NEW DEVELOPMENTS FOR THE HOROWITZ REACTOR'S NEUTRONICS MODELIZATION AND VALIDATION

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ABSTRACT

The definition and the validation of the neutronics route of the HORUS3D package, based on the codes APOLLO2 [1] and CRONOS2 [2], is described. HORUS3D is dedicated to the design studies of the future European MTR, called Jules Horowitz Reactor.
A rigorous methodology, based on the decomposition of the validation problem in a series of benchmarks, is applied from the self-shielding effect to the whole core calculation. Moreover, a nuclear data uncertainty propagation method has been developed [3].
Hence, the HORUS3D neutronics route allows the neutronics modeling of the Horowitz reactor with a great confidence : compared to expensive reference calculation the discrepancy on the initial reactivity level is less than 200 pcm, the maximum difference on the assembly power distribution is 1.4% at the beryllium reflector interface (hot spot) and reactivity discrepancies don't exceed 150 pcm along the burn-up.

1. INTRODUCTION

The future European Material Testing Reactor, called Jules Horowitz Reactor [4] will allow very high performances. Its special fuel assembly geometry and its small dimensions particularly characterize the JHR. This leads to neutronics and thermohydraulics modeling problems : specific geometry, neutronics streaming effects, "flow redistribution rate", etc.
These difficulties, combined to the lack of specific integral experimental data, require a rigorous methodical approach. To overcome these problems, an adapted and consistent neutronics/ thermohydraulics code package, named HORUS3D (HOrowitz Reactor simulation Unified System) is developed.
This paper presents the methodology and the development of the neutronics route, as well as the elementary validation against reference Monte Carlo results.

2. JHR DESCRIPTION

The JHR project is split in different phases. Preliminary design studies allowed to define of the main options of the core and its elements, and to characterize a reference configuration. The Definition Studies will optimize the JHR performances by testing modifications from the reference configuration. The JHR assembly would be composed of 3x6 cylindrical fuel plates maintained by 3 stiffeners (Fig. 1). The external diameter of the assembly is close to 8 cm with an active height of 60 cm.

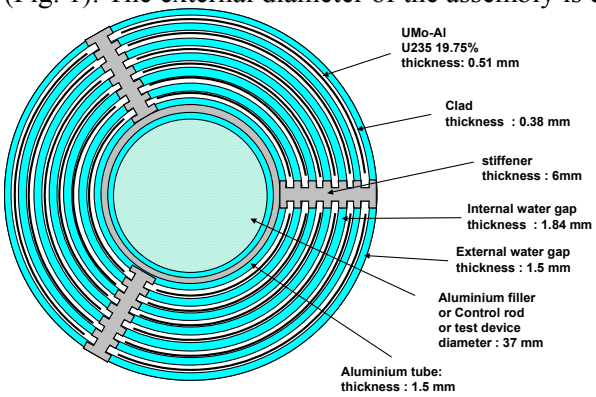


Figure 1 **:** Cross-section of the JHR assembly

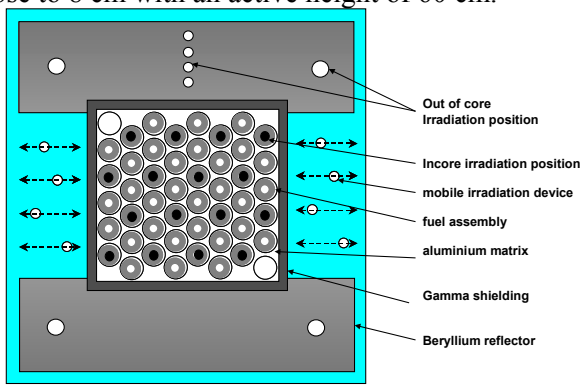


Figure 2 : Cross-section of the JHR core

The fuel is composed of a dispersion of UMo powder in an aluminium matrix. The fuel plates are obtained in a rolling mill process. The uranium-235 enrichment, less than 20%, respects the non-proliferation agreement. The central cavity can host either aluminium filler, a hafnium control rod or an irradiation test device.

The preliminary core consists of 46 assemblies, arranged in a triangular lattice inside a rectangular aluminium matrix (Fig. 2). It is boarded on two sides by a beryllium reflector. The other two sides are left free in order to introduce mobile irradiation devices. These characteristics would be confirmed by the detailed studies.

With a maximum thermal power of 100MW, the specific power in the core amounts to 600kW/l.

