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EXECUTIVE SUMMARY OF THE THESIS

Extending OpenMC for Molten Salt Fast Reactors: Implementation and Benchmark Comparison

TESI MAGISTRALE IN NUCLEAR ENGINEERING – INGEGNERIA NUCLEARE

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1 Introduction

Molten Salt Fast Reactors (MSFR), being circulating fuel reactors, present some peculiar features that make them very attractive in the context of Generation IV reactors. Among other things, they allow to perform an online removal of fission products (FPs), to keep the composition of the salt close to the eutectic - thus preserving a constant melting temperature, suitable thermophysical properties, chemical stability and, indirectly, the neutronic characteristics of the reactor - and to control the long-term reactivity of the system by tuning the injections of fertile (^{232}Th) and fissile (^{233}U) nuclides. However, standard burnup tools, developed for solid-fueled reactors, do not allow to model the mass-exchange processes that come into play in the aforementioned procedures. Hence, the development of suitable MSFR simulation tools has always been a central point in the research projects aimed at promoting the advancement of the technology. In this context, the Monte Carlo code OpenMC represents an interesting candidate for MSFR simulations, thanks to its open-source nature, high-fidelity neutron transport capabilities and wide adoption within the nuclear research community. In a previous study, the code had already been tested in the framework of the SAMOSAFER Benchmark [1], a benchmark developed during the SAMOSAFER project to compare MSFR depletion codes. In particular, Steps 0 and 1 were run, showing a good agreement with partner's results, although some relevant discrepancies were found [2]. However, among the MSFR mass-exchange processes, Steps 0 and 1 consider only FPs removal, which can already be modelled in OpenMC using the method "add_transfer_rate" [3]. Hence, it is necessary to assess the capability of OpenMC to correctly predict the evolution of the nuclide inventory in more complex configurations, involving also eutectic control and reactivity control. To do that, algorithms developed for this purpose for Serpent 2 at Polimi were implemented also in the OpenMC source code. Then, Steps 2, 3 and 4 of the SAMOSAFER Benchmark were run and results were compared with the partner's ones. Moreover, this work allowed also to perform a general simplification of the benchmark itself, by discarding those Steps which were not considered useful to observe possible differences between the

codes. In the future this should allow for a faster verification of new MSFR burnup tools.

2 Modelling of mass-exchange in OpenMC

The modelling of mass exchange processes in a MSFR requires to modify in the system of Bateman equations, which describes the evolution of the nuclide inventory during burnup.
The simplest, but still effective approach to simulate the transfer of a nuclide i, whose concentration in a generic material α is $N_i^{\alpha}(t)$, to a material β, where the nuclide concentration is $N_i^{\beta}(t)$, consists in adding a fictitious decay term within the Bateman equations of nuclide i, negative for material α and positive for material β. In this way, it is assumed that the transfer occurs at a constant rate over time, defined by the fictitious decay constant $\lambda_i^{\alpha\beta}$ $[s^{-1}]$:

$$\frac{dN_i^{\alpha}}{dt} = \sum_j \sigma_{j\to i}\phi N_j^{\alpha} + \sum_j \lambda_j b_{j\to i} N_j^{\alpha} - \sum_j \sigma_{i\to j}\phi N_i^{\alpha} - \lambda_i N_i^{\alpha} - f_i \lambda_i^{\alpha\beta} N_i^{\alpha} \quad (1)$$

$$\frac{dN_i^{\beta}}{dt} = \sum_j \sigma_{j\to i}\phi N_j^{\beta} + \sum_j \lambda_j b_{j\to i} N_j^{\beta} - \sum_j \sigma_{i\to j}\phi N_i^{\beta} - \lambda_i N_i^{\beta} + f_i \lambda_i^{\alpha\beta} N_i^{\alpha} \quad (2)$$

Where f_i represents the effectiveness of the process of transferring nuclide i from material α to material β (assumed to be equal to 1 for the purpose of this work).
This is the approach used also by the OpenMC's method "add_transfer_rate" to model FPs removal.

2.1 Eutectic control

Two algorithms were implemented in OpenMC to simulate the continuous control of the eutectic composition: Thorium Mass Control (ThMC) and Molar Fractions Control (MFC), both initially developed for Serpent at Polimi [4] [5].

