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Cyril Patricot, Roland Lenain, Dominic Caron. Upgrade of apollo3® internal thermohydraulic feedback model with THEDI, and application to a control-rod ejection accident. M&C2019, ANS, Aug 2019, Portland, United States. cea-02623807

**HAL Id: cea-02623807**

**<https://cea.hal.science/cea-02623807>**

Submitted on 26 May 2020

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# UPGRADE OF APOLLO3<sup>®</sup> INTERNAL THERMOHYDRAULIC FEEDBACK MODEL WITH THEDI, AND APPLICATION TO A CONTROL-ROD EJECTION ACCIDENT

Cyril PATRICOT<sup>1</sup>, Roland LENAIN<sup>1</sup>, and Dominic CARON<sup>1</sup>

<sup>1</sup>DEN-Service d'études des réacteurs et de mathématiques appliquées (SERMA)  
CEA, Université de Paris-Saclay, F-91191, Gif-sur-Yvette, France

cyril.patricot@cea.fr, roland.lenain@cea.fr, dominic.caron@cea.fr

## ABSTRACT

In the frame of APOLLO3<sup>®</sup> project (new generation CEA code system for core physics analysis based on deterministic neutron transport), it was decided to develop a new internal thermohydraulic feedback model: THEDI, a multi-1D, two-phase flow solver. This paper is dedicated to the presentation of the integration of THEDI in the APOLLO3<sup>®</sup> code. After a brief presentation of THEDI and of its APOLLO3<sup>®</sup>'s interface, some code-to-code verification cases are presented. First, APOLLO3<sup>®</sup>, using THEDI, is compared to CRONOS2 (a neutronic CEA code of the previous generation with its own feedback model) for steady-state and depletion calculations on a small PWR core. Then, APOLLO3<sup>®</sup> is compared to a CRONOS2 – FLICA4 (a two-phase, four-equation three-dimensional thermohydraulic CEA code) coupling for control-rod ejection accidents, on a similar core. The objective of these comparisons is to verify the coupling between APOLLO3<sup>®</sup> neutronic solvers and THEDI. They are therefore all made with identical models and data, and they all lead to very close results. Thanks to THEDI integration, APOLLO3<sup>®</sup>'s capabilities to model a nuclear reactor core are improved. Thermohydraulic feedbacks can now be taken into account, in both steady-state and transient, for possibly diphasic flows.

KEYWORDS: APOLLO3<sup>®</sup>, THEDI, multi-physic coupling, control-rod ejection, CORPUS<sup>SALOME</sup>

## 1. INTRODUCTION

Data used in neutron transport calculations vary with the temperatures and the densities of media, issued from thermohydraulics. In the same time, thermohydraulics needs the power distribution in the core, which is provided by neutronics. As a consequence, it is mandatory to couple these two physics in order to correctly compute a nuclear reactor.

The strategy followed by CEA to address this issue is twofold. On the one hand, specialized codes are developed, for example APOLLO3<sup>®</sup> [1] (new generation CEA code system for core physics analysis based on deterministic neutron transport) and FLICA4 [2] (a two-phase, four-equation three-dimensional thermohydraulic code), coupled in the multi-physics platform CORPUS<sup>SALOME</sup> [3] ("external" coupling). On the other hand, and complementarily with the previous approach, neutronic codes dedicated to core calculations often have their own simplified thermohydraulic model ("internal" coupling). It simplifies routine nuclear reactor calculations which do not always need a very accurate thermohydraulic model. In

that respect, CRONOS2 [4], the production CEA deterministic neutron transport code, dedicated to PWR core analysis, uses THERMOC, a three-equations multi-1D model.

In the frame of APOLLO3<sup>®</sup> project, it was decided to develop a new thermohydraulic model for internal coupling: THEDI (*THErmohydraulique DIphasique*) [5]. THEDI is a multi-1D, two-phase flow solver. It improves the modeling, compared to THERMOC, thanks to a four-equation model (instead of three), and to some new system modeling capabilities. Moreover, THEDI is written in C++ (instead of FORTRAN) with the objective to improve code flexibility, maintainability and performance. It was also conceived as an independent tool in order to allow future sharing with other neutronic codes (like the Monte Carlo code TRIPOLI-4<sup>®</sup> [6]). It is linked as an external library by client codes.

The integration of THEDI in APOLLO3<sup>®</sup>, its coupling with neutron transport solvers and the new abilities provided to APOLLO3<sup>®</sup> by this work are presented in this paper. Some verification cases are also presented: comparisons with CRONOS2, using THERMOC or coupled with FLICA4 within the multi-physics platform CORPUS<sup>SALOME</sup>, for control-rod ejection accidents on a small PWR core.

## 2. THEDI MODELING

THEDI is presented in a dedicated paper [5]. Some elements are recalled here.