3. STRATEGY AND METHODOLOGY

The JHR assembly and core design does obviously not allow the direct application of validated neutronics route such as PWR schemes. Nevertheless, present codes are built of modules performing specific tasks (geometry, self-shielding, flux solver, etc.) and a user language is used to link the operators at run time. This allows a very flexible and powerful use of the codes, but leads to a more complex validation. Moreover, not only do the present JHR characteristics reduce the representative experimental data set, but the future design studies will also lead to important modifications. Therefore, the HORUS3D development strategy follows 3 axes :

1. process splitting : an anticipating analysis of the modelization requests and the planning is essential to define the three different processes : Code developments, Scheme definition and validation, and the realization of a dedicated Experimental program.
2. the use of existing experimental validation studies, elaborated for other reactor types, is essential due to the lack of directly representative experiments. Therefore, the same options must be used in the JHR scheme as far as possible.
3. incremental approach : The qualification process is based on well-identified steps (Figure 3). The Verification guarantees the correct numerical resolution of the implemented models according to unitary tests. The Elementary Validation allows verifying that the scheme uses the suitable

physical model and the best options. Successive benchmarks and the comparison of tested scheme results to reference results obtained by an exact resolution (like a Monte Carlo simulation code which uses the same Nuclear Data) are then performed. The benchmarks are defined in order to emphasis elementary physical problems, allowing to determine numerical and model biases and to avoid error compensations. The final step, called the Global Validation, consists in testing the scheme results against representative experimental data. The numerical procedures and the nuclear database are evaluated. In the case of lack of experiment results, a propagation method can be used to give an order of magnitude of the bias due to the potential nuclear data errors [3].

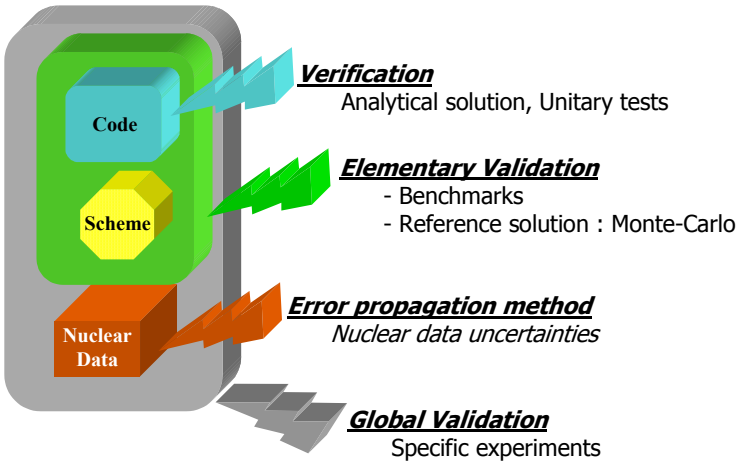


Figure 3 : Qualification process step

In this paper, we focus on the development of the neutronics route and the elementary validation.

4. ASSEMBLY NEUTRONIC SCHEME

The JHR assembly neutronics route is performed with the APOLLO2 [1] code and its 172 groups library. The complex geometry (Figure 1) necessitates the use of the exact 2D collision probability method. The optimized slowing-down model with a Doppler cross-section broadening for the first resonance [5,6], developed for PWR UOX fuels, can be used. Nevertheless, many options have to be re-defined.

On terms of validation, we can identify three different physical problems : the self-shielding calculation, the flux resolution, the burn-up calculation, and that for the assembly with or without the absorber. Hence, six benchmarks have been defined, and a reference solution for each has been determined.

Moreover, in order to avoid compensation effects, the calculations have to be compared on relevant parameters. The multiplicative factor k_∞ results from a physical sequence that can be separated into the well-known 6 factor formula ($k_\infty = \chi_{n,2n} \times \varepsilon_{even} \times \varepsilon_{odd} \times p \times f \times \eta$) composed of the (n,2n) factor $\chi_{n,2n}$, the fast fission factor ε_{even} , the odd fast fission factor ε_{odd} , the resonance escape probability p, the thermal utilization factor f and the thermal fission factor η.

We add the comparison of the absorption rate and the fission rates determined on an adapted 13 groups energy mesh, separating the most important resonances (Figure 4).

We will present first the developments of the standard assembly scheme, without control rod, and secondly the studies of the control rod assembly route.

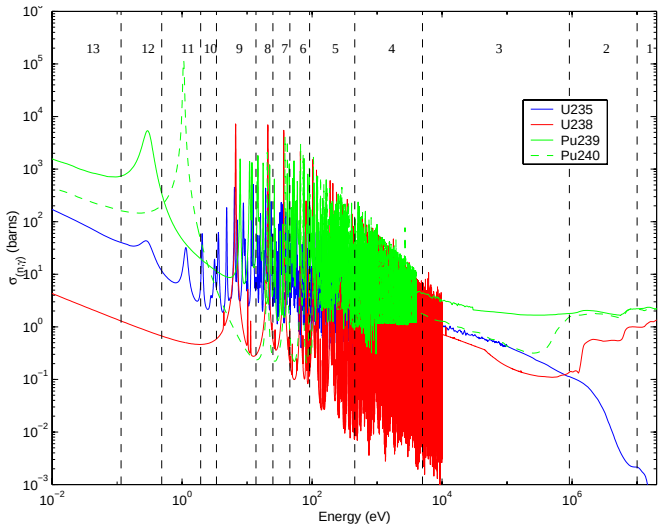


Figure 4 : Capture cross sections and the 13 groups energy mesh

4.1 Standard Assembly

4.1.1 Self-shielding problem

In order to identify a potential bias in the self-shielding calculation, a 1D benchmark is sufficient as the Pij/Flux calculation are unproblematic. Moreover, the spectrum of this 1D model is completely representative of that found between the stiffeners. The Monte Carlo code TRIPOLI4 [7] is used to determine the reference solution of the problem.