In the Thorium Mass Control (ThMC) algorithm, the total mass of ^{232}Th in the fuel is maintained at a constant value during the entire simulation. This is accomplished by forcing the Bateman equation for ^{232}Th in the fuel as:

$$\frac{dN_{^{232}Th}}{dt} = 0 \quad (3)$$

implying that any thorium lost through transmutation or decay is instantaneously replenished. However, in long-term depletion calculations, an artificial increase in the total actinide mass may occur. This happens because the algorithm involves the injection a new ^{232}Th atom independently from the type of the nuclear reaction that consumes the old ^{232}Th atom. Specifically, if a capture reaction occurs, and eventually it does not lead to the production of a nuclide that undergoes fission, an increase in the overall actinide mass is observed.

The MFC algorithm, instead, directly targets the molar ratio between light and heavy fluorides and is based on two complementary actions:

1. Replacement of consumed actinides with ^{232}Th: every time a heavy nuclide undergoes fission, leading to a reduction of the heavy fluoride fraction, an equivalent amount of ^{232}Th is introduced into the system.
2. Adjustment of light fluoride content in response to FPs generation and removal: each fission event is associated with the formation of two fission products, which displace part of the LiF fraction. To maintain the original light/heavy molar ratio:
    - one ^{7}Li atom is removed for each fission product atom generated
    - when fission products are removed during reprocessing, the corresponding quantity of ^{7}Li is re-injected to restore the baseline composition.

2.2 Reactivity control

Reactivity control is a fundamental requirement for molten salt fast reactors, as the continuous evolution of the fuel composition leads to long-term reactivity variations that must be compensated through controlled injections and

removals of fertile and fissile nuclides. In this work, an off-diagonal reactivity control strategy, originally developed for Serpent at Polimi [4], was implemented also in OpenMC. The control algorithm adjusts the concentration of a fissile nuclide based on the deviation of the system from criticality, while coupling its action to the concentration of a low-feed fertile nuclide, thus enhancing numerical stability and convergence.
The implementation of reactivity control in OpenMC is non-trivial due to the structure of the depletion solver, which provides nuclide inventories only at discrete burnup steps and does not allow for intermediate solutions of the Bateman equations, thus preventing from performing a finer control. To account for these limitations, the control strategy has been adapted to operate consistently within the OpenMC burnup framework, while preserving the physical meaning of the control action and respecting the characteristic times of the fuel treatment unit (FTU). This required introducing intermediate solutions (sub-steps), modifying the material handling routines and extending the standard depletion workflow to allow controlled, step-wise mass exchange operations.

3 Benchmark analysis

To assess the correct implementation of the control strategies in OpenMC, the benchmark developed in the framework of the Work Package (WP) 3 of the EURATOM SAMOSAFER project [1], was considered. In particular, OpenMC results were compared with the ones obtained at the Paul Scherrer Institut (PSI, Switzerland) with the MATLAB-based EQL0D procedure [6] and with the ones obtained at Polimi with a modified version of Serpent 2 specifically developed for MSFR simulations [4] [5]. In this framework, to reduce the number of possible sources of discrepancies, it is better to compare results from different codes obtained with the same nuclear data library, thus OpenMC results were compared mainly with the EQL0D ones, as Sepent simulations were performed with different libraries.
The SAMOSAFER Benchmark has an incremental structure and is divided into 4 Steps, each internally subdivided in a certain number of sub-steps: Step 0 considers only decay and FPs removal for a simple fuel cube, Step 1 adds irradiation, Step 2 control strategies, Step 3 the blanket, while Step 4 considers a real MSFR geometry. The Steps that are mainly of interest in the context of this work are Steps 2, 3 and 4, as they foresee the implementation of control actions. However, also a revaluation of Steps 0 and 1, which had already been run using OpenMC in a previous study [2], was carried out. The aim was to identify the reasons beyond the discrepancies that appeared in those Steps, in order to be able to discard between them and possible new discrepancies introduced by different implementations of the control actions. Moreover, this allowed also to reduce the number of sub-steps in Steps 0 and 1, by discarding those that were not found valuable to observe possible differences between different MSFR simulation tools.

