Burnup impact of an ASTRID-like core during a ULOF with SIMMER-III

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Abstract. Innovative Sodium-cooled Fast Reactors (SFRs) are currently investigated in the ESNII+ European project. The goal of the WP6 "Core safety" of this project is to support the development of the ESNII roadmap, the implementation of the ESNII deployment strategy and the licensing of the ESNII systems. This is done by identifying the experimental and theoretical R&D activities which are necessary for improving the present designs, as well as the existing methods, tools and databases for static and transient safety analysis of the ESNII critical reactor cores. One of the main issues of the WP6 "Core safety" of the ESNII+ project, as for ASTRID development, is to assess the behavior of the ESNII+ core (ASTRID-like core) in severe accidents at a representative stage, ie. the end of equivalent cycle (EOC), as the sodium voiding effect is less favorable at this moment. Consequently, the SIMMER-III code system (coupled thermohydraulics, pin mechanics and neutronics) is used as it can represent the accident up to an advanced core degradation. However, it has been developed to perform neutronics calculations at the beginning of life (BOL, without irradiation). This gives good results for homogeneous cores at EOC, but a new methodology needs to be implemented to perform EOC calculations for heterogeneous ones.

The aim of this paper is to present the behavior of the ESNII+ heterogeneous core at EOC, so as to highlight the importance of burnup in the accident scenario. Thus, a new methodology developed in the framework of the ESNII+ project to perform neutronics calculations at EOC is presented. Then, Unprotected Loss Of Flow (ULOF) calculation, with a 22s primary flow-rate halving time, is performed at EOC. The sodium boiling and the pin degradation happen earlier at EOC than at BOL, but the core degradation is slow in both calculations.

Despite less favorable feedback coefficients at EOC, and thanks to its heterogeneous geometry, the ESNII+ core in ULOF with a 22s halving time, does not lead, with the given hypotheses, to a power excursion.

Key Words: ASTRID-like, SIMMER, ULOF, burnup.

1 Introduction

In the framework of the ESNII+ project, an ASTRID-like CFV (heterogeneous) core is studied in the WP6.1.4 dedicated to the study of ASTRID-like core behavior under design-extension conditions. KIT-IKET, CEA, JRC, CIEMAT, KTH and EDF R&D take part to this benchmark. This document describes the work performed by EDF R&D on this subject.

The ESNII+ core corresponds to the CFVv1 core. This study aims at modelling the unprotected loss of flow accident (ULOF) with a 22s halving time of the ESNII+ core at the end of equivalent cycle (EOC).

To do so, a methodology is proposed and evaluated to model the CFV core at the EOC.

Then, it is used to perform a ULOF calculation with a 22s halving time as asked by the project.

2 The ESNII+ core

The main dimensions of the ESNII+ core, defined by CEA [1] [2], are given in TABLE **I**.

TABLE I: MAIN DIMENSIONS OF THE ESNII+ CORE

Nominal thermal power (MW)	1500
Number of fuel elements (inner/outer/total)	177 / 114/291
Pin diameter (mm)	9.7
Number of pins/SA	217
Inner/outer zone fissile height (cm)	60/90
Fertile plate height (cm)	20

The cross section of the ESNII+ core is given in *FIG. **1***.

The core is described at end of equivalent cycle (EOC), the fuel EOC compositions are given as input data. The rods are not inserted in the core, they are located at the level of the outer core pin plugs.

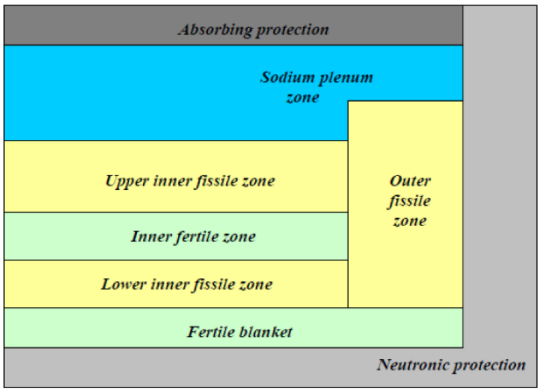


FIG. 1. General scheme of the CFV-v1 core [1]

