Hot Zero and Full Power Validation of PHISICS RELAP-5 Coupling

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INTRODUCTION

PHISICS is a reactor analysis toolkit developed over the last 3 years at the Idaho National Laboratory. It has been coupled with the reactor safety analysis code RELAP5-3D. PHISICS is aimed at providing an optimal trade off between needed computational resources (in the range of 10~100 computer processors) and accuracy. In fact, this range has been identified as the next 5 to 10 years average computational capability available to nuclear reactor design and optimization nuclear reactor cores.

Detailed information about the individual modules of PHISICS can be found in [1]. An overview of the modules used in this study is given in the next subsection. Lately, the Idaho National Laboratory gained access plant data for the first cycle of a PWR, including Hot Zero Power (HZP) and Hot Full Power (HFP).

This data provides the opportunity to validate the transport solver, the interpolation capability for mixed macro and micro cross section and the criticality search option of the PHISICS package.

The current paper will first briefly recall the structure of the different PHISICS modules used, then illustrate the modeling process for the PWR HZP/HFP and finally present some preliminary results of this validation effort.

THE PHISICS MODULES USED FOR THE MODELLING

The following sections present the PHSICS toolkit involved in this simulation and a brief description of its capabilities and modules.

INSTANT

INSTANT [2] is the neutron transport solver. It is based on the spherical harmonics approximation of the angular dependence of the neutron flux. Currently the following nodal spatial meshes are available: Cartesian, hexagonal, and extruded triangle.

MIXER

The MIXER is tasked to perform the interpolation of the microscopic or macroscopic cross sections. It also generates the macroscopic cross sections used by INSTANT.

PHISICS offer a noticeable flexibility in the treatment of cross sections, since both microscopic and macroscopic cross sections can be combined together in the same simulation. Macroscopic cross sections are treated as microscopic ones with the atomic density equal to one. Cross sections can be tabulated for an unbounded number of parameters and an unbounded number of tabulation points for each parameter. The interpolation of the cross sections within the parameter grid is linear.

Criticality Search Module

The Criticality Search (CS) adjusts isotope densities (user defined) for a specified location in the geometry until a prescribed value of k_{eff} is reached (or the densities would be outside user specified boundaries).

A classical usage of this module is to search for critical boron concentration, fissile enrichment, or control rod positioning.

To speed up the process, the user can also specify whether (in case the concentration of an isotope is also a tabulation parameter) to use just a first order approximation, i.e. the user can specify that a) only the variation in density of the specific isotope impacts the macroscopic cross sections or b) the isotopes (user provided information) need to be re-evaluated to account for the change in the tabulation coordinate.

RELAP5 coupling

The coupling between RELAP5 and PHISICS allows for thermal-hydraulic feedbacks such as water density, fuel temperature, soluble poisons concentration and control rods positioning.

THE MODELLING APPROACH

Microscopic Cross Section Library Generation

Figure 1 shows the core layout indicating the different assembly types (enrichment is given in the legend while the number on each assembly indicates the number of fuel rods with burnable poison). Starting from that layout, a set of 30 libraries has been generated in order to account not only for assembly type but also for neighboring effects. Figure 2 shows the library correspondence to the 2D octant core (circle indicates presence of instrumentation channels). The chosen energy structure involves 8 groups with the following upper bounds: 2.0E+07, 2.2313E+06, 8.2085E+05, 9.11884E+03, 1.3007E+02, 3.9279E+00, 6.2506E-01 and 1.4572E-01 eV. Each fuel library has ~300 isotopes (only 200 are tracked) while each reflector library contains 24 isotopes (all tracked). For the 3D full core analysis, to compare with experimental results, a total of 64 libraries have been used. Other 30 are identical to the ones

described but located in a plane with grid spacers, while the remaining 4 are for the axial reflectors (top and bottom).

Table 1 reports the tabulation parameters, the number of points and the values for each parameter and the total number of points. The burn-up has been added as an additional tabulation dimension for the HFP only, since for HFP, following the first and second depletion cycle is part of the benchmark (second part).

