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Document Title

COMPARATIVE SYNTHESIS AND ANLYSIS OF THE EUROPEAN RESULTS ON THE HTTR's CORE PHYSICS BENCHMARKS

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INTRODUCTION

HTR appears as a promising concept for the next generation of nuclear power reactor. In this context, the European scientific community must have operational tools to perform as well conceptual design studies, industrial calculations as best-estimate or reference calculations. This imply to use in a near future, besides Monte Carlo codes, the multigroup diffusion method with FEM to model a HTGR core with its reflector, with taking into account the thermal feedbacks and the inserted control rods in the reflector, treating of non diffusing regions (cavities), … in a core depletion calculation and all of that whatever the concept is (pebble or prismatic).
Therefore, validation and qualification steps are always needed. Of course code to code comparison and critical facilities have been used for validation in the past but, only a small amount of validation is available at elevated temperature or from comparisons at operating plants. Moreover, on one hand the codes and associated methods may have progressed and on the other hand, the HTGR design evolutions and changes lead today to some new core configuration (geometry, fuel, …) for which reference does not exist.
Core physics calculation tools are available in the participating organisations both for pebble bed and block-type fuel and are validated for the former HTR concept conditions and a limited set of fuel types, such as uranium or thorium. New annular core configurations, ultra high-burn-up, actinide burning or waste minimisation strategies impose additional requirements. For all these reasons decribed above, the objectives of the Work Package 1 (WP1) are:

- to contribute to the code validation
- to qualify and improve the methods for modeling the HTGR

This work is based on the HTTR and HTR-10 reactors recently started-up and for which benchmarks have been proposed through the IAEA (CRP-5). The HTTR with annular core configurations at first criticality and the HTR-10 provide experimental data for the validation of the codes in an extended spectrum of fuel cycles and core geometries.

This report constitutes a deliverable for the European contract HTR-N. It provides a summary of the works performed in the work package 1 during one and half year. Three partners are involved in this work package: FZJ in Germany, NRG (and IRI) in Netherlands and the CEA (work package manager). The synthesis presented in this report concerned the *HTTR's start-up core physics benchmark*. This benchmark proposed through the Coordinated Research Programme of the IAEA (CRP5), has been calculated by nine countries with large discrepancies in the results. Both the diffusion and the Monte Carlo codes used within the CRP5 underestimate the number of fuel columns needed to get critical the HTTR. Two tasks of the WP1 are concerned by the HTTR. In the following report, the results of task 1.1 and task 1.2 are presented together to obtain a consistent description.

Task 1.1: HTTR First Criticality Discrepancies

The HTTR gathers several potential difficulties to model ; small size core, high heterogeneity and core/reflector interface problems, double geometric heterogeneity, large streaming effect, control rods inserted in the reflector...
The reasons for the discrepancies observed in the preliminary performed calculations have been investigated further. Another approach with some Monte Carlo calculations gave

better results; the codes used by European organisations were MCNP, KENO and TRIPOLI4. So, there is a great evidence that, along with HTTR mass balance uncertainties (e. g. graphite impurities), there may also be a real challenge in the improvement of the calculation methods. For instance the description of double heterogeneous fuel in the cell calculations. And it could be necessary to perform a more local homogenisation of HTTR assemblies, with equivalence adjustments, to take into account the voided control rod channels, with their neutron streaming, in 3D diffusion core calculations. It should be mentioned that the predicted critical configurations of the HTTR where rather asymmetrical. Thus there is a great interest in analysing symmetrical core geometries as described in task 1.2.

Task 1.2: HTTR New Configurations

With the experience gained in task 1.1 only the annular core configuration obtained for the first criticality is tackled. In this task, some selected new configurations that have already been realised during the step-wise fuel loading of the HTTR are calculated and the results are compared with measured values. New configurations from the annular to cylindrical core geometry with completed fuel loading at room temperature are concerned.

The present comparative synthesis of the calculations performed with different codes systems commonly used in Europe relies on the works of H. Brockmann and U. Ohlig from FZJ, Han de Haas and E.J.M. Wallerbos from NRG and F. Damian at CEA.

After a brief presentation of the calculation scheme used to model the HTTR, the former results obtained in 98 and 99 are reminded and discussed. Then, some important physical phenomena involved in this reactor have been identified. Their impact on the model assumptions quantified by the different code systems allowed improving the methods and getting better results as well the first criticality is concerned as the others core configurations.

NUCLEAR DATA

As for the pointwise cross section used in the Monte Carlo calculations, the 123 and 172-group cross section (XS) libraries come from the JEF2.2 evaluated nuclear data file and treated by NJOY. For the present calculations, the existing multi-group libraries have been used without specific reprocessing with NJOY. Therefore, the multi-group cross sections are weighted by classical Maxwell+1/E+fission spectrum.

THE MONTE CARLO CALCULATIONS

Two MC codes have been used in Europe to model the HTTR. First, the KENO (IRI) code associated with a multigroup approximation (172 gr). The KENO calculations should then be considered as transport calculations and as an alternative to the core diffusion calculations. The second code named TRIPOLI-4 (CEA) comes near to the reference calculation whilst pointwise cross sections are used everywhere in the core except in the fuel rod region where an assumption is necessary due to the presence of the coated fuel particles (CFP). Indeed, codes like MVP and MCNP contain models, which allow taking into account the stochastic position of the CFP. Another possibility to treat this fuel region would be to place regularly the CFP in the fuel rod zone. The last way that has been adopted with TRIPOLI-4 consists in generating multigroup cross sections (172 gr) with the transport code APOLLO-2 (CEA) in which a model is available to treat the double geometric heterogeneity. Therefore pointwise and multigroup cross sections are used simultaneously in one run.

CROSS SECTION GENERATION FOR THE DIFFUSION CALCULATIONS

The general methods and assumptions used to model fuel and block elements and to generate the cross sections for the core calculations are gathered in Table 1. Some illustrations are also provided in annexe.

As far as the core diffusion models are concerned, the streaming effect is treated by the uses of anisotropic diffusion coefficients ($Dz \neq Dr$). These diffusion coefficients can be estimated by the way of an heterogeneous neutron leakage model included in the transport code as it is the case for WINS-7 (NRG). The homogenised fuel block regions contain therefore anisotropic diffusion coefficients taking into account the presence of large coolant channels or control rod guides which increases neutron streaming in the axial direction. Not available in the SCALE-4 (IRI) system, the heterogeneous leakage model of APOLLO-2 (CEA) did not run at this time with the 2D-generalised-geometry module used for the HTTR calculations. Consequently, the group constants provided to CRONOS-2 (CEA) and BOLD VENTURE (IRI) have only homogeneous diffusion coefficients. Finally, The MARCOPOLO (FJZ) code has been used to adjust the homogeneous diffusion coefficients calculated by TOTMOS (FZJ) and thus given to CITATION (FZJ) in form of correction factors.

Table 1 : Cross Section Generation for the Diffusion Calculations

<table>
<tr><th>WIMS 7</th><th colspan="2">SCALE 4</th><th colspan="2">APOLLO 2</th><th colspan="2">NITAWL/ TOTMOS</th></tr>
<tr><td></td><td colspan="2">172 gr
1D spherical cell
Self shielding + Dancoff</td><td colspan="2"></td><td colspan="2">123 gr
1D spherical cell
Self shielding + Dancoff</td></tr>
<tr><td>69 gr - Pij
1D cyl. fuel cell
Double hete.
<u>Self shielding</u>
B^2 crit.</td><td colspan="2">172 gr – Pij
1D cyl. fuel cell

B^2 crit.</td><td colspan="2">172 gr - Pij
1D cyl. fuel cell
Double hete.
<u>Self shielding</u>
B^2 crit.</td><td>123 gr - Pij
1D cyl. fuel cell

$B^2 = 0$</td><td>123 gr - Pij
1D cyl. BP cell

$B^2 = 0$</td></tr>
<tr><td>16 gr - Pij
2D ‘multi-pin’
B^2 crit.
hete. leakage
no equivalence#</td><td rowspan="3"></td><td rowspan="2"></td><td>172 gr - Pij
2D
B^2 crit.
homo. leakage
no equivalence#</td><td rowspan="3"></td><td rowspan="3"></td><td rowspan="2"></td></tr>
<tr><td></td><td rowspan="2"></td><td rowspan="2">123-gr cell averaged
$\sigma_{123gr}(^{10}B)$ adjusted from
S_n R-Z BP cell.</td></tr>
<tr><td></td><td>172-gr cell averaged
σ_{172gr}(isot)
172 gr – Pij 1D cyl. core</td><td></td></tr>
<tr><td>2-gr <u>block region averaged</u>
Σ_{2gr}(isot) for PANTHER</td><td>172-gr <u>fuel averaged</u>
σ_{172gr}(isot) for KENO</td><td>13-gr <u>core reg. averaged</u>
σ_{13gr}(isot) for BOLD VENT.</td><td>8-gr <u>block averaged</u>
Σ_{8gr}(isot) for CRONOS</td><td>172-gr <u>fuel averaged</u>
σ_{172gr}(isot) for TRIPOLI</td><td colspan="2">4-gr <u>cell averaged</u>
σ_{4gr}(isot) for CITATION</td></tr>
</table>

 # as a first approach no equivalence factor has been applied between the tr. 16gr -> diff. 2gr calculations (WIMS-PANTHER) and the tr 172 gr -> diff. 8 gr calculations (APOLLO-CRONOS)

THE FORMER CORE CALCULATIONS

Calculations performed with the different codes systems are presented below. Four diffusion codes have been used. The KENO calculations can be considered as a 3D transport calculations whereas the TRIPOLI-4 runs are simultaneously a Monte Carlo calculation with pointwise cross sections and a 172 gr transport calculation on the fuel compact region.