3 The new methodology to describe burnup cores

3.1 Existing method in SIMMER [3]

The isotopic composition of a cell is calculated using the Pu content (which can be specified for each cell) and the average density of "fertile" (UO_2) and "fissile" (PuO_2), following this formula:

$$V_i = t_i V_{fissile} + (1 - t_i) V_{fertile} \qquad i \in [1, number\ of\ fuel\ cells]$$

With t_i Pu content of the cell i, and $V_{fissile}$ and $V_{fertile}$ the isotopic vectors of PuO_2 and UO_2 respectively.

When calculating an isotopic composition at beginning of life (BOL), these parameters enable to represent exactly the core. Up to now, most of the neutronics calculations with SIMMER have been performed at BOL, as it is the only state which could be perfectly represented. However, the BOL state is not representative of the core during its operation as the feedback effects are different (the sodium voiding effect is more favourable for instance). A representative state is the end of equivalent cycle (EOC). In this case, the composition is different in each cell because of the irradiation, which depends on the flux. If the core is homogeneous, the description with the existing SIMMER models gives good results, but with a heterogeneous core, the problem is much more intricate.

Thus, another way must be found to model the core at the EOC. It is not possible to give one composition for each cell in the SIMMER model. Therefore, to simplify the problem, the isotopic compositions are averaged on a given area. For the CFV core for instance, 4 regions are considered: inner fissile core, outer fissile core, intern axial blanket and lower axial blanket. The problem, now, results in the representation of 4 given isotopic compositions with SIMMER, and in the ability to follow the variations of compositions when they are mixed (e.g. when the fertile plate is mixed with the inner fissile core).

The ESNII+ project gives the isotopic compositions for each region. It can be underlined that there is no fission product in this EOC composition. Indeed, for the ESNII+ benchmark, the fission products have been replaced by an equivalent absorber, Molybdenum.

The approach, presented in the document, aims at modelling the ESNII+ core at EOC, using the specified isotopic compositions (or at least a good approximation).

3.2 Application of the Principal Component Analysis method

The Principal Component Analysis [4] (PCA) is a statistical procedure which uses an orthogonal transformation to convert a set of observations of possibly correlated variables into a set of values of linearly uncorrelated variables called principal components.

This method is widely used to reduce a large amount of data into a small quantity, much easier to deal with. It must be highlighted that this method approximates the initial data with an accuracy which depends on the considered case.

In this case, we want to approximate 4 uncorrelated vectors (4 isotopic compositions, as seen previously) using 2 principal components V_1 and V_2 (eigenvectors of the covariance matrix):

$$V_i \sim V_{mean} + \alpha_i V_1 + \beta_i V_2 \qquad i \in [1,4]$$

With V_{mean} the mean vector of the 4 initial vectors, α_i and β_i the principal factors (eigenvalues of the covariance matrix). α_i and β_i are independent from each other.
A Python script automatically calculates V_{mean}, V_1, V_2, α_i and β_i ($i \in [1,4]$), when given the 4 initial vectors.

TABLE II shows the result of the PCA on the ESNII+ case. Indeed, the relative error between the initial data and the result of the PCA is given (in %). The main isotopes, with a concentration greater than 10^{-4}at./barn.cm, are calculated with a good accuracy in the fissile region (less than 3.7%). In the fertile region, the Pu239 and Pu240 are calculated with a very important error (20-300%), but their importance in the region is 10 times less than U238, which is calculated with a 0.1% accuracy. Actually, the main isotope in the core, U238, is calculated with a very good accuracy, less than 0.1%.