Figure 1: Core overview

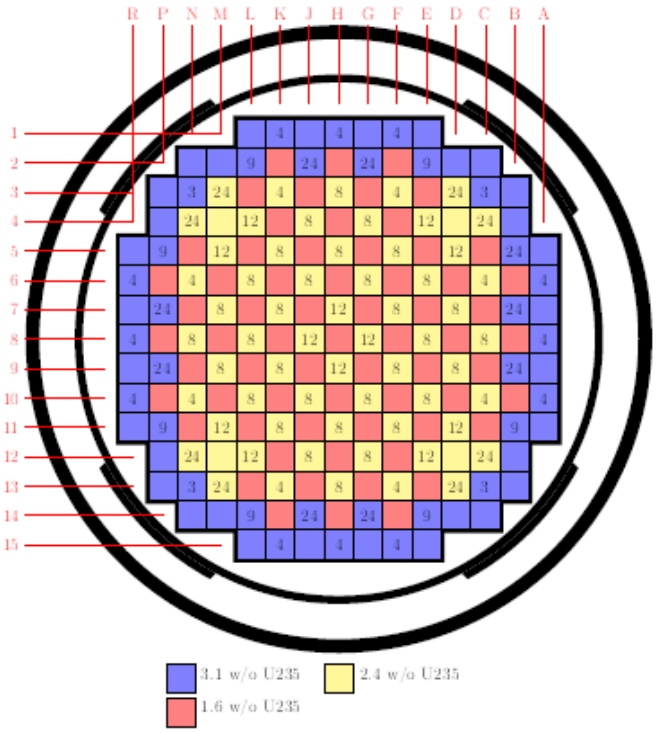


Figure 2: Material placement

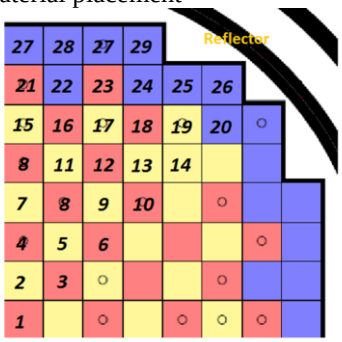


Table 1: HZP Tabulation

Library Type	HZP	HFP
Boron Tabulation (ppm)	1700, 1150, 1000, 1.0E-06	1150,1000, 1.0E-06
Fuel Temperature (°C)	286.66, 291.66	300, 800, 1300
Moderator Density (kg/m^3)	752.705, 733.36	752.705, 733.36
Burn-up (GWd)	--	0.150, 15.0
Tabulation points	16	108

Description of the Boron Modeling

The presence of boron both, as burnable poison and in the coolant to control the reactivity swing required some modeling effort, especially due to the direct usage of microscopic cross sections in the simulation.

In fact, the boron in the water is not depleted and its density follows both, the water density and the ppm of soluble boron maintained in the water by the plant control system while the boron in the poison locations is burnable. Correct prediction of the critical soluble boron concentration in the water (as a function of moderator temperate and burn-up) is a key value for reactor control.

In order to properly take into account this features in the PHISICS framework, we have generated two cross section sets for the boron in the water and in the burnable absorbers with HELIOS 2. Care needs to be taken since the cross sections generated in this way are normalized with respect the average flux in the water and in the burnable absorbers, while when used in the nodal simulation of the core, the reaction rates are computed using the average assembly fluxes. To eliminate this discrepancy the cross sections have been rescaled using the following formula:

$$\sigma^r_{iso} = \sigma^r_{iso}\left(\frac{\phi_{subreg}}{\phi_{regtot}}\right)$$

Where *r* is the reaction type index, *iso* is the isotope index and the fluxes are representative of (*subreg*) the sub-region where the homogenization has been made and (*regtot*) the whole region (usually the one used in the full core calculation for the reactor being considered).

