# 3-D MODELLING OF A SUPERPHÉNIX BENCHMARK WITH SERPENT AND PARCS FOR COUPLED SIMULATION WITH PARCS/ATHLET

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## ABSTRACT

Most of the safety criteria for Sodium cooled Fast Reactors (SFR) are local core parameters. Thus, application of 3-D neutron kinetic and thermal-hydraulic coupled codes including detailed modelling of core expansion effects is mandatory for best estimate evaluations of safety margins. A recently published benchmark related to Superphénix offers the opportunity to validate codes and methods for SFR safety assessment. This requires the generation of few-group cross-sections. Since whole core Serpent Monte Carlo models for production of such cross-section libraries would be computationally costly (and the standard 2-D approach may introduce unnecessary large approximations), 3-D models of each sub-assembly type in infinite radial lattice configurations have been created with Serpent. To simplify the handling of temperature dependent geometric changes, a pre-processor for generation of temperature driven expansion of geometry and material densities has been developed and implemented in the GRS core simulator KMACS. These cross-sections are then used to evaluate effective multiplication factors and 3-D distributions of power density using PARCS for different core configurations. The results are compared with the reference calculation and with experimental data provided with the benchmark. In the next step, a simple ATHLET parallel channel open core model has been developed for coupled PARCS/ATHLET first transient test calculations. This paper describes in detail the models and techniques used for the generation of the few-group parameterized cross section libraries, the PARCS model and the ATHLET open core model and first transient test calculations.

KEYWORDS: Thermal expansion, Cross-section generation, SERPENT, PARCS, ATHLET, SFR

## 1. INTRODUCTION

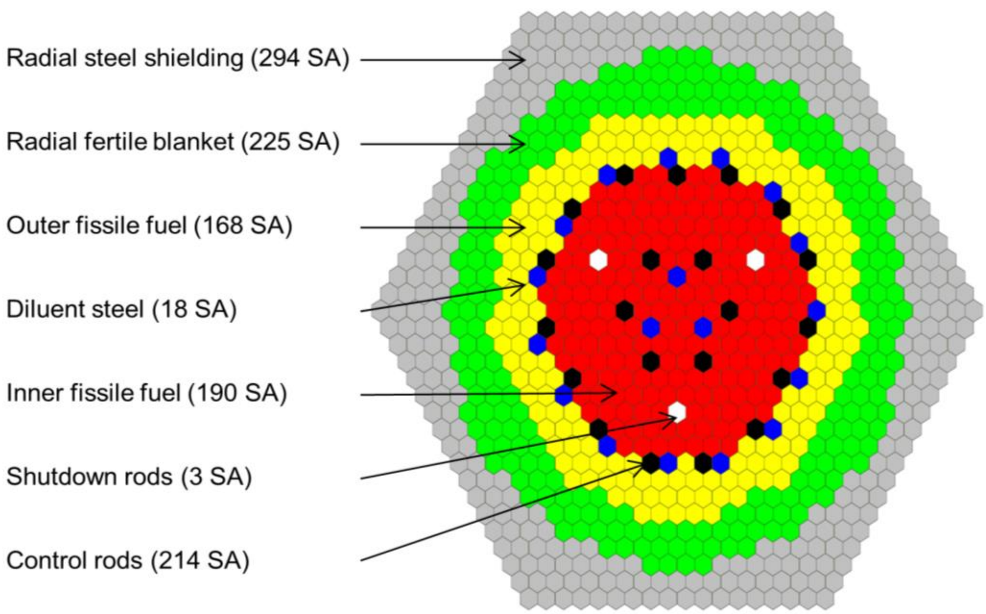
Superphénix (SPX) is a 2990 MW Sodium cooled Fast Reactor which was operated between 1985 and 1997 in Creys-Malville (France) [1, 2]. During that time, data on the physical properties of the core such as reaction rate distributions and feedback coefficients were measured and can be used in order to validate methods and codes for SFR simulations. In the framework of the ongoing ESFR-SMART EU project [3], a benchmark based on the Superphénix reactor core was recently proposed [4] to take advantage of these experimental results.