TABLE II: Discrepancy in the isotopic composition between the ESNII+ data and the PCA results (%) for the main isotopes (concentration > 10^{-4}at./barn.cm)

	Inner fissile core	**Intern axial blanket**	**Outer fissile core**	**Lower axial blanket**
O16	0.0	0.0	0.0	0.0
Mo	-0.1	0.4	0.1	-0.9
U238	0.0	-0.1	0.0	0.1
PU239	2.1	-10.5	-1.7	19.7
PU240	-2.5	73.5	2.3	-258.3
PU241	-3.1	352.4	2.7	-1910.4
PU242	-3.7	11073.7	3.2	-124408.3

For the SIMMER calculations, only the isotopes with a concentration greater than 10^{-10}at./barn.cm are kept. 20 isotopes remain in the SIMMER library.

3.3 Steady-state results

To evaluate the bias between a reference ERANOS calculation and a SIMMER calculation, 6 calculations were compared:

- ERANOS calculation using the ESNII+ composition per area, and 33-energy-groups heterogeneous cell calculation (1968 groups self-shielding) ⇒ Impact of the composition per area
- ERANOS calculation using the PCA composition per area, and 33-energy-groups heterogeneous cell calculation (1968 groups self-shielding) ⇒ Impact of the PCA composition
- ERANOS calculation using the PCA composition per area, and 33-energy-groups homogeneous cell calculation (1968 groups self-shielding) ⇒ Impact of the homogeneous cell calculation
- ERANOS calculation using the PCA composition per area, and 16-energy-groups homogeneous cell calculation (16 groups self-shielding) ⇒ Impact of the 16-energy-groups mesh (and 16 groups self-shielding)
- SIMMER calculation, using the PCA composition per area, and 16-energy-groups homogeneous cell calculation (16 groups self-shielding) ⇒ Impact of the

SIMMER cell scheme (i.e. self-shielding using Bondarenko factors).
The core calculation is, for each case, performed in S4 transport 2D-RZ.

The comparisons are performed on the nominal reactivity value, and three reactivity effects:

- Sodium voiding in the fissile zone and in the intern axial blanket,
- Sodium voiding in the fissile zone, the intern axial blanket, the pellets upper plugs and the sodium plenum,
- The Doppler effect from the initial temperature (here 900 K to 1500 K for both fertile and fissile).

TABLE III gathers the results of the comparisons. The following conclusions can be drawn:

- Impact of the PCA composition: it is negligible
- Impact of the homogeneous/heterogeneous cell calculation: this impacts the leakage in the core, so the Doppler is unchanged, and there is a slight modification (~100pcm) on the core and total voiding. The initial reactivity is very different (-650pcm).
- Impact of the energy mesh: this causes a major change in the voiding values, as it decreases by 200pcm in the core. This difference is kept in the total voiding, which means the estimation of the voiding in the sodium plenum is the same. The Doppler effect is not affected.
- Impact of the SIMMER cell calculation scheme: compensations make the core voiding unchanged, but there is 180pcm difference in the sodium plenum voiding, and 80pcm on the Doppler. This difference comes from the cell calculation scheme used in SIMMER, where the leakage is treated differently and the self-shielding is calculated using Bondarenko factors (vs. probability tables in ERANOS).

TABLE III: Reactivity values for sodium voiding and Doppler effect for the different cases

		Reactivity	Reactivity effect		
		Nominal	Core voiding	Total voiding	Doppler 1500K
SIMMER	PCA 16G homogeneous	4575	950	-217	-416
ERANOS	PCA 16G homogeneous	6950	913	-353	-509
	PCA 33G homogeneous	666	1177	-142	-523
	PCA 33G heterogeneous	1318	1295	-46	-494
	ESNII compo. 33G heterogeneous	1278	1279	-56	-494

This comparison shows that finally, despite all the differences of model, the new SIMMER model gives a rather correct approximation of the main reactivity effects at EOC, that is to say the core voiding, the total voiding and the Doppler effect.
The Doppler is correctly evaluated. The total voiding is very close, mainly due to error compensations. The main discrepancy relies in the core voiding, with a difference of about 300pcm. This difference is mainly due to the energy mesh used in the SIMMER calculation, and a solution to improve this result could be to better adapt the energy mesh.

