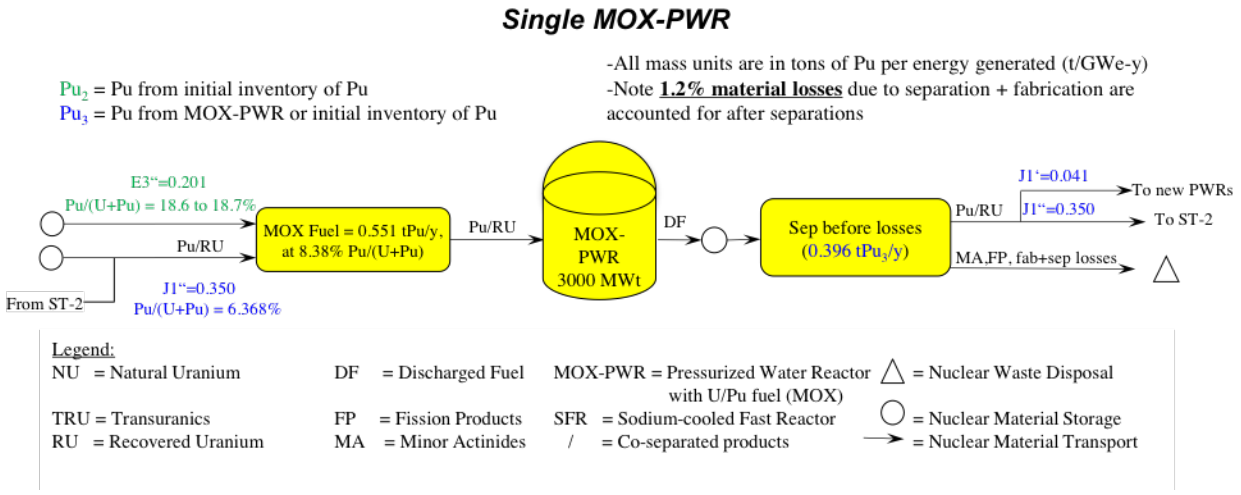

Figure 1: Schematic of Pu mass flow for Case 1.x

Case 1 is subdivided into three sub-cases corresponding to calculations of increasing fidelity:

- 1: without isotopic composition,

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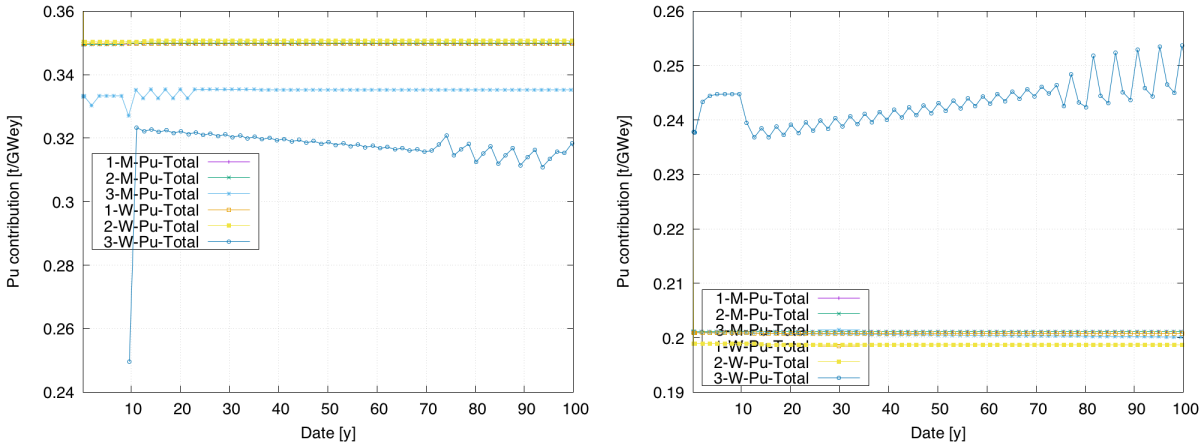
- 2: with isotopic composition and no decay,
- 3: with isotopic composition and decay.

2 Fixed mixing ratio vs Pu-equivalent theory

The first part of this memo is dedicated to the comparison between fixed ratio mix and Pu-equivalent theories for the fuel fabrication process.

Two variations on fuel-building were calculated for each sub-case (1.1 to 1.3). The first calculation used a standard mixing fab (in Cyclus, the "cycamore::mixer"). This mixed the E3 and the J1 streams using a constant mixing ratio to build MOX fuel for the PWR, labeled M. The second calculation used plutonium equivalent theory to determine the mixing fraction of each stream to build the MOX fuel, labeled W.