Since most of the safety criteria for SFR are local core parameters, application of 3-D neutron kinetic and thermal-hydraulic coupled codes including detailed modelling of core expansion effects is mandatory for best estimate evaluations of safety margins. This requires the generation of few-group cross sections for the individual subassemblies' (SA) axial zones which also depend on temperature dependent changes of material densities and geometry (pin and subassembly pitch, inter-assembly gap, axial cladding and fuel expansion, radial grid plate expansion). This is accounted for by appropriate neutron kinetics model extensions in PARCS for the 3-D simulation of axial and radial thermal expansion effects in connection with an appropriate parametrization of the few-group cross section libraries [5, 6].

This paper describes the solution of this benchmark using the deterministic 3-D neutron kinetics code PARCS [7]. In the first part of this paper, the reference SERPENT benchmark model is presented. The methodology used to produce assembly homogenized few-group cross-section libraries for PARCS using SERPENT [8] driven by the KMACS [9] core simulator is described. In the third part of the paper, assessment of the cross-sections is done by comparing PARCS results with measurements and reference SERPENT predictions. Finally, an open core ATHLET model of SPX for coupled PARCS/ATHLET calculations is described and tested for a simple coolant temperature transient in SPX accounting for explicit radial core expansion.

## 2. THE SERPENT BENCHMARK MODEL

The SPX benchmark core is arranged in a hexagonal lattice with a nominal pitch of 17.9 cm (Figure 1 left). Every SA is modelled in detail, meaning that heterogeneous axial and radial structures of every SA, besides diluent and shielding, are explicitly modelled. The reader can have an overview on the level of details on the example of the axial section of the model of a fissile fuel SA shown in Figure 1 (right). All dimensions and material compositions are presented in the benchmark specification [4].



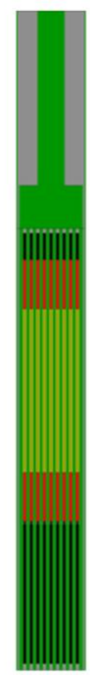



**Figure 1. Top view of the SERPENT benchmark model of SPX (left) and side view of a fuel SA (right)**

## 3. FEW-GROUP CROSS-SECTION GENERATION FOR DETERMINISTIC CALCULATION

### 3.1. Full scale 3-D subassembly models

The first step in a deterministic calculation is to generate parameterized assembly homogenized few-group macroscopic cross-section libraries. This task is usually done with deterministic (2-D) lattice codes, but in the past few years SERPENT has shown its ability to generate accurate few-group homogenized cross-section without approximations, neither on the geometry nor in the nuclear data [10]. To this aim, full scale 3-D subassembly models are developed for the generation of cross-sections for every sub-assembly (SA) axial section. The advantage of such 3-D models is to take into consideration the influence of neighbouring axial regions for the calculation of the neutron flux and so for the homogenization process over a certain axial zone. Different subassembly models are used:

- For fuel (fissile and fertile), a single fuel SA is considered with reflective boundary conditions (Figure 2 left).
- For non-fuel SAs (e.g. diluent), small scale supercell models consisting of the respective non-fuel SA surrounded by six half fuel SAs with reflective boundary conditions (Figure 2 right).

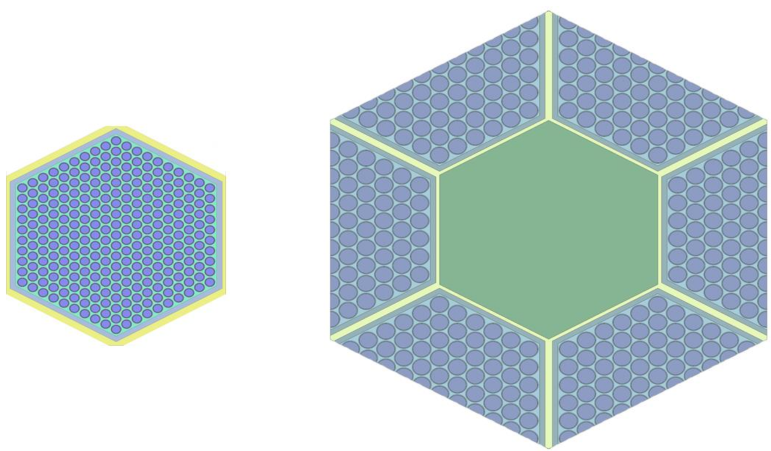


**Figure 2. Mid-plane cut of the 3-D mini model for a fuel SA (left) and for non-fuel SA (right)**

**Table I. : 12-group energy structure.**

| Group number | Upper energy limit (MeV) | Group number | Upper energy limit (MeV) |
|---|---|---|---|
| 1 | 2.00E+01 | 7 | 4.09E-02 |
| 2 | 6.07E+00 | 8 | 1.50E-02 |
| 3 | 2.23E+00 | 9 | 5.53E-03 |
| 4 | 8.21E-01 | 10 | 2.03E-03 |
| 5 | 3.02E-01 | 11 | 7.49E-04 |
| 6 | 1.11E-01 | 12 | 1.49E-04 |