3.4 Fuel movement mainstreaming during the transient

A very simplified method to follow the movements of materials has been implemented. Indeed, inter-cell movements are taken into account, i.e. the mass transfer between cells is evaluated, and then, it is used to weigh and calculate new α_i and β_i coefficients in the mesh. To evaluate the mass variation, the following method is used:

- The mass in the cell at each time step is known. They are called $MASS_{t=0}(I,J)$ and $MASS_{t=1}(I,J)$ for the cell (I,J) at the time steps t=0 and t=1.
- As we perform the calculation at a given time between two time steps, we need to calculate the mass variation at the moment we perform the evaluation of the α_i and β_i coefficients. Thus, we use:

$$MASS_{t=0} = MASS_{t=1} - \Delta MASS_{exiting\ from\ the\ cell\ between\ t=0\ and\ t=1}$$

- The needed information is the origin of each mass. Hence, the fuel mass flux ("fertile" and "fissile") at each interface is calculated (example of the left interface):

$$Fuel\ mass\ variation\ at\ the\ left\ interface$$
$$= Fuel\ macroscopic\ density\ of\ the\ left\ cell$$
$$\times\ fuel\ radial\ velocity\ in\ the\ left\ cell\ (if\ positive, otherwise\ 0)$$
$$\times\ surface\ between\ cells\ \times\ time\ step.$$

- With all these informations, the updated values of α_i and β_i can be calculated.

The reevaluation of the α_i and β_i coefficients takes into account the inter-cell fuel movements with a slight error, as all the elements in the formula are not calculated at the same time step. Thus, this creates a bias in the result, which increases with the calculated time. This modification is not reliable after the first fuel break-up. Moreover, it does not take into account intra-cell material phase change, what is very important.

4 ULOF calculation of a CFV-type core at EOC

4.1 SIMMER model of the ESNII+ core

The ESNII+ core has been modelled with SIMMER at hot state and at EOC, using the methodology described in Section 3.

Geometry

As there is no thermal axial expansion and no solid steel radial expansion in SIMMER, the geometry has been given at hot state. The mass balance is kept.

The definition of materials in SIMMER does not enable to describe different steel materials for the claddings and the hexcans. Thus, the choice has been made to model all the steel in the core with AIM1 (claddings material).

Moreover, B_4C enriched at 20% in B10 is chosen for the absorber material. The results given in TABLE III were calculated using this hypothesis.

A sketch of the geometry described in SIMMER is given in FIG. 2.

