

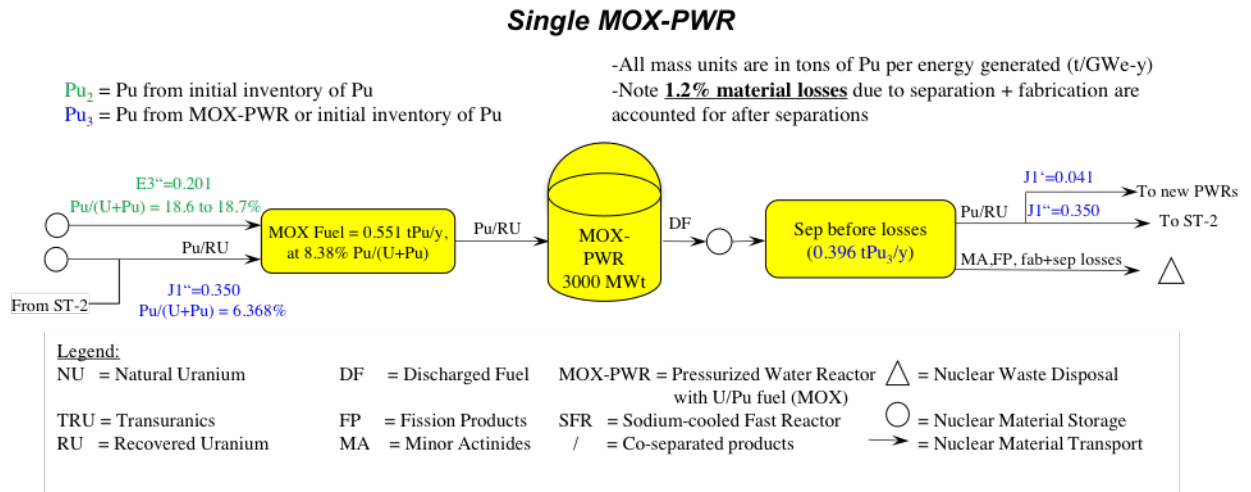
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## 1 Intro/specification

This memo presents the modeling results of cases 1.1 to 1.3 of the EG29 scenario, induced 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,
- 2: with isotopic composition and no decay,
- 3: with isotopic composition and decay.

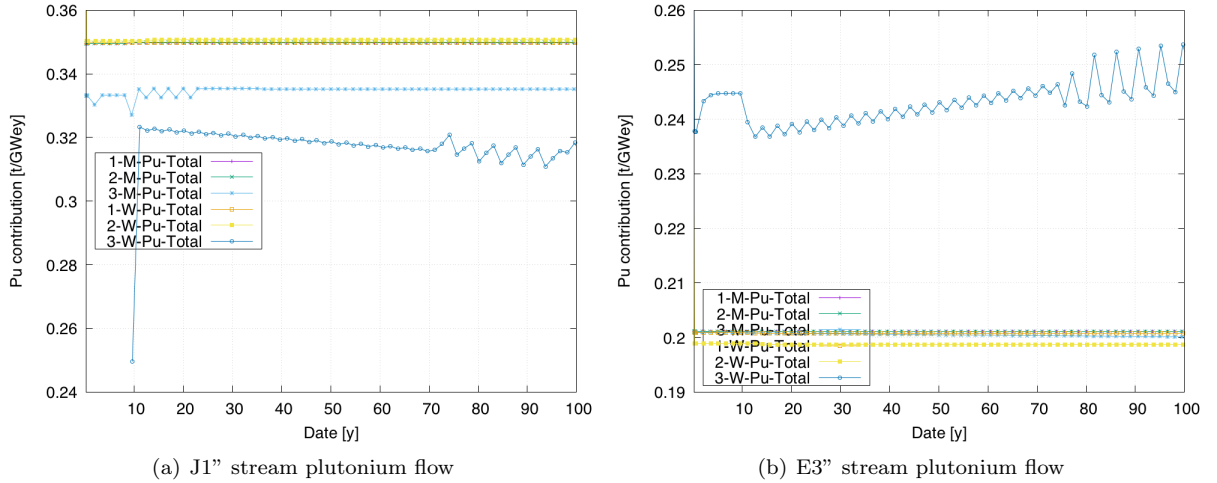
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## 2 Fix mixing ratio vs Pu-equivalent theory

