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ARTICLE

Benchmarking Molten Salt Reactors Modelling for Americium Transmutation in Fuel Cycle Simulation Studies

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The ISAC Project (Innovative System for Actinide Conversion) is a collaboration between five French nuclear corporations and institutions (CEA, CNRS, EDF, Framatome and Orano). It aims to identify the potential and the technological limitations of minor actinides transmutation – americium in particular – in molten salt reactors. This project, started in 2022, is partially funded by the "France 2030" investment plan – for a total budget of 26 M€. As part of this project, a benchmark on fuel cycle simulation tools is carried out to compare the modelling of molten salt reactors in each participant's code on simplified trajectories. Their impact on the fuel cycle, when used for americium transmutation, is then assessed. This work presents the hypotheses used for this benchmark and a comparison of the first results of interest.

KEYWORDS: MSR, transmutation, nuclear fuel cycle, fuel cycle simulation tools, benchmark, waste inventory

I. Introduction

Molten Salt Reactors (MSR), especially when used as a transmutation option, have rarely been modelled in fuel cycle simulation studies. A benchmark on the modelling of MSR in this kind of studies has therefore been included in the ISAC Project (Innovative System for Actinide Conversion) - a collaboration between five French nuclear corporations and institutions (CEA, CNRS, EDF, Framatome and Orano), aiming to identify the potential and the technological limitations of the use of MSR for minor actinides transmutation. The different codes compared are COSAC[1)] (Framatome), COSI[2)] (CEA), ISF[3,4)] (CNRS) and Tirelire-Stratégie[5)] (EDF). This benchmark has two objectives: to build knowledge around MSR modelling in fuel cycle simulation codes and to assess the performances of MSR compared to other transmutation strategies. Most fuel cycle simulation tools compared in this work are first and foremost designed for "solid-fuel reactors" modelling – except for ISF. To reach the first objective, most participants either need to simplify the modelling of molten salt reactors, so that they fit their tool's logic, or to implement designated routines in their codes - highlighting the benchmark importance in building trust in the newly developed models. To reach the second objective, similar hypotheses to the one used to carry out an extended review of transmutation options for the French nuclear cycle in 2012 - to which most current participants had taken part[6,7)], have been selected. They are also less complex than the hypotheses usually used in industrial fuel cycle studies, enabling the contribution of a wider variety of simulation tools with different maturity levels.

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II. Work Organization

1. Methodology

Because the various codes involved in this benchmark rely on significantly different calculation logics, this work is divided in 2 steps:

- a control trajectory (without MSRs), to assess the discrepancies between codes that are not related to the modelling of MSRs;
- a transmutation trajectory (with MSRs) where MSRs are used to transmute the americium produced by the rest of the fleet.

The second trajectory has first been studied by CEA using COSI: the scenario has been built with the objective of stabilizing Pu and Am at the end of the transition, while respecting constraints on the maximum masses of separated Pu (55 t) and Am (10 t). This trajectory has then been reproduced by the other participants, using the same number of MSRs and the same deployment rhythm - to the best of each code's ability.

The discrepancies between the participants are then analysed – with a special focus on the inventories of minor actinides and of Pu and Am – while taking into account the gaps identified during the control study and the modelling used for MSRs. Two types of modelling are highlighted:

- Static modelling, where the inputs and outputs of a reactor have a fixed value, independent from the fuel's isotopy - and thus known at the beginning of the calculation;
- Dynamic modelling, where the inputs and outputs of a rector are computed at each cycle, and are therefore evolving with the isotopy of the fuel.

2. Hypotheses

As stated above, the hypotheses used for this benchmark are strongly similar to the one used in[1,6] 2012, which used the French nuclear fleet as a framework (note however that these hypotheses are out of date with the current national strategy). Calibration data regarding used fuel inventories are provided for the year 2005. The studied trajectory is described in **Fig. 1**: the historical French nuclear fleet is gradually replaced by an EPR2 fleet of 40 Gwe,[8] implementing mono-recycling. All fuel must cool at least 5 years before being reprocessed and fresh fuel fabrication takes 2 years. Starting 2040, a 20 GWe SFR fleet (the design used here is the SFR V2B[9]) is deployed, transitioning soon after into a 60 GWe SFR fleet – which should stabilise Pu - as the EPR2 fleet closes.