Table 2 : Core Calculations

	CITATION	PANTHER	B. VENT.	KENO	TRIPOLI	CRONOS
	Diffusion 4 groups	Diffusion 2 groups	Diffusion 13 groups	M. Carlo 172 gr	M. Carlo 172 gr & pointwise	Diffusion 8 groups
	3D triang.	3D hexag.	RZ	3D	3D	3D hexag.
	1 reg/block	7 reg/block	6 rings			1 reg/block
	finite diff.	*finite elem.*	*finite diff.*			*finite elem.*
	6 mesh/bl.	7 mesh/bl.				24 mesh/bl
30 col.	**1.1607**	**1.1595**	***1.1925*#**	**1.1600 ± 0.0005**	**1.1503 ± 0.0009**	**1.1738**
18 col.	**1.0254**			**1.0240 ± 0.0005**	**1.0211 ± 0.0009**	**1.0620**

#*corrected for the BP effect from the KENO calculations*

The experiments give the following values for both core configurations :

$\Delta k/k = 12 \pm 3.3$ % for the first one and **barely subcritical** for the simple core arrangement. The first value leads to a multiplication factor of **1.1363** but with an important uncertainty that must be emphasized. In these conditions, the differences between calculation and experiment are comparable and correspond to an overestimation of the core reactivity ranges from **$\Delta k = 0.014$ to 0.056** for the fully loaded core and **$\Delta k = 0.021$ to 0.062** near the first criticality.

Due to the large experimental uncertainty on the full-core excess reactivity, the following discussions will be first focus on the explanations of the discrepancies between diffusion and Monte Carlo calculations. Moreover, new data are now available to re-calculate the HTTR-FC and should permit to get nearer to the experiment.

MAIN COMMENTS

First of all, it seems to be important to note that the CITATION given values include the control rods insertion in the top of the side reflector for which a reactivity effect of $\Delta k = 0.004$ has been considered. Besides, the control rods insertion has been taken into account in the core modelling performed with PANTHER and KENO.

The higher discrepancies of the values evaluated by both BOLD VENTURE and CRONOS-2 are explained by the fact that the streaming effect is not taken into account here. Moreover, as it will be noticed below the rough axial representation of the boron pin in CRONOS-2 compensates the streaming effect, which is not modelised.

The relatively good accordance ($\Delta k < 0.003$) in the simple core configuration between both MC codes disappears in the fully loaded core configuration (Δk # 0.01). One explication could be that the P1 approximation describing interaction between neutrons and the graphite would have a higher impact on the neutron leakage in case of the harder neutron spectrum of the fully loaded core.

AXIAL HOMOGENISATION OF THE BURNABLE POISON (BP)

The BPs in the fuel blocks present an axial heterogeneity. The B_4C pellets are stacked with graphite disks put between them and can be modelled explicitly or not, throughout the cross section generation process. In order to evaluate the impact of these model assumptions, two comparisons have been done on core calculations performed with CITATION and TRIPOLI-4.

In the Monte Carlo calculation only the BP rods have been homogenised (B_4C-C) in the 3D detailed geometry and compared to the reference case given above (Table 2). As far as the CITATION diffusion calculation is concerned, it is in course of the cross section generation process that the BP adjustment, based on the S_n-RZ cell calculation, is considered (see Table 1). The cell averaged cross sections with and without BP adjustment have been then used in the core calculation.

Table 3 : Axial homogenisation of the BP

	reactivity effect - $\Delta k_{eff}/k_{hete}$ (pcm#)	
	TRIPOLI-4	CITATION
30 columns	**0.0220** (2224 pcm)	**0.0226** (2292 pcm)
18 columns	**0.0145** (1460 pcm)	**0.0198** (2000 pcm)

$10^5.ln(k_1/k_2)$

The spatial self-shielding effect of the B_4C is clearly highlighted. The homogenisation of the BP rods leads to an overestimation of the boron absorption, which is amplified with the number of fuel blocks loaded in the core although the neutron spectrum is harder. It is noteworthy that this effect is less emphasis by the diffusion calculation in the 18-columns related case for which it is more difficult to get flux weighted cross sections well representative of the core conditions.

Although less important it is interesting to note that if this effect is applied to the multiplication factor evaluated by CRONOS-2 model (Table 2) for which the BP are homogeneous, a $k_{eff} = 1.1996$ is obtained. This value is very close to the one calculated by BOLD VENTURE.

Besides, this overestimation has also been underscored in the spectrum calculations. The effect on the infinite multiplication factor ranges from 0.015 to 0.033 depending of the fuel block enrichment and is smaller for harder neutron spectrum (higher enrichment). The Δk values calculated by DORT for a BP cell (Table 4) lead to comparable Δk values than those obtained with TRIPOLI-4 on a 3D/2D fuel block geometry (Table 5).

Table 4 : Impact of the BP correction factor on the fuel block reactivity

R-Z BP CELL WITH DORT	Fuel block 993120 (enrichment 9.9 %)	Fuel block 343320 (enrichment 3.4 %)
$\Delta k_\infty/k_{hete}$	**0.0155**	**0.0335**

Table 5 : Fuel block MC calculations. BP homogenisation impact

Fuel block 993120 with TRIPOLI-4	3D hete. BP	2D homog. BP
k_∞ ($B^2 = 0$)	1.4187 ± 0.0005	1.3994
$\Delta k_\infty/k_{hete}$		**0.0136**
$\Delta(\Sigma_a\Phi)_{BP}$		*+ 11.1 %*

The comparison of the reaction rates between both calculations displayed in Table 5 lead to an overestimation greater than 10 % of the total absorption rate in the BP rods axially homogenised or not. On the contrary, similar absorption rates in the fuel compact are obtained between both cases.

FUEL BLOCK HOMOGENISATION

Two consequences due to the fuel element homogenisation in the core diffusion calculations can be identified:

- this can lead to an overestimation of the core reactivity by neglecting the neutron streaming in the cylindrical and annular holes in the core regions if the diffusion coefficients have not been adjusted or calculated precisely.
- the anomalies in the blocks like BP and their positions smeared over the entire block does not allow good representation of local absorptions. A solution, which consists in considering several regions in the block with different group constants allows to take into account block heterogeneities. However, this solution often requires equivalence factors to respect either the flux or the absorption rates between fine multigroup transport calculations on the heterogeneous block and broad group diffusion calculations with several homogenised regions per blocks. This point will be discussed later.

RADIAL HOMOGENISATION EFFECT

This last point has been evaluated with TRIPOLO-4 and CRONOS-2 in a 2D radial core configuration (without axial leakage). In this case the streaming effect and the BP axial homogenisation are not considered. Therefore, the results given in Table 6 point towards the radial homogenisation of each block in one region a piece. Beside, for the homogenised case, the 2D-diffusion core calculations give results close to those obtained by the Monte Carlo where the fuel blocks are represented by homogeneous 172 group cross sections.

Table 6 : Fuel block radial description impact on the core reactivity

	k_{eff}(2D) simplified core (no axial leakage, *<e=9.4%>*)			**$\Delta k/k_{hete}$**
	TRIPOLI-4 hete.	**TRIPOLI-4 homog.**	*CRONOS-2 homog.*	TRIPOLI-4
30 columns	1.28837 ± 0.00069	1.31985 ± 0.00063	*1.32675*	**0.0244**
18 columns	1.14040 ± 0.00087	1.18554 ± 0.00075	*1.18630*	**0.0396**
	k_{eff}(2D) simplified core (26 gr, no streaming and BP adjust.)			**$\Delta k/k_{hete}$**
	CITATION hete.	**CITATION homog.**		CITATION
18 columns	1.0419	1.0840		**0.0388**

As far as the CITATION calculations are concerned the first results were given for homogenised fuel blocks with only six triangular meshes per block as indicated in Table 1. When taking into account a detailed radial description of the fuel blocks with 24 radial meshes and its associated new fuel and BP cell models, the multiplication constant decreases significantly as can be seen also on Table 6. Once again, the physical effect observed here with two different codes and methods leads to very close results.