The first part of this memo is dedicated to the comparison between fixed ratio mix and Pu-equivalent theory 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 the 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. The



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

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

For both stream (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  $^{241}\text{Pu}$  decay: the E3" is not affected much by the decay process as it contains mainly  $^{239}\text{Pu}$ , J1" stream contains a higher  $^{241}\text{Pu}$  content 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 predicted using different kind of models. The model used can be divided in two categories, the one able to mix any stream to another (fix mixing ratio and Pu-equivalent based model) and the one allowing only to mix a plutonium stream into a uranium stream.

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

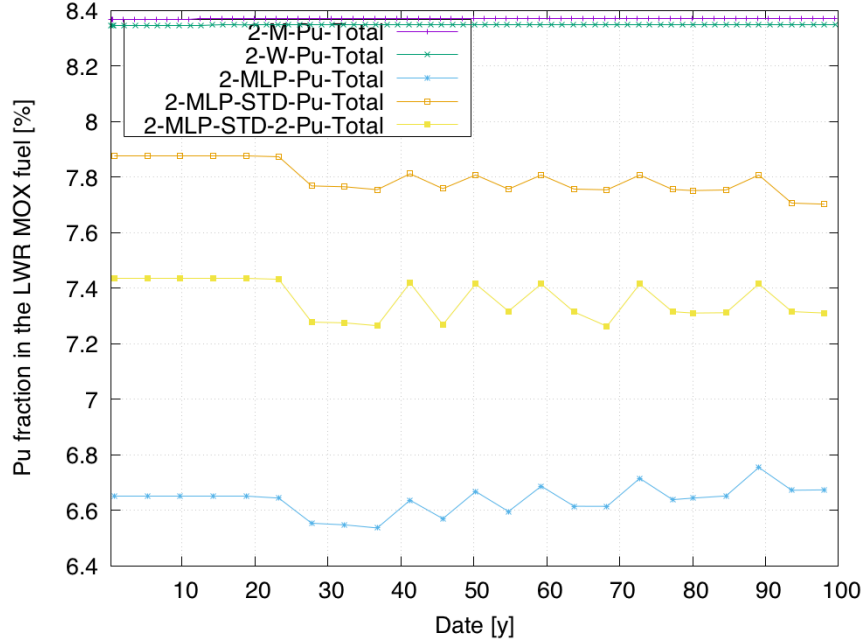
The different model used are:

- fix 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, CLASS model based on neural network have 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 composition are close at the fix recipe calculation equilibrium).

