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ARTICLE

Initial Benchmark Comparison of the Open-Source Cyclus and NMB Fuel Cycle Simulators

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Verification exercises between fuel cycle simulators are important for understanding how the methodology and capability differences between the simulators affect the results. This work performs an initial verification exercise with the Cyclus and NMB fuel cycle simulators. The exercise compares the results of the two codes in three simple fuel cycle scenarios: a once-through scenario with a pressurized water reactor, a limited recycle scenario with a pressurized water reactor, and a continuous recycle scenario with a pressurized water reactor and a sodium fast reactor. The results of this exercise highlight the differences in the codes' methodologies to determine when fresh fuel is fabricated and to model fuel depletion. These differences affect where material is located in a scenario but do not greatly affect the total amount of material in a scenario.

KEYWORDS: Cyclus, NMB, fuel cycles, verification

I. Introduction

Nuclear fuel cycle simulators are important computational tools for modeling and understanding various nuclear fuel cycles. They have been used for a variety of purposes, including modeling potential high assay low enriched uranium (HALEU) demand,[1)] analyzing the transitions between fuel cycle options,[2,3)] performing sensitivity analysis on a fuel cycle transition,[4,5)], and assisting in nonproliferation studies.[6,7)] With such a great variety of uses, multiple fuel cycle simulators have been developed over the years. Many of these simulators were developed independently and use different methodologies, which leads to the need for benchmarks and comparisons between the different codes to identify how the implemented methodologies might affect the results of a simulation. For example, previous efforts[8,9)] identified that the differences in how the simulators model reprocessing (e.g., continuous vs. instantaneous) can lead to different timelines for the recovery of fissile material for reprocessing used nuclear fuel. Another benchmark comparison of different codes identified that as the scenario complexity increases, it is more likely for differences in the results to appear.[10)]

This work builds upon previous work by benchmarking Cyclus and Nuclear Material Balance (NMB), two open-source fuel cycle simulators. The first objective of this work is to identify how the different methodologies and capabilities of these two simulators affect the modeling of hypothetical fuel cycle scenarios. The second objective is to improve both codes based on the results in the scenarios selected to investigate plutonium management and minimization. The Cyclus and NMB codes were chosen for this work because they are both open-source codes and have not been directly compared against each other in previous benchmarks. Additionally, there were different focuses in their development that led to different modeling methodologies in the two codes, such as how facilities interact and trade material. Finally, they are the most widely used open-source fuel cycle simulator in the US (where Cyclus was developed) and Japan (where NMB was developed). The open-source nature of the codes facilitated the information exchange, and there is flexibility and accessibility in the development of open-source software.

II. Simulator Information

1. Cyclus

Cyclus[11)] is a dynamic, open-source, agent-based fuel cycle simulator. Cyclus uses the notion of an *agent* to represent different components in the simulated fuel cycle, such as a facility or a material. The agent-based modeling paradigm employed by Cyclus allows agent-level modeling and for independent definitions for different fuel cycle facilities while still allowing interaction with each other in the simulation. Generic facility types are modeled through archetypes (or type/class of agent with common features) that implement physics calculations and specific behaviors for different types of agents. These archetypes can model fuel cycle facilities such as material sources (e.g., mines), fuel fabrication, reactors, or separations. The Cycamore archetype library provides a variety of archetypes that can be dynamically loaded into Cyclus for use in a simulation.[11-12)]

Agents in Cyclus trade materials through the built-in dynamic resource exchange (DRE),[11,13)] which defines the supply-demand communication framework. The DRE treats

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facilities as black boxes so the solution strategy is agnostic to the resource types being exchanged.