The reduction of the homogenisation effect for the fully loaded core is essentially due to the hardening spectrum observed in this case. This reduce the impact of the underestimation of the BP

absorption and moreover, the neutron spectrum becomes closer to the one existing in the 2D transport calculations carried out on the blocks with a white boundary condition.

In the 18 columns core configuration, the neutron spectrum seen by the BP during the 2D transport calculations are very different from the one observed in the core conditions. A next step in the calculations to explain the discrepancies with the experiment will have to take into account surrounding regions for the fuel block under study as it has been done with WIMS-7. However, this has the disadvantage to increase the complexity of the transport calculations and to multiply the number of cases to be treated.

To complete this analysis of the impact of the radial description of the fuel block, new finite elements recently implemented in CRONOS-2 has been used. They allow taking into account the exact position of the burnable poison in the fuel blocks. Indeed, from the 2D transport calculations illustrated on the Figure 1, the fuel element was initially homogenised in one hexagonal finite element. Then, with the help of the new available finite elements, two different meshes were considered to describe the fuel elements with 24 radial meshes : 24 equilateral triangles (type I) or the cutting out depicted below (type II). Only the last one has been kept in the final model because of the fact that it is the only one that allows homogenising the poison with its associated graphite without homogenising partially the fuel compacts.

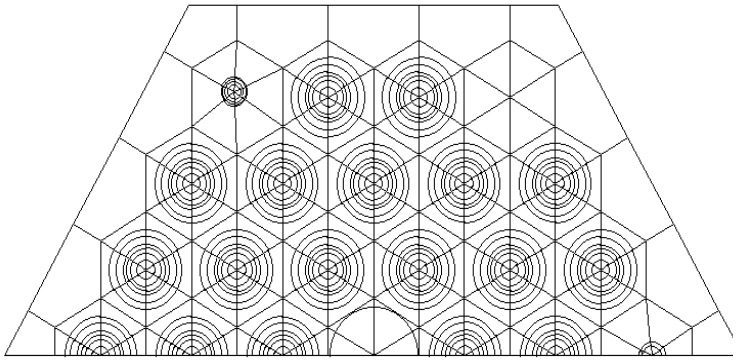
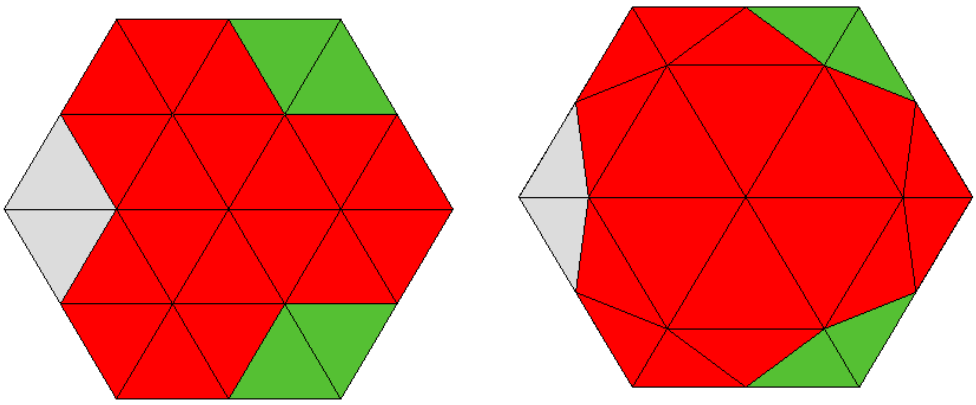


Figure 1: P_{ij}-2D transport calculation

Figure 2 : Finite element mesh type I and type II



The quantified effect is presented in the chart below. It has been evaluated for both configurations, 18, 24 and 30 columns, on the basis of a 2D simplified core with no axial leakage and an average uranium enrichment. As previously mentioned, the most important impact is obtained for the 18 columns core loading. The Figure shows the differences observed between the diffusion calculations and the Monte Carlo calculations already cited in Table 6.

Figure 3 : 2D calculations, 18 columns

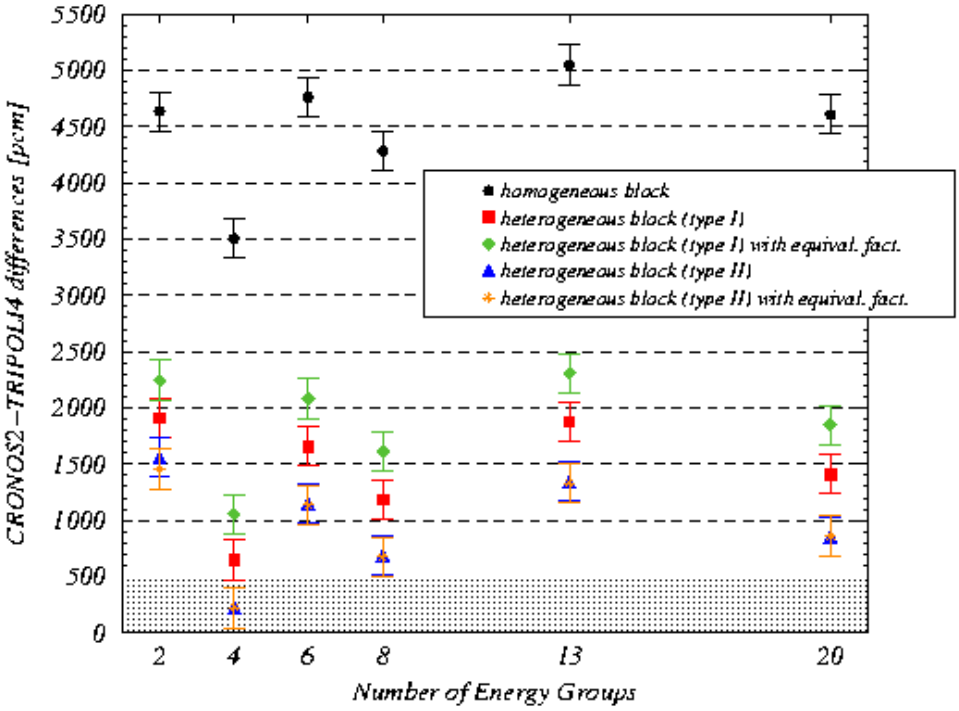
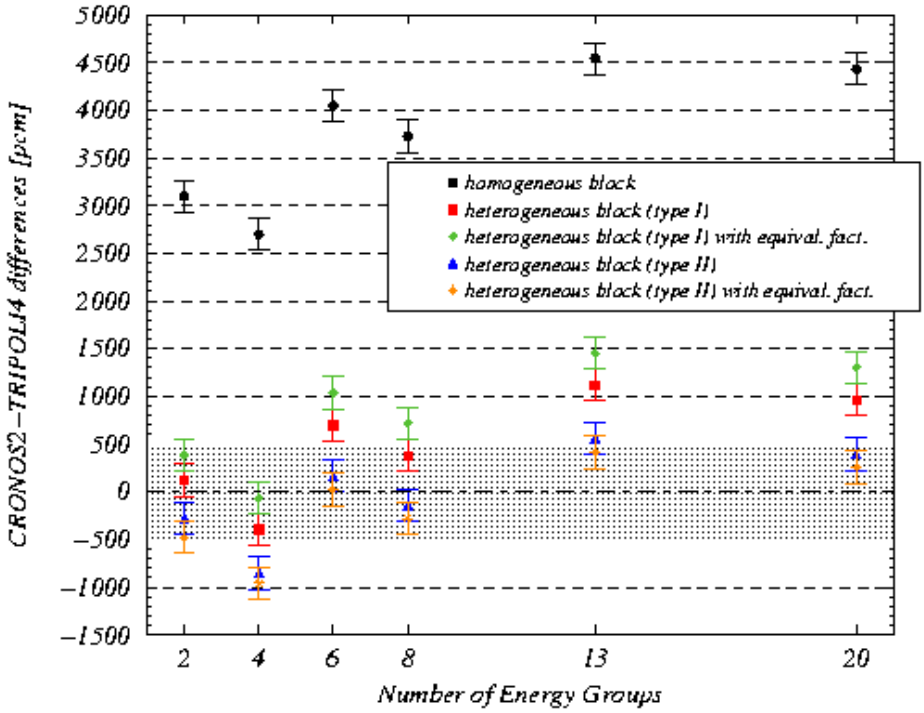