### 3.1 No decay

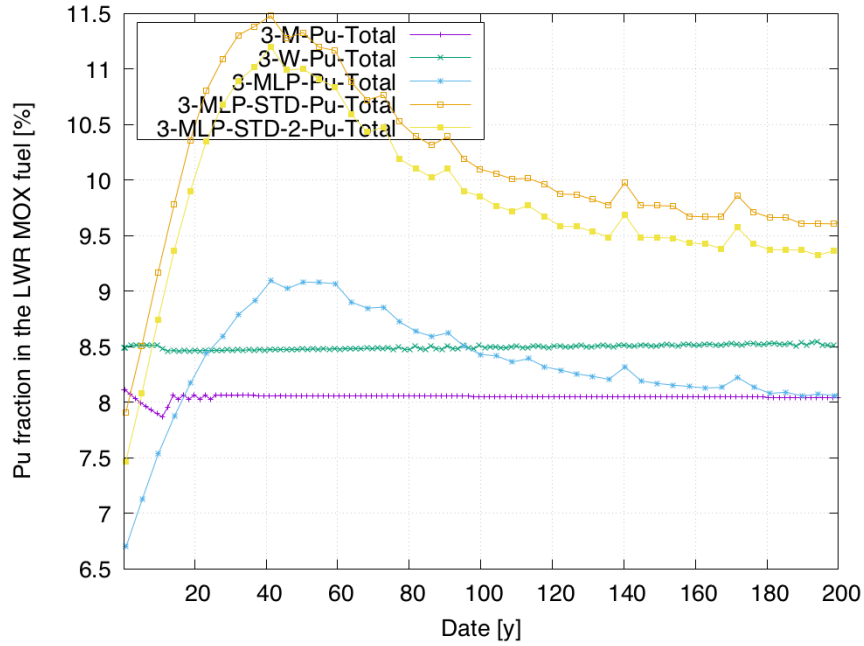


**Figure 3:** Evolution of the plutonium fraction in the MOX fuel loaded in PWR. Those calculation did not include decay process.

On Figure 3, one can observe the evolution of the plutonium enrichment loaded in the PWR fuel depending of the model considered for the fabrication. The Neural network model using a k of 1.01 clearly under estimate the amount of plutonium require comparatively to the other models: the require reactivity is lower. We can observe the effect of the batching (3or 4) on the neural network models using a k of 1.034, which predict an initial enrichment close to the one use on the more standard models: 7.5% versus 7.8%. Those models

predict a enrichment slightly lower than the one use with the fix mixing fraction and the Pu-equivalent. The Pu-equivalent try to mix both stream to reach the composition of the fuel used in the fixing-fraction method. So it is expected to match it or to be very close. For all fabrication model used, the behavior without decay very closed to expected: we observe a small variation of the amount of plutonium: the composition of the plutonium is constant with allow the equilibrium to be maintain.

### 3.2 Decay

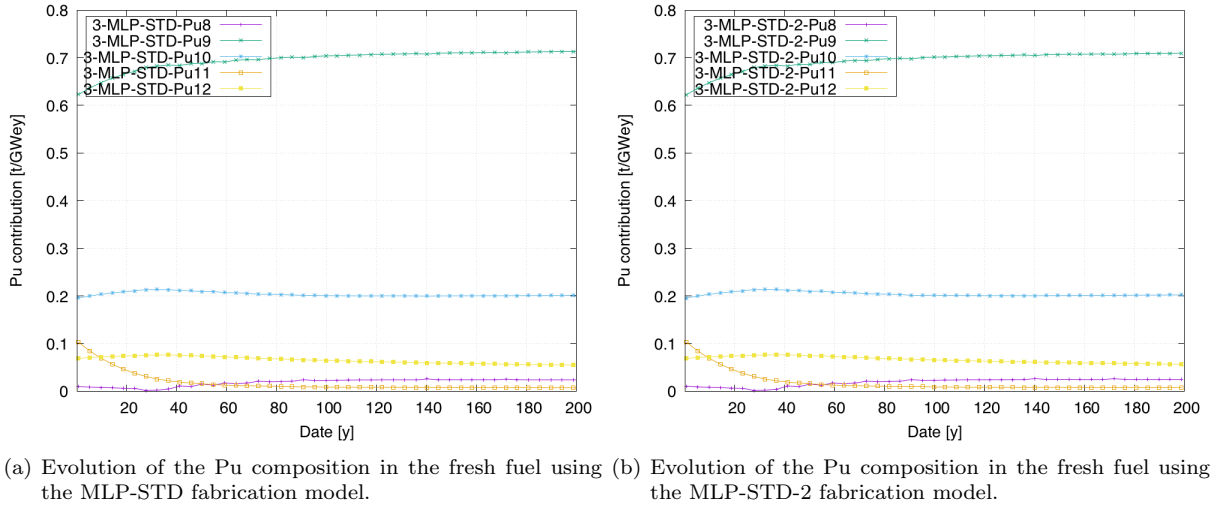


**Figure 4:** Evolution of the plutonium fraction in the MOX fuel loaded in PWR. Those calculation did include decay process.