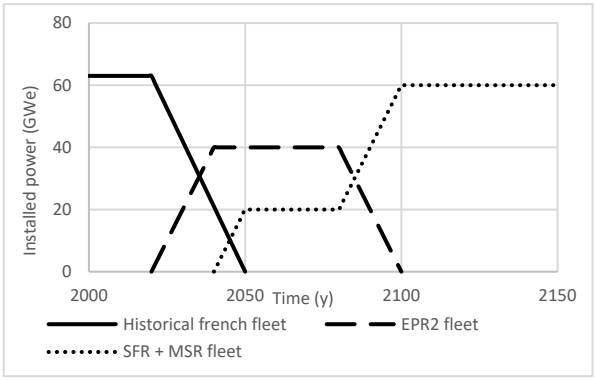

Fig. 1 Installed power per reactor technology (GWe)

In the study that includes them, MSRs are introduced simultaneously with SFRs – starting 2040. The installed SFR power is adapted so to keep a total power as close to 60 GWe as possible. The MSR design considered here is ARAMIS-A (300 MWth fast chloride reactor, fueled with both plutonium and americium)[10] also developed in Project ISAC. Starting the commissioning of MSRs, the flows of matter follow the directions described in **Fig. 2**, with the goal of stabilising both Pu and Am inventories.

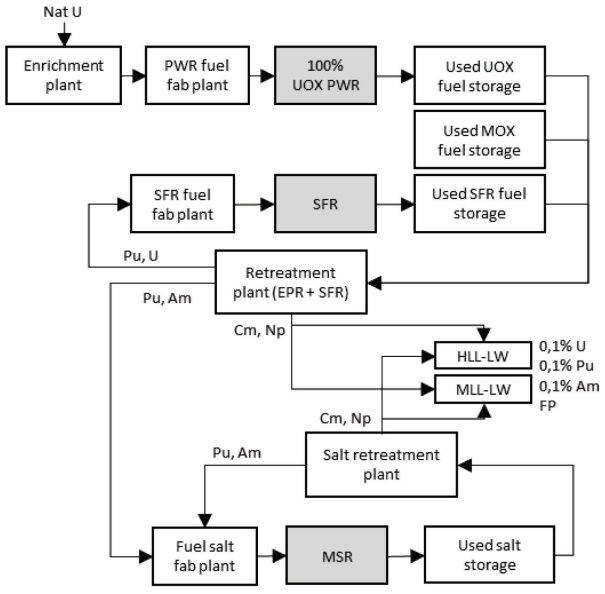

Fig. 2 Flow chart describing the cycle including transmutation in MSR

3. Code Particularities

The main characteristics of each codes are summarized in **Tabl**. Most scenario codes taking part in this benchmark generally use dynamic modelling in simulations involving "solid fuel" reactors. They rely on two types of metamodels: the equivalence model – which links the isotopy of the available matter and the composition of the fresh fuel; and the irradiation model – which computes the isotopy of the used fuel based on the fresh fuel's isotopy. The main hypothesis behind the use of these models is that they can be applied to a single load of fuel, without taking into account the environment of the rest of the core.

This hypothesis falls short in the case of a liquid fuel: even when the reactor is refuelled with a consistent isotopy, the content needed to ensure criticality as well as the used salt composition change with each cycle. Since it is not possible to single out a batch of salt in an homogenous mixture, the history of the core has to be taken into account.

Hence the need to develop new modelling methodologies – be they static or a dedicated dynamic metamodel – for most participating codes.

(1) COSAC – Framatome

In COSAC, the irradiation of solid fuels is modelled using a dedicated evolution matrix. The content of plutonium in fresh MOX assemblies (be they used for PWR, EPR2 or SFR) is constant over time (and therefore not dependent on the isotopy).