Figure 4 : 2D calculations, 24 columns

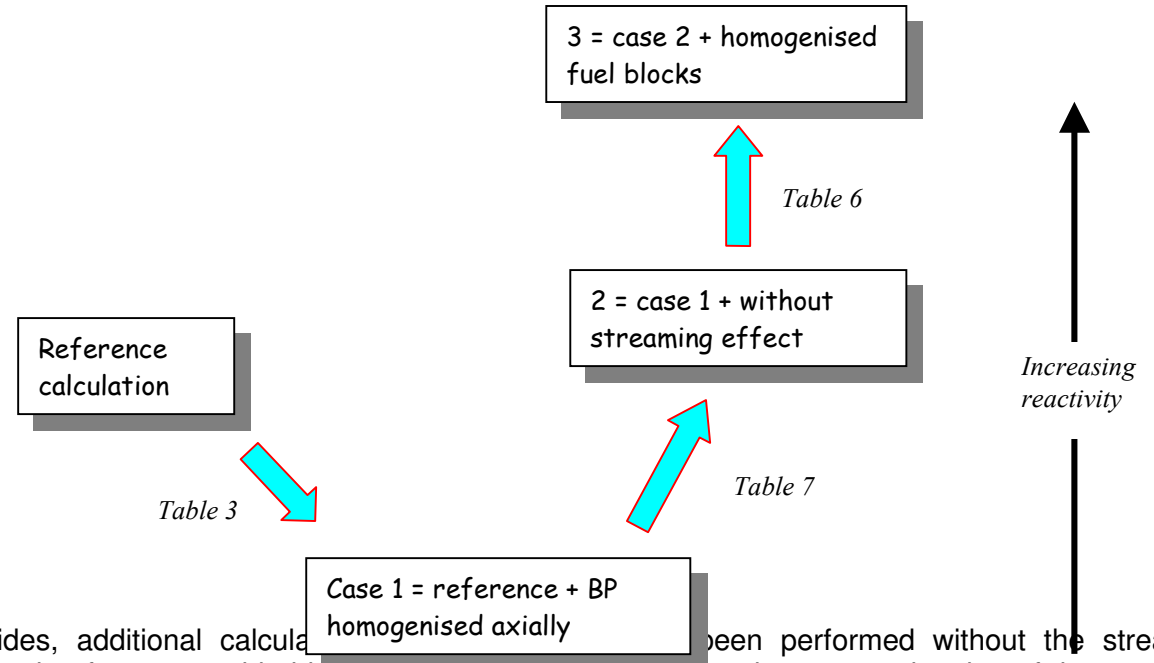


Compared to the previous homogeneous hexagonal model for which an effect of about 4 % (depending on the number of energy group) can be seen, the new heterogeneous (type II) model leads to some discrepancies ranging from 1 to 1.5 % with the reference calculation (TRIPOLI-4). This more realistic model leads to a higher absorption in the burnable poison in the fuel element but nevertheless the resulting gain (~ 3 % as can be seen in Figure 3 and 4) is less important than the ones expected and mentioned in Table 6.

Finally, the use of equivalence factors has been implemented in order to respect the global absorption rate between the APOLLO-2 transport calculations (172 groups) and the CRONOS-2 diffusion calculations with a few groups. This option has not been considered afterwards because of its small impact (Figure 3 and 4) on the finite element of type II.

STREAMING EFFECT

All the obtained values for tentatively quantifying this effect are gathered in Table 7. The former CRONOS-2 model does not take into account the streaming effect, the axial heterogeneous composition of the BP and the heterogeneities of the blocks (case 3 in Figure below). Both last cases have been quantified previously (Table 3 and 6). The streaming effect indicated Table 7 is then deduced from these last two points.



Besides, additional calcula been performed without the streaming correction factors provided by MARCOPOLO. This permit to have an estimation of the streaming effect alone.

Table 7 : Streaming Effect

	$\Delta k/k_{st}$ - 30 columns	$\Delta k/k_{st}$ - 18 columns
CITATION with and without streaming	**0.0132**	**0.0176**
KENO *simplified core <e=5.2%>, no BP* detailed and homogenised model	**0.0256**	**-**
KENO – BOLD VENTURE *no BP* detailed and R-Z homogenised model	**0.0280**	**-**
Estimated values deduced from TRIPOLI-4 / CRONOS-2 calculations	***0.0152***	***0.0185***

Finally, a comparison between the detailed core model of KENO and an homogenised core model of KENO and BOLD VENTURE has been carried out on a core configuration without BP. In this condition, the problem of the BP axial homogenisation is withdrawn and the differences between the obtained values provide indication on the streaming effect.

It appears that the $\Delta k/k_{st}$ evaluated from KENO and BOLD VENTURE can not be attributed to the streaming effect only. Homogenisation effect as described in the previous section obviously take place here. A 172 gr 3D transport calculations on the fully detailed core is compared to an 13 gr R-Z diffusion calculations with 6 homogenised rings. The R-Z and diffusion related assumptions have a small impact if it is compared to the $\Delta k/k_{st}$ obtained with a KENO det./KENO homog. assessments on a simplified core. Therefore, cross sections provided by the spectrum calculations and the homogenisation of the different kind of blocks in the rings should explain the above values.

If one assumes that the 0.0256 value obtained by KENO correspond to both the streaming and homogenisation effect and taking into account the order of magnitude of the streaming effect given by CITATION and TRIPOLI-4, the homogenisation effect would be near 0.01. This value is smaller than the one given in Table 6 (0.0244) and should be explained by the absence of BP in the KENO calculations.

IMPACT OF THE NUMBER OF ENERGY GROUP AND NEUTRON LEAKAGE ITERATION IN THE DIFFUSION CALCULATIONS

The use of few energetic group collapsed cross sections in the diffusion calculation and the application of a white boundary condition without critical buckling search in the spectrum calculation (fuel cell calculations) might be possible reasons for explaining the discrepancies.

Therefore, a study of the influence of neutron leakage feedback and different energy group structures on k_{eff} has been carried out with the CITATION code on a simplified 1 D cylindrical core model with 3 spectrum zones [6]:

- an inner graphite zone representing the dummy fuel blocks,
- an annular core zone with 18 fuel columns (fuel block type 633325: e = 6.254 %),
- and an outer annular graphite zone representing the permanent and the outer replaceable reflector.

Several iterations between the CITATION core calculations and the cylindrical cell calculations were performed. At the beginning of iteration all leakage terms are zero (white boundary condition and $\mathbf{B^2 = 0}$). In the subsequent iterations, leakage terms are provided by the CITATION calculations in different forms:

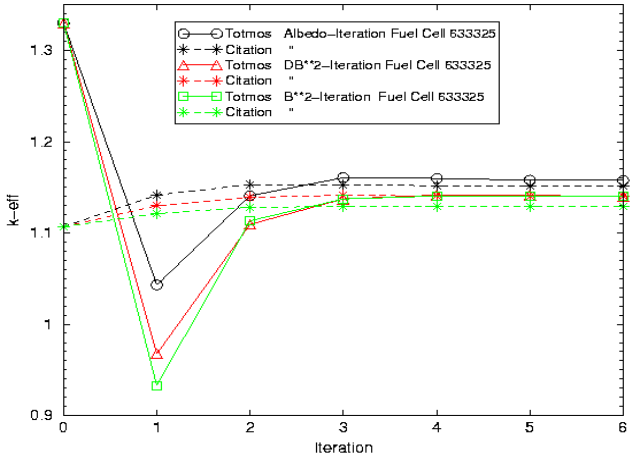
- DB^2 iteration (the leakage in each fine group is input in form of $L_i = (DB^2)_g$ where i is the fine group number in a broad group g)
- B^2 iteration (the leakage in each fine group is input in form of $L_i = D_i B^2_g$)
- Albedo iteration (the leakage is input in form of albedos α_i, where
-

$$\alpha_i = \frac{1 - 2(DB^2)_g \phi_g^c V_c / \phi_g^s A_s}{1 + 2(DB^2)_g \phi_g^c V_c / \phi_g^s A_s}$$

with Φ_c = average cell flux, Φ_s = flux at cell boundary, V_c = cell volume and A_s = cell surface).

The assumption of the same leakage/absorption ratio in the unit cell and the corresponding diffusion spectrum zone has been made. The figure below illustrates the different methods of iteration.

Figure 5 : k_{eff} behaviour for the several type of iteration



All the results are gathered in the following Table 8. It turns out that a 4 groups calculation with neutron leakage feedback is consistent with a 26 or 123 groups calculation ($B^2 = 0$). Therefore, the 26 groups energy structure has been retained as an optimum in the final CITATION model between a finer energy structure option with CPU time consuming and the 4 groups with leakage feedback option slightly difficult to manipulate. However, the main tendency that can be observed here is an increase of the discrepancies (by more than 2 %) related to an improvement of the model whatever is the method retained for enhancing this model.