Another problem, connected to the soluble boron modeling that had to be addressed, was the water density feedback on its number density.

In fact, the atomic density of the born in the water is not only linked to the ppm value but also to the density of the water itself.

The macroscopic cross section of the coolant (water + boron) could be written as:

$$S^r_W = N_B(r_{H_2O}, ppm)s^r_B + N_{H_2O}(r_{H_2O})s^r_{H_2O},$$

where the density of the Boron (N_B) is a linear function of the ppm value and water density r_{H_2O}.

Given that none of this two components will be depleted and that the water density and ppm are already tabulation parameters, it is more convenient to use directly the S^r_W with unitary densities. In this way, the water density variation computed by RELAP5, given as a feedback to PHISICS, directly impact the effective amount of soluble boron present in the core.

The criticality searching, used to find the critical value of the Boron, is then performed on a dummy isotope with 'zero' cross sections while S^r_W is the only

isotope for which the values of the cross section are recomputed at each iteration of the CS.

SPH Factors Calculation

To further improve results, the super-homogenization technique (SPH) [3] can be implemented in order to have reaction rates of the lattice calculation equal to the ones obtained in a 2D nodal representation of the core. SPH could be applied at different levels of resolution; in the present case, SPH factors by assembly and by energy group are used. Generally speaking, the SPH is a non-linear methodology where the unknowns are a) the average fluxes in each assembly computed by the nodal core simulator and b) the cross sections to be used in the nodal simulation. The average assembly core fluxes are provided by the INSTANT solver for a given set of homogenized cross-sections. These values have to be scaled by an unknown common scaling factor. In standard calculation this scaling factor is provided by the power normalization. In the case of the SPH set of equations, this normalization does not provide an additional constraint. In fact, this is equivalent to imposing the sum of all fission rates (volume weighted) to be equal between the lattice and the nodal simulation. This is a linear combination of a part of the second set of equations that are used in the SPH methodology, where all the reaction rates are forced to be the same between the lattice calculation and the nodal core calculation. The additional constraint we decided to use, is given by forcing the neutronic population given by the nodal solution to be equal to the one in the lattice solution.

The solution of the non-linear system of equations (nodal core P1 equation, neutron population and reaction rates) is performed using a simple fixed-point scheme described in the following:

1. An initial set of homogenized cross section is used to compute the average assembly fluxes by PHISICS.

2. Normalization of the average fluxes of the core calculation to the ones of the lattice.

$$\phi_g^{norm,i} = \phi_g^i \frac{\left(\sum_g \sum_i \phi_g^{i,lattice} V_i\right)}{\left(\sum_g \sum_i \phi_g^i V_i\right)}$$

Where *i* is the region index and *g* the macro energy group index while V is the region volume. The lattice index identifies the flux of the lattice calculation.

3. Use the new flux to calculate the correction factors α.

$$\alpha_g^i = \left(\frac{\phi_g^{i,lattice}}{\phi_g^{norm,i}}\right)$$

This can be proved to be equivalent to force the macro reaction rate to be the same in the lattice and core calculation when the cross section are scaled by the factor α_g^i.

4. Correct the cross sections by the factor α.

$$\tilde{\Sigma}_{g,iso}^{i,r} \leftarrow \alpha_g^i \Sigma_{g,iso}^{i,r}$$

$$\tilde{\Sigma}_{s0,g\to g',iso}^{i,r} \leftarrow \alpha_g^i \Sigma_{s0,g\to g',iso}^{i,r}$$

where the tilde indicates the corrected cross sections, *iso* is the particular isotope and *s0* the zero order of the scattering cross section.

Steps 1 to 4 are repeated until convergence is achieved in the correction factors.