To achieve acceptable statistical uncertainties in cross-section generation, SERPENT calculations were performed with 4000 cycles of $2 \cdot 10^5$ neutron histories each; the first 100 batches were discarded. The cross-sections have been generated using the 12 energy groups structure shown in Table I as used in [7] and are based on the JEFF3.1.1 continuous energy library.

### 3.2. Super homogenization (SPH) method

The previously described methodology could be also applied to the control rods and diluent SA. However, the diffusion approximation is questionable for such cases. To correct potential related errors, the SPH method can be envisaged. The aim of this method is to conserve the reaction rates of a reference heterogeneous solution in a diffusion calculation [11]. The method and its iterative process is described in [12]. The same algorithm was implemented at GRS in order to calculate the SPH corrected cross-sections with DYN3D [13]. Significant improvement has been observed with PARCS for power distribution and effective multiplication factor predictions as shown in Table II.

**Table II. : PARCS results without and with SPH corrected cross sections.**

| $k_{eff}$ SERPENT | Relative multiplication factor difference ($1-k_{PARCS}/k_{SERPENT}$, pcm) | | |
|---|---|---|---|
| | No SPH correction | SPH for control rods SA | SPH for control rods and diluent SA |
| 0.99791 | 382 | 260 | 130 |

### 3.3. Parameterization of the few-group cross-section library

In SFR, major negative feedback effects are due to thermal expansion of the materials. In order to correctly predict this effect, core structures dimensional changes must be considered according to their thermal expansion correlations. Furthermore, to ensure mass conservation, the corresponding material densities are modified accordingly. In order to simplify the handling of temperature dependent geometric and material density changes in the SERPENT model, a pre-processor for generation of temperature driven expansion of geometry and material densities has been developed and implemented in the GRS core simulator KMACS [9] (Kernsimulator Modular Adaptable Core Simulator). The SERPENT inputs generated by KMACS allow for the generation of parameterized few-group homogenized cross-section libraries with SERPENT for SPX. The library is functionalized with respect to fuel temperature, cladding temperature, sodium density and subassembly pitch in order to account for radial diagrid expansion and corresponding increase of the inter-assembly gap using the radial core expansion model implemented in PARCS. The support points for each parameter, used for the transient presented in section 5, are shown in Table III. For every specific combination of those parameters a set of cross-sections homogenized over each subassembly axial region was generated.

**Table III. : The parametrization of the few-group homogenized cross-section library.**

| Parameter | Value |
|---|---|
| fuel temperature (K) | 300, 600, 900, 1200 |
| sodium density (kg/m3) | 941, 874, 805 |
| cladding temperature (K) | 600 |
| diagrid pitch (cm) | 17.90, 17.98, 18.05 |

## 4. PARCS SOLUTION OF THE STATIC-NEUTRONIC PART OF THE BENCHMARK

### 4.1. The PARCS benchmark model and results for different core states

The deterministic code selected for the SPX benchmark model is the US-NRC code PARCS which has been recently extended by explicit models for axial and radial core expansion effects [5,6]. The SPX core configuration is modelled as full core in PARCS according to Figure 1.

Different core configurations represented by different material temperatures and by the positions of the CSD control rods (0 cm means that CSD are completely withdrawn and 100 cm completely inserted) as specified in the benchmark have been considered to investigate thermal expansion effect on the reactivity. For every case, a set of cross-sections at a given temperature homogenized over each SA region was generated.

Table IV presents the multiplication factors for every case calculated by PARCS and provides the reactivity difference with respect to the corresponding benchmark reference. For the cases with CSD withdrawn, the maximum discrepancy is less than 120 pcm; for cases with inserted CSD, the discrepancies are up to 509 pcm. However, the deviations between PARCS and the SERPENT reference results remain smaller than discrepancies arising from nuclear data libraries that can be up to 600 pcm while comparing results obtain with JEFF3.1.1 and ENDFB7.0.