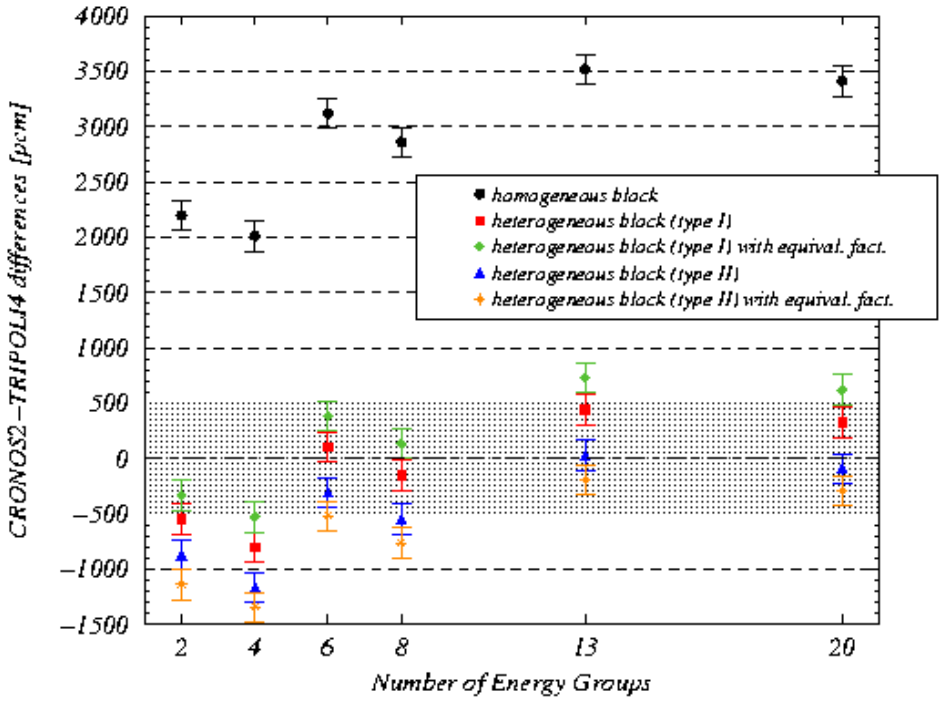
Table 8 : Simplified core k_{eff} depending of the iteration method

	4 groups no leak. iter.	4 groups six DB^2 iter.	4 groups six B^2 iter.	4 groups six alb. iter.	26 groups no leak. iter.	123 groups no leak. iter.
k_{eff}	1.10704	1.14013	1.12912	1.15145	1.13573	1.13685
$\Delta k^{\#}$	- 0.02981	+ 0.00328	- 0.00773	+ 0.01460	- 0.00112	-

$^{\#}$ *reference calculation with 123 energy groups*

To complete the analysis on the impact of the number of group taken into account in the diffusion calculation, it should be noticed that the calculations performed with CRONOS-2 does not lead to the same conclusion than the one observed with CITATION. Indeed, the comparison between the 2D diffusion and Monte Carlo calculations presented on the previous Figures 3 and 4 leads to some discrepancies, which seem to not indicate a specific trend depending on the number of groups. This is also illustrated in the Figure 6 below for the fully loaded core configuration where the number of considered energy groups range from 2 to 20.

Figure 6 : 2D calculations, fully loaded core



Moreover, as shown hereafter in the following section, the discrepancies observed with CRONOS-2 in 2D calculations may disappear in 3D (e.g. the 3D results with 4 groups is in very good accordance with the reference TRIPOLI-4). The none apparent dependency of the number of group in the CRONOS-2 calculations is likely due to the fact that the collapsed cross sections come from P_{ij}-2D transport calculations on the whole fuel or control blocks (with **critical B^2** search option) and this might reduce the impact of the white boundary condition and the number of energy groups used to collapse the cross sections.

PRELIMINARY CONSIDERATIONS ON THE CORE IMPURITIES

A simple exercise has been carried out with TRIPOLI-4 on the thin annular core configuration in order to estimate the impact of the graphite impurities on the reactivity. The impurity rate of only the 12 dummy fuel blocks at the centre of the core has been multiplied by a factor 1.5 and 2. As shown in the Table 1.9 below the latest value might lead to a barely critical state.

Table 9 : MC calculation results as a function of the impurity level

Dummy fuel block Impurity:	k_{eff}
Benchmark data: I_{ref}	**1.02110±0.00090**
150 % of I_{ref}	**1.01350±0.00090**
200 % of I_{ref}	**1.00070±0.00090**

Seeing that these impurity rates seem to be not realistic but that only 12 central blocks were considered this exercise might mostly explain the discrepancies with the experiments. However, new data (HTTR-FC2 benchmark) has been released considering new graphite impurities and the presence of air (N, O) in the graphite porosities of the fuel blocks, CR guide blocks, reflector and matrix of the fuel compact. According to the absorption cross section and the concentration of N^{14} in the pores of the graphite, the presence of air in the core amounts to saying that 1 ppm of natural boron equivalent will be added in each component of the core. The HTTR-FC2 re-calculation benchmark was a good opportunity to implement the new enhanced methods coming from all the previous analyses presented above.

A similar exercise has been performed with the help of the PANTHER code, considering the impurity level available in the HTR-10 benchmark data (Table 10). With all the control rods out, the difference in term of reactivity observed in the 3D core calculation is **$\Delta\rho$ = -0.013**.

Table 10 : Diffusion calculation results as a function of the impurity level (#weight fractions)

Impurity in	HTTR-FC specifications#	HTR-10 specifications#
Matrix	0.82e-6	1.35e-6
Sleeve	0.37e-6	1.30e-6
Block	0.40e-6	1.30e-6
Repl. refl.	0.37e-6	4.85e-6
Perm. refl.	1.91e-6	4.85e-6

HTTR FIRST CRITICALITY RE-CALCULATIONS (HTTR-FC2)

MONTE CARLO COMPUTATIONS

New reference calculations (Table 11) with TRIPOLI-4 were performed with and without taking into account the presence of the control rods slightly inserted in the upper part of the axial reflector. The impact of these CR, about **Δk ~ 0.003**, evaluated only in the 18 columns core configuration, is in accordance with the one evaluated by the Japanese with MVP (Monte Carlo), about **0.004**. Moreover, the presence of the detectors never considered here, has been evaluated with MVP to **Δk ~ 0.002**.

Nevertheless, the TRIPOLI-4 Monte Carlo results let always appear a deviation with the experiment at first criticality. It ranges from about **Δk/k = 1.9 %** for this thin core configurations. On the other hand, a quite acceptable **Δk/k of 0.4 %** is observed for the full core configuration. According to the large uncertainties on the experimental values especially in the 24 and 30 columns core configurations, the method improvement in the diffusion calculations should be validated and compared in priority to the reference Monte Carlo results.

Table 11 : : Reference calculation with TRIPOLI-4 (new available data)

Core configuration (**CR inserted into the axial reflector**)	$k_{eff} \pm \sigma$	**Experiment with inserted CR**
18 columns ***(without)***	1.01376±0.00039	
18 columns ***(with)***	**1.01055±0.00040**	**.9913**
19 columns ***(without)***	1.03292±0.00043	**1.0152**
30 columns ***(without)***	1.14433±0.00030	**1.1363**

DIFFUSION RESULTS

The final results coming from the CRONOS-2 calculations are partially gathered in the Figure 7 below. It is noticeable that the number of fuel columns needed to achieve criticality increases by about 7 in comparison with the former results (Table 2). Furthermore, some last additional calculations are in progress and will permit to conclude.

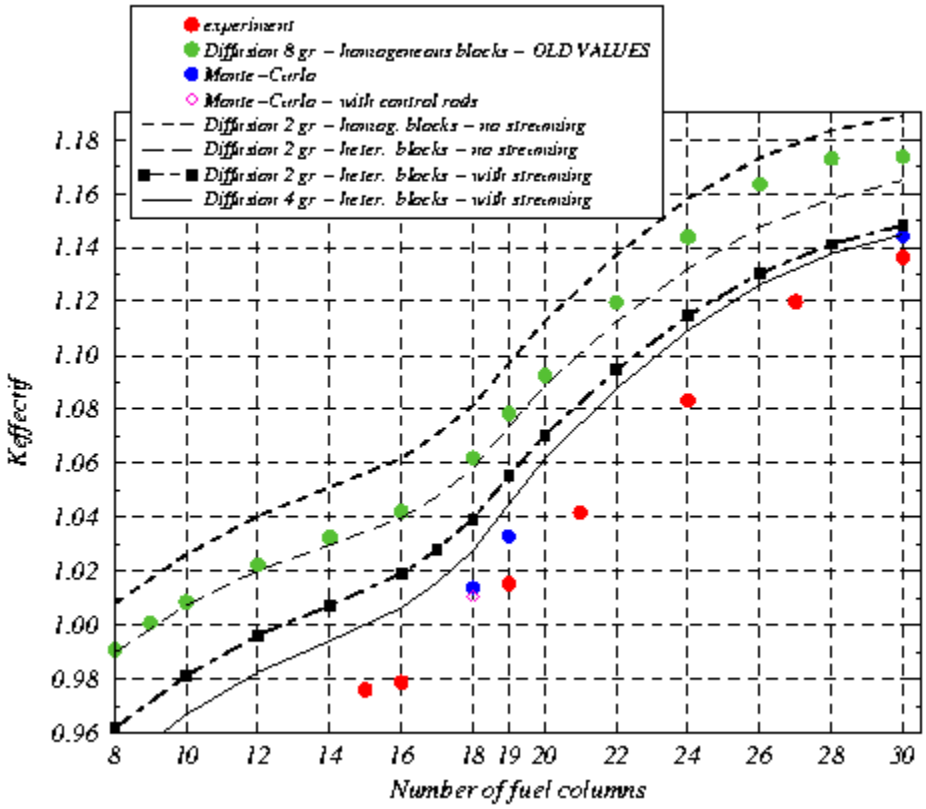
By comparing the 2-group diffusion calculations, the previous effects can be observed again as the model become more and more detailed. The 4-group model give better results particularly for the fully loaded core configuration for which the result is in total agreement with the reference calculation.