The main thermohydraulic model is one-dimensional and treats a four-equation system composed of total mass conservation, vapor mass conservation, total motion equation and total internal energy conservation. The core is therefore divided into separated 1D channels sharing consistent boundary conditions: this is the “multi-1D approach”, already used by THERMOC. Each mesh of each thermohydraulic channel can contain several solid objects, such as fuel rods. THEDI computes the temperature distribution in each of them, by solving one-dimensional heat transfer diffusion equation. THEDI is also able to compute the power evolution during a transient by solving the neutronic point kinetic equations.

THEDI is, at the moment, able to model light water and sodium-cooled reactors in normal and accidental (with possible two phase flow) conditions.

## 3. INTEGRATION OF THEDI IN APOLLO3<sup>®</sup>

APOLLO3<sup>®</sup> is a multipurpose neutronic code which permits to carry out lattice calculations (self-shielding and flux calculations used to produce multi-parametrized cross-section libraries) up to full core calculations (from multi-parametrized cross-section libraries) with several solvers using different angular approximation (Sn, PN, SPN and diffusion).

APOLLO3<sup>®</sup> has integrated THEDI as its internal thermohydraulic module since September 2018. An interface to THEDI has been developed in APOLLO3<sup>®</sup>, based on APOLLO3<sup>®</sup> data model, to initialize THEDI module (definition of a coherent geometry between neutronics and thermohydraulics) and to manage coupled calculations (it transfers power to thermohydraulics and temperatures and densities to neutronics). The interface proposed allows specifying a 2D-1D thermohydraulic grid, in which each column is a hydraulic channel. This grid forms a 3D unstructured mesh where each region can receive specific hydraulic properties. Each mesh of the hydraulic grid can receive solid objects. The assignment of solid objects within each hydraulic region can be done with a spatial distribution over the mesh allowing modeling every fuel rod distinctly in the core. This forms an unstructured solid object grid.

The inputs for THEDI’s interface are 3D power distributions for each grid: hydraulic and solid object ones. THEDI outputs are given on the different grids. All the quantities exchanged are based on APOLLO3<sup>®</sup> data model, allowing easy use in APOLLO3<sup>®</sup> framework. Consequently, the final user does

not need to know THEDI's data model to run coupled calculation as the interface is in charge of format conversion between APOLLO3<sup>®</sup> data model and THEDI's. Moreover, coupling calculation can be carried out with every neutronic solver of APOLLO3<sup>®</sup> without any additional effort.

#### 4. COMPARISON WITH CRONOS2

In order to verify the integration of THEDI in APOLLO3<sup>®</sup>, a comparison has been made with CRONOS2.

CRONOS2 is the CEA neutron transport code, dedicated to core scale PWR applications, of the previous code generation. CRONOS2 is particularly relevant for this code-to-code benchmark because its neutron diffusion solver (MINOS) has been ported in APOLLO3<sup>®</sup>. Neutronics results should therefore be in very good agreements (as long as diffusion solver is used in APOLLO3<sup>®</sup>).

CRONOS2 has its own thermohydraulic module, THERMOC. Like THEDI, THERMOC is multi-1D. However, THERMOC's thermohydraulic model is three-equation instead of four (no vapor mass conservation equation). Correlations can be used in order to compute the gas volume fraction. Vapor and liquid have the same velocity. Only steady-state THERMOC calculations are presented in this paper.

##### 4.1. Benchmark Definition

A small PWR core, with 32 assemblies (Fig. 3 shows a sketch of the core), is considered for this benchmark. Each assembly has a reduced height, but is otherwise representative of a standard PWR. This core is not functional and is only used for numerical benchmarks. The comparison is made first for a beginning of life steady-state calculation, and then for a simple depletion calculation.

Neutron transport computations are made, by the two neutronic codes, in diffusion with 4 energy groups, on homogenous rod-cell mesh. Cross-sections were generated by APOLLO2 [7] with Method Of Characteristic calculations [8] and 281 energy groups [9]. No control-rods are considered here.

Thermohydraulic computations are made with one channel per assembly. Fuel temperatures are calculated on a mean fuel rod per assembly for the code-to-code comparisons. APOLLO3<sup>®</sup> results with the calculation of all fuel rods are also included for physical analysis. Exchanged data are, here, always pin averaged. Rowland formula [10] is used to compute the fuel effective temperature, used by neutronic solvers, from the radial temperature distribution calculated in fuel pellets by THERMOC or THEDI.

The axial mesh is shared by all physics, and is made of meshes of about 3 cm.