**Table IV. : Effective multiplication factor for different core configuration.**

| Case ID | CSD insertion (cm) | Temperature for XS/geometry [K] | | | C | |
|---|---|---|---|---|---|---|
| | | Fissile | Fertile | Other | k-eff PARCS | 1-PARCS/Benchmark (pcm) |
| 1 | 0 | 453/453 | 453/453 | 453/453 | 1.03647 | -22 |
| 2 | 0 | 673/673 | 673/673 | 673/673 | 1.02851 | -33 |
| 3 | 0 | 1500/1500 | 900/900 | 673/673 | 1.01781 | -117 |
| 4 | 0 | 300/300 | 300/300 | 300/300 | 1.04341 | -22 |
| 5 | 0 | 300/453 | 300/453 | 300/453 | 1.04234 | -11 |
| 6 | 0 | 300/673 | 300/673 | 300/673 | 1.04060 | -18 |
| 7 | 0 | 600/673 | 600/673 | 600/673 | 1.03019 | -32 |
| 8 | 0 | 900/673 | 900/673 | 900/673 | 1.02443 | -38 |
| 9 | 0 | 600/673 | 600/673 | 300/673 | 1.03022 | -110 |
| 10 | 40 | 300/673 | 300/673 | 300/673 | 1.00666 | -155 |
| 11 | 40 | 600/673 | 600/673 | 600/673 | 0.99716 | -179 |
| 12 | 40 | 673/673 | 673/673 | 673/673 | 0.99564 | -180 |

A comparison between these multiplication factors enables the evaluation of the isothermal temperature coefficient. Results are summarised in Table V

**Table V. : Isothermal temperature coefficients (ITC) and its components.**

| Parameter | Benchmark | PARCS | Measured |
|---|---|---|---|
| ITC (case 1 and 2) [pcm/C] | 3.341 | 3.39 | 2.87 ± 0.14 |
| Expansion component (case 5 and 6 )k [pcm/C] | 0.695 | 0.73 | 0.74 ± 0.15 |
| Doppler component (case 6 and 7 ) k_D [pcm] | 1381 | 1401 | 1180 ± 118 |

It can be observed that PARCS results are in good agreement with the reference calculation.

## 4.2. Feedback Coefficient

For every coefficient presented here below, the reference is case 11 in Table IV, every geometrical dimension is calculated at 673 K and every isotope is taken at 600 K. Control rods are 40 cm inserted into the core. For every effect, a corresponding set of few-group cross-sections for PARCS was evaluated with SERPENT.

### 4.2.1. Fuel Doppler effect

First the Doppler effect of the fuel was investigated. For each case, a criticality calculation was performed and only the fuel isotope temperature was changed (from 600 K to 1500 K) in the mentioned axial zone (i.e. in the fissile part of the inner core). For every case, the predicted multiplication factor was compared to the one of the reference case 11 (Table IV) in order to deduce the Doppler constant contribution of this axial zone. Results are presented in Table VI.

**Table VI. : Fuel Doppler effect.**

| Fuel isotope temperature changed in: | Sodium effect (pcm) |
|---|---|
| Inner Core fissile | -789 |
| Outer Core fissile | -263 |
| Radial Blanket | -28 |
| Lower Axial Blanket | -51 |
| Upper Axial Blanket | -17 |
| Total | -1169 |

It can be observed that two third of this the fuel Doppler effect arise from the fissile part of the inner core. The second major contributor is the fissile part of the outer core while the fertile part plays a very little role.

### 4.2.2. Sodium density effect

The sodium density effect in the fuel assembly was also investigated. To do so, the reactivity effect due to a sodium heat-up by 400 K was studied. Different criticality calculations were performed to investigate the sodium density effect zone-wise. Results are presented in Table VII

**Table VII. : Sodium density effect.**

| Sodium density changed in | Sodium effect (pcm/K) |
|---|---|
| Inner Core total height | 0.207 |
| Outer Core total height | 0.006 |
| Radial Blanket total height | -0.012 |

It can be observed again that the main contributor is the inner core. An interesting observation is the negative behaviour of the radial blanket.