The reprocessing of matter is carried out "on demand", meaning that the code automatically reprocesses as much used fuel as necessary to provide plutonium for the fabrication of new assemblies. In consequence, there is no accumulation of separated plutonium in Framatome's scenarios (although there can be accumulation of separated americium), which comes at the cost of a strong variation of reprocessing capacities over time.

The modelling of MSRs is static: the repartition between Pu and Am is fixed to 45 % and 55 % respectively (reference repartition for ARAMIS-A), and the fueled mass of heavy nuclei (HN) as well as the content of the used salt are constants. The value used are the equilibrium values obtained for ARAMIS-A, after it has been fueled all its life with the same reference isotopy.

(2) COSI – CEA

In COSI, the irradiation of solid fuels is modelled using the evolution code CESAR.[11] The content of plutonium in fresh MOX assemblies (be they used for PWR, EPR2 or SFR) is dependent on the isotopy.

The reprocessing of matter is carried out "on line", meaning that the user specifies how much fuel is reprocessed each year. This means that the reprocessing capacities can be kept constant over significant periods of time, but that separated matter (Pu or Am here) accumulates in stocks, which have to remain capped.

The modelling of MSR is static: the repartition between Pu and Am is fixed to 45% and 55% respectively (reference repartition for ARAMIS-A), and the fueled mass of HN as well as the content of the used salt are constants. The value used are the averaged inputs and output obtained for

ARAMIS-A after it has been fueled all its life with the same reference isotopy.

(3) ISF – CNRS

ISF is a very fast running code where the reactors are modelled statically without using metamodels. Being developed for systematic studies of MSR deployment, ISF is strongly connected to the in-house REM depletion code[12]. The values used as inputs and outputs for the solid fueled reactors have been chosen based on estimations of the isotopy of matter in the cycle at a given moment in time and external depletion calculations computed prior to the fuel cycle simulations. The modelling of MSR has been done in a similar fashion, with the additional possibility of implementing yearly variations in the inputs and outputs.

(4) Tirelire-Strategie – EDF

In Tirelire-Strategie (T-S), the irradiation of solid fuels is modelled using the evolution code STRAPONTIN[13]. The content of plutonium in fresh MOX assemblies (be they used for PWR, EPR2 or SFR) is dependent on the isotopy. Matter reprocessing is managed in the exact same way as in COSI.

The modelling of MSR is dynamic: the mass of fueled HN is considered constant – and chosen as the refueling mass at equilibrium for the reference isotopy for ARAMIS-A – but the repartition between Pu and Am is computed at each cycle and thus differ from ARAMIS-A reference configuration. Pu is first computed so that the refueled core reaches a criticality criteria (estimated using a Baker & Ross approach, for the first cycle and for a reference fueling isotopic composition)[14], and Am is used as a complement so that the sum of both elements equals the fixed total HN mass. Irradiation is modelled using an evolution matrix.

Table 1 Summary of the codes particularities

	COSAC	COSI	ISF	T-S
Solid fuel irradiation	Evolution matrix	Evolution code	Static	Evolution code
Pu content in MOX	Constant	Calculated	Constant	Calculated
Reprocessing	On demand	On line	On demand	On line
MSR modelling	Static	Static	Static	Dynamic

III. Control Study Results, without MSR Deployment

In this section, a comparison is made between trajectories that do not include MSRs, to assess the discrepancies that are only related to the different codes and not to the modelling choices made for MSRs.

1. Plutonium Inventory

Figure 3 shows the repartition of the plutonium inventory in the cycle. Results show similar trends and numerical results. In ISF's, the detail of the repartition of Pu inventory is not accessible: only the reactor inventory and a sum of the rest of the cycle are available. Data related to plants and waste are not differentiated from the used fuel either. Except in T-S's case, a slight increase can be observed in the total Pu inventory. In COSI's case, it is because the exact equilibrium isotopy has not yet been reached, so the V2B core behaves as slightly breeder. In COSAC's and ISF's case, the fixed Pu content at fresh fuel fabrication might be lower than the equilibrium value as well, hence an increase in spent fuel inventory.