When decay is taking into account, all model base on neural network increase the enrichment in plutonium by 2.5 – 3%. The  $^{241}\text{Pu}$  decay and change in the final isotopic composition of the fuel. The decay of  $^{241}\text{Pu}$  is causing the degradation of the plutonium quality and to the production of  $^{241}\text{Am}$  (acting as a neutronics poisons), both of those effect tends to increase the amount of plutonium require to build the fuel. The effect of the presence of the initial inventory which is required to start the calculation, is as limited as possible: all calculation have been tuned to reduce at the minimum the amount of initial storage (which depends on the model used). We can observe (see Figure 4 and Figure 5) that as the  $^{241}\text{Pu}$  fraction decrease and the  $^{239}\text{Pu}$  fraction increase in the used MOX composition, the amount of plutonium in the fresh fuel reaches an equilibrium closer to the initial fix ratio.

Even if the different model predictions fail to agree on a common equilibrium, the point of the study is not determining which calculation is correct or not (both are probably correct), but to highlight the sensitivity of the equilibrium state to the isotopic composition and the modeling choice (particularly on thermal reactor): having too strong constrains on the definition of the fuel cycle might lead us on the wrong path...

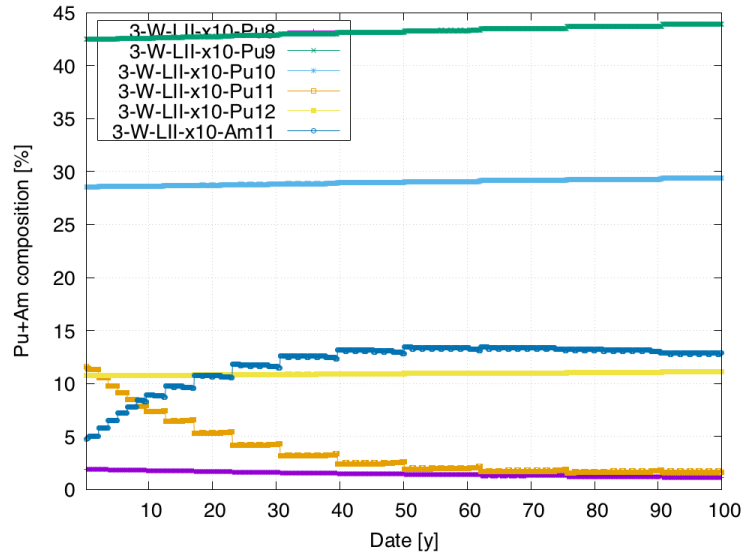
In order to support this statement, 3 addition calculations have been performed using the plutonium equivalent theory. In this calculation the fuel cycle is the same as the one described as Case 1.3, but the initial inventory has been increased by a factor 2, 5 and 10.