### 4.2.3. Diagrid radial expansion effect

The last effect studied is the diagrid radial expansion effect. To investigate it the SA pitch was increased by 1 % resulting of an increase of the inter assembly gap. As a result, it was observed a decrease of the reactivity by more than 700 pcm. The Diagrid radial expansion coefficient was evaluated to be -0.917 pcm $K^{-1}$.

## 4.3. Power distribution

Additionally, assembly power distributions have been compared. The case considered in this section is a near criticality core configuration. The temperature of every structure and isotope is at 673 K, and CSD are inserted for 40 cm. The PARCS result has been compared to the reference SERPENT solution .

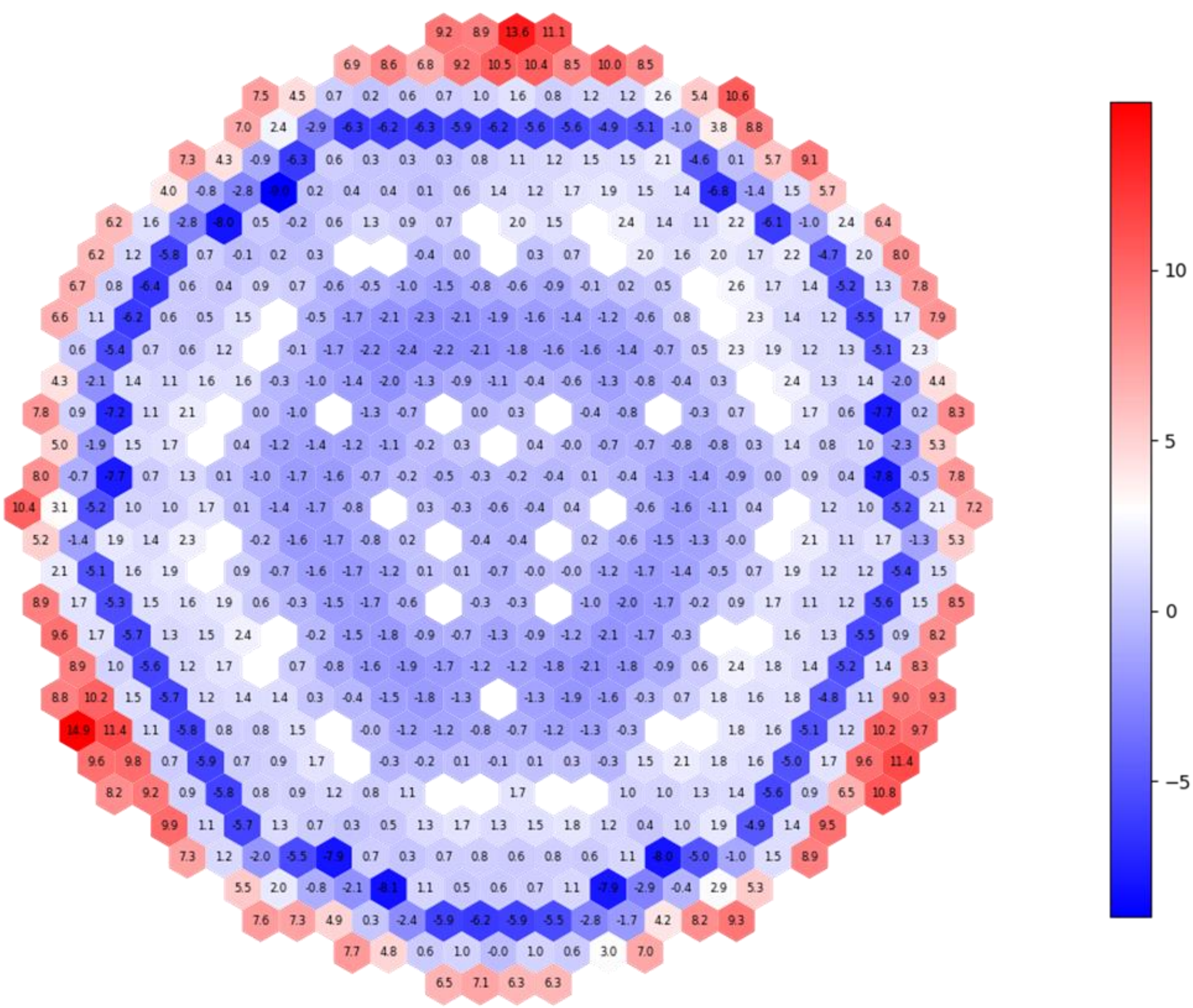



**Figure 3. Relative difference (in %) of the assembly power distribution between PARCS and SERPENT**

Figure 3 shows the relative difference between PARCS and SERPENT. In the fissile part of the core (Figure 1), discrepancies are below 2 % while in the fertile part they are up to 15 %. However, power is mainly generated in the fissile part and so the absolute discrepancies in the fertile part, 1 to 2 kW, per assembly has no significant effect on the maximum fuel and cladding temperature in the core.

In summary, the PARCS benchmark model demonstrates its capability to reproduce accurately integral and local quantities as shown by comparisons to the reference SERPENT calculation. Furthermore, parameterized few-group cross-section libraries for SPX have been successfully generated in order to perform 3-D neutron kinetic and thermal-hydraulic coupled calculation. In the following, a thermal-hydraulics open core ATHLET model of SPX is presented as well as coupled PARCS/ATHLET test calculations.

## 5. COUPLED 3-D PARCS/ATHLET SIMULATIONS

### 5.1. ATHLET model

For coupled 3-D neutron-kinetic/thermal-hydraulic PARCS/ATHLET simulation of SPX, a parallel-channel open core model was developed with the current version of GRS thermal-hydraulic system code ATHLET. ATHLET (Analysis of THermal-hydraulics of LEaks and Transients) [14] is being developed by GRS for the safety assessment of the whole spectrum of leaks and transients in light water reactors (PWRs and BWRs) without core degradation, small modular reactors (SMR) as well as in GEN-IV reactors with helium or liquid metal (Na, Pb, LBE) coolants.