(a) J1" stream plutonium flow

(b) E3" stream plutonium flow

Figure 2: Evolution of the plutonium content in the J1" and E3" stream

The difference between J1" and E3" for all 6 calculations can be observed in Figure 2. Note that for this study one should only consider the time after 15 and 75y, as the calculation needs almost 12y to reach an equilibrium.

For both streams (J1" and E3"), the 2 cases without decay are similar in the 2 calculation methods (W and M). When decay is taken into account, one can observe a small reduction of the plutonium from J1" stream as well as a small increase of the plutonium from E3" stream directly due to ^{241}Pu decay: the E3" is not affected much by the decay process as it contains mainly 239Pu, while the J1" stream contains a higher ^{241}Pu content and is very sensitive to decay. The decay tends to decrease the reactivity potential of the J1" stream, which is compensated by the increase of the E3" stream in the mix.

3 Model enrichment prediction

The second part of this memo is dedicated to the comparison of the plutonium fraction in the fresh PWR-MOX fuel as predicted by different kind of models. The models can be divided in two categories, one category for those able to mix any stream with another (fixed mixing ratio and Pu-equivalent based models) and another category that only allows a plutonium stream to be mixed into a uranium stream.

For the first kind, the EG29 specification are applied as is (except for the fuel fabrication). For the second kind, the plutonium and uranium from J1" and E3" streams are separated. Then the plutonium from J1" and E3" are mixed according to the ratio provided in EG29 specifications. The model is used to determine what proportion of this J1" + E3" plutonium stream is required to build the PWR-MOX fuel to achieve the EG29 specifications (LWR, 50GWd/t, 1/3 batching).

The different models are:

- fixed mixing ratio between J1" and E3" stream, (M)
- Pu-equivalent based model to mix J1" and E3" stream, (W)
- Neural Network (NN) trained with irradiation stopped at a k_∞ of 1.01 (mean k_∞ of all batches), 3 batches, (MLP)
- NN with irradiation stopped at a mean a k_∞ of 1.034, 3 batches, (MLP-STD)
- NN with irradiation stopped at a mean a k_∞ of 1.034, 4 batches. (MLP-STD-2)

In addition to the fuel fabrication, a CLASS model based on neural network has been used to recalculate the proper evolution during the irradiation of the fuel in the PWR reactor.

Note that some calculation based on neural network usage have been extended 200y in order to allow the calculation to reach the equilibrium (since the initial compositions are close to the fixed recipe calculation equilibrium).

3.1 No decay

In Figure 3, one can observe the evolution of the plutonium enrichment loaded in the PWR fuel depending on the model considered for the fabrication. The Neural Network model using a k_∞ of 1.01 clearly underestimates the amount of plutonium required compared to the other models: the required reactivity is lower. We can observe the effect of batching (3 or 4) on the neural network models using a k_∞ of 1.034, which predict an initial enrichment close to the one used in the more standard models: 7.5% versus 7.8%. Those models predict