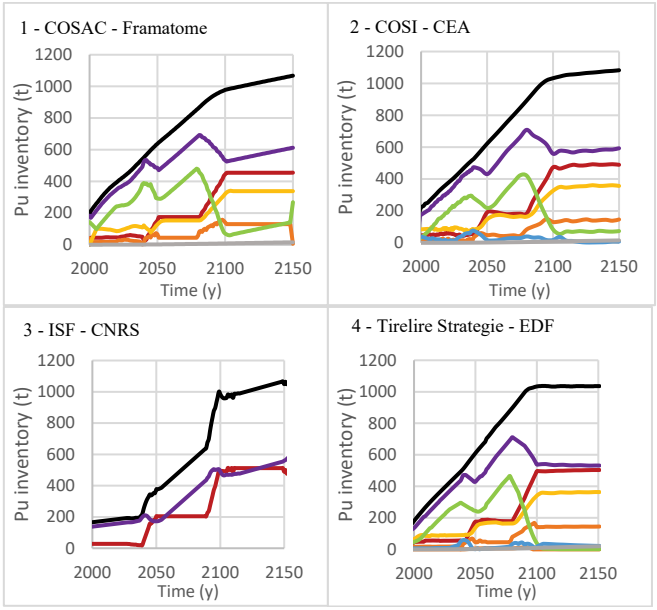

Fig. 3 Plutonium inventory in the cycle; Shared label: Black: Total - Red: Reactors – Green: Cooled spent fuel – Yellow: Cooling spent fuel – Orange: Plants – Blue: Stocks – Grey: Waste – Purple: all the cycle except for reactors

2. Minor Actinides Inventory

Figure 4 shows minor actinides inventories for each participant. Since Am separation is not implemented in this scenario, most of the americium of the cycle is here concentrated in waste.

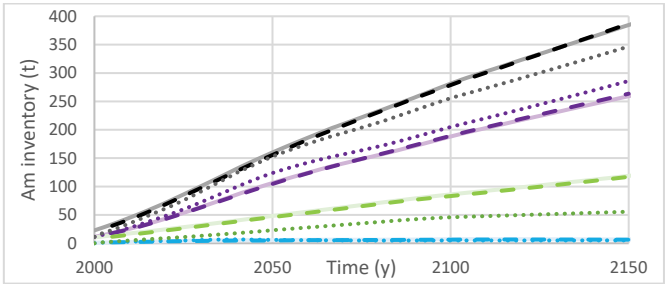

Fig. 4 Minor actinides inventory;
Shared label, colours: Black: Total - Purple: Am – Green: Np – Blue: Cm
Shared label, line: Dots: COSAC - Dashes: COSI – Full line: ISF – Faded line: T-S

This shows very good correspondences between COSI and T-S's results – which was expected, since they are the closest tools amongst the participants. It is worth noting that the difference in the Am estimation between all the participants seems to have been accumulated before the deployment of SFRs and that the slope in the increase of Am seems consistent between all codes once the 100% SFR fleet has been deployed. ISF's results are the most different compared to the other participants: the annual Am production of the EPR2 reactors seems to be significantly underestimated and the annual production of Cm significantly overestimated.

Other gaps, especially on Np and Cm are attributed to

differences in the reactors irradiation models. These discrepancies will need to be taken into account when analysing the results of the MSR study.

3. Intermediary Conclusion

Table 2 compiles the main results of the control study at equilibrium (2150). All codes show good correspondences, especially on natural uranium consumption and Pu inventory. It is worth noting that the minor actinides estimation can differ significantly between the different participants, which would need to be taken into account when analysing the MSR study results. Nevertheless, all participants converge towards a close annual increase value.