3.1 Revaluation of Steps 0 and 1

The revaluation of Step 0 allowed to assess that the main discrepancies are related to the EQL0D procedure. In particular, there is an error in the decay matrix construction, that leads to errors in the prediction of the concentrations of some actinides decay products, and there is a mistake in the input file, as H, He and O were not included among the elements that should be removed by the off-gas.
Step 1 introduces irradiation, and here the main cause of discrepancies is related to OpenMC. Indeed, to calculate the independent fission yields OpenMC considers the average energy at which nuclear fissions occur, while Serpent (used also in the EQL0D procedure to retrieve the reaction rates for the burnup matrix construction) computes one yield for each energy at which the yields are tabulated in the nuclear data library. This allows to better account for those fissions caused by neutrons at the extremes of the energy distribution, particularly for highly energetic fissions, that have higher yields for nuclides at the extremes at the mass number distribution and in the neutron-deficient region. On the other hand, OpenMC systematically underestimates the concentrations of these nuclides. This is shown also in Figure 1, which reports the distribution in the nuclides of the relative differences between OpenMC and EQL0D after 5 years of burnup.
Furthermore, in Figure 1 one can notice that discrepancies appear also on the left side of the

actinides region and in the light nuclides region. The affected nuclides are generally produced in threshold reactions, such as (n,2n) reactions, caused only by highly energetic neutrons. In this framework, the discrepancies are mainly due to statistical uncertainty, as the right tail of the energy distribution is not sufficiently explored in the considered Monte Carlo simulations. Moreover, due to limitations in computational resources, the number of simulated particles in OpenMC was even lower compared to EQL0D, thus increasing the uncertainty.

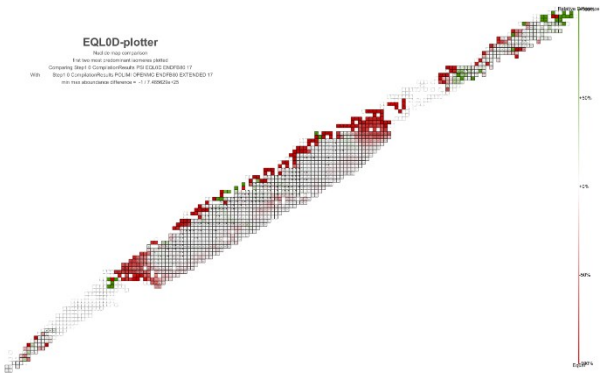

Figure 1: Relative differences between OpenMC and EQL0D after 5 years of burnup (Step 1.0)

The last cause of discrepancies that was identified in the revaluation of Step 1 is related to the integration scheme. Indeed, in OpenMC simulations the predictor-corrector CE/CM integrator was adopted, while in EQL0D the simple predictor integrator was used, thus providing slightly less precise results, especially for actinides produced in successive capture reactions starting from ^{232}Th and ^{233}U.

3.2 Step 2 results

Step 2 allowed to assess the correct implementation of the control algorithms in OpenMC. Specifically, Step 2.0 enabled to verify the correct implementation of the ThMC algorithm, as one can notice in Figure 2 and in Figure 3, and Step 2.1 the correct implementation of the MFC algorithm, shown in Figure 4 (Serpent results were not available for this Step). Concerning the former, OpenMC predicts exactly the same ^{232}Th concentration as Serpent, while PSI values are slightly lower and decrease very slightly in time, although the difference is practically negligible.
Concerning Step 2.1, while in OpenMC there is just a very slight increase in the actinides concentration in the final burnup steps, in EQL0D the concentration decreases. This happens because EQL0D simulations were run controlling the mass of actinides instead of their concentration. Hence, to compensate for heavy actinides buildup and to keep the total mass constant, the amount of removed ^{232}Th is higher compared to concentration control (MFC algorithm), as ^{232}Th is lighter compared to the nuclides it has to compensate for. Nevertheless, the difference is very small.