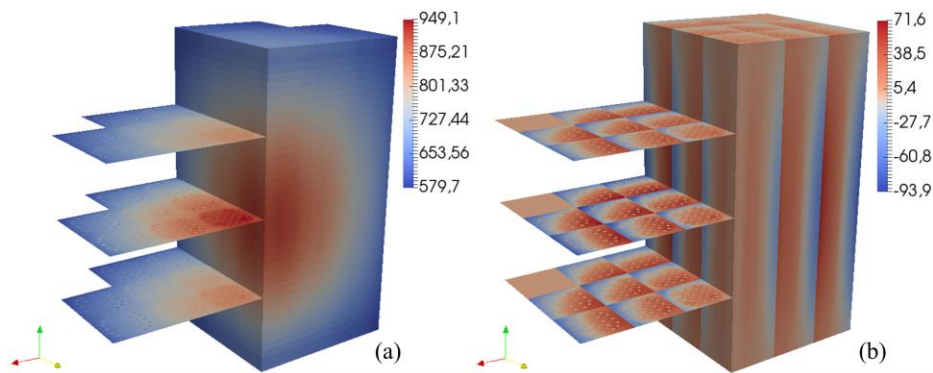
##### 4.2. Beginning of Life Steady-State

Without feedback, APOLLO3<sup>®</sup> and CRONOS2 both give a reactivity of 14718 pcm and a 3D power peaking factor of 2.945. Results with feedback are given in the Table I and show a good agreement between codes. The effect on reactivity of the calculation of every fuel rod is small here, about 17 pcm.

**Table I. Reactivity and pressure loss from APOLLO3<sup>®</sup> and CRONOS2 in steady-state.**

	Reactivity (pcm)	Peaking factor	Pressure loss (Pa)
APOLLO3 <sup>®</sup> , with mean fuel rods	14916	2.832	17603
CRONOS2, with mean fuel rods	14916	2.832	17626
APOLLO3 <sup>®</sup> , with all fuel rods	14899	2.828	17603

Fig.1.a shows the fuel effective temperature from APOLLO3<sup>®</sup> calculation with every fuel rods, and Fig.1.b shows the map of the difference of fuel effective temperature between calculations with one mean fuel rod per assembly and with every fuel rods in the core. In Fig.1.b, the effect visible in each assembly is directly linked to the gradient of power. This effect is found to be quite important here, up to 100 K, although the impact on the reactivity, visible in Table I, is small. This new capability of APOLLO3<sup>®</sup> improves its ability to compute local phenomena.

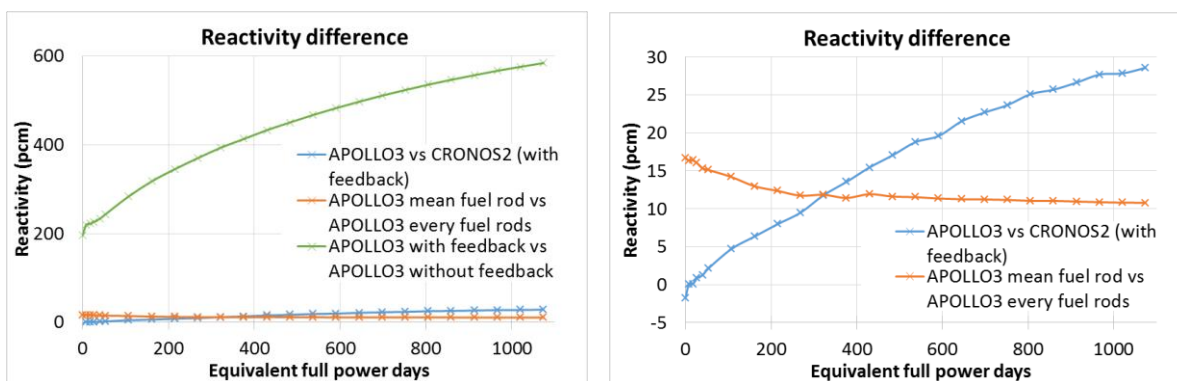


**Figure 1. (a) Fuel effective temperature (K). (b) Fuel effective temperature difference (K) between one mean fuel rod per assembly and the calculation of every fuel rods.**

### 4.3. Depletion

A very simple depletion calculation is done here: macroscopic cross-sections (generated by APOLLO2) are parametrized with respect to the local burnup. At the core scale, the burnup is computed at each time step and is used to update the cross-sections. The process is repeated until a criterion is reached (here, a given mean burnup). No depletion chain is thus needed at the core level. When a thermohydraulic feedback is used, a coupled computation is made at each time-step, instead of a simple neutronic one.

During the depletion, the multiplication factor varies from 1.17 to 0.92 (that is to say, a variation of about 25,000 pcm). An initial reactivity drop of about 2,500 pcm is foreseen, corresponding to absorbing fission product (<sup>135</sup>Xe) production. The differences in reactivity of different calculations are given in Fig. 2 (the first two curves are repeated with an adapted scale on the right). The effect of the thermohydraulic feedback varies from 200 pcm to 600 pcm here. The agreement between APOLLO3<sup>®</sup> and CRONOS2 with thermohydraulic feedback is very good: the difference in reactivity is always less than 30 pcm. The reactivity effect of the calculation of every fuel rod is pretty constant during the depletion.