Cyclus has undergone a verification exercise to compare its performance against other fuel cycle simulators and a benchmark analytical solution.[9)] This work identified that Cyclus fully resolves discrete batches of fuel discharge, while the other simulators in the exercise do not. Cyclus has been used to model various fuel cycles and transition scenarios, including the transition from light water reactors (LWRs) to HALEU-fueled reactors[1)] and the transition from LWRs to sodium fast reactors (SFRs). [3)]

2. NMB

Nuclear Material Balance (NMB)[14)] is developed as a collaboration between Institute of Science Tokyo (former Tokyo Institute of Technology) and the Japan Atomic Energy Agency (JAEA). Some of the distinguishing features of NMB include its dynamic and "integrated analyses of the nuclear fuel cycle", dynamic depletion, material balance calculations, thermal analysis of a geologic repository, and nuclide migration from the repository to the environment.[14)] The material tracking in NMB consists of 26 actinide and 153 fission product nuclides, selected based on their half-lives, association with burnup and decay chains, and reproducibility of results from ORIGEN. NMB is an open-source code that runs on Microsoft Excel®.

NMB divides the fuel cycle into three modules: the front-end, the reactor, and the back-end. The front-end module encompasses mining, enrichment, and fuel fabrication. The fuel fabrication component determines the enrichment for uranium oxide (UOX) and the plutonium content for mixed oxide (MOX) fuel based on k_∞ calculations. In the reactor module, NMB models the depletion of fuel given operating conditions such as burnup and cycle length. Depletion is calculated through the Okamura explicit method (OEM), which is a kind of first-order approximation matrix exponential method that achieves sufficient accuracy with low calculation cost. [14)] Similar to Cyclus, NMB resolves discrete batches of fuel discharge. Finally, the back-end module models reprocessing, partitioning, stabilization, storage, and geologic disposal. The back-end module of NMB includes thermal evolution and thermal limits for a geologic repository, nuclide migration between the repository and the environment, and the number of radioactive waste canisters required to store the waste. Each of the back-end elements of NMB provides an extensive suite of capabilities to provide a detailed understanding of waste management strategies.

NMB was compared against the performance of other fuel cycle simulators by recreating a Nuclear Energy Agency (NEA) benchmark study.[10)] This work showed that the results from NMB have good agreement with the other codes, but differences were identified.[14)] For example, differences in the annual reprocessing amount arose because of different interpretations in fuel loading.[14)]

III. Fuel Cycle Scenarios

The first stage of this benchmark considers three different fuel cycle scenarios, Scenarios A, B, and C. shows the facilities and material flows in each of these scenarios. Scenario A is a once-through fuel cycle with one pressurized water reactor (PWR) fueled with UOX fuel. The used UOX fuel is disposed of in a repository after a cooling period. Scenario B is a limited recycle fuel cycle, in which used UOX fuel from the PWR is reprocessed and used to create MOX fuel (referred to as L-MOX when the MOX is used in a PWR). The used L-MOX fuel is disposed of in a repository, after a cooling period. Finally, Scenario C involves a transition from 3 PWRs to an SFR. The used UOX fuel from the PWRs is reprocessed to create L-MOX that is placed in the PWRs. The used L-MOX fuel from the PWRs is reprocessed to create MOX fuel for use in the SFR. The used MOX fuel and blanket material from the SFR is then continuously reprocessed to produce MOX fuel. These scenarios are modeled after fuel cycle scenarios used in previous verification exercises. [10)]