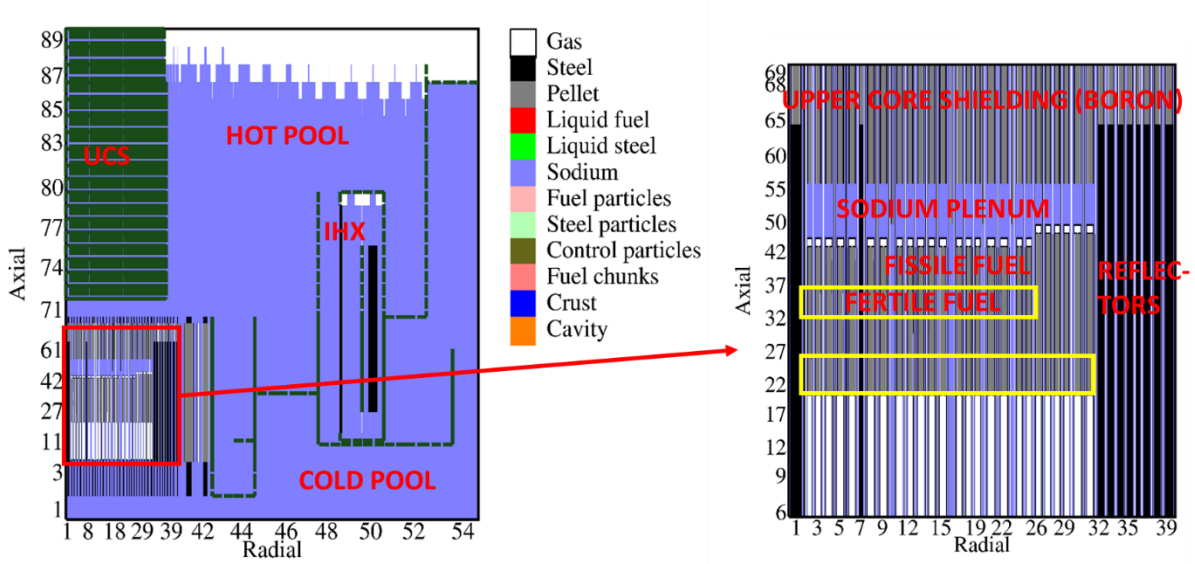


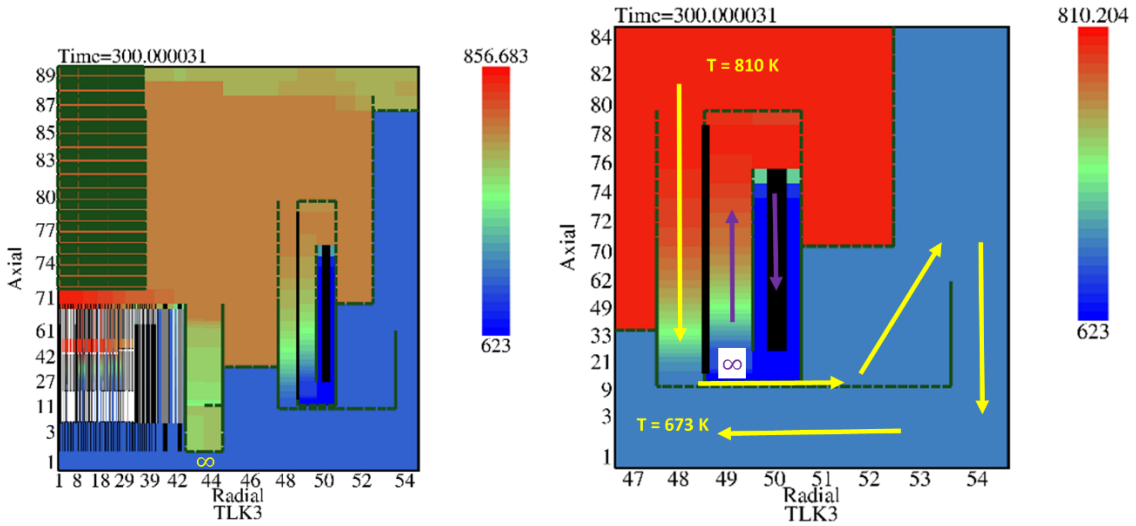
FIG. 2. Sketch of the SIMMER model of the ESNII+ core (UCS stands for Upper Core Structure, IHX for Intermediate Heat Exchanger).

Heat exchangers

The model (see FIG. 3) aims at describing the decrease in the core inlet sodium temperature that occurs during a ULOF transient. It is modelled using 2 sodium circuits:

- one with a thermostat at 623 K, and a pump, corresponding to the secondary loop,
- one corresponding to the primary sodium circuit, with another pump.

The exchange between both circuits is done thanks to a hexcan, which length has been calculated for the sodium inlet temperature at steady state to be 673 K.



a) General overview b) Zoom on the heat exchanger

FIG. 3. Geometry with primary and "secondary" sodium circuits (temperature variations in K)

Boundary conditions

There is one boundary condition, at mesh (54,89), corresponding to a 1 bar-pressure value.

Additional models

Three additional models have been used with the standard SIMMER version (SIMMER III v3E) to perform the study:

- β_{eff} calculation using the Keepin formula [5],
- Pin plug collapse leading to the pin plug break-up once the pin has collapsed,
- Control rod driveline expansion, using a model from KIT given in the ESNII+ framework.