**Figure 2. Reactivity differences between the different depletion calculations.**

## 5. COMPARISON WITH CORPUS<sup>SALOME</sup>

APOLLO3<sup>®</sup> can model multi-physic transients by coupling THEDI with kinetic neutron transport solvers. In order to verify this new APOLLO3<sup>®</sup>'s capability, a comparison has been made with CORPUS<sup>SALOME</sup>, for control-rod ejection accidents on a small PWR core.

CORPUS<sup>SALOME</sup> is a coupling platform developed by CEA for reactor physics analysis. It is based on Salome, an open source platform which provides, among others, generic tools for code coupling.

The main CEA codes for core physics analysis can be coupled within CORPUS<sup>SALOME</sup>:

- Core neutronics can be computed by either CRONOS2 or APOLLO3<sup>®</sup>,
- Core thermohydraulics can be computed by FLICA4,
- Reactor system computations can be done by either CATHARE2 [11] or CATHARE3 [12],
- Fuel physics simulations can be performed by ALCYONE2 [13].

CORPUS<sup>SALOME</sup> was first made for PWR applications, but fast reactor capabilities are under-development.

In the following, CORPUS<sup>SALOME</sup> is used to couple CRONOS2 and FLICA4. As already mentioned, CRONOS2 is chosen because its diffusion solver is identical to APOLLO3<sup>®</sup>'s one. The time-schemes used for kinetics calculations are, here, nevertheless slightly different. Similarly, the set of equations solved by THEDI and FLICA4 are the same (but the solver implementations are different). They should thus provide a similar answer to the same problem. FLICA4 was already used to verify THEDI in [5].

### 5.1. Benchmark Definition

For this benchmark, a core similar to the one used in section 4 is considered. The core geometry is the same, but the detailed compositions are different. The following calculations are always made with a core at beginning of life.

In order to have quick calculations, we use a coarser discretization, identical in both APOLLO3<sup>®</sup> and CORPUS<sup>SALOME</sup>. Neutronics is computed with diffusion and 2 energy groups, on a homogenous assembly mesh. Cross-sections were generated by APOLLO2 using the process presented in the previous section. Thermohydraulic computations are made with one channel per assembly. Fuel temperatures are calculated on one mean fuel rod per assembly. The axial mesh is common and fixed, and meshes are about 3cm.

The mass flow in each assembly is imposed (the same for all assemblies), and does not vary during the accidents. The core pressure drop is therefore not precisely defined.

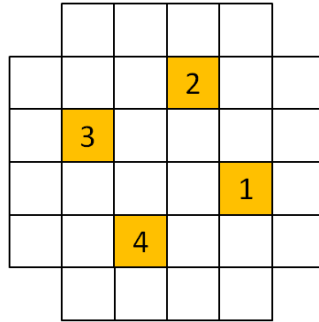
For the code-to-code benchmark, FLICA4 model used in CORPUS<sup>SALOME</sup> calculations uses "closed" channels in order to reproduce the multi-1D modelling of THEDI. However, CORPUS<sup>SALOME</sup> results with open channels in FLICA4 are also included for physical analysis. It is important to note that a 3D thermohydraulic best estimate calculation would not only use open channels, but also refined radial mesh.

Two control-rod ejection accidents are considered:

1. The core is initially at a full power steady-state (100 MW), with the control-rod 1 fully inserted (see Fig. 3). This control-rod is then ejected in 0.1 s. Sub-cooled vapor production correlations are not used, the transient is strictly monophasic.

2. The core is initially at a full power steady-state (100 MW), with the four control-rods fully inserted (see Fig. 3). The control-rod number 1 is then ejected in 0.1 s. Two-phase flows with high void fractions are observed during this transient.

In both cases, the initial reactivity is made equal to 0 by dividing fission cross-sections by the multiplication factor of the initial steady-state.



**Figure 3. Control-rod position.**

Both transients are computed with  $10^{-4}$  s time-steps for both neutronics and thermohydraulics. An explicit time-scheme is used for coupled variables.

## 5.2. Ejection Scenario 1

### 5.2.1. Steady-state

The main results on the initial steady-state are given in Table II. APOLLO3<sup>®</sup> and CORPUS are in perfect agreement. The ejected control-rod weight is about 1 \$ here. The opening of channels in CORPUS has no impact (the forced convection is dominant at the assembly scale here).

**Table II. Main results on the initial steady-state of the 1<sup>st</sup> ejection.**

	Reactivity (pcm)	Peak power	Ejected control-rod weight (pcm)
APOLLO3 <sup>®</sup>	17091	2.733	800 (0.99 \$)
CORPUS	17092	2.733	800 (0.99 \$)
CORPUS with open channels	17092	2.733	800 (0.99 \$)

The initial power map (from either APOLLO3<sup>®</sup> or CORPUS) is given in Fig. 4. On the left, a 2D slice of the middle of the core is shown, and, on the right, the axial power distribution in the hot fuel assembly is given. The control-rod position is indicated with a yellow square. The impact of the control-rod on the power distribution is clearly visible.