The impact of the spatial description of the fuel plates for the self-shielding calculation, to take into account the Dancoff effect, was tested first. Because of the small fuel plate thickness, the RIM effect can be neglected. The number of regions in the moderator was also analyzed, leading to a three-point mesh in the water gap (δe=0.6mm). The number of iterations in the self-shielding resolution was also tested, in order to take into account the mutual shielding between isotopes. Results are summarized in Table 1. The last column gives the TRIPOLI4 statistical uncertainty σ (standard deviation).

Table 1 : APOLLO2 self-shielding model discrepancies with the 1D TRIPOLI4 results

δ (pcm)	1 region / fuel plate	1 region	3 points water gap	2 iterations	σ
χ	45	45	44	45	38
ε_{even}	2	2	6	2	1
ε_{odd}	-19	-19	-12	-21	19
p	-159	-160	-206	-140	15
f	69	69	44	69	5
η	2	2	5	2	10
k_∞	-100	-100	-159	-82	*36*

We can observe that only the water interval spatial description has a perceptible impact with regards to the simulation uncertainties.

The comparison of the Uranium-238 reaction rates (Figure 5) shows that the high Uranium-235 enrichment emphasizes the mutual shielding problem between these isotopes and the discrepancies with the TRIPOLI4 results increases for the 20.9eV resonance of the Uranium-238.

The important Molybdenum concentration makes more difficult the self-shielding calculation. The effective cross section of the natural isotope (MoNat) has recently been introduced in the APOLLO2 library (CEA93.V7); the precedent library version (V6) allowed only computing the self-shielding effect for the Molydbenum-95.

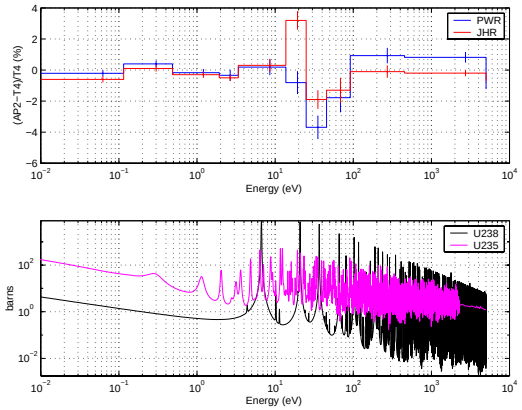


Figure 5 : APOLLO2 Uranium-238 absorption rate discrepancies with TRIPOLI4 results

Table 2 : Molybdenum absorption rate discrepancies with TRIPOLI4 results

	CEA93V6		V7
Energy (eV)	Mo (total)	Mo95	MoNat
1.96E+07	9.9%	-0.5%	-2.8%
1.00E+07	20.5%	-0.1%	-0.1%
9.07E+05	14.2%	-0.3%	-0.2%
5.01E+03	8.4%	-0.3%	0.4%
454	239.3%	-1.2%	-0.1%
91.66	1.4%	-0.8%	-0.3%
45.52	1.6%	1.6%	2.2%
24.98	3.2%	-0.7%	-0.9%
13.71	1.1%	-0.7%	-0.1%
3.381	4.1%	-0.4%	-1.0%
1.93	3.4%	-0.4%	-0.4%
0.485	3.6%	0.0%	0.1%
0.115	2.7%	-0.7%	-0.7%
Total	17.8%	0.6%	0.7%

4.1.2 Flux calculation

A second benchmark was performed, modeling the actual geometry of the assembly and TRIPOLI4 was used to obtain a reference solution. APOLLO2 can easily handle the complexity of the geometry thanks to its exact 2D collision probability module, TDT [8]. The optimal ray tracing parameters have first been determined (angle between rays $\Delta\Phi=\pi/24$ and step between rays $\Delta R=0.05$cm). The geometry data were generated by the graphic software SILENE [8] that was developed for this purpose. We present the results for two spatial meshes, azimuthally split and uniform, in Table 3:

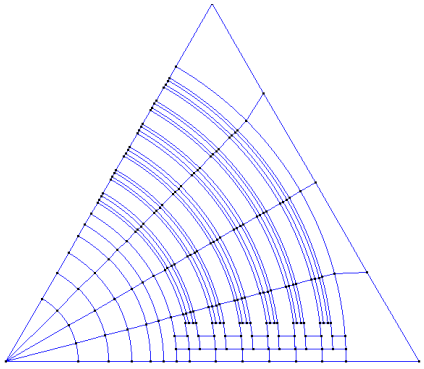


Figure 6 : Azimuthally split spatial mesh (1)

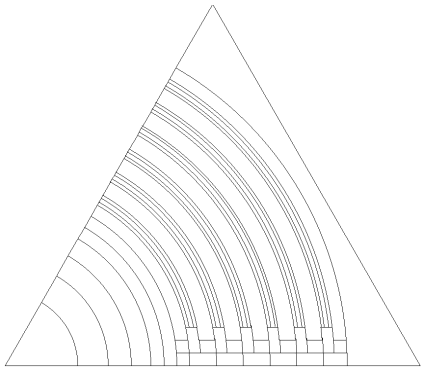


Figure 7 : Azimuthally regular spatial mesh (2)