To conclude with the CRONOS-2 diffusion calculations, it turns out that the only remaining way to improve again the model would be :

- to take into account the CR inserted in the axial reflector (this has been done for the 18 columns configuration and give a similar effect than the one observed with the Monte Carlo, Δk ~ 0.003)

- to consider an other streaming effect related theoretical model. The Benoist method used for the treatment of the neutron streaming might not be applicable in the large channel of the dummy fuel blocks (18 columns) and underestimate this effect. In the other analytical model one allows to get new anisotropic diffusion coefficients has been tested (with 2 groups) for the thin annular core and seems to give better results ($\Delta k \sim 0.004$).

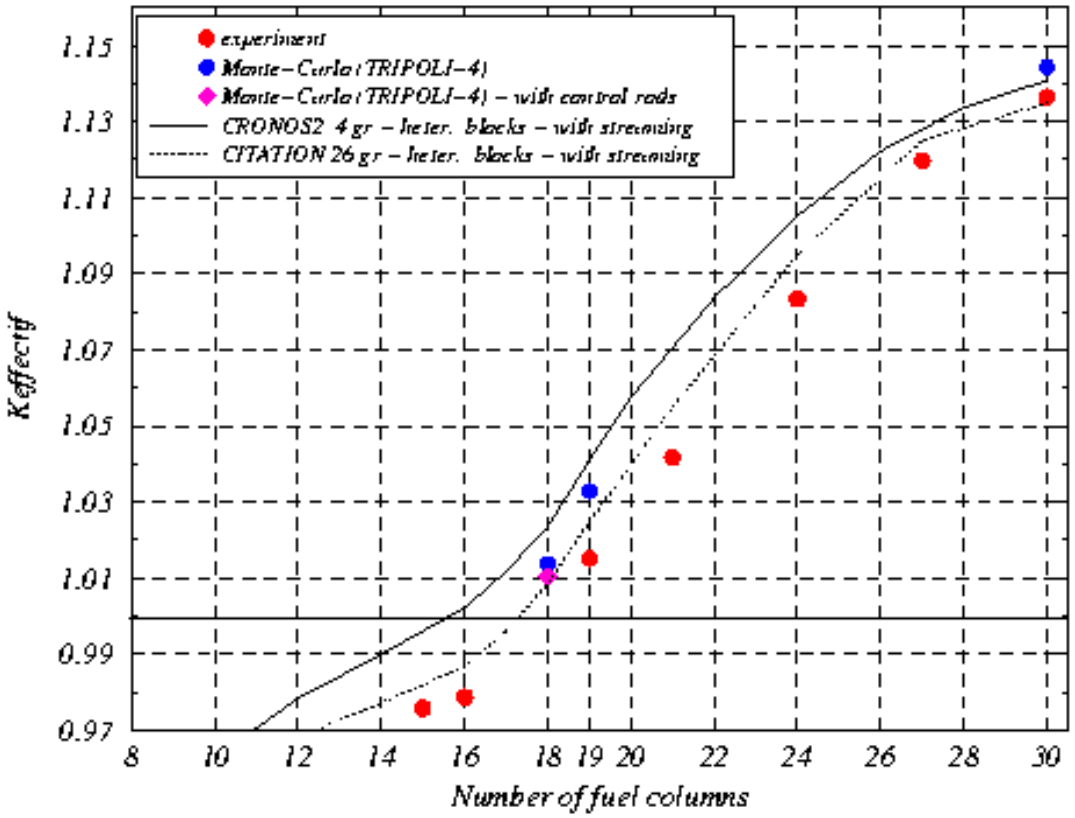
Figure 7 : CRONOS-2 results obtained with new available data (without CR inserted)



Nevertheless cumulating these both effects, the remaining discrepancy could only be explained by the fact that a method based on a cross section homogenisation from a fundamental mode calculations (infinite medium) is barely pertinent for the 18 columns core configuration. The actual environment (reflector blocks) should be considered and should take place instead of the white boundary condition in the 2D APOLLO-2 transport calculations, before homogenising and collapsing locally the cross sections inside the fuel elements.

This important remark is confirmed by the impact of the neutron leakage iteration emphasized with the TOTMOS-CITATION code system. Finally, it is noteworthy that this effect tends of course to disappear for the fully loading core configuration where all the discrepancies become smaller.

Figure 8 : Last HTTR results including a $\Delta k = 0.004$



As far as the CITATION results are concerned, those coming from the detailed annexe are presented in Figure 8 with the experiment, the TRIPOLI-4 and the CRONOS-2 values. An important point concerns the efficiency of the control rods inserted in the axial reflector, $\Delta k = 0.004$, that is included to the diffusion results shown in this chart.
The final model used in CITATION incorporates :

- a 26 group energy structure
- an heterogeneous fuel blocks description (4 vertical and 24 horizontal meshes per element)
- a neutron streaming correction remaining unchanged
- but an unchanged treatment of the BP poison

The CITATION results seem to be quite acceptable. However, as mentioned in annexe a more realistic model of the fuel burnable poison has been developed but increases again the discrepancy at the first criticality. However, a too small streaming effect also suspected (as with CRONOS-2) might counterbalance the effect of the refined model of the BP. These considerations will have to be confirmed by further investigations.

CONCLUDING REMARKS

Based on the revised data of the HTTR benchmark, the recalculation of the first criticality with the TRIPOLI-4 **Monte Carlo** code allowed to reduce the discrepancy by about a factor two (from ~ 2 % to 1 % Δk/k). On the other hand, the result obtained for the fully loaded core configuration is quite acceptable taking into account the uncertainties associated with the experimental values. The remaining deviation for the thin annular core (first criticality) might be explained by the uncertainties of the graphite impurities for which the impact is very important in this core configuration (dummy fuel blocks in pure graphite in the central part of the core).

From these considerations, the Monte Carlo results should be used to compare and to qualify the methods employed in the **diffusion calculation**. New implemented methods coupled with new benchmark data allowed obtaining good enough results for all the 3D diffusion calculations in the full core configuration. Near the first criticality, the number of fuel columns needed to achieve criticality increases by about 7 (CRONOS-2) and 2 (CITATION) in comparison with the former results.

The CITATION calculations seem to be in good accordance with TRIPOLI-4 but with a well-identified underestimated streaming effect and without considering the most realistic model to describe axially the BP. As far as the CRONOS-2 calculations are concerned, further investigations in progress should permit to conclude.

All the final results are gathered in the following Table:

Tableau 12 : The new core calculations together with the experimental results

	CITATION	TRIPOLI	CRONOS	EXPERIMENT
	Diffusion 26 groups	M. Carlo 172 gr & pointwise	Diffusion 8 groups (4 gr.)	
	3D triangular	3D	3D hexagonal	
	3 reg./block		3 reg/block	
	finite difference		finite element	
	24 meshes/block		24 meshes/block	
30 col.	**1.1336** [1]	**1.13833** [2] ***± 0.00090***	**1.1451 (1.1362)** [2]	**1.1363 ± (*> 3.6 %*)**
24 col.	**1.0944** [1]	**-**	**1.1096 (1.1000)** [2]	**1.0834 ± (*> 2 %*)**
19 col.	**1.0263** [1]	**1.02692** [2] ***± 0.00043***	**1.0432 (1.0351)** [2]	**1.0152 ± ?**
18 col.	**1.0080** [1]	**1.00855** [2] ***± 0.00090***	**1.0275 (1.0178)** [2]	**subcritical**

[1] *CR inserted considered Δk = 0.004 and detector impact included Δk = 0.002*
[2] *detector impact included Δk = 0.002*

All calculational results obtained for the fully loaded core configuration agree well with each other and with the experiment, moreover when taking into account the experimental uncertainties. Furthermore, it is seen that there is an excellent agreement between the diffusion CITATION and Monte Carlo TRIPOLI calculational results. Altogether it turns out that the following procedures seem to be necessary for a better approach to the experimental results:

- detailed heterogeneity of the BP- and fuel-region in the whole core calculation,

- use of fine group constants in the whole core (FZJ) diffusion calculation or the consideration of the actual environment of the fuel blocks in the (CEA) transport cell calculations in order to describe the core/reflector coupling accurately,
- consideration of the axially heterogeneous distribution of the BP by 2d cell calculations (FZJ) or by 3d diffusion calculations (CEA and NRG)
- treatment of the enhanced neutron streaming whether by an adaptation of the diffusion constants to Monte Carlo calculations (FZJ) or by a leakage model combined with an analytical model (CEA).