Table 1 Fuel cycle scenario diagrams

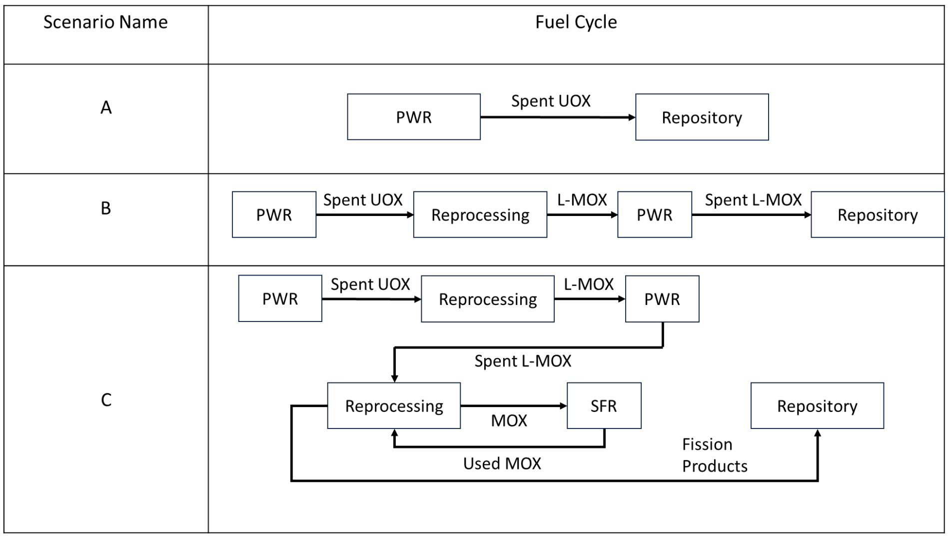


Table 2 reports some of the reactor design specifications, and **Table 3** defines some of the scenario parameters. The cycle length in Table 2 is the combined duration for the operating and outage time in calendar years. Scenario A runs for 120 years, with 1 PWR deployed at year 0. Scenarios B and C run for 150 years, with one PWR deployed at year 0 in Scenario B, and three PWRs deployed at year 0 and one SFR deployed at year 60 in Scenario C.

Table 2 Selected reactor design specifications

Design Characteristic	PWR	SFR
Power (MWe)	1000	1000
Reactor life (yr)	60	60
Thermal efficiency	33%	40%
Load factor	85%	95%
Enrichment	4.1% ^{235}U, 9% Pu	18% Pu
Burnup (GWd/MTHM)	45	150
Batches	3	4
Cycle length (yr)	1.288	2.193
Assembly mass (tHM)	0.4614	1

Table 3 Scenario specific reactor parameters

Parameter	Scenario A	Scenario B	Scenario C
Duration (yr)	120	150	150
Number of PWRs	1	1	3
Number of SFRs	0	0	1
PWR deployment year	0	0	0
SFR deployment year	N/A	N/A	60

Table 4 contains scenario-specific details. To meet the LMOX loading limit in the PWRs the LMOX fabrication was limited at the fabrication facility.

For modeling all three scenarios in Cyclus, we used archetypes from the Cycamore library. The Cycamore Reactor archetype uses static recipes to model depletion. We generated the fuel recipes by averaging the fuel compositions in NMB. The fresh UOX, L-MOX, and MOX compositions are based on the k_∞ calculations performed in NMB. The PWR UOX and L-MOX used fuel compositions came from averaging the PWR spent compositions during years 30-50 in Scenarios A and B. The MOX spent fuel composition came from the averaged used MOX composition between years 80-100 in Scenario C.

In NMB, all three scenarios use a time step size of 0.01 year. In Cyclus, Scenario A uses a time step size of 0.01 year, while Scenarios B and C use a time step size of 0.1 year because of limited computational resources. The different time step sizes in Cyclus allow for investigation of how this parameter may affect the results.

IV. Results

The results from each simulator are compared based on the beginning-of-year plutonium inventory in different materials (e.g., spent UOX fuel, fresh MOX fuel, etc.) in the fuel cycle, as applicable. Comparisons based on these metrics are good indicators of code performance and demonstrate how these

Table 4 General scenario definition fuel cycle parameters

Parameter	Value	Scenario applied
UOX fabrication time (yrs)	5	A, B, C
L-MOX fabrication time (yrs)	2	B, C
MOX fabrication time (yrs)	2	C
UOX cooling time, before reprocessing (yrs)	15	B, C
UOX cooling time, before disposal (yrs)	50	A
LMOX cooling time before reprocessing (yrs)	3	C
LMOX cooling time, before disposal (yrs)	75	B
UOX reprocessing	20 tHM/yr	B
UOX reprocessing	60 tHM/yr	C
L-MOX reprocessing (after year 45)	24 tHM/yr	C
MOX reprocessing (after year 60)	10 tHM/yr	C
U and Pu separation efficiency	99.8%	B, C

simulators can be used for evaluating different fuel cycles for plutonium management.