Table 3 : 2D APOLLO2 discrepancies with the 2D TRIPOLI4 results depending on the geometry spatial mesh

δ (pcm)	Geo. (1)	Geo. (2)	σ
χ	-26	-26	38
ε_{even}	-10	-10	1
ε_{odd}	-41	-44	17
p	-61	-63	15
f	174	178	5
η	1	1	10
k_∞	-11	-11	36

We can observe that the stiffeners do not perturb the flux to an extent which requires an azimuthally spatial mesh. The error of the resonance escape probability is significantly different on this benchmark than the 1D benchmark. A compensation occurred for the self-shielding determination between slowing down model and Pij calculation. Hence, the error on the thermal utilization factor increases. Nevertheless, the resulting precisions are within the precision targets and close to the error observed in PWR rod modeling (about -300 pcm for p and +300 pcm for f).

4.1.3 Burn-up calculation

As the Bateman equation integration is exactly solved by the APOLLO2 burn-up calculation module, only a numerical bias might occurred. So, a reference solution can be easily obtained by dividing the time variable in small enough steps. Hence, for the reference solution the self-shielding and the flux is computed at the following burn-up values : 0, 37.5, 75.0, 112.5, 150, 325, 500, 750, 1000, + every 500 MWd/t until 150 GWd/t (307 points in all). The flux and the self-shielding computations (to take into account the isotope concentration evolution) were optimized.

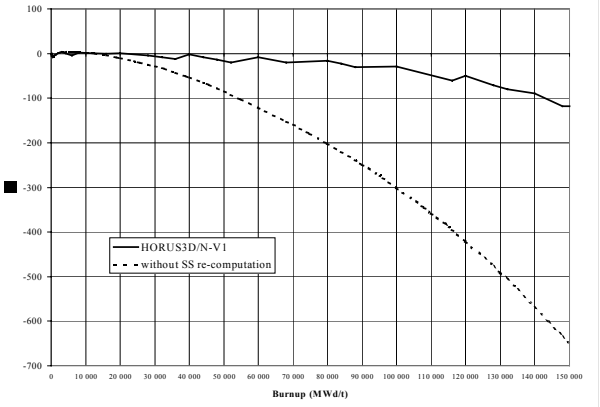


Figure 8 : Evolution reactivity discrepancies with regard to the reference calculation

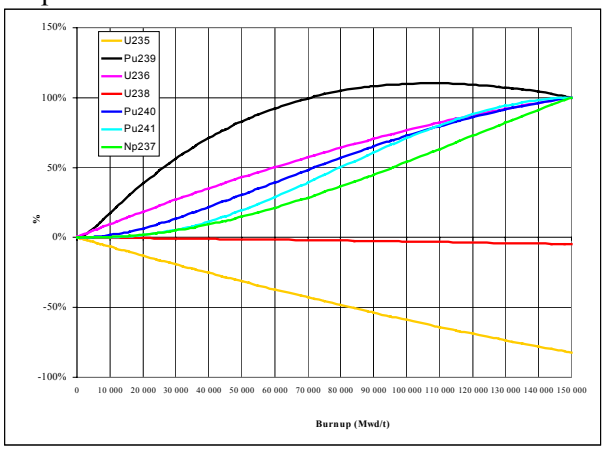


Figure 9 : M.A. concentration evolution (consumption or production relative to initial or final concentration)

The evolution of the major actinides concentrations (Figure 9) forces to re-compute the self-shielding correction at 4, 8, 12, 20GWd/t, and then every 20GWd/t, otherwise a bias of up to –600 pcm could arise at 150GWd/t (Figure 8). The optimized set of time integration points, defining the HORUS3D/N-V1 scheme, allows to determine the assembly reactivity with a bias of under 100 pcm.
This optimized set of integration points unfortunately leads to prohibitive calculation times. Thanks to the APOLLO2 modularity, however, a two level scheme has been developed. The self-shielding effect is calculated with the 172 groups library. The macroscopic cross-sections are then collapsed on an optimal 6 groups mesh to compute the Pij and the evolution of flux and nuclide concentration in time. In order to keep the precision, the self-shielding effect is re-computed every 8GWd/t (with 172 groups). Hence, the assembly cross-section data is obtained in 10 minutes instead of 2 hours, without loss of precision (Table 4, Figure 10).

Table 4 : HORUS3D/N-V1 discrepancies with reference burn-up calculation at 150GWd/t

	Ref.	6G+/Ref (pcm)
χ	1.00030	1
ε_{even}	1.02903	38
ε_{odd}	1.10553	-14
p	0.67937	85
f	0.84398	-40
η	1.47231	-58
k_∞	0.96066	13