Table 2 Control study - Main results

At equilibrium	COSI	T-S	COSAC	ISF
Nat U (kt)	728	733	636	747
Plant capacity (t/y)	445	445	441	-
Pu inventory (t)	1082	1036	1068	1048
MA inventory (t)	387 + 2.2 t/y	368 + 2.05 t/y	346 + 1.88 t/y	322 + 1.99 t/y
Am inventory (t)	263 + 1.5 t/y	248 + 1.39 t/y	286 + 1.68 t/y	194 + 1.66 t/y

IV. MSR Study Results

As explained in subsection **II.1**, this study has first been performed by CEA with the objective of adding ARAMIS-A reactors in order to stabilize Pu and Am at the end of the transition. During the transition, separated Pu stocks should remain below 55 t and separated Am stocks under 10 t. Since MSRs are fueled with both Pu and Am and since the deployment of SFRs also requires large amounts of Pu, it is allowed to have a plutonium deficit - although no Am deficit. Other participants have then reproduced this scenario to the best of their codes functionalities. Discrepancies are then analysed.

1. Plutonium Inventory

Figure 5 shows the repartition of the plutonium inventory in the cycle. Compared to the control study, results show much more differences: COSI and COSAC's results are stabilized or almost so – depending on the equivalence model they use to compute fresh SFR fuel fabrication. However in COSI's case, it is necessary to import 71 t of Pu from outside the cycle during the transition, which is not the case in other scenarios. The transition is therefore not sustainable even though the equilibrium state is.

Since T-S's results were very similar to COSI's in the control study, we can conclude that the differences are here first and foremost explained by the modelling of MSR. As a matter of fact, since T-S's model takes into account the isotopy of the available matter and since the plutonium grade increases in a SFR fleet, the MSRs need less Pu in this dynamic modelling than in the COSI scenario. As a result, Pu accumulates in used fuel stocks, which in turn decreases the need to reuse Pu coming from used salt, and strengthen this good Pu grade effect. Even though this phenomena is credible, a precise full core evolution study should be performed so as to state the accuracy of the T-S model.

Like in the control study, the detail of the repartition of the inventory outside of the reactors is not accessible in ISF's case. At the end of the transition the total inventory is not stabilized, for the same reason as in the control study – which is that the fixed modelling of SFRs is slightly breeder.

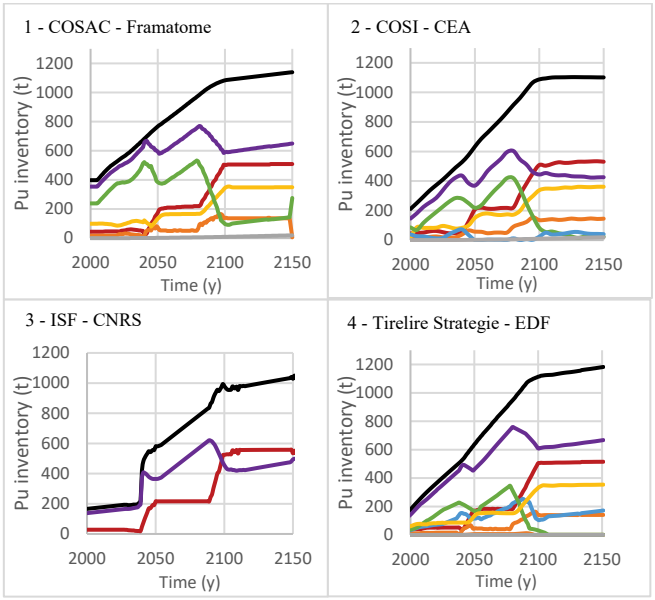

Fig. 5 Plutonium inventory in the cycle; Shared label: Black: Total Red: Reactors – Green: Cooled spent fuel – Yellow: Cooling spent fuel – Orange: Plants – Blue: Stocks – Grey: Waste – Purple: all the cycle except for reactors

2. Americium Inventory

Figure 6 shows the repartition of the americium inventory in the cycle.

