CODE AND METHODS IMPROVEMENT IN HTGR MODELLING AT CEA

F. DAMIAN, X. RAEPSAET, F. MOREAU
CEA – Saclay
DEN/DM2S/SERMA
91191 Gif-sur-Yvette Cedex France
fdamian@cea.fr; xraepsaet@cea.fr; fmoreau@cea.fr

ABSTRACT

Following the present tendency of the international community, the French industrial partners are greatly interested in the technical and economical potential performances of the HTGR (High Temperature Gas cooled Reactor) concept that appears as a promising reactor for the future nuclear power applications. However, the next nuclear program related studies will rely on a major part on the intensive use of computational calculations rather than experimental results. Therefore, the codes will have to be reliable and well prepared to calculate a wide range of applications. The computational tools will have to serve as well for conceptual studies and industrial calculations as for best estimate and reference calculations. Taking advantages of the benchmark problems of the HTTR's start-up core physics experiments initially proposed by JAERI through the IAEA in a Co-ordinated Research Program, CEA has performed calculations in order to validate and qualify the codes that will serve to evaluate the future HTGR generation. For the analysis, two different calculation schemes based on a deterministic or a probabilistic approach are used. It turns out that all calculation results obtained for the fully loaded core configuration fit well each other and with the experiment, considering the experimental uncertainties. As far as the diffusion calculations are concerned, the number of fuel columns needed to achieve criticality increases by about 7 or 8 in comparison with the results obtained with a simplified Transport – Diffusion calculation scheme (homogenized fuel elements and no streaming effect taken into account in the diffusion calculations).

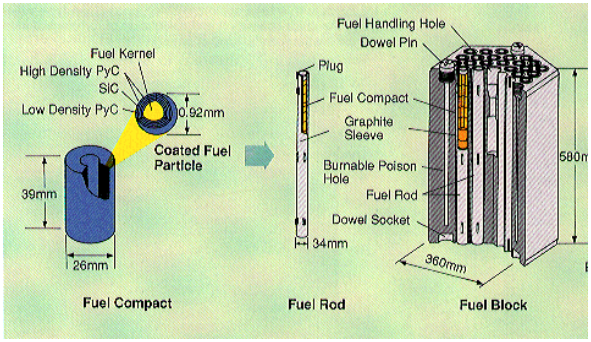
INTRODUCTION

Several validation and qualification steps have been carried out in the past for the code used in the HTGR applications (code to code comparisons and critical facilities). But only a small amount of validation is available on operating plants. The High Temperature Test Reactor (HTTR) gathers

several potential difficulties that can be encountered during HTGR core physical studies. It is a small core with large heterogeneities and interface problems, a double geometric heterogeneity (fuel in form of coated particles), a large streaming effect and control rods inserted in the reflector. This paper provides an analysis of the calculations performed in the framework of the benchmark problems of the HTTR's start-up core physics experiments. Among all the calculations, the first part of the benchmark (HTTR-FC) proposes to evaluate the number of fuel columns necessary to achieve the first criticality while the second part (HTTR-EX) proposes to evaluate the excess reactivity for 18, 24 and 30 fuel columns loaded into the core, described in detail in [1].

1. HTTR CORE CHARACTERISTICS

The structure of the HTTR core is presented in Figure 1. It is a small core (2.30 m in diameter and 2.90 m in height) with control rod blocks (graphite) inserted in the active core. As it is described in the Figure below, in order to achieve the first criticality, the fuel elements are loaded into the core from the outer ring to the inner ring. This fuel-loading scheme leads to intermediate core configurations with a single ring of fuel columns (thin annular core). This configuration is characterized by a strong neutron flux gradient at the core/reflector interface and represents a challenge for the reactor core modelling.



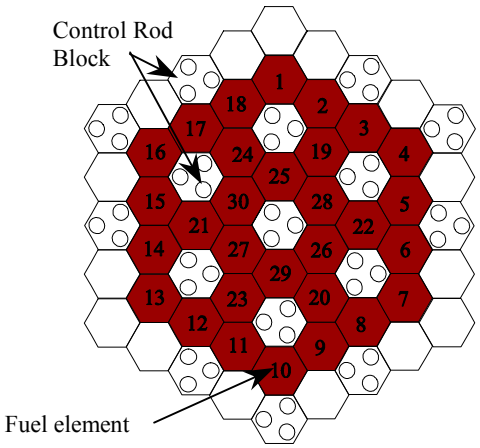


Figure 1: Structure of the High Temperature Test Reactor (HTTR) and fuel-loading scheme

2. COMPUTATIONAL METHODS AND NUCLEAR DATA

For the following calculations, the French reactor physics code system SAPHYR is used. SAPHYR gathers several CEA codes like APOLLO2 [2] (transport) based on a database produced with THEMIS/NJOY, CRONOS2 [3] (diffusion-transport), FLICA4 (3D- thermal hydraulics), ..., which are interconnected. This code system, initially dedicated to PWR calculations, has been transposed to HTGR calculations. The Monte-Carlo code TRIPOLI4 [4] has also been used.