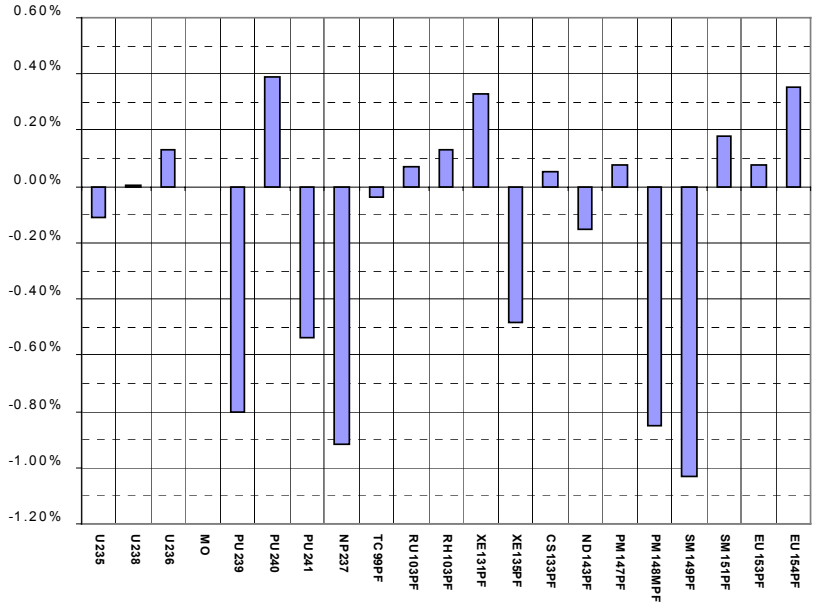
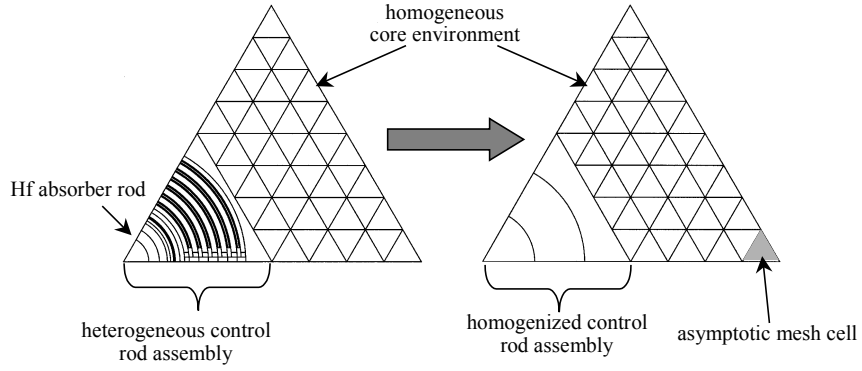


Figure 10 : Nuclide concentration discrepancies
with reference depletion calculation at 150GWd/t

4.2 Control Rod Assembly

The control rod assemblies are subject of a particular treatment in order to take into account the important self-shielding in the solid hafnium rods. This strong localized absorption necessitates the use of a heterogeneous/homogeneous equivalence procedure, a unique feature of the APOLLO2 code [9,10]:



a) heterogeneous-homogeneous model b) homogeneous model

Figure 11 : calculational models of the heterogenous/homogenous equivalence procedure

As for the standard fuel assembly (STD) , the heterogeneous fluxes of the control rod assembly (CNT) are calculated in an exact 2D transport calculation, the geometry of which takes advantage of the 1/6 symmetry (Figure 11 a). This model comprises additionally a homogenous zone representing the core environment, composed of homogenized STD assemblies.
After homogenization and condensation to 6 energy groups, a transport calculation in an equivalent homogeneous model of control rod assembly and core environment (Figure 11 b) is performed. The actual equivalence procedure consists now in an iterative process, in which the cross sections of the homogenized control rod assembly are modified by so-called equivalence factors in such a manner, as to obtain the same reaction rates in the homogeneous as in the original heterogeneous calculation. The conservation of the fission rate in an asymptotic mesh cell of the core environment is used as closing condition.

Figure 12 shows the resulting equivalence factors [1] EQV(E), which are to be applied to the homogenous CNT cross-sections, along with the absorption cross section of Hafnium177, the dominating isotope. Values of EQV(E) < 1 indicate an over-estimation of the corresponding cross section by the straight-forward homogenization.

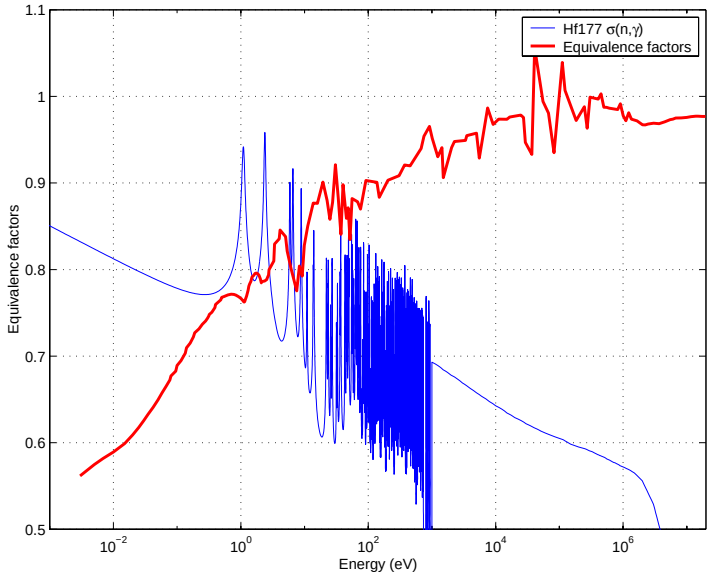


Figure 12 : equivalence factors of the CNT control rod assembly homogenization (in 172 energy groups) and the Hf177 absorption cross section

By virtue of this equivalence procedure, the difference in the reactivity worth of the control rod in an APOLLO2-CRONOS2 benchmark amounts to only 1.7%, against 15.3% without equivalence. Figure 13 depicts the local power density in the control rod assembly and the neighboring STD assembly in this benchmark as calculated with APOLLO2 and the error in the corresponding CRONOS2 calculation.