Options

Options have been used to perform the study. They are listed below:

- The fuel pellet breaks up when the cladding is lost and the pin structure in the lower cell does not exist
- Chunks creation when the pellet breaks up
- Activation of the intra-cell heat transfers
- Activation of the inter-cell axial heat transfer between fluids and lower/upper structures
- P1 scattering model (approximate treatment): the transport cross section is derived from the cross-section library.

5 velocity fields for the liquid and gaseous components are considered: 1 for liquid fuel, 1 for liquid steel, 1 for liquid sodium, 1 for fuel, steel and absorber particles, as well as fuel chunks, 1 for vapor mixture.

To be consistent with the fuel pin collapse model, the value of maximum packing fraction for defining the particle viscosity is set to 0.9 instead of the standard value which is 0.62.

Finally, the sodium equations of state are described according to specifications given by KIT. This impacts directly the sodium heat capacity.

4.2 Steady-state results

Neutronics

The SIMMER neutronics calculation scheme consists in:

- a homogeneous cell calculation at 16 energy groups, with a self-shielding at 16 groups obtained using Bondarenko factors,
- a Sn transport core calculation with 16 angular directions and a Diamond scheme.

The JEFF3.1.1 library is used. Neutronics libraries for SIMMER are created using the ERANOS/SIMMER interface [5], and the cell flux used to condensate the cross-section is an inner core cell of the ESNII+ core at EOC.

The TABLE **IV** gives the initial reactivity obtained for the SIMMER calculation, as well as a comparison with 2 results from the ESNII+ neutronics benchmark. The 2 results from the benchmark are very close, with a reactivity of about 400pcm. However, the calculations performed at EDF give very different results. This is due to the different modelling of the materials that exists in SIMMER. Indeed, in SIMMER, there is only one steel material and only one absorber material. There is thus no distinction between claddings and hexcans, or B_4C with 20% B10 and B_4C with 90% B10. This has an important impact on the initial reactivity, which goes up to 4575 pcm. The initial reactivity obtained with SIMMER is even higher, and this is due to the homogeneous cell calculation, the self-shielding method and the decrease in the number of energy groups.

Concerning the core voiding effect (no voiding of the sodium plenum), they are analogous except for the SIMMER calculation, where the lower number of groups in the energy mesh leads to an important decrease of 331 pcm in the reactivity effect.

TABLE IV: Comparison of initial reactivity and voiding effect (pcm) between EDF, CEA and PSI

	Initial reactivity	Core voiding effect
PSI SERPENT (Monte Carlo)	429	1258
CEA ERANOS 33G heterogeneous cell calculation	430	1297
EDF SIMMER 16G homogeneous cell calculation	4575	950

Despite the fact that SIMMER does not represent the same materials as was specified in the core data file, the radial power profile obtained with SIMMER was compared to the ones from the neutronics benchmark. The SIMMER power profile (see FIG. **4**) fits very well with the results of the other codes. The SIMMER power profile is thus validated.

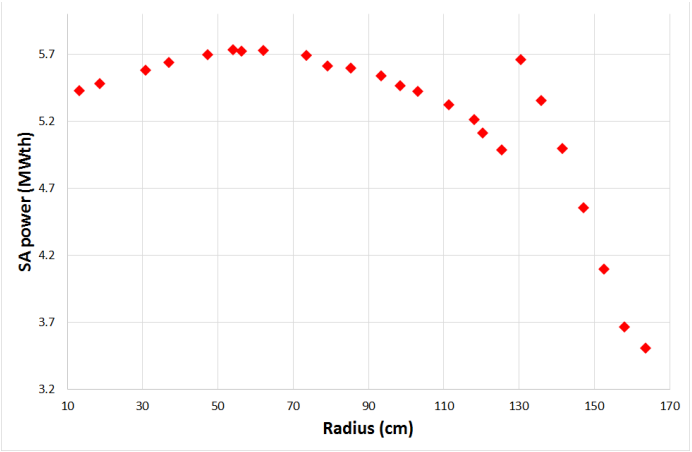


FIG. 4. Radial power profile of the core calculated by SIMMER

Thermohydraulics

The cooling scheme which has been used in the SIMMER calculations corresponds to the one given by PSI, with 3 groups. The flow rates calculated by SIMMER are close to the PSI values:

- in the inner core (cooling group 1), the flow rate is less important in SIMMER, which is logical as the power in the SA of the inner core is lesser in SIMMER. Thus, the sodium outlet temperature should be close to the PSI values.
- In the outer core (cooling groups 2 and 3), the flow rate is slightly greater as the power in these SAs is also greater.