All the problems proposed in the framework of the benchmark have been treated considering two calculation methods: one based on a Transport – Diffusion calculation scheme and a second one based on a Transport – Monte-Carlo calculation scheme. As far as the Transport – Diffusion calculation scheme is concerned, two different modelling have been used. The first one is a simplified modelling that is also used for physical and parametrical analyses and in which the diffusion calculations are performed with a homogenized fuel element and without taking into account the streaming effect. The second one is an improved modelling in which both effects (radial heterogeneity and streaming effect) are taken into account.

The Figure 2 illustrates the general procedure. The standard 172-groups or pointwise cross sections library issued mainly from JEF-2.2 are used for the calculations.

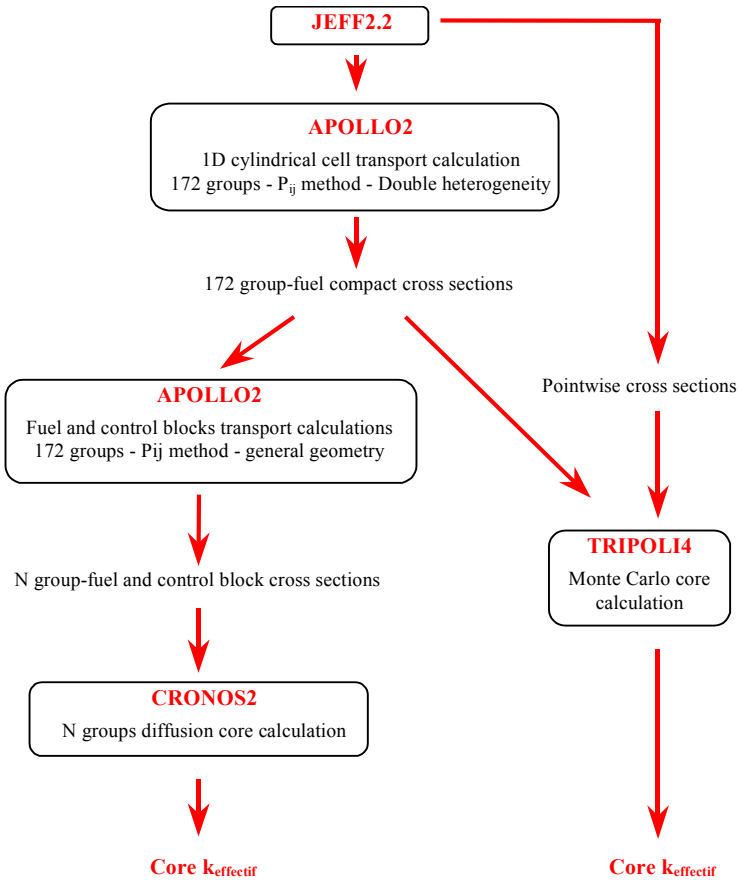


Figure 2: Description of both calculation schemes

For both calculation schemes, the double heterogeneity calculations of the coated fuel particles and the self-shielding in the resonance region are taken into account in a fuel cell calculation performed with APOLLO2. Knowing that the stochastic geometries calculations (coated fuel particles randomly distributed in the fuel compact) is not available in the Monte-Carlo code, this first step provides homogenized and multigroup cross sections for both Monte-Carlo core calculations (TRIPOLI4) and fuel element calculations (APOLLO2). Thus, for the core calculations performed by TRIPOLI4, pointwise cross sections are used everywhere in the core except in the fuel rod region where the multigroup cross sections have been generated by APOLLO2 calculations. As far as the Transport – Diffusion calculation scheme is concerned, the fuel element is calculated with APOLLO2 by a P_{ij}

method in a 2D-general geometry (calculation performed in infinite medium with a critical buckling search).

3. ANALYSES OF THE RESULTS OBTAINED WITH A SIMPLIFIED TRANSPORT – DIFFUSION MODELLING

The calculations performed with the two different code systems are presented in Table I [5]. All the preliminary calculations underestimated the number of fuel columns needed to achieve the first criticality (Diffusion calculations: 9 columns; Monte-Carlo calculations: 17 fuel columns). As it can be seen in Table I, the discrepancy between the calculations and the experiment at least ranges from $\Delta k = 0.0171$ to 0.058 at 18 fuel columns loading and from $\Delta k = 0.01$ to 0.033 at full core.

Table I: Experimental, Monte-Carlo and simplified diffusion results

	CRONOS2 (simplified modelling) • *Diffusion 8 gr* • *Fuel block homogenised* • *No streaming* • *BP axially homogenised*	**TRIPOLI4** *Monte-Carlo* *172 gr & pointwise*	**EXPERIMENT**
30 col	1.16980	1.14630 ± 0.0009	1.13630 ± (> 3.6%)
18 col	1.05800	1.01710 ± 0.0009	subcritical

It is noteworthy that the observed discrepancies decrease with increasing number of fuel columns in the core. Due to the large experimental uncertainty at 30 fuel columns loading, the differences between the calculations and the experiment are within the error bar, whereas at the thin annular core assembly the discrepancies are significant. A reason for the latter circumstance can be the consideration of another boron impurity in the dummy fuel blocks than the actual (dummy fuel blocks replace the fuel columns during the criticality approach) and of helium instead of residual air in the graphite pores. Indeed, the impurity of one dummy fuel block has been re-measured by JAERI and revised data [6] have been recommended for the recalculation of the first criticality (HTTR-FC2).