1. Scenario A

The plutonium in Scenario A is in the spent UOX fuel as it cools for 50 years and in the repository. **Figure 1** shows the total plutonium inventory in Scenario A. The inventory from each code is consistent in their general patterns and magnitude.

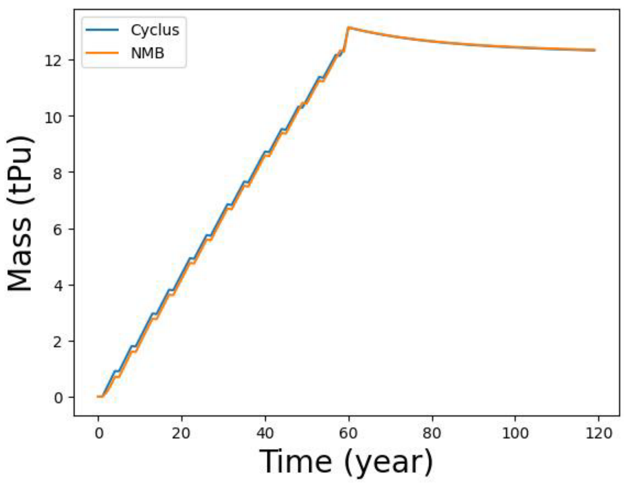


Fig. 1 Total plutonium (all in UOX fuel) in Scenario A

The inventories from both codes increase during the PWR operation time (years 0–60) and there are small differences (up to 0.21 tPu difference). The differences in the inventory during this time comes primarily from the different depletion methods from each code: NMB dynamically depletes the fuel, while the Cycamore Reactor archetype in Cyclus uses static recipes for fuel depletion. The difference between the results decreases during the PWR operation, suggesting that the SNF compositions in each code become more similar. This behavior matches expectations based on how the recipes used in Cyclus were created.

There are one-year long increases in the difference between the results, such as years 49, and 58. These increases are a result of how each code models time steps. Cyclus uses discrete time step modeling (i.e., integer time steps) while NMB does continuous time modeling. Therefore, some small approximations made in the scenario definition to account for the different time step modeling can affect the results from the codes. These are small differences that do not affect the overall trend of the result.

After the PWR is decommissioned in year 60, the two results differ by at most 0.016 tPu, a 1% difference. The agreement in this period of the results highlights how the different depletion methods produce similar results in the total amount of plutonium that enters the scenario.

2. Scenario B

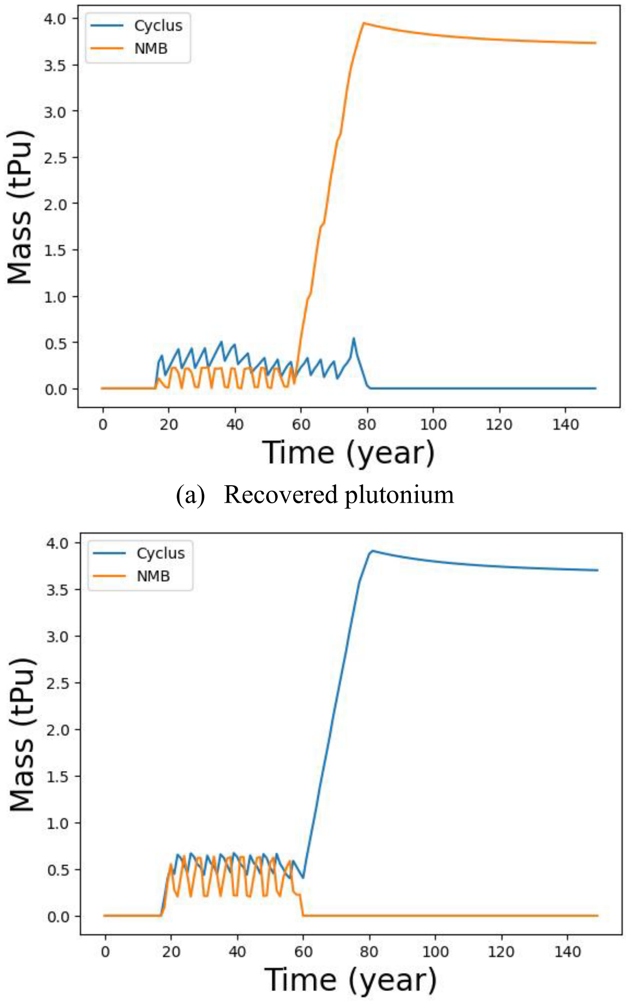
The plutonium inventories in Scenario B include the used UOX, the recovered plutonium from the used UOX fuel, the fresh, in-core, and spent L-MOX fuel, and the waste material inventories. The spent L-MOX fuel is divided into what is cooling for 75 years (spent L-MOX) and what is sent to a repository (L-MOX repository).