### 5.2.2. Transient

The global power and max fuel effective temperature evolutions are given in Fig. 5, and the main results are repeated in Table III. A very good agreement is found between APOLLO3<sup>®</sup> and CORPUS<sup>SALOME</sup>. The opening of channels in CORPUS has no impact on this transient. We recall that there is no sub-cooled vapor production here, this transient is strictly monophasic.

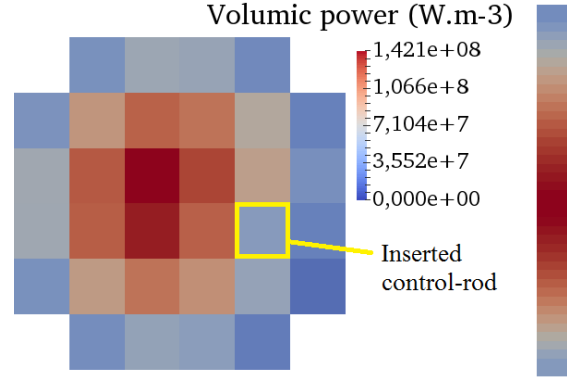


Figure 4. Initial power map of the 1<sup>st</sup> ejection.

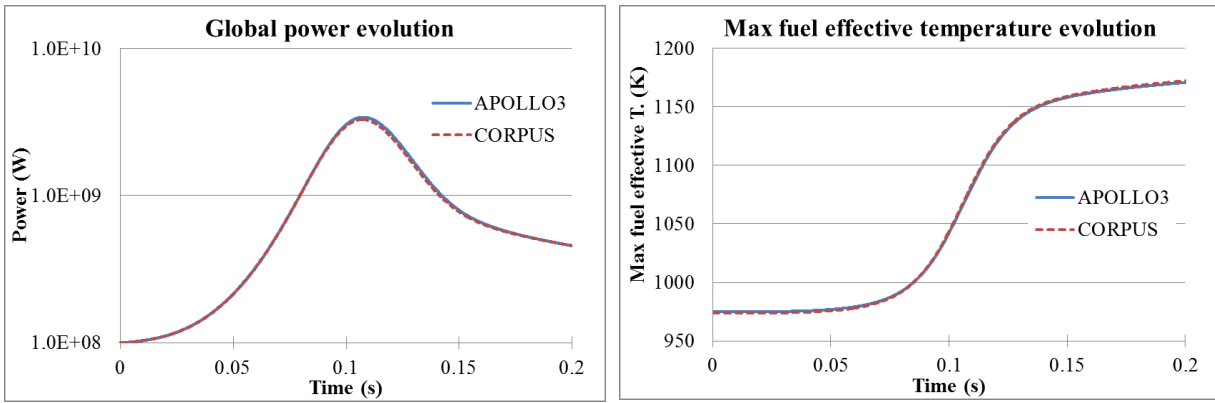


Figure 5. Total power (left) and max fuel effective temperature (right) evolutions during 1<sup>st</sup> ejection.

Table III. Main results of the 1<sup>st</sup> ejection.

	Max power (W)	Max fuel effective temperature (K)
APOLLO3	$3.41 \cdot 10^9$	1171
CORPUS	$3.28 \cdot 10^9$	1172
CORPUS with open channels	$3.28 \cdot 10^9$	1172

In order to analyze the local difference during the transient, the maximum and average differences between the power maps renormalized to the same value at each time step are given in Fig. 6. These quantities are given as a ratio to the average power. They are defined in equations (1) to (3), with  $P_i$  being the power density of mesh  $i$  for each time step, and  $V_i$  the volume of mesh  $i$ .

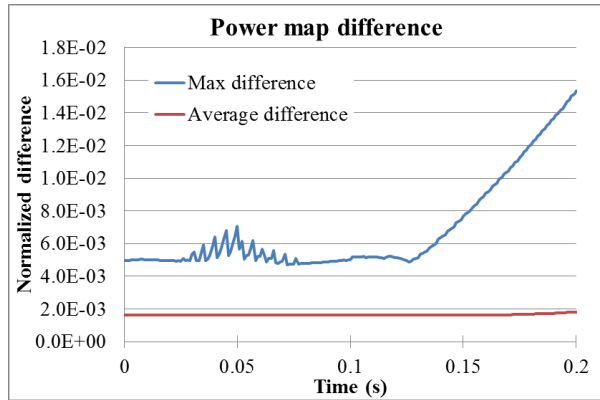
$$P_{average} = \frac{\sum_i P_i V_i}{\sum_i V_i}, \quad (1)$$

$$Max\ difference = \max_i \left| P_i^{CORPUS} \frac{P_{average}^{APOLLO3}}{P_{average}^{CORPUS}} - P_i^{APOLLO3} \right| / P_{average}^{APOLLO3} \quad (2)$$

$$Average\ difference = \frac{1}{\sum_i V_i} \sum_i V_i \left| P_i^{CORPUS} \frac{P_{average}^{APOLLO3}}{P_{average}^{CORPUS}} - P_i^{APOLLO3} \right| / P_{average}^{APOLLO3} \quad (3)$$