Moreover, in the course of the studies, the following reasons for the above mentioned discrepancies (especially for the simplified Transport – Diffusion calculation scheme) have been identified and quantified (Figure 3):

1 / A non-adequate treatment of the axial self-shielding in the Burnable Poison rods,

2 / An underestimation of the neutron streaming (due to voided channels),

3 / The neglect of the detailed structure of the HTTR fuel block in the core calculations.

Therefore, the HTTR-FC2 benchmark has been a good opportunity to implement the new enhanced methods coming from the analyses of all post-test studies and to evaluate the progress considering the new data.

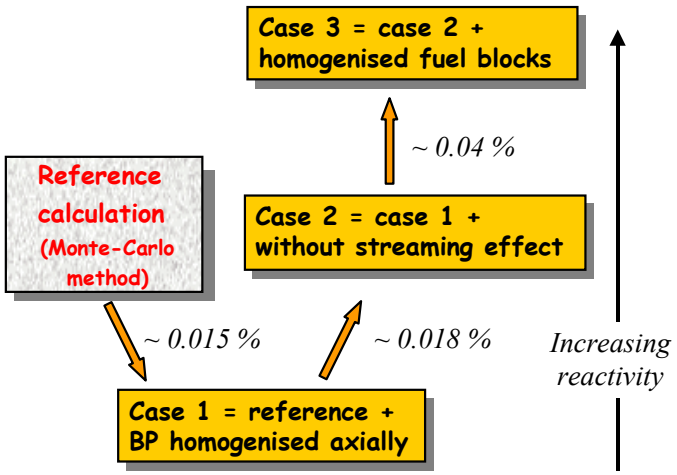


Figure 3: Impact of models on diffusion calculation results for the 18 fuel columns configuration (thin annular core)

4. MODELS IMPROVEMENT AND VALIDATION IN THE TRANSPORT - DIFFUSION CALCULATION SCHEME

4.1. NEW FINITE ELEMENTS

The new finite elements have been used in the code CRONOS2 in order to improve the description of the fuel element radial heterogeneity in the core calculations [7]. In CRONOS2, the core is described with hexagonal meshes corresponding to the fuel element size. The heterogeneities are taken into account by building as much geometry as there can be different mediums in a mesh (Figure 4).

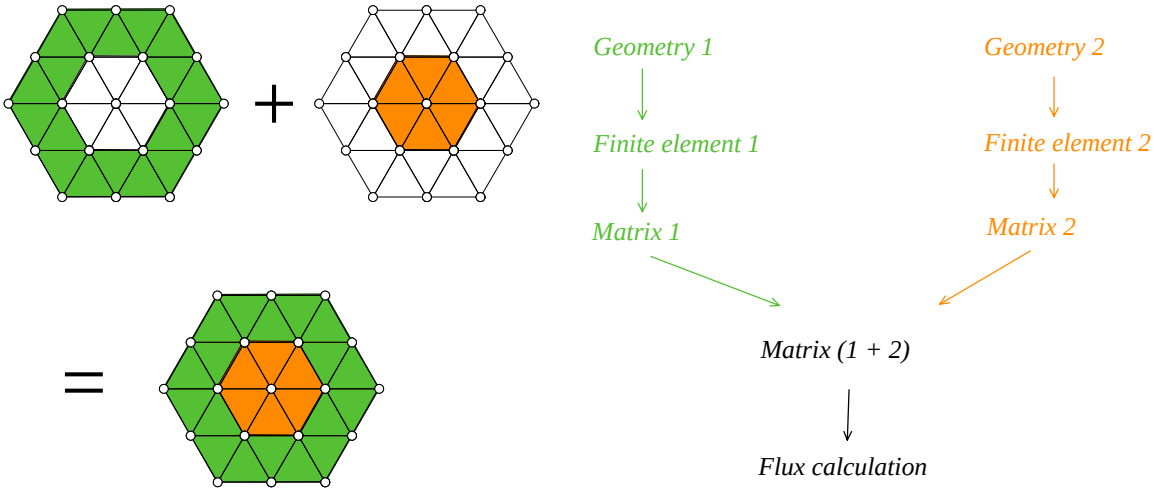


Figure 4: Geometry description in CRONOS2

Each different medium is also associated with a specific finite element that allows taking into account only the contribution of the triangles containing the medium considered. Therefore, each finite element is also associated with a matrix. The global matrix used for the flux calculation is obtained by summing each matrix described above.

The fuel element description used in the Transport – Diffusion calculation scheme is presented on Figure 5. This description allows taking into account the radial position of the burnable poison and the fuel element orientation in the core. In diffusion calculations, the fuel element structure is described by using three different mediums and the flux is calculated for each point described in the figure (61 points for the hexagonal element). Calculations performed on a simplified core configuration (2D) showed that this fuel element description was better than the one consisting in describing the hexagonal