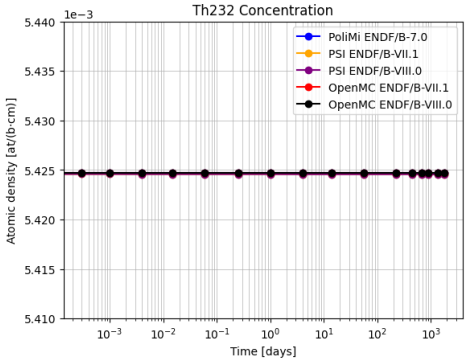

Figure 2: Evolution of the ^{232}Th concentration (Step 2.0)

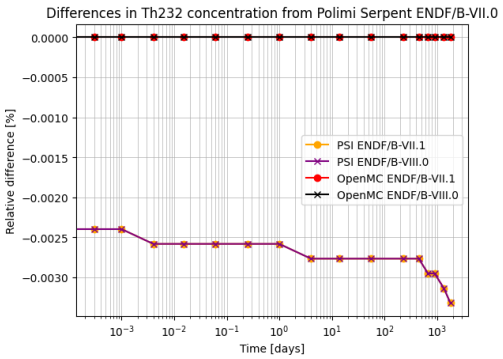

Figure 3: Relative differences in ^{232}Th concertation compared to Polimi Serpent ENDF/B-7.0

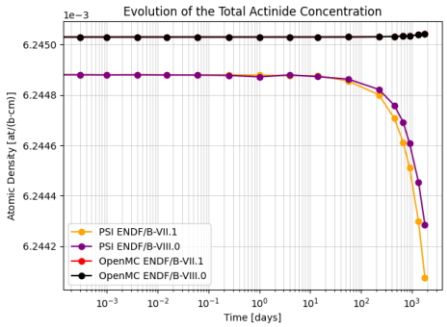

Figure 4: Evolution of the total actinide concentration (Step 2.1)

Step 2.4 allowed to assess the correct implementation of reactivity control, as one can notice in Figure 5, which shows the evolution of the multiplication factor during the simulation, comparing it with the one obtained with Serpent at Polimi. EQL0D results are not reported, as EQL0D sets the composition to be equal to the one required to have a critical system already after the first burnup step, thus providing different results in the first steps. However, as one can notice in Figure 6, eventually both algorithms converge to the same values.

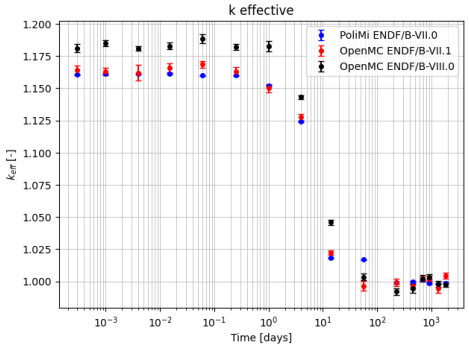

Figure 5: Evolution of the k_{eff} (Step 2.4)

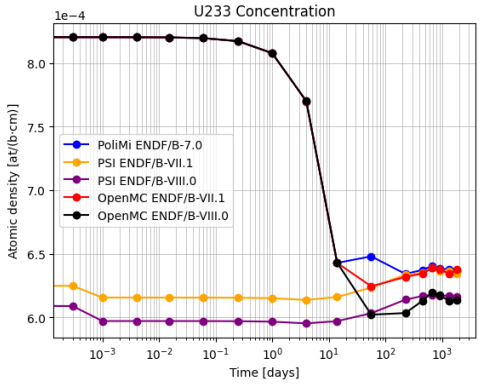

Figure 6: Evolution of the ^{233}U concentration (Step 2.4)

Apart from the discrepancies related to the different implementations of actinides control and reactivity control, it is important to underline that in this Step the main causes of discrepancies remained the same ones of the previous benchmark Steps.

3.3 Steps 3 and 4 results

Step 3 adds a blanket layer on one side of the fuel cube geometry considered in the previous Steps. Moreover, on the external surface of the blanket vacuum boundary conditions are imposed, thus allowing to partially account also for neutron leakages, while reflective boundary conditions are still imposed on the other external surfaces.
An important discrepancy emerged in Step 3.1: EQL0D significantly underestimates the flux and the ^{232}Th capture cross section in the blanket, thus causing a lower ^{233}U buildup and, hence, a lower fission rate. No differences were found in the input files, thus the reason for the discrepancy seems to lie inside the EQL0D procedure.
Nevertheless, apart from this, no new discrepancies were found in Step 3 simulations.
Also in Step 4, which considers the complete MSFR geometry, no new discrepancies appeared.