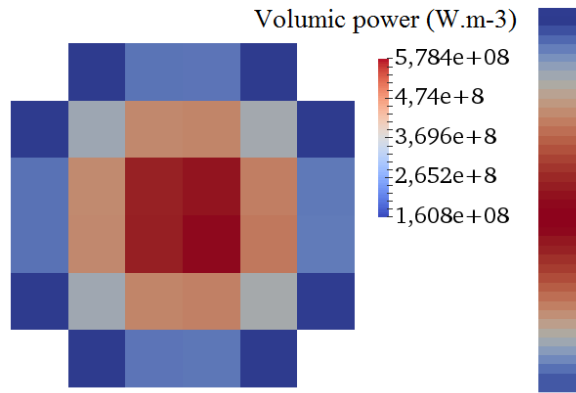


It can be seen that local differences are always small during the transient, and stay below 1.5%. This shows the good agreement between APOLLO3<sup>®</sup> and CORPUS<sup>SALOME</sup> on local power. The shape of the max difference curve may be due to differences in the time-integration techniques of the neutron diffusion solvers (in particular for precursor concentrations from 0.13 s).



**Figure 6. Power map max and average differences during 1<sup>st</sup> ejection**

The final power map (from either APOLLO3<sup>®</sup> or CORPUS) is given in Fig. 7 (slice in the middle of the core on the left and the axial distribution in the assembly with the power peak on the right). It is interesting to note that the final power map is not perfectly symmetric. The power is maximized nearby the initial position of the control-rod: the core was initially cooler there, leading to a more reactive zone. A longer calculation would obviously lead a symmetric final state.



**Figure 7. Final power map of 1<sup>st</sup> ejection.**

### 5.3. Ejection Scenario 2

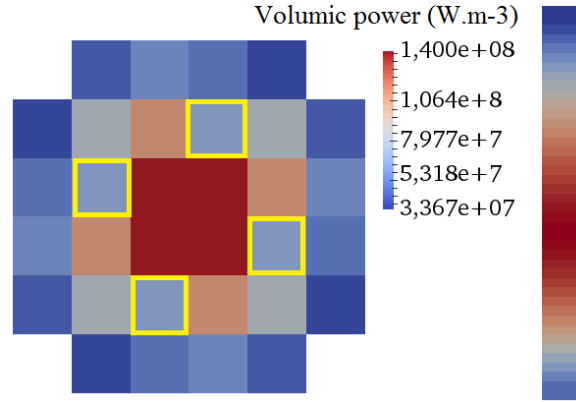
#### 5.3.1. Steady-state

The main results on the initial steady-state are given in Table IV. Here again, APOLLO3<sup>®</sup> and CORPUS are in perfect agreement, and the opening of channels has no impact. The ejected control-rod weight is very strong here, about 2 \$. The reader has to keep in mind that this reactivity is not injected instantaneously: the control-rod is ejected in 0.1 s (as in the 1<sup>st</sup> ejection).

The initial power map (from either APOLLO3<sup>®</sup> or CORPUS) is given in Fig. 8, and is perfectly symmetric. Yellow squares indicate the control-rod positions.

**Table IV. Main results on the initial steady-state of the 2<sup>nd</sup> ejection.**

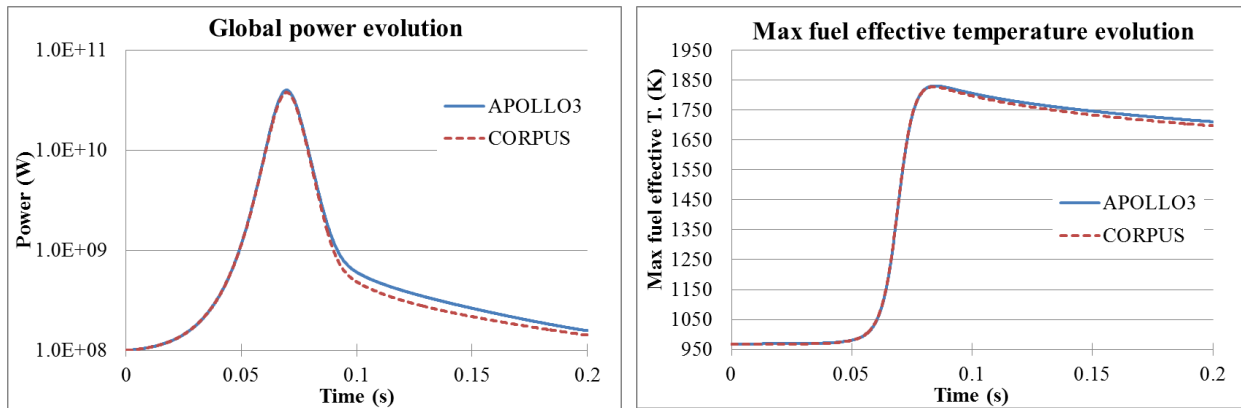
	Reactivity (pcm)	Peak power	Ejected control-rod weight (pcm)
APOLLO3	13457	2.694	1648 (2.05 \$)
CORPUS	13457	2.694	1648 (2.05 \$)
CORPUS with open channels	13457	2.694	1648 (2.05 \$)