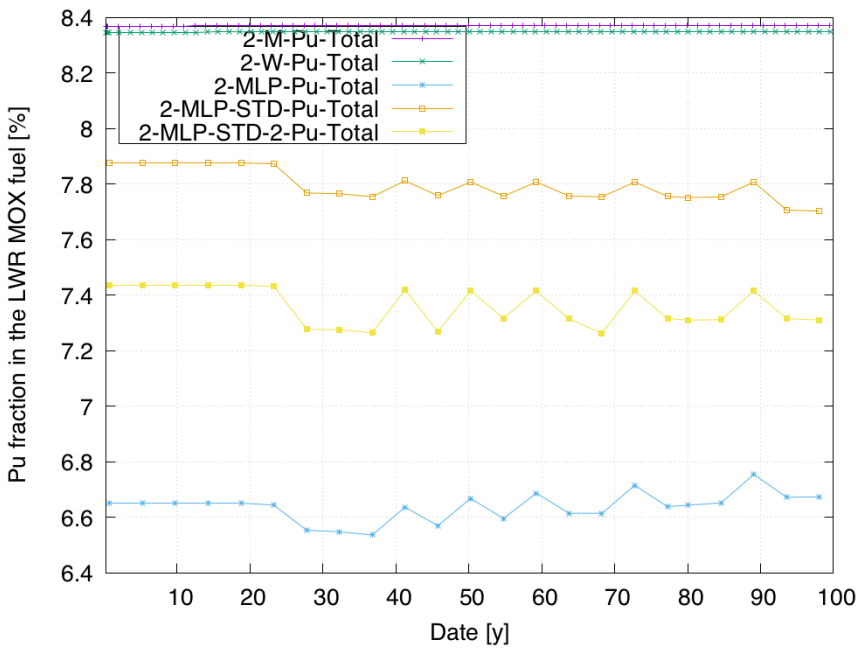


Figure 3: Evolution of the plutonium fraction in the MOX fuel loaded in PWR. These calculations do not include decay process.

an enrichment slightly lower than the ones using the fixed mixing fraction or Pu-equivalence. The Pu-equivalent model tries to mix both streams to reach the composition of the fuel used in the fixed mixing-fraction method. So it is expected to match or to be very close. For all fabrication models used, the behavior without decay is very close to expected: we observe a small variation in the amount of plutonium: the composition of the plutonium is constant, which allows the equilibrium to be maintained.

3.2 Decay

When decay is taking into account, all models based on the neural network increase the enrichment in plutonium by $2.5 - 3\%$. The ^{241}Pu decays and changes the final isotopic composition of the fuel. The decay of ^{241}Pu is causing the degradation of the plutonium quality and the production of ^{241}Am (acting as a neutronics poison), both of those effects tend to increase the amount of plutonium required to build the fuel. The effect of the presence of the initial inventory that is required to start the calculation, is as limited as possible: all calculation have been tuned to minimize the amount of initial storage (which depends on the model used). We can observe (see Figure 4 and Figure 5) that as the ^{241}Pu fraction decreases and the ^{239}Pu fraction increases in the used MOX composition, the amount of plutonium in the fresh fuel reaches an equilibrium closer to the initial fixed ratio.

Even if the different model predictions fail to agree on a common equilibrium, the point of

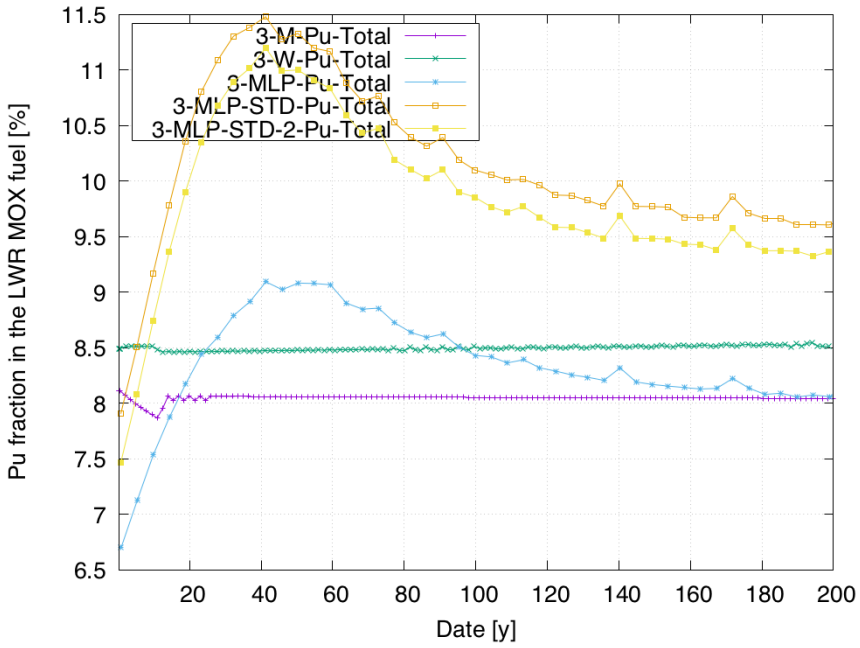
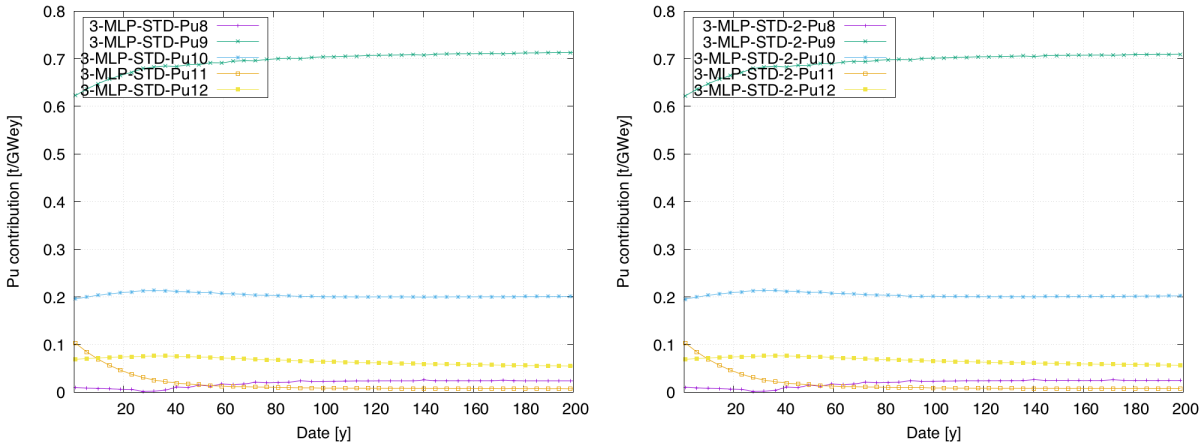