4 Benchmark simplification

The revaluation of the SAMOSAFER Benchmark carried out to verify the capability of OpenMC to correctly predict the evolution of the nuclide inventory in a MSFR allowed also to perform a general simplification of the benchmark itself, by discarding those Steps which were not considered valuable to observe possible discrepancies between the different tools.
In this framework, Step 0, which aims to assess Bateman solutions with decay only and the correct implementation of FPs removal, was reduced to only two sub-steps (0.1 and 0.4), which were considered sufficient for this purpose.
Step 1 aims to assess the behavior of the fuel cube under irradiation, firstly alone and then combined with reprocessing. For this purpose, Step 1.1 (which considers only irradiation) and 1.4 (which implements also the FTU reprocessing and the off-gas) were found to be sufficient, since no relevant differences appeared in Step 1.2 (which considers

only the FTU reprocessing) and the ones noted in Step 1.3 (which considers only the off-gas) remained the same in Step 1.4.
Step 2, instead, aims to assess the correct implementation of the MSFR control strategies. Each simulation is repeated twice, one assuming a burnup time equal to 5 years and another assuming a burnup time equal to 200 years. By comparing results from the two simulations at 5 years, if a predictor-corrector integrator is used, no relevant differences were found, thus suggesting that it will be possible to skip the 5 years simulation, as long as a predictor-corrector integrator is adopted. Moreover, Step 2 comprehends also two sub-steps that prescribe the implementation of thorium control without considering FPs removal. However, they were not considered valuable, as it is possible to assess the correct implementation of thorium control even with FPs removal enabled. Also the Steps which prescribe the implementation of reactivity control without controlling actinides mass were discarded, since the lack of a refill led to the progressive consumption of all the fissile and fertile inventory and, eventually, to the failure of the simulation.
Concerning Step 3, only Step 3.1 was kept, as it was considered valuable to observe how the different codes manage power distribution between fuel and blanket. The possible reasons why different codes may provide different results in the next sub-steps were already assessed in the previous ones, so they were all discarded. The only new physical phenomenon they introduce compared to the corresponding Step 2 sub-steps is the presence of neutron leakages. However, to completely account for them it will be better to consider directly Step 4, as in that case vacuum boundary conditions are imposed on all the external surfaces.
Thanks to this work, the number of sub-steps was reduced form 30 to 12, with the possibility of performing just 6 of them for a preliminary assessment.

5 Conclusions

This work allowed to develop an extended version of the OpenMC Monte Carlo code able to model MSFR eutectic control and reactivity control. Indeed, the Thorium Mass Control (ThMC) algorithm and the Molar Fraction Control (MFC) algorithm for eutectic control, and the off-diagonal reactivity control algorithm, originally developed for Serpent at Polimi were implemented also in the OpenMC source code. The successful extension of the code was assessed by running Steps 2, 3 and 4 of the SAMOSAFER WP3.1 Benchmark and by comparing results with the ones obtained at PSI with the EQL0D procedure and with the ones obtained at Polimi with Serpent. In this framework, the only new discrepancies compared to Steps 0 and 1 are related to the fact that EQL0D controls actinides mass instead of concentration and to the faster convergence speed of the EQL0D reactivity control algorithm. Nevertheless, both reactivity control algorithms converge to the same values and, concerning actinides control, the difference in controlling mass or concentration is very low.
However, the discrepancies which had been observed in Steps 0 and 1 were still present, and are due to:

- Errors in the management of decay data in the EQL0D procedure
- H, He and O were not included among the nuclides that should be removed by off-gas in EQL0D
- Poorer OpenMC fission yield treatment
- Stochastic nature of the calculation
- Use of different integration schemes (predictor vs predictor-integrator)

Moreover, the revaluation of the SAMOSAFER Benchmark carried out to verify the capability of OpenMC to correctly predict the evolution of the nuclide inventory allowed also to perform a general simplification of the benchmark, by discarding those Steps which were not found to be valuable to observe possible discrepancies between the different MSFR simulation tools. Eventually, the number of sub-steps was reduced from 30 to 12, with the possibility of performing just 6 of them for a preliminary assessment. In the future, this should allow for a faster verification of new MSFR burnup tools.

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To my family, who always supported me during all this incredible journey.