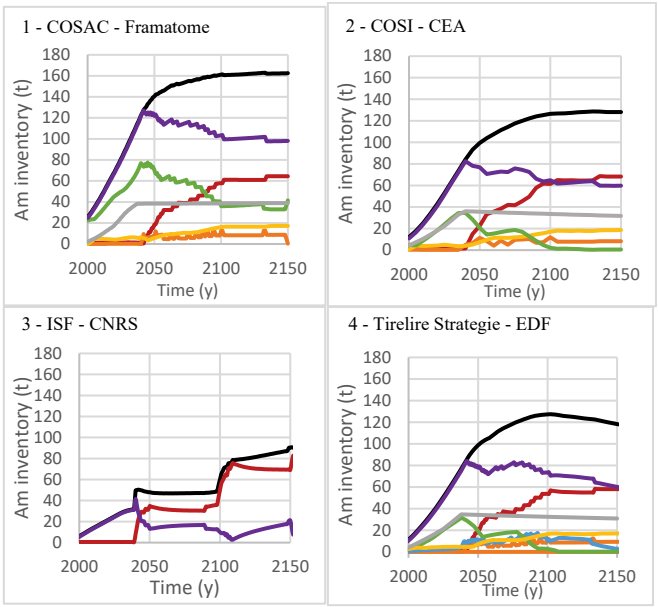

Fig. 6 Americium inventory in the cycle; Shared label: Black: Total - Red: Reactors – Green: Cooled spent fuel – Yellow: Cooling spent fuel – Orange: Plants – Blue: Stocks – Grey: Waste – Purple: all the cycle except for reactors

Only COSI and COSAC's trajectories reach Am stabilization at the end of the transition. This is coherent with the facts that they have the closest modelling of MSR and a

very similar slope of increase of Am inventory in the control study. However, in COSAC's case, the constraint on the maximum separated Am mass is not verified. This is related to differences in the reprocessing choices: in COSAC's case, reprocessing is only Pu-driven, and Am is only a subproduct of this reprocessing. In COSI's case, the general strategy is similar (Pu is the limiting element for fueling the fleet), but the MSR deployment rhythm was tailored specifically to respect the constraint. One can also note that the initial Am inventory in used fuel is not the same for the two codes. The control study also highlighted a different annual production of Am in SFR between COSI and COSAC. These two effects explain the reason why the two codes do not stabilise Am at the same value.

In T-S's case, the Am inventory slightly decreases over time – 450 kg of Am need to be imported yearly from outside the fleet, which represents a total of more than 43 t; the trajectory is thus not sustainable. Contrary to the scenarios previously discussed, Am is the limiting element here. Reprocessing aims first at accessing it, hence the accumulation of Pu in separated stocks (which are hard to manage) instead of in cooled spend fuel. This result is a direct consequence of the chosen MSR model: with a fixed total mass of HN, and a Pu content that decreases over time due to an increase of its grade, and, as a result, the Am complement increases until reaching an equilibrium over the course of the life of the reactor. This means that Am is stabilised inside the core but not in the cycle. It is worth noting that this modelling does not actualize the impact on reactivity of the increase of Am in the refueling salt and in the core.

In ISF's simulation, the waste item has not been modelled: this means that contrary to other trajectories, the Am reprocessed before 2040 is not vitrified and therefore available for use in MSR. With this modelling, 18 ARAMIS-A reactors doesn't seem enough to stabilize the Am inventory, but deploying more would entail a shortage of matter incompatible with the code's functionalities.

3. Minor Actinides Inventory

Figure 7 shows the minors actinides inventories for each participant.

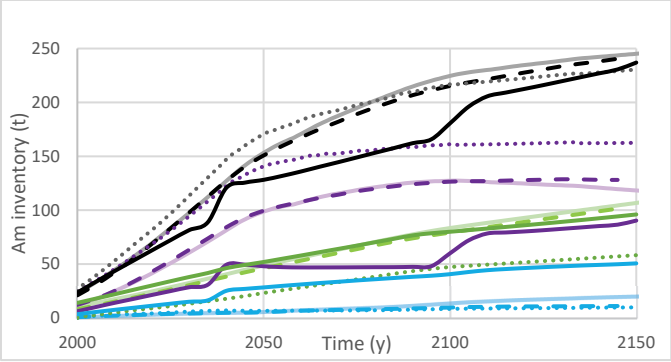

Fig. 7 Minor actinides inventory;
Shared label, colours: Black: Total - Purple: Am – Green: Np – Blue: Cm
Shared label, line: Dots: COSAC - Dashes: COSI – Full line: ISF – Faded line: T-S

As seen in the previous part, Am is stabilized in both COSI and COSAC's case. The discrepancies are coherent with the control study - and with a different initialization value in the case of Am.