The ATHLET model developed for SPX uses a 1-by-1 mapping scheme between ATHLET and PARCS, i.e. each subassembly is represented by an individual thermal-hydraulic parallel channel. First test calculations involving radial core thermal expansion induced by a variation of the sodium inlet temperature are shown in the following. In this test case, axial thermal expansion is not considered, i.e. the axial meshes remain unchanged. No expansion effects have been considered in the thermal hydraulic model. Finally, the parametrization of the few-group homogenized cross-section library chosen for the transient described in the next section is shown in Table III.

### 5.2. Results

In order to demonstrate the effect of radial core thermal expansion for SFR based on the SPX neutron kinetic and thermal hydraulic models described in this paper, a simple transient test case, initiated by a variation of the core coolant inlet temperature, is performed. As shown in Figure 4, the sodium temperature at the inlet (blue curve) rises from 400 °C to 500 °C for 5 seconds and stay constant during the next 10 seconds before returning to the initial value of 400 °C. The radial core expansion effect is investigated by comparing prediction of the coupled model in two different cases. In the first case, the temperature of the diagrid remains constant at 400 °C while in the second case, the temperature of the diagrid varies as shown in Figure 4 (orange curve).

Figure 5 presents the evolution of the power level when only the sodium inlet temperature perturbation is accounted for, and the temperature of the diagrid is kept constant (blue curve). The orange curve describes the evolution of the power level when both the sodium inlet temperature and the diagrid temperature vary. As a result, one can see that by the radial expansion of the diagrid – due to increased available coolant volume causing more neutron absorptions by sodium – the power decreases more than in the case where expansion of the diagrid is not considered.