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[2] *Analysis of the HTTR with Monte Carlo and Diffusion theory. An IRI-ECN intercomparison*. – J.B.M. de Haas, E.J.M. Wallerboos – Report ECN-I-98-056 and IRI-131-99-004.

[3] *HTTR criticality, physical parameters calculations and experimental results* – J.B.M. de Haas, E. Turkcan – ICENES 2000 (September 2000).

[4] *Calcul du benchmark neutronique de démarrage du Coeur HTTR* – F. Damian, X. Raepsaet – CEA Report : SERMA/LCA/RT/99-2658/A.

[5] *CEA's benchmark calculation results of the HTTR's start-up core physics tests* – X. Raepsaet, F. Damian – CEA Repport : SERMA/LCA/RT/99-2648.

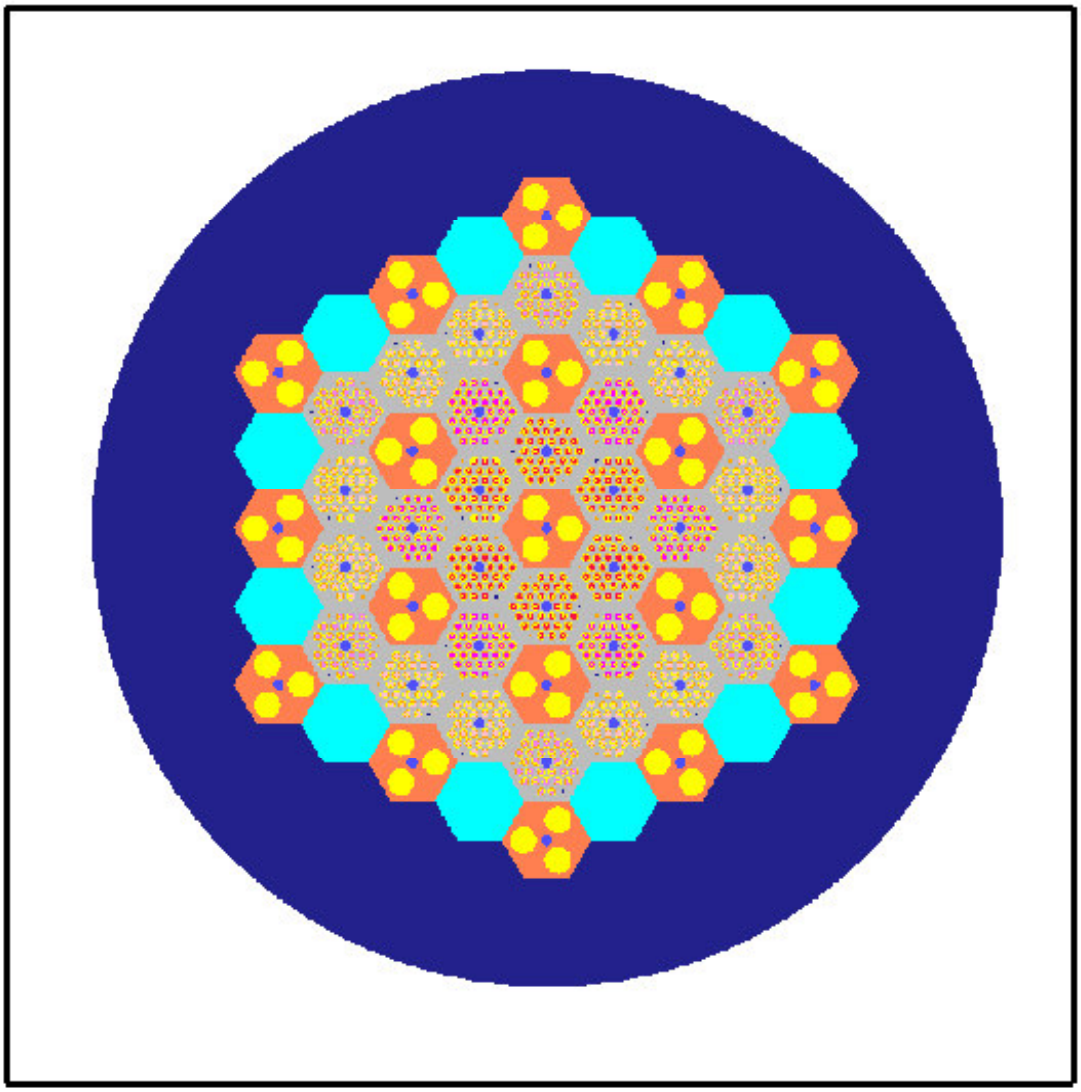
[6] *Scoping studies on the first criticalityof the HTTR* – H. Brockmann, U. Ohlig – FZJ contribution to the 2nd Research Co-ordinated Meeting of the CRP-5 (IAEA) – Nov. 2000.

[7] *Recalculation of the first criticality of the HTTR* – H. Brockmann, U. Ohlig – FZJ contribution to the 3rd Research Co-ordinated Meeting of the CRP-5 (IAEA) – March 2001.

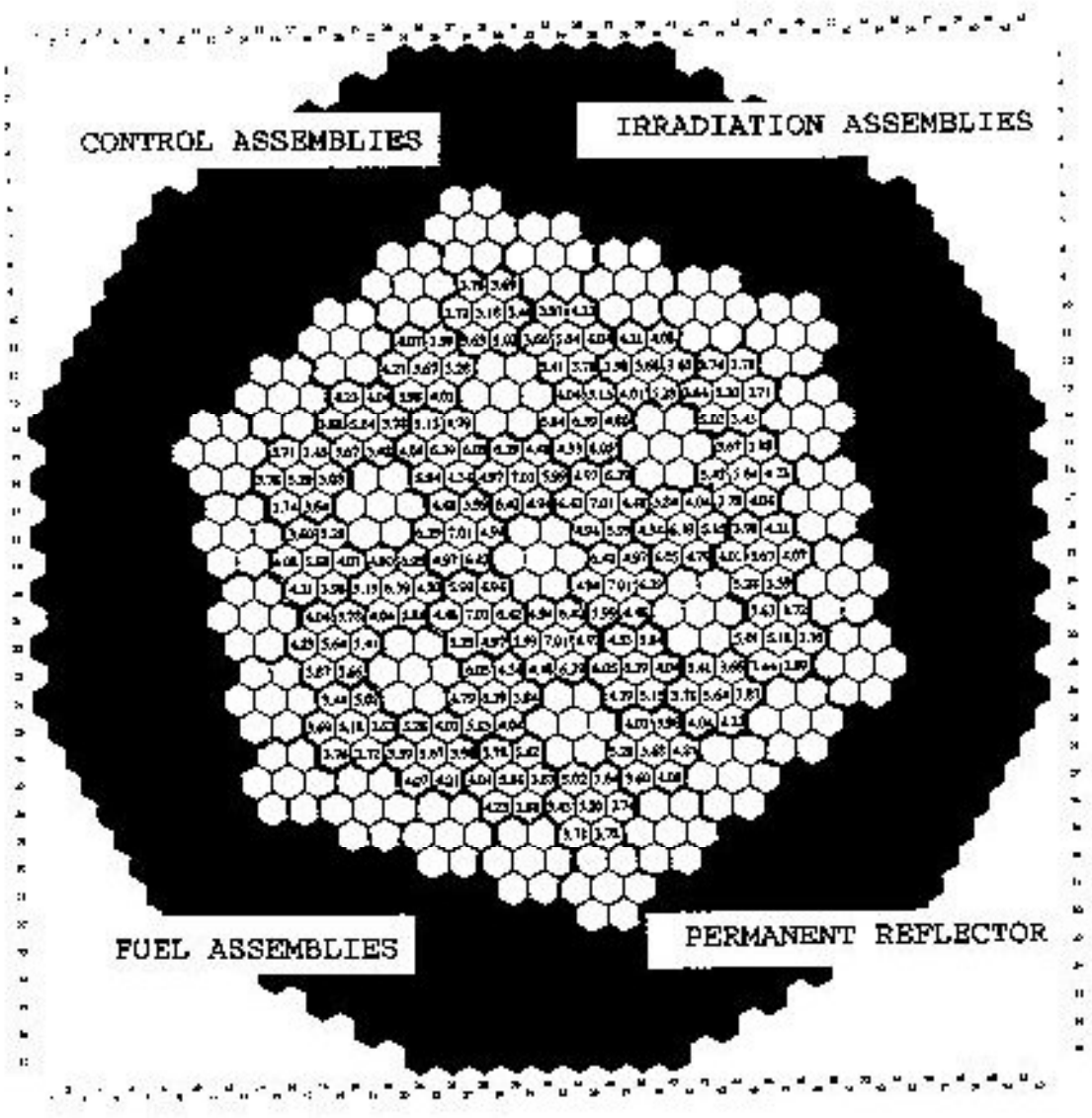
[8] *Present status of the FZJ work within WP1* – H. Brockmann, U. Ohlig – July 2001.