Figure 4: Evolution of the plutonium fraction in the MOX fuel loaded in PWR. These calculations include the decay process.



(a) Evolution of the Pu composition in the fresh fuel using the MLP-STD fabrication model.

(b) Evolution of the Pu composition in the fresh fuel using the MLP-STD-2 fabrication model.

Figure 5: Evolution of the isotopic composition of the plutonium in the fresh MOX fuel.

the study is not determining which calculation is correct (in fact both are probably correct), but to highlight the sensitivity of the equilibrium state to the isotopic composition and the modeling choice (particularly for thermal reactors): having overly strong constraints on the definition of the fuel cycle may lead us on the wrong path...

In order to support this statement, 3 additional calculations have been performed using the plutonium equivalence theory. In these calculations the fuel cycle is the same as the one described as Case 1.3, but the initial inventory has been increased by a factor of 2, 5 or 10.

4 Plutonium stacking effect

In the following calculation, the inventory of J1" has been increased by a factor 2, 5, or 10, in order to probe the effect of the of material stacking on the J1 storage.

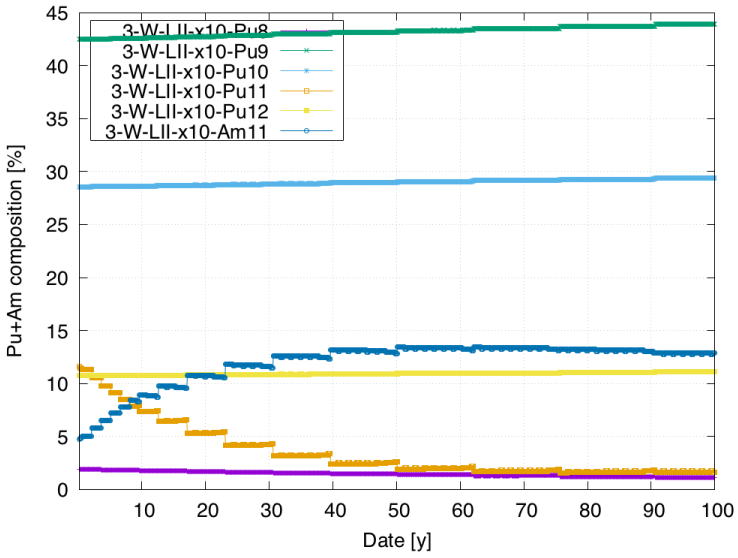
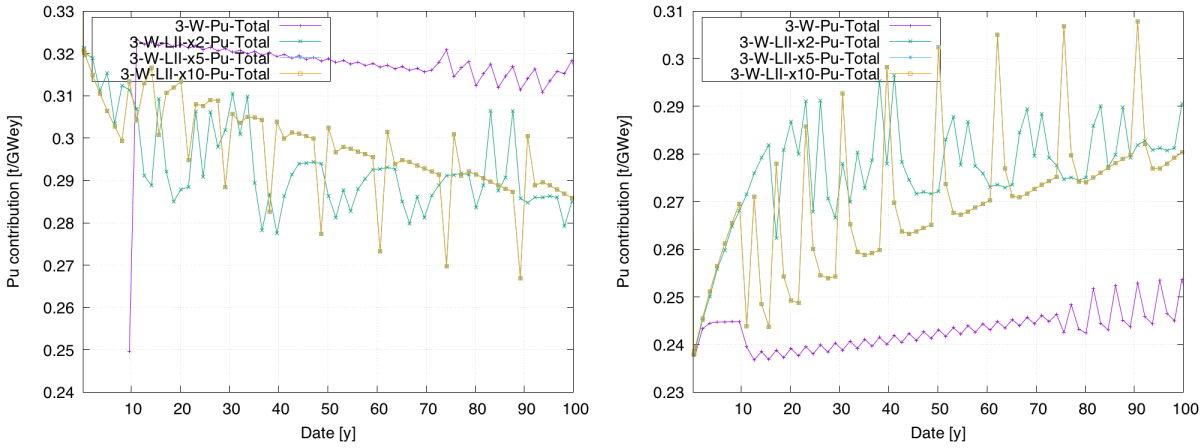