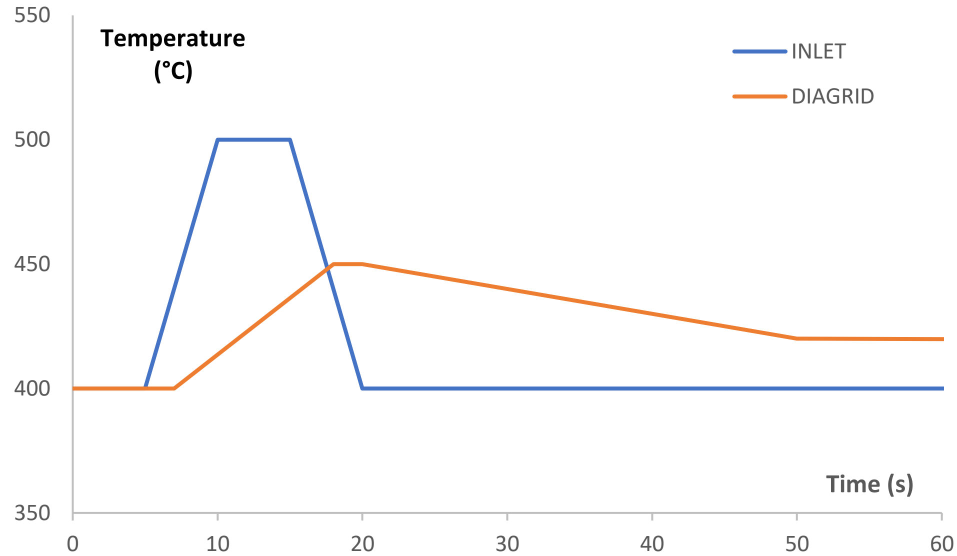



Figure 4.  Diagrid and core inlet temperature evolutions during the transient

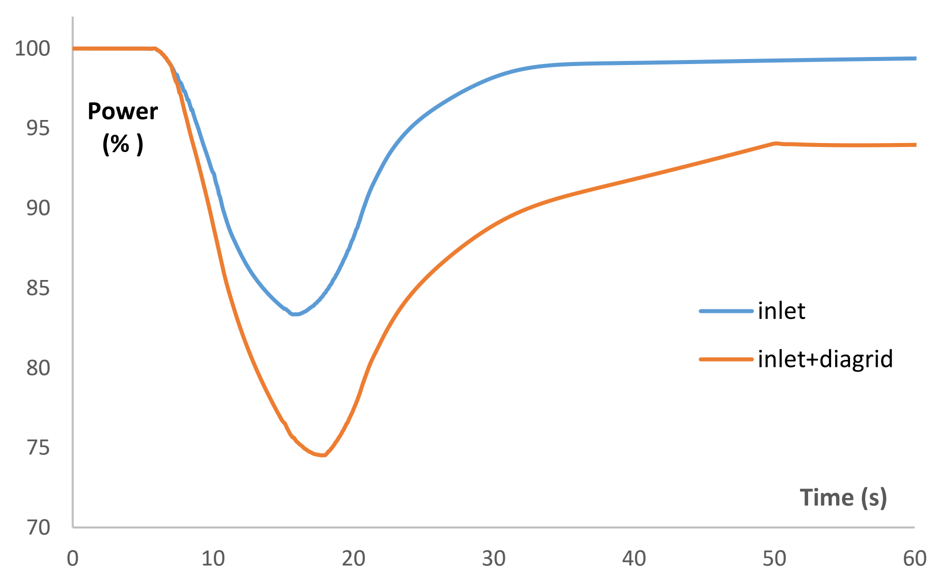



Figure 5.  Power evolution during the transient accounting for diagrid expansion

These SPX coupled PARCS/ATHLET test calculations are physically plausible as they reproduce the expected behaviour during the transient. This first step paves the way toward validation of the PARCS neutron kinetics model extensions for radial core expansion implemented by GRS for the safety assessment of SFR.

## 6. CONCLUSIONS

Detailed modelling of core expansion effects is mandatory for sodium cooled fast reactors. In this paper, the 3-D radial core expansion model implemented in PARCS by GRS was applied to the Superphénix static-neutronic benchmark.

First, a full core SERPENT benchmark model has been created. Results obtained agree well with measurements and reference calculations. In order to simplify the handling of temperature dependent geometric changes, a pre-processor for generation of temperature driven expansion of geometry and material densities has been developed and implemented in the GRS core simulator KMACS.

In addition, 3-D full scale subassembly models of the SPX core have been developed in SERPENT to generate few-group cross-sections were then used with the deterministic code PARCS to evaluate integral parameters, feedback coefficients and 3-D distributions of power density. Results obtained were in good agreement with reference calculation.

Finally, a simple ATHLET parallel channel open core model has been developed for coupled PARCS/ATHLET calculations. A simple first transient test was performed, in which the temperature at the core inlet was changed. The corresponding transient was simulated with and without considering the radial thermal expansion of the diagrid in PARCS. Results agree with the expected behaviour of the reactor and are physically plausible.

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