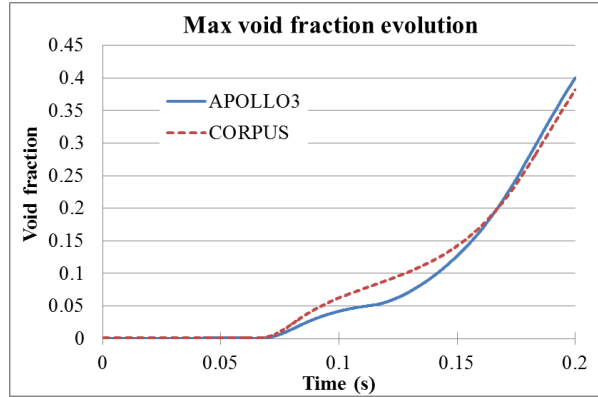
**Figure 8. Initial power map of the 2<sup>nd</sup> ejection.**

### 5.3.2. Transient

The global power, max fuel effective temperature and max void fraction evolutions are given in Fig. 9 and 10, and the main results are repeated in Table V. A good agreement is found between APOLLO3<sup>®</sup> and CORPUS<sup>SALOME</sup>. Some little differences can be suspected in the treatment of diphasic flow between FLICA4 and THEDI. The opening of channels in CORPUS has a small impact on the results here.



**Figure 9. Total power (left) and max fuel effective temperature (right) evolutions during 2<sup>nd</sup> ejection.**

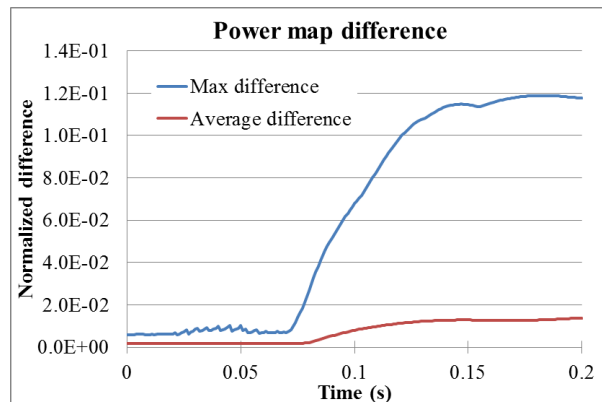


**Figure 10. Max void fraction evolutions during 2<sup>nd</sup> ejection.**

**Table V. Main results of the 2<sup>nd</sup> ejection.**

	Max power (W)	Max fuel effective temperature (K)	Max void fraction
APOLLO3	$3.98 \cdot 10^{10}$	1830	0.40
CORPUS	$3.78 \cdot 10^{10}$	1827	0.38
CORPUS with open channels	$3.75 \cdot 10^{10}$	1816	0.44

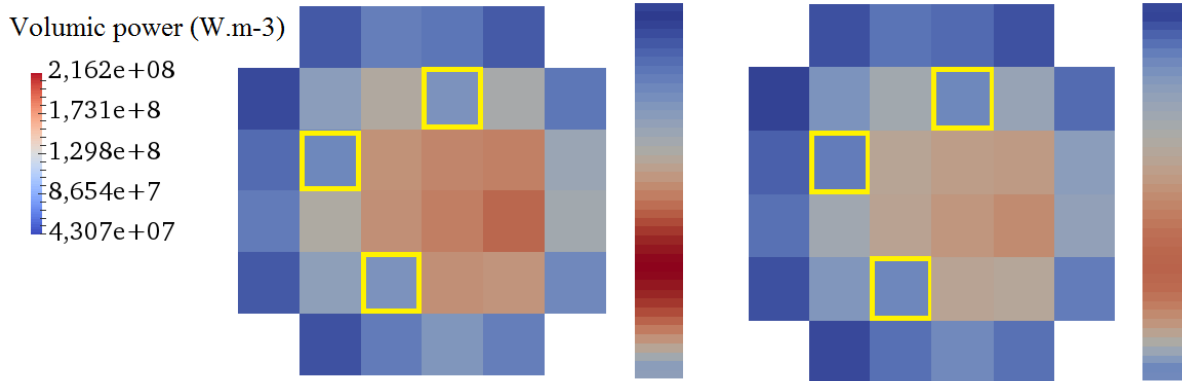
The maximum and average differences between the normalized power maps are given in Fig. 11 (these quantities are defined in equations (1) to (3)). The differences are higher than in the first ejection, but are still small: the average power difference reach a maximum of about 1.5%, while the maximum difference goes up to 12% at the end of the transient. These differences are probably due to thermohydraulic effects.