Most of the inventories in this scenario are in good agreement, with maximum differences for most of the inventories reported in

The recovered plutonium and fresh L-MOX inventories are discussed in more detail below.

Table 5 Maximum difference in select Scenario B inventories

Inventory	Difference (tPu)	Rel. Diff
Used UOX	0.58	16.9%
In-core L-MOX	0.27	42.7%
Spent L-MOX	0.30	6.4%
Waste	0.0010	4.1%
L-MOX repository	0.22	22.3%



(a) Recovered plutonium

(b) Fresh L-MOX

Fig. 2 Recovered plutonium and fresh L-MOX inventories in Scenario B

(1) Recovered Plutonium and Fresh L-MOX

The recovered plutonium and fresh L-MOX inventories do not show good agreement (**Figs. 2 (a)** and **(b)**). The results show some agreement near the beginning of the scenario. Before year 60, there are some differences in these Pu inventories: the Cyclus results have more recovered plutonium and the peaks in each inventory do not have consistent alignment. These differences can be directly attributed to the different time step approaches used by the two codes (0.1y time step in Cyclus versus 0.01 y time step and continuous time modeling in NMB). However, in year 60 the results start to diverge. The NMB inventory for recovered plutonium increases and the fresh L-MOX inventory goes to zero, while the Cyclus results have the opposite pattern. It was discovered that this behavior arises because of differences in how each code determines when fresh fuel is fabricated. In NMB, the fuel fabrication part of the front-end module will only produce fresh fuel if there is demand for it from a reactor.

The PWR is decommissioned in year 60, which removes the demand for fresh L-MOX fuel and results in the plutonium remaining in the recovered plutonium inventory. In Cyclus, the agent- based methodology of the system means that the fuel fabrication agent will continue to produce fresh fuel as long as there is sufficient input material available. Therefore, the material continues to move from the recovered plutonium inventory to the fresh L-MOX inventory after the reactor is decommissioned.

Figure 3 shows the summed the recovered plutonium and fresh L-MOX inventories. The summed inventory shows good agreement after year 60, with a maximum difference of 0.35 tPu (9.82%), supporting that the difference in the methodology to determine when fresh fuel is created leads to the large differences in the individual inventories.

(2) Total Plutonium

Figure 4 shows the major inventories in Scenario B. The largest difference in the total inventory is 0.21 tPu. Figure 4 highlights how the different fuel fabrication methodologies impact the total L-MOX fuel and recovered plutonium inventories, but the total material inventories are similar.