Special care needs to be taken in dealing with the corrective factors to be applied to the transport cross sections. In fact, the transport cross-section adjustment tries to preserve the assembly leakage rather then a reaction rate. In this case, the right weighting function is not anymore the average scalar flux but one over its gradient cross the assembly. Using the gradient in the 2D plane will lead to a correction coefficient for the transport cross-section that is directional dependent. In the present case, PHISICS (which is based on a coherent spherical harmonics approximation) does not use the transport cross sections but the effect is emulated by altering the within group anisotropic scattering cross section as suggested in [4]. As a result the SPH factor for the $\Sigma_{s1,g\to g,iso}^i$ is computed as follows:

- Point 3 in the above iteration scheme is replaced by:

$$\frac{1}{\tilde{\sigma}_{T,g}^i - \beta_g^i \sigma_{s1,g\to g}^i} = \frac{\alpha_g^i}{\sigma_{T,g}^i - \sigma_{s1,g\to g}^i}$$

where this formula implicitly defines the correction factor.

- Point 4 in the above iteration scheme is replaced by:

$$\tilde{\sigma}_{s1,g\to g,iso}^i \leftarrow \beta_g^i \sigma_{s1,g\to g}^i$$

where $\tilde{\Sigma}_{T,g}^i$ is the total cross section.

Currently, the out-scattering anisotropic cross sections are left unchanged.

Even if this approach converges and gives satisfactory results using the P1 approximation in the core simulation, the correction on the border assemblies and especially in the reflector can become significant because of the simplification used in the preservation of the leakage that is a dominant effect in these regions.

Besides that, the general accuracy of the calculation can be considerably increased by using the SPH factors.

RESULTS

The SPH correction has been performed for only one tabulation point and then applied to the whole library. The approximation is acceptable if for different points of the tabulation the relative magnitude of the fluxes in space and energy are reasonably preserved. The final corrective factors averaged over energy for the HZP and HFP conditions are shown in Table 2 with also the reaction rate

relative errors averaged over energies are shown in Table 3.
As can be seen from the errors, acceptable convergence can be reached with a reasonable amount of iterations (between 10 and 20).

Table 2: SPH factors energy averaged and relative error

Material	Factors		Error	
	HZP	HFP	HZP	HFP
1	0.94361	0.93266	1.4676E-02	1.5996E-02
2	0.91596	0.90558	1.4745E-02	1.5869E-02
3	0.92790	0.91873	1.4676E-02	1.5855E-02
4	0.91999	0.91254	1.4811E-02	1.5924E-02
5	0.90693	0.89993	1.4810E-02	1.5924E-02
6	0.92096	0.91640	1.4858E-02	1.6028E-02
7	0.90775	0.90336	1.4885E-02	1.6106E-02
8	0.92601	0.92361	1.4934E-02	1.6159E-02
9	0.91644	0.91497	1.5178E-02	1.6235E-02
10	0.94211	0.94568	1.5404E-02	1.6249E-02
11	0.92309	0.92333	1.5162E-02	1.6323E-02
12	0.93664	0.94043	1.5307E-02	1.6386E-02
13	0.93858	0.94734	1.5767E-02	1.6628E-02
14	0.99478	1.01220	1.6194E-02	1.6509E-02
15	0.95501	0.95933	1.5604E-02	1.6438E-02
16	0.96671	0.97303	1.5524E-02	1.6475E-02
17	0.96837	0.97675	1.5797E-02	1.6575E-02
18	0.97240	0.98753	1.5956E-02	1.6653E-02
19	0.95972	0.97865	1.6489E-02	1.6588E-02
20	1.07209	1.09028	1.6747E-02	1.6465E-02
21	0.99968	1.01190	1.6330E-02	1.6645E-02
22	0.96904	0.97928	1.6376E-02	1.6610E-02
23	0.99895	1.01304	1.6252E-02	1.5996E-02
24	1.05531	1.06646	1.6379E-02	1.5869E-02
25	1.13983	1.14627	1.6160E-02	1.5855E-02
26	1.19367	1.19248	1.5873E-02	1.5924E-02
27	1.14728	1.14730	1.6452E-02	1.5924E-02
28	1.15148	1.15189	1.6499E-02	1.6028E-02
29	1.24804	1.23865	1.5950E-02	1.6106E-02
Reflector	1.80192	1.67313	1.4449E-02	1.6159E-02

The corresponding power distributions are shown in Figures 3 and 4.