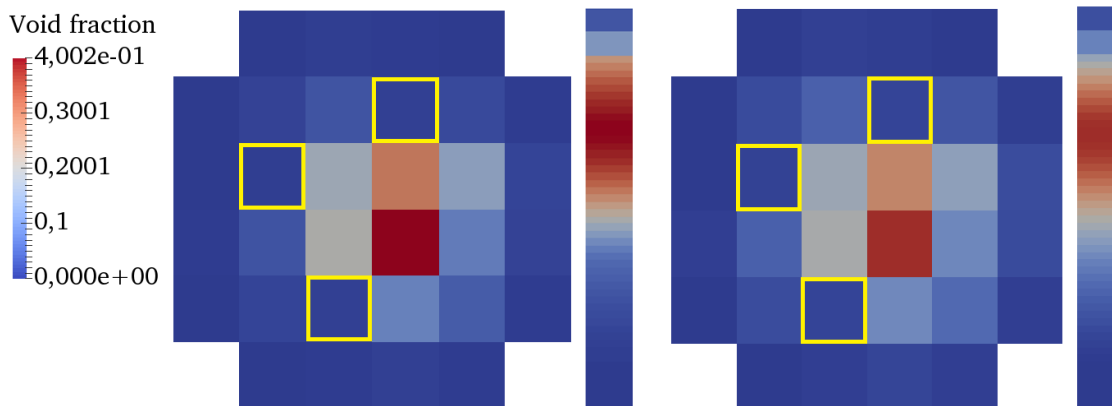
**Figure 11. Power map max and average differences during 2<sup>nd</sup> ejection.**

Final power and void fraction maps (from APOLLO3<sup>®</sup> on the left of figures and CORPUS on the right) are given in Fig. 12 and 13. Yellow squares indicate the control-rod positions. The power maps are given on a slice in the middle of the core, together with the axial distribution in the assembly with the maximum power. The void fraction maps are given on a slice at the height of the maximum void fraction, together with the axial distribution in the assembly with the maximum void fraction.

The shapes of these maps are in good agreement, although the differences in the power distribution are maximize at this time (end of transient) according to Fig. 11. The small difference in total power and maximum void fraction, visible in Fig. 9 and 10 is visible in the color shift of these maps. The final power map is here clearly shifted to the bottom of the core. This is due to the heating of the upper part of the core, and is thus a good example of the impact of thermohydraulic convection on neutronics.



**Figure 12. Final power maps of the 2<sup>nd</sup> ejection (left: APOLLO3<sup>®</sup>, right: CORPUS)**



**Figure 13. Final void fraction maps of the 2<sup>nd</sup> ejection (left: APOLLO3<sup>®</sup>, right: CORPUS)**

## 6. CONCLUSIONS

This paper presents the integration of THEDI in APOLLO3<sup>®</sup>. THEDI is a thermohydraulic solver developed to enhance the internal thermohydraulic models of CEA neutronic codes. A more detailed presentation of THEDI can be found in [5].

This integration is verified by a comparison with CRONOS2 in steady-state and CORPUS<sup>SALOME</sup> (used to couple CRONOS2 and FLICA4) in transient.

CRONOS2 is a CEA neutron transport code of the previous generation. It also has an internal thermohydraulic module, THERMOC. The comparison is made for coupled neutronic and thermohydraulic steady-state and depletion calculations, on a small PWR core. Models and data are the same (in particular, only monophasic flows are considered), leading to very close results.

CORPUS<sup>SALOME</sup> is a CEA coupling platform dedicated to reactor physics analysis. Main CEA codes for reactor physics can be coupled within CORPUS<sup>SALOME</sup>. A coupling between CRONOS2 and FLICA4 (a two-phase, four-equation thermohydraulic code) is used in this case. Two rod-ejection accidents are considered. Coupled neutronic and thermohydraulic kinetic calculations are compared. Here again, models and data are the same, and results found by APOLLO3<sup>®</sup> and CORPUS<sup>SALOME</sup> are very similar. This time, strongly diphasic flows are studied.

Thanks to THEDI integration, APOLLO3<sup>®</sup>'s capabilities to model nuclear reactor cores are improved. Thermohydraulic feedbacks can now be taken into account, in both steady-state and transient, for possibly diphasic flows and with local fuel rod temperature calculation. However, THEDI is a simplified tool, and should be substituted by specialized thermohydraulic codes when a multi-1D four-equation model is not adequate.

## ACKNOWLEDGMENT

The authors wish to thank Framatome & EDF for financial support on APOLLO3<sup>®</sup>.

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