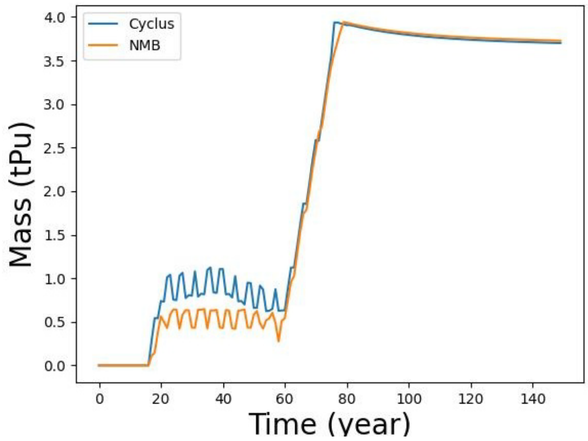


Fig. 3 Sum of recovered plutonium and fresh L-MOX

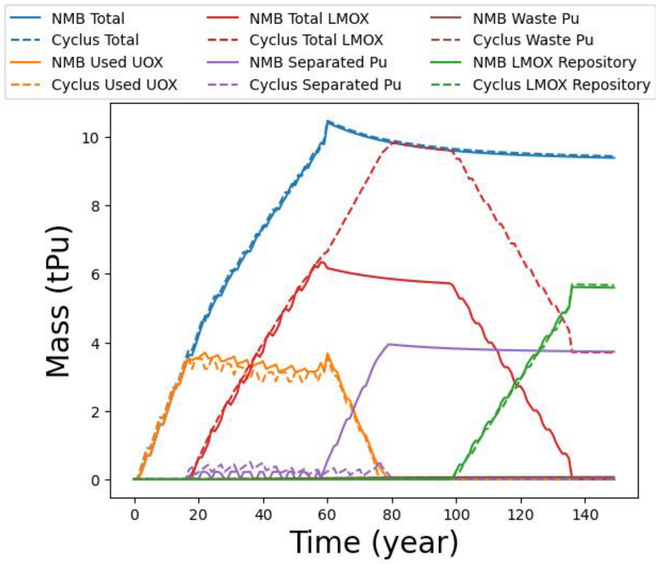


Fig. 4 All major material inventories in Scenario B

3. Scenario C

Scenario C has many plutonium inventories: used UOX fuel, recovered plutonium from UOX fuel, fresh L-MOX fuel, in-core L-MOX fuel, used L-MOX fuel, recovered plutonium from L-MOX fuel, fresh MOX fuel, in-core MOX fuel, used MOX fuel, used SFR blanket, recovered plutonium from MOX, and waste. Like the results of Scenario B, some of the inventories have good agreement while others differ because of the different methodologies to determine when fresh fuel is fabricated. Specifically, the recovered plutonium from used UOX and fresh L-MOX fuel inventories differ.

Table 6 reports the maximum difference in some of the inventories in Scenario C. This scenario has three PWRs deployed, compared with only one in Scenarios A and B. The additional PWRs in Scenario C leads to larger inventories and thus larger differences in the PWR-related inventories.

(1) Recovered Plutonium from L-MOX and MOX and Fresh MOX Fuel

Similar to the recovered plutonium from UOX fuel and the fresh L-MOX fuel inventories, the recovered plutonium from the used L-MOX fuel, recovered plutonium from the used MOX, and the fresh MOX fuel inventories are different

Table 6 Maximum difference in select inventories in Scenario C

Inventory	Difference (tPu)	Rel. Diff (%)
Used UOX	1.69	16.4%
In-core L-MOX	0.57	30.9%
Used L-MOX	1.07	18.1%
In-core MOX	0.21	2.5%
Used MOX	2.86	100%
Used blanket	0.32	26.3%
Waste	0.082	12.4%

because of the fresh fuel fabrication methodologies. All three inventories show differences because material from the used L-MOX and used MOX fuel is used to fabricate fresh MOX fuel.

Figure 5 shows these three inventories when they are summed. There is good agreement in the summed inventory, but the difference slowly increases with time between years 60-132. The increase in the difference is primarily an effect of the different depletion methodologies. In a continuous recycling fuel cycle, there is more variation in the composition of the fresh and used MOX fuel, which impacts the amount of plutonium recovered from the used fuel. The dynamic depletion in NMB capture these changes, but the static recipes used in Cyclus here do not.