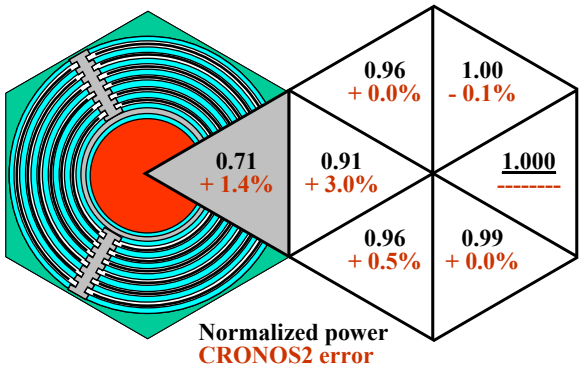


Figure 13 : Local normalized power and CRONOS2 error in the APOLLO2-CRONOS2 benchmark of a control rod assembly

Due to the thickness of the absorber rod and the multiple absorption resonances of the different Hf isotopes, particular attention had to be paid on the self-shielding effect. The optimization process, based on a 1D-benchmark with TRIPOLI4 results, results in a set of recommendations allowing to calculate the absorption rate with a bias of only 0.4%.

[1] For the sake of illustration, this equivalence calculation was performed in 172 groups, instead of 6 groups in the HORUS scheme.

5. CORE CALCULATION

5.1 Geometry description and reflector constant scheme

The 3D core neutronics route uses the new finite elements developments in the CRONOS2 code [2], allowing splitting the hexagonal cells in several triangles (6 or 24). A first study showed that a 6-triangle discretization is enough and gave the number of hexagon rings to represent the JHR core. This leads to 145 000 prisms and the tedious task of constructing the core geometry is assumed by the procedural possibilities of the CRONOS2 code.
The triangular spatial mesh allows the correct representation of the fuel part (Figure 14). The reflector parts would necessitate a rectangular mesh. Therefore, an adapted flux homogenization is made in APOLLO2 using the exact 2D Pij solver TDT on a quarter section of the core (Figure 15). 22 homogenized media are so handled in the radial CRONOS2 geometry.
For the axial modeling, 10 homogenized media are computed with a 1D plane geometry.