The same SPH technique has been applied to the grid spacer planes libraries while for the axial reflector the same factors for the radial one have been used.

Table 3 summarizes the differences between the nodal core simulation versus the 2D lattice calculation and experimental results for k_{eff} and the critical boron concentration. For the 3D calculation, a total of 64 libraries have been used. The same SPH technique has been applied to the grid spacer planes libraries while for the axial reflector the same factors for the radial one have been used.

Table 3: difference in 2D (code to code) and 3D (experimental to code)

Reference	PHISICS (PHISICS-Reference)	
	Critical Boron (ppm)	K_{eff} (pcm)
2D HELIOS (HZP)	Not calculated	127
3D Experimental (HZP)	34	406
3D Experimental (HFP)	30	355

Figure 3: HZP power distribution after SPH correction

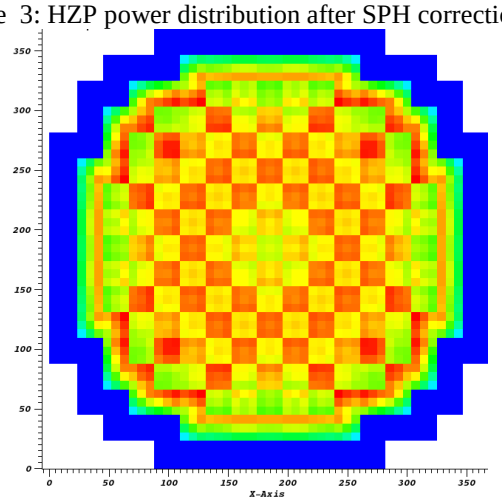
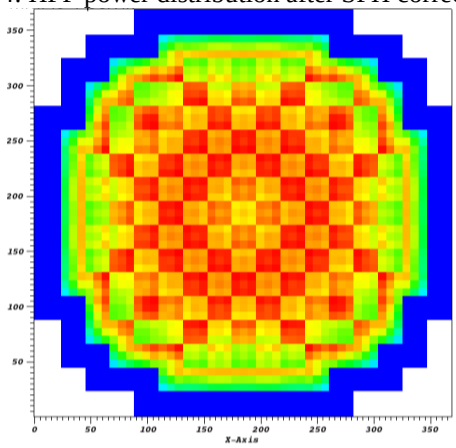


Figure 4: HFP power distribution after SPH correction



This initial attempt to model a realistic PWR core with the PHISICS package reveals a good robustness of the code and its flexibility for multiple usages. Results compare in a satisfactory way with experimental results and further improvements are possible and considered for the second part of the benchmark, when the simulation and comparison with operational data will be performed over two reactor cycles.

ENDNOTES

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REFERENCES

1. C. RABITI, Y. WANG, G. PALMIOTTI, H. HIRUTA,J. COGLIATI, A. ALFONSI, A. EPINEY, T. GRIMMET "PHISICS: New Features and Advancements", *2011 Annual Winter Meeting*, Washington, D. C., USA, October 30-November 3 (2011).
2. A. EPINEY, C. RABITI, A. ALFONSI, Y WANG, J. COGLIATI, G. STRYDOM "PHISICS multi-group transport neutronic capabilities for RELAP5", Proc. 2012 ICAPP'12, Chicago, Illinois, USA, June 24-28, (2012).
3. A. HEBERT "A Consistent Technique for the Pin-by-Pin Homogenisation of a Pressurized Water Reactor Assembly", *Nucl. Sci. Eng.*, **113**, 227 (1993)
4. U. GRUNDMANN, S. MITTAG "Super-homogenisation factors in pinwise calculations by the reactor dynamics code DYN3D", *Annals of Nuclear Energy*, Volume 38, Issue 10, October 2011, Pages 2111–2119 (2011).