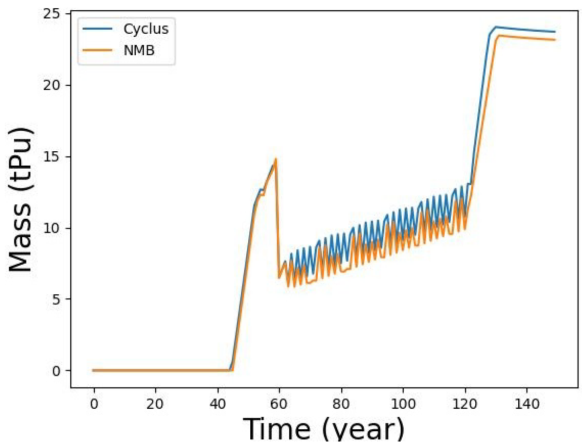


Fig. 5 Summed recovered plutonium from L-MOX and MOX fuel and fresh MOX fuel inventories in Scenario C

(2) Total Plutonium

Figure 6 shows each of the primary inventories in Scenario C. This figure highlights the differences in the various recovered plutonium, L-MOX, and MOX inventories. However, the differences in these inventories do not lead to large differences in the total inventory because they are just differences in the location of the material. Similar to Scenario B, there are more one-year variations in the difference between the Cyclus and NMB results than in the Scenario A results because of the different time step sizes.

Figure 6 also shows an increase in the difference between the total inventories between years 60-120, which stem from the different depletion methodologies. This effect from the depletion methodologies was not observed in Scenarios A and B because only this time segment in Scenario C uses a multi-recycling fuel cycle, when fuel depletion accuracy has the most impact on the material inventories.

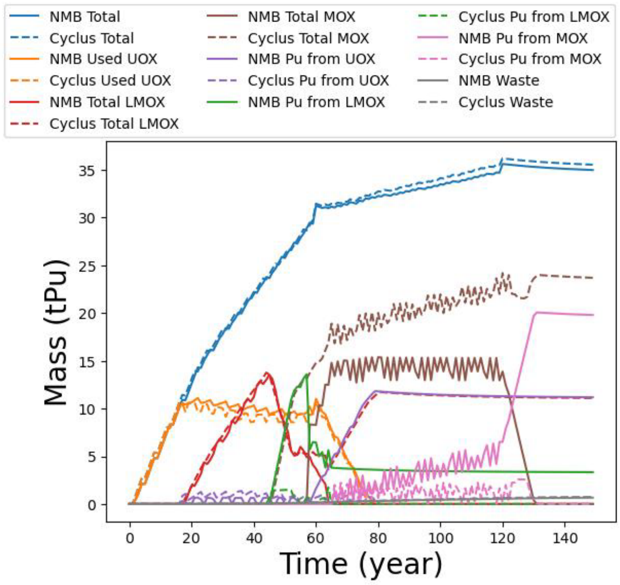


Fig. 6 All major inventories in Scenario C

V. Conclusions

The results of these verification simulations highlight two main differences in Cyclus and NMB: the methodology to determine when fresh fuel is created and the depletion methodology. In Cyclus, fresh fuel is continuously fabricated if there is sufficient material available because of the agent-based nature of the code. In NMB, fresh fuel is fabricated only when there is demand from a reactor because of the more integrated nature of the code. This methodology difference affects where material is located in a fuel cycle scenario but does not impact the total amount of material in the scenario. The depletion methodology difference impacts the amount of plutonium present in the scenario. This difference has a minimal effect on once-through or mono-recycling fuel cycle scenarios, but a greater effect in the continuous recycling scenario. There are also some observed one-year variations in the difference in the results because of different time step sizes and how each code models time, but those contribute little to the total difference. Future steps in this collaboration involve improving both codes after additional detailed scenarios are run to form a complete list of modifications that will be prioritized.

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