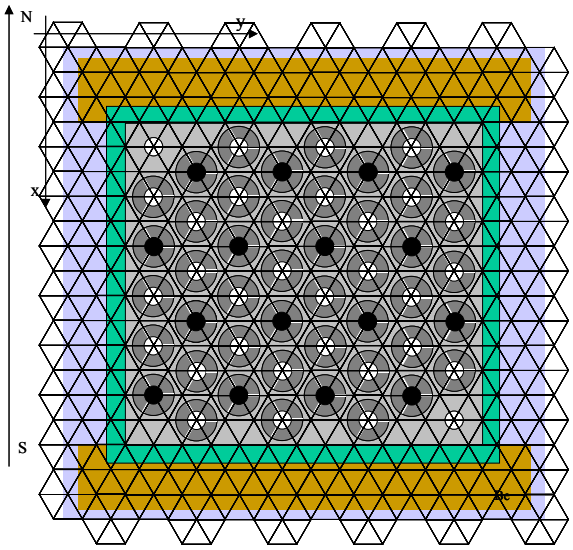


Figure 14 : JHR core and triangular mesh view

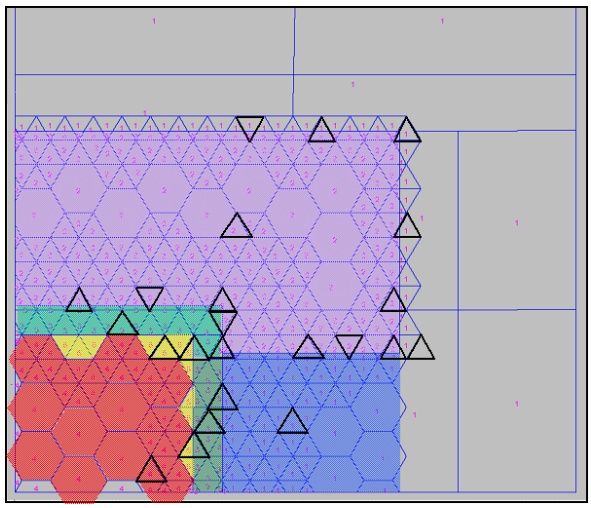


Figure 15 : 2D geometry of reflector constant calculation

5.2 BOL results

Two configurations have been considered to validate BOL whole core calculation : without control rod and with 12 Hafnium control rods.
The reference Monte Carlo calculations were obtained with the TRIPOLI4 code without any simplifications; all geometry details has been represented and punctual cross sections were used. 50 Millions of particles were generated. The multiplicative factor is so determined with a precision of about 15 pcm (1σ) and the radial fuel plate power uncertainty arises to only 0.15%. This TRIPOLI4 simulation requires 10 hours on a Parallel Compaq Alpha Server using 8 processors.
First, the degree of the polynomial element and the integration type were analyzed. A parabolic element is required and the Gauss integration method gives better results than the Gauss-Lobatto's one. A 3D core calculation requires then about 10 minutes.
Several possibilities for the definition of the diffusion coefficient are given in CRONOS2. The standard B_1 homogeneous diffusion coefficient cannot be used due to the assembly and reflector scheme based on heterogeneous zone homogenizations. Therefore, the homogenized transport cross section for each media is used to determine the diffusion coefficient ($D=1/3\Sigma_{tr}$).

The comparison of the HORUS3D/N-V1 results with the TRIPOLI4 reference are presented Table 5, Figure 16, Figure 17, Figure 18 and Figure 19. One can observe that the multiplicative factor is particularly well determined in both cases, the efficiency of the control rods is determined with a very satisfactory accuracy.
Besides, these good results can also be observed for the flux in the water reflector and also in the Beryllium reflector that causes an important increase of the thermal flux.

Table 5 : Comparison of HORUS3D/N-V1 and TRIPOLI4 multiplicative factor with control rods

	Keff With control rod assemblies	Keff Without control rod assembly	Control rod efficiency
CRONOS2	1.02669	1.18552	-13049 pcm
TRIPOLI4	1.02525 ± 15.10^{-5}	1.18279 ± 16.10^{-5}	-12991 ± 18pcm
discrepancy	137 ± 14 pcm	195 ± 11 pcm	-0.4 ± 0.2%

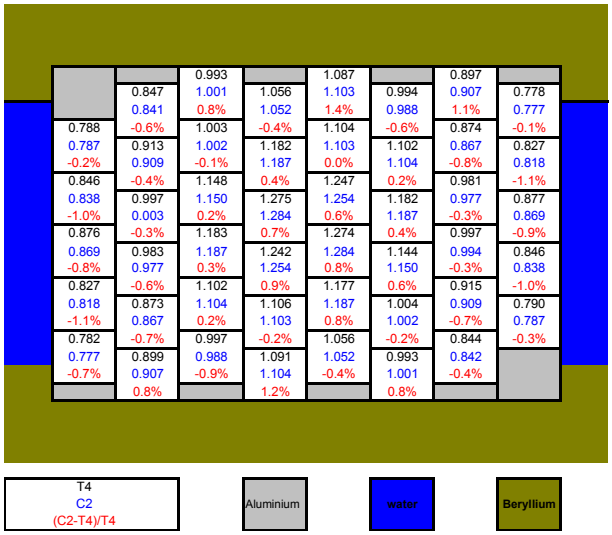


Figure 16 : Assembly power map discrepancies with TRIPOLI4 results – Without CRA

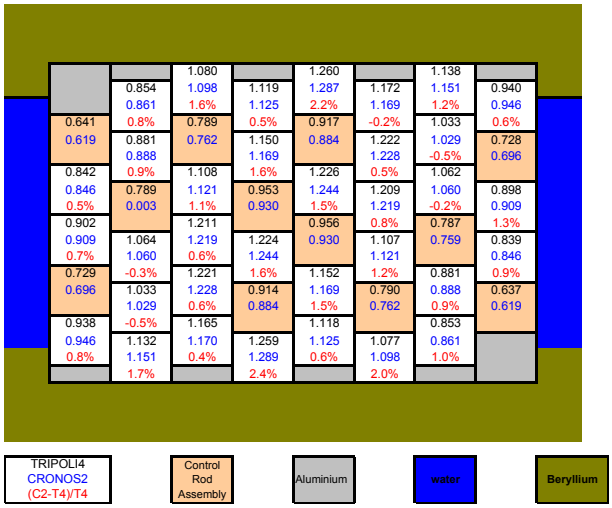


Figure 17 : Assembly power map discrepancies with TRIPOLI4 results – With CRA

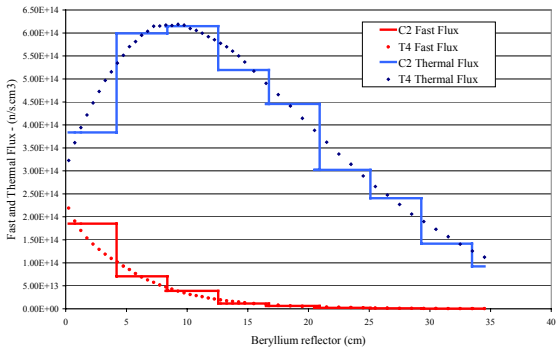


Figure 18 : Flux discrepancies in the Beryllium reflector (without CRA)