ANNEXE

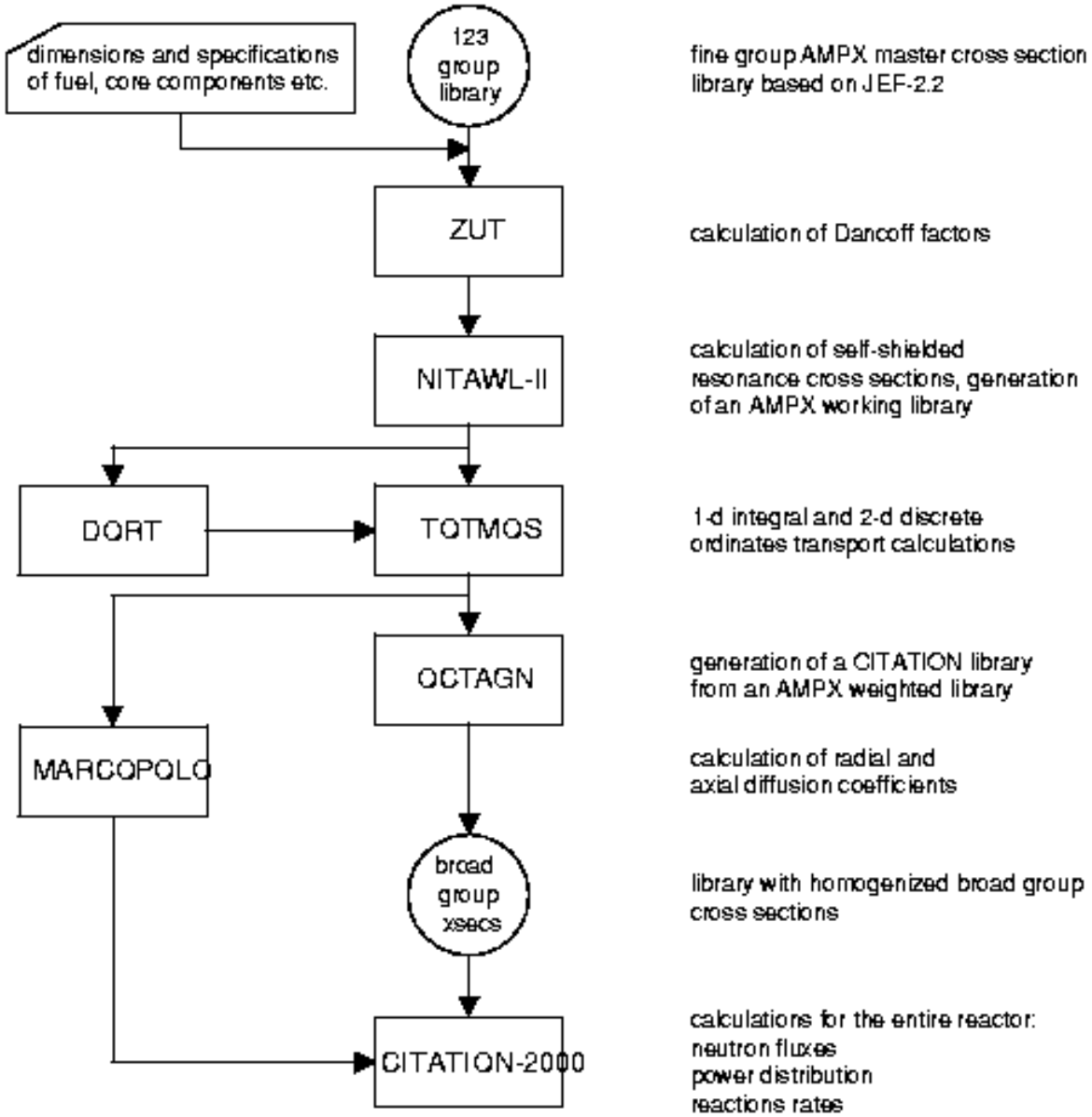
Radial description used in TRIPOLI4



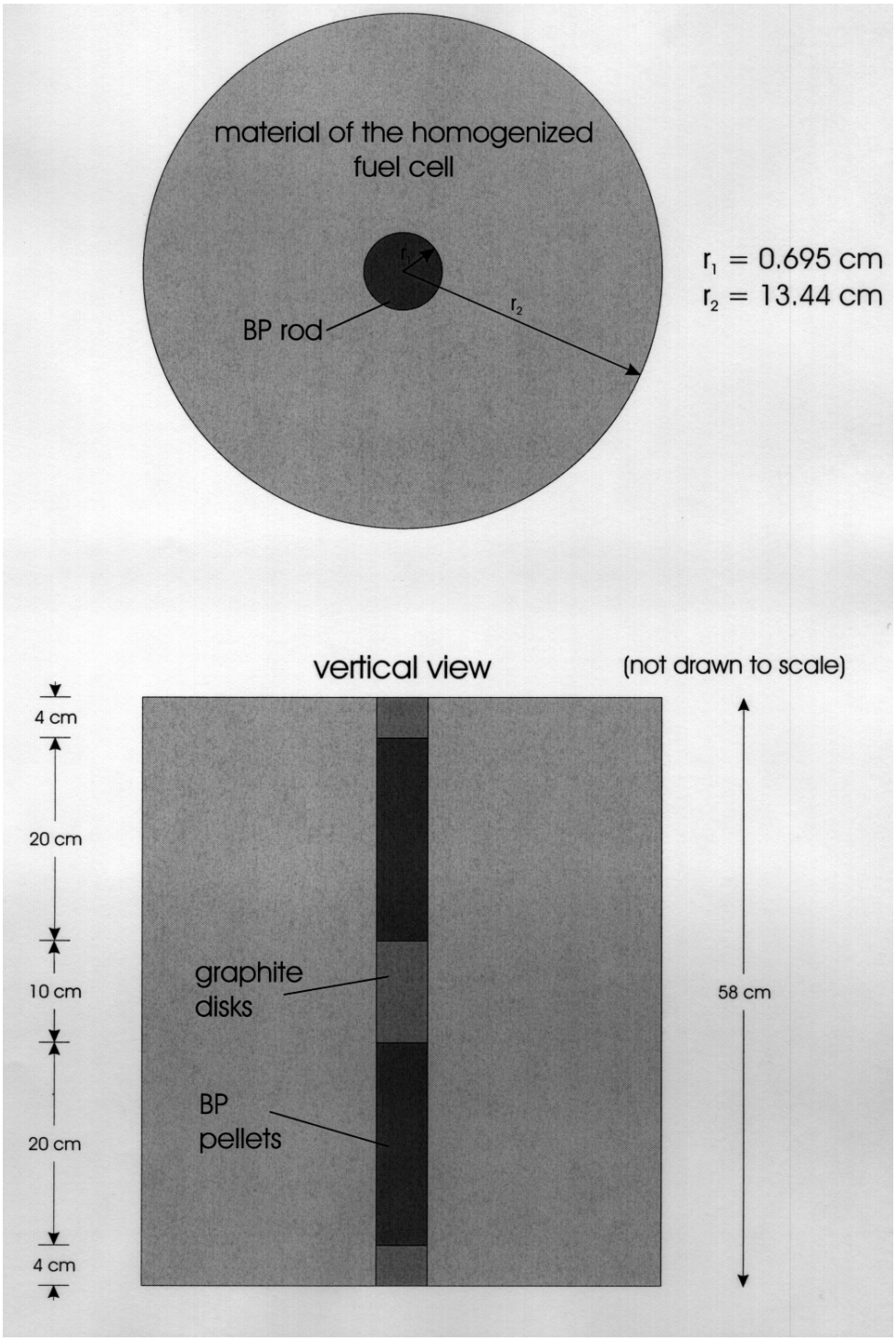
Radial description used in PANTHER



Programme structure for the HTTR calculations with CITATION



1D and 2D cell in TOTMOS and DORT



1D fuel cell representation in TOTMOS