In T-S's case, Am appears stabilized but it is only thanks to the addition of 450 kg of matter from outside the fleet every year – so the situation is in fact far from an equilibrium. This scenario is the one for which the Cm production has changed the most – which seems coherent with a dynamic model, since transmutation tends to increase the amount of Cm produced during irradiation.

In ISF's case, the total amount of minor actinides is much closer to the other participants than in the control study. However it's probably because the amount of Cm is overestimated compared to the other participant – which was already the case in the control study - and the amount of Am underestimated – especially since the vitrification of Am in waste is not modelled here, which means that the matter that should have been immobilised in waste before 2038 is absent.

4. Intermediary Conclusion

Table 3 compiles the main results of the MSR study at equilibrium (2150). Natural uranium consumption is, coherently, not affected by the addition of ARAMIS-A. The reprocessing and fabrication plants capacities of SFR are slightly modified to accommodate the small decrease in the installed SFR power. The results obtained amongst participants who were able to compute that data are close.

Table 3 MSR study - Main results

At equilibrium	COSI	T-S	COSAC	ISF
Nat U (kt)	728	733	636	747
SFR plant capacity (t/y)	429	422	419	-
MSR plant capacity (t/y)	14	5 (HN[1])	14	-
Pu inventory (t)	1120	1182	1139	1028
Pu deficit	71 t	0	0	0
MA inventory (t)	243 + 0.5 t/y	245 + 0.3 t/y	230 + 0.3 t/y	237 + 1.1t/y
Am inventory (t)	128	118 – 0.45 t/y	162	90 + 0.6 t/y
Am in waste (t)	31	31	38	-
Am deficit	0	43 + 0.45 t/y	0	0

Regarding actinides inventories, even if the final global results are satisfyingly close to each other, the uses and needs for matter differ significantly depending on the modelling choices of MSRs. The most explicit example of this is visible in the comparison between COSI and T-S results – which had almost identical data in the control study: in the former case, both Pu and Am are stabilized but a significant deficit of Pu appears during the transition due to a usage conflict between SFRs and MSRs; in the later, the modelling of MSR entails a

[1] In T-S, only the HN are modelled, contrary to COSI and COSAC which take into account an averaged value of inert salt. Hence a difference in reprocessing capacities.

much smaller need of Pu in the refueling of MSR, which in turn strongly increases the complementary need for Am: as a result, Pu accumulates and Am goes lacking.

Other differences are also explained by the host fleet itself: in COSAC case, there is no matter shortage despite using almost the same modelling as COSI. This has more to do with the characteristics of the SFR reactors fleet than with the MSR modelling.

One final explanation comes from differences in the hypotheses: in ISF's case, the absence of waste modelling entails a different use of Am - and therefore a different final inventory.

Consequently, it should be highlighted that each code would have led to different optimized trajectories.

V. Conclusion

In a context of growing interest around MSRs – especially when it comes to their use in transmutation – a benchmark has been proposed on fuel cycle simulation studies in the framework of Project ISAC. Since most fuel cycle simulation tools participating in this work - except for ISF – were not initially designed to account for this technology, this requires either simplifications of the MSR modelling or significant code adaptations. One of the main objectives of this benchmark is therefore to build knowledge around MSR modelling in fuel cycle simulation codes.

Two studies have therefore been performed: first a control study, based on hypotheses used in a prior collective project[6)7)], to assess discrepancies linked to the codes themselves ; second a study including the MSR ARAMIS-A, to assess the possibility of stabilizing both Pu and Am inventories depending on the modelling choices.

Results show rather satisfying similarities between codes in the control study but notably significant results in the MSR one – with a notable impact of the modelling choices made by the different participants.

This conclusion calls for further investigation on the modelling of liquid fuel reactors that are refueled during their lifetime with matter that evolves over time, as they represent a relatively new problem – one that questions most hypotheses used by dynamic models - for the fuel cycle simulation community.

Acknowledgment

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