Figure 6: Evolution of the plutonium composition in the J1" storage in the case where the initial inventory has been increased by a factor 10.

As shown figure 6, the fraction of ^{241}Pu drops from about 12% to less than 2% in about 60y, while the ^{241}Am rises from 5% to about 12%. To illustrate this effect one only show the configuration with the strongest. ^{241}Pu and ^{241}Am find their respective equilibria around 11% and 1% for the normal calculation, 10% and 2% in the "x2" calculation and, 3% and 10% in the "x5" case. This conversion of the ^{241}Pu into ^{241}Am increases the average time the separated plutonium spends in storage before being used to build fresh MOX fuel.

As observed in Figure 7, the decay of the ^{241}Pu has a direct impact on the different contributions of the E3" and J1" streams. The model is trying to balance the loss of reactivity of the J1" stream by increasing the amount of E3" stream in the mix. The variation can be up to 10% after 100y in the worst case.



(a) J1" stream flow.

(b) E3" stream flow.

Figure 7: Evolution of the J1" and E3" stream flow according to the size of initial inventory.

5 Discussion

In conclusion, this study has shown the impact of different ways to model the MOX fuel fabrication, including whether or not decay is considered. The Pu-equivalence theory reaches an equilibrium (in the mixing ratio of E3" and J1" stream) very close to the fixed mixing ratio when the decay is not activated. This was expected: the Pu-equivalent model tried to build a MOX fuel with the same initial reactivity as the one used in the fixed mixing ratio calculation, so it used the same mixing ratio...

Nevertheless we can observe a variation of 20% in the contribution of E3" and J1" streams when taking the decay process into account. This variation is a direct consequence of the decay of ^{241}Pu producing ^{241}Am, which decreases the reactivity potential of J1" (loss of the ^{241}Pu reactivity and neutronic poisoning of the ^{241}Am). The E3" reactivity barely changes: the ^{241}Pu is negligible in E3" composition.

The main difference between the calculation using the CLASS model and the other calculation is the recalculation of the fuel evolution during irradiation.

The calculation using the CLASS model based on a neural network supports this observation. Without decay, this model predicts a constant plutonium enrichment in the MOX fuel 6.6%, 7.4% or 7.8%, depending on the model used, versus about 8.4% for the mixing ratio. This disagreement of a few percent in the plutonium enrichment is a direct consequence of the modeling assumptions in the different models. But this common flat behavior highlights that the steady state is well-described by all simulations when decay is not considered. Even if the CLASS model did not exactly agree on the plutonium enrichment required in the fuel to get the correct reactivity properties, the output composition recalculated by the CLASS

model was very close to the out recipe used by the other calculation because the equilibrium did not change.

When considering decay, all the CLASS models need about 180y to reach a proper equilibrium. This is because the composition of the plutonium strongly impact its enrichment in the fresh fuel (as shown in the Pu-equivalent case). The fresh fuel composition will likewise strongly impact the plutonium composition at the end of irradiation.

Moreover, the last part of the study shows the impact of the stacked plutonium on its composition and on fuel fabrication. This kind of material stacking could the consequences for disruption if the material flow in a real cycle. Having very strong constraints might cause such a disruption effect to be overlooked. In order to mimic a potential material stacking, the same steady state calculations have been perform three times, increasing the amount of initial inventory required to start the calculation by a factor 2, 5 or 10. In all cases, ^{241}Pu stacking induces ^{241}Am production which strongly impacts the mixing ratio between E3" and J1" (5% to 10%). This may have a strong effect on the used fuel composition, specially with thermal reactors,if the different cross sections are so sensitive to the composition of the fuel.