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

## 4 Plutonium stacking effect

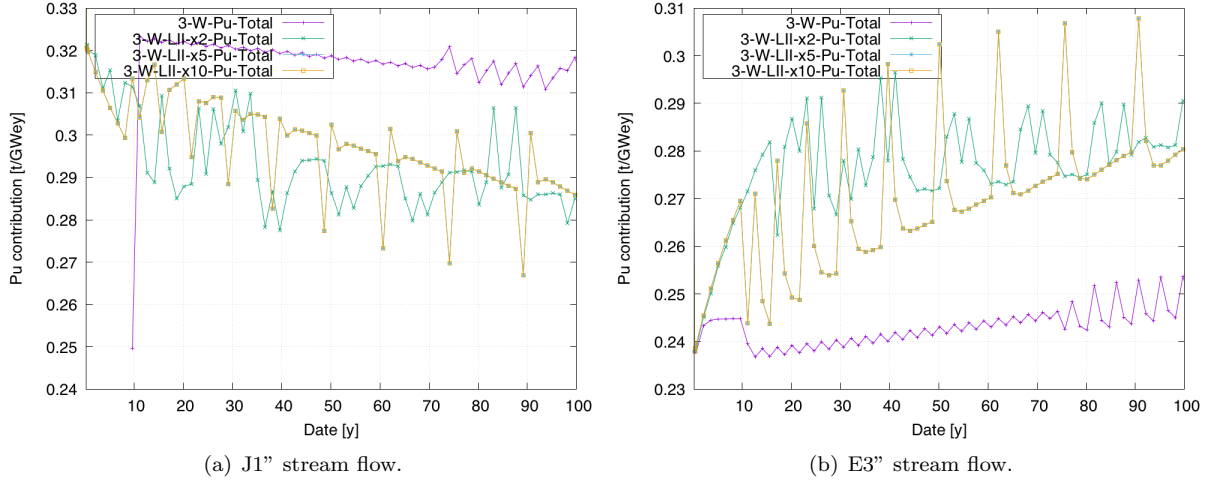
In the following calculation, the inventory of the J1" have been increase by a factor 2, 5, and 10, in order to probe the effect of the of material stacking in the J1 storage.



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

As shown figure 6, the fraction of  $^{241}\text{Pu}$  drops from about 12% to less than 2% in about 60y, while the  $^{241}\text{Am}$  rises from 5% to about 12%. To illustrate this effect one only show the configuration with the strongest.  $^{241}\text{Pu}$  and  $^{241}\text{Am}$  finds a respective equilibrium 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  $^{241}\text{Pu}$  into  $^{241}\text{Am}$  induce an increased average time the separate plutonium spend in storage before being used to build fresh MOX fuel.



**Figure 7:** Evolution of the J1'' and E3'' stream flow accordingly to the size of initial inventory.

As observed on Figure 7, the decay of the  $^{241}\text{Pu}$  has a direct impact on the different contribution of E3'' and J1'' stream. The model 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% in the worse case after 100y.

## 5 Discussion

In conclusion, this study has show the impact of different way to model the MOX fuel fabrication considering decay or not. The Pu-equivalence theory reach an equilibrium (in the mixing ratio of E3'' and J1'' stream) very close to the fix mixing ratio, when the decay is not activate. This was expected: the Pu-equivalent model try to build a MOX fuel with the same initial reactivity as the one used in the fix mixing ratio calculation, so it used the same mixing ratio. . .

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

The main difference, between 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 neural network support those this observation. Without decay, those model predict a constant plutonium enrichment in the MOX fuel 6.6%, 7.4% and 7.8% depending on the model used versus about 8.4% for the mixing ratio. This disagreement of few percents in the plutonium enrichment, is directly a consequence of the modeling differences between the models. But this common flat behavior highlight that the steady state is well described by all simulation when the decay are not considered. Even if the CLASS model did not exactly agree on the plutonium enrichment require in the fuel to get the correct reactivity properties, because the equilibrium did not change, the output composition recalculated by the CLASS model if very close the out recipe used by the other calculation.

When considering the decay, all the CLASS model 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). And the fresh fuel composition will 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 then on the fuel fabrication. Those kind of material stacking could the consequences of disruption if the material flow of in a real cycle. Having very strong constrains might lead to ignore such disruption effect. In order to mimic a potential material stacking, the same steady state calculation have been perform three times increasing the amount of initial inventory require to start the calculation by a factor 2, 5 and 10. In all cases,  $^{241}\text{Pu}$  stacking induce  $^{241}\text{Am}$  production which impact strongly the mixing ration between E3" and J1" ( 5% to 10%), which might have a strong effect on the used fuel composition, specially with thermal reactor, were the different cross section are so sensitive to the composition of the fuel.