Indeed, the FIG. 5 shows the profile of the sodium outlet temperature and confirms the tendency given by the cooling groups values:

- In the inner core, the values obtained by SIMMER are close to that of PSI, except in the centre of the core where the sodium outlet temperature is lesser.
- In the outer core, the SIMMER values are also close to the PSI ones.

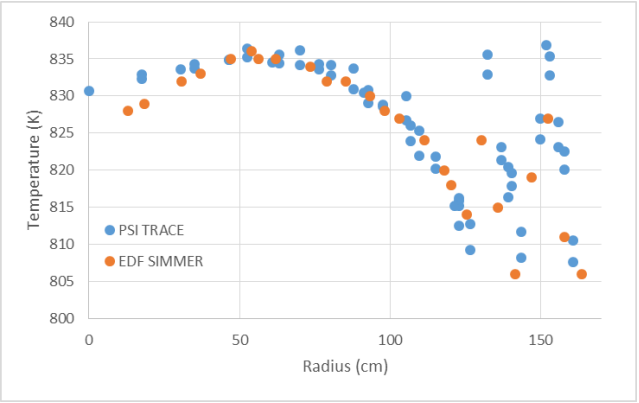


FIG. 5. Radial profile of the sodium outlet temperature between PSI and EDF

4.3 Transient results

The mass flow rate decrease has a 22s halving time. The SIMMER flow rate is close to the theoretical one. The error is 3% at 60s. After this time, boiling occurs and there can be no further comparison between the SIMMER result and the theoretical value. The error is considered small enough for the result to be correct.

To check the consistency of the IHX model in SIMMER, the variation of the sodium inlet temperature was validated according to the thermohydraulics benchmark of the ESNII+ project. The result obtained with SIMMER is a bit lower than that of the other codes (-4°C at 120s), but gives a correct order of magnitude and decreases at approximately the same moment. The SIMMER model for the IHX is considered satisfying.

The transient starts at t=300s and is described on FIG. 6. The power variation is given on FIG. 6. The main events of the scenario with respect to the start of the transient are:

- t=102.5s: boiling onset in channel 9, followed by channels 5, 6, 8, 10, 11, 13, 2 and 3 ⇒ reactivity and power decrease
- t=118.2s: sodium plenum refilling in channels 2, 3 and 5 ⇒ reactivity increase.
- t=127s: voiding of channels 2, 3 and 5 ⇒ reactivity decrease
- propagation of voiding in the fuel zone ⇒ reactivity increase.
- t=143.5s: first cladding break-up in channel.
- t=151s: general voiding of the core ⇒ reactivity decrease
- t=164s: cladding movement outside the flux zone ⇒ important reactivity increase and slight power excursion ($t = +176.18s, P = 19P_0, \rho = 0.92\$$)
- t=177s: fuel melting and fuel ejection outside the core.

The calculation was stopped because there was no time left to pursue the calculations, but a power excursion is expected, as only part of the fuel has melted.