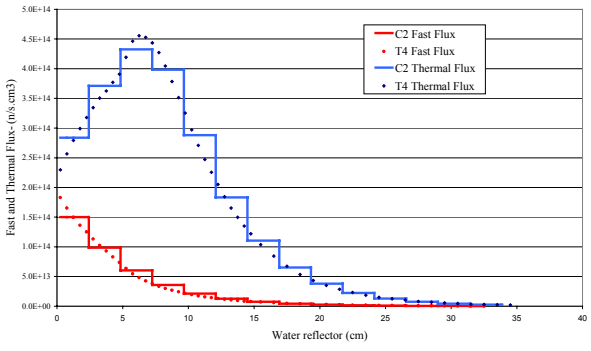


Figure 19 : Flux discrepancies in the Water reflector (without CRA)

5.3 Burn-up calculation

Due to the fuel assembly homogenization, a macroscopic depletion calculation is used in HORUS3D/N. Nevertheless, the evolution of Xenon and Samarium concentrations is directly taken into account by there microscopic cross sections.
In the same way than the assembly burn-up scheme validation, a reference calculation has been made dividing the time variable in small enough steps in the CRONOS2 code. An optimal time mesh has been determined in order to follow the evolution of Xenon and Samarium concentrations and also the 3D spatial burn-up variations.
The optimal time integration points are 0, 150, 500, 1000, 2500, 4000, 7000, 12000, 18000, 24000, + every 8 GWd/t. The residual bias is under 10 pcm along the burn-up.
Nevertheless, one can observe strong spatial gradient of the flux in fuel assemblies at the core/reflector interface. The homogenization could introduce bias in the burn-up calculation. Soon, the next APOLLO2 developments will allow a whole detailed core calculation in order to determine the potential bias. A fine Monte Carlo depletion calculation cannot be presently used according to the required running time to achieve the uncertainty target.
Otherwise, the important flux level in the reflector leads to the production of Lithium-6, which is a significant neutronics poison. A specific procedure has been so developed in HORUS3D in order to take into account the Beryllium depletion that could be more or less important according to the Zirconium shield dimension (Figure 2). This part of the core drastically reduces the fast flux that determines the Lithium production.

ACKNOWLEDGEMENTS

The authors are greatly indebted to the code development teams of Saclay and acknowledge the support of the JHR project team (Cadarache).

CONCLUSION

The preliminary design studies led to the definition of the main options of the future European MTR : Jules Horowitz Reactor, and a reference configuration has been designed. The Definition Studies, just starting, will optimize the JHR performances, testing modifications from the reference configuration. The computational tools, required for these studies, have to face up three difficulties : the specific characteristics of the JHR lead to modeling problems, the running time of the developed schemes has to be short enough for the design studies and the results have to be guaranteed by Validation studies. These difficulties, combined to the lack of specific integral experimental data, require a rigorous methodical approach. An adapted and consistent neutronics/thermohydraulics code package: HORUS3D (HOrowitz Reactor simulation Unified System) is developed. The neutronics route has been presented with the Validation methodology based on successive benchmark definitions.
The assembly neutronics route is performed with the APOLLO2 code and its 172 groups library and an exact 2D collision probability method. Thanks to the APOLLO2 modularity, a two level scheme has been developed, allowing appreciable time saving without loss of precision: Two successive benchmarks, for which a reference solution has been given by a polycinetic Monte Carlo simulation (TRIPOLI4), allowed the definition of the optimal options for the self-shielding and the flux calculation. Initial assembly reactivity is so determined with a residual bias of about 100 pcm. A depletion calculation reference calculation gave the right step size to integrate the Bateman equation and to compute the self-shielding along the burn-up.
The control rod assemblies have been subject of a particular treatment in order to take into account the important self-shielding in the solid hafnium rods. This strong localized absorption necessitates the use of a heterogeneous/homogeneous equivalence procedure, a unique feature of the APOLLO2 code.

The 3D core neutronics route uses the new finite elements developments in the CRONOS2 code. The tedious task of constructing the core geometry with 145 000 prisms is assumed by the procedural possibilities of the CRONOS2 code. The reflector constants are obtained by an exact 2D transport resolution on a quarter section of the core, thereby taking into account the strong heterogeneity of the core reflector interface.
The use of a 6 triangles decomposition with parabolic polynomial integration gives excellent results in comparison with reference heterogeneous polycinetic TRIPOLI4 results. The discrepancy on the initial reactivity level is less than 200 pcm and the maximum difference on the assembly power distribution is 1.4% at the beryllium reflector interface (hot spot).
Hence, the first version HORUS3D/N package allows the modeling of JHR core with a great confidence and will be used for the Definition Studies of the Horowitz Reactor.
This Validation will be followed by the comparison of HORUS3D results against experimental results. In order to complete the experimental database, an ambitious experimental program is in preparation. The first phase, foreseen during 2003, will focus on the fuel reactivity qualification by analyzing the effect of an UMoAl rod in an adapted critical UOX lattice. The second phase, planed for 2007, consists of criticality experiments with a small lattice of fuel assemblies in reference and off-reference conditions. This phase, much more extensive than the first, will allow the qualification of the assembly power map, control rod efficiency, reactivity coefficients, Beryllium reflector effect with the actual characteristics of the JHR assemblies.

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