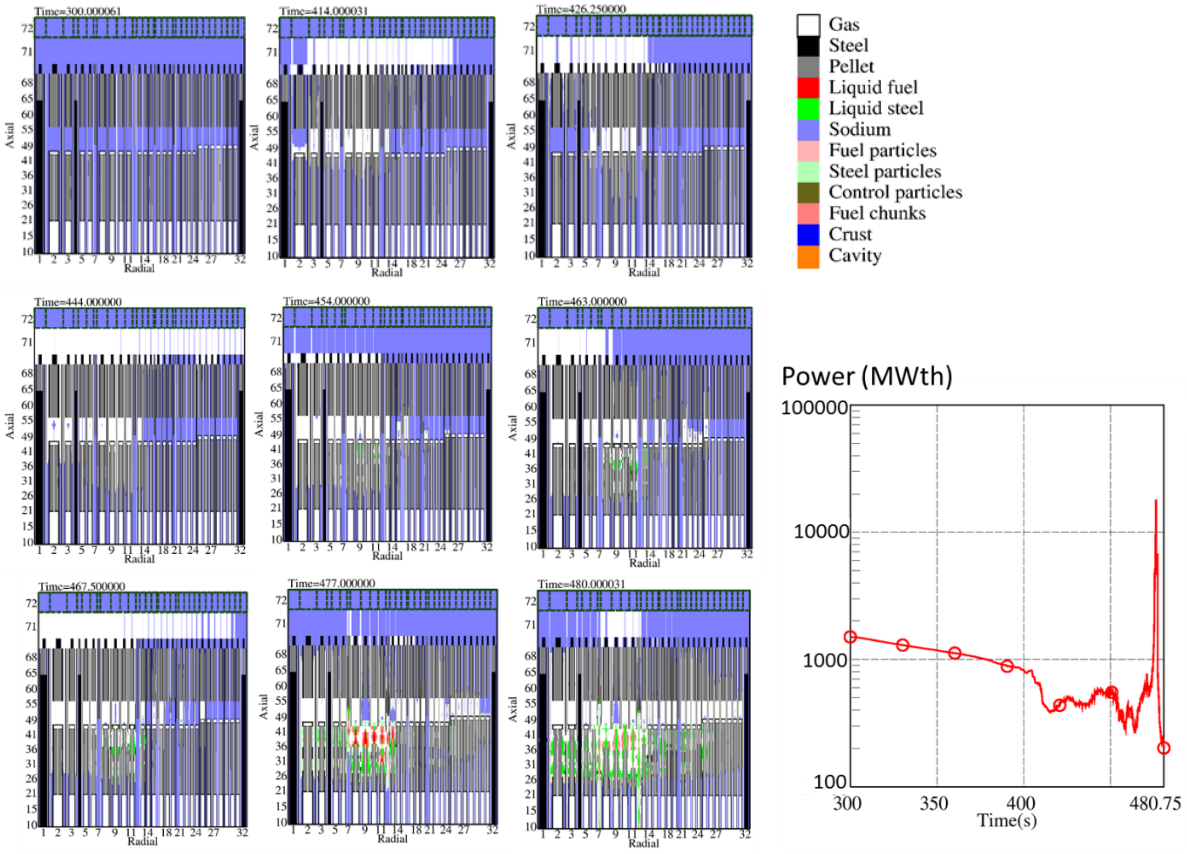


FIG. 6: Scenario of the transient and power variation

5 Conclusions and prospects

The Unprotected Loss Of Flow of the ESNII+ core was modelled with a 22s halving time, which is what was asked for the benchmark. A more severe and also more representative halving time could have been chosen. This would have led to the same scenario of the accident, with a reduced time of occurrence of the events.

The ESNII+ core was modelled at the end of equivalent cycle (EOC). Because of the heterogeneity of the core, a new methodology had to be developed to perform this calculation. The evaluation of the neutronics reactivity effects were not as satisfying as expected at first, but these results could have been improved by additional modifications. Indeed, it must be outlined that this methodology was the most precise to represent the burnup of the core that we could ever try for heterogeneous cores, but the problem was much more intricate than expected and could not be led further. This methodology needs to be developed to calculate the CFV core with precision, but much more effort and time is required. At EDF R&D, we choose to continue in the standard way and will follow our studies by improving our actual results using the SIMMER models in their standard use. To do so, we need:

- to increase the number of energy groups in the neutronics library mesh,
- use the SIMMER code in its standard mode and use the CPA method with one degree of freedom to approximate the absorption macroscopic cross sections in the different areas of the core.

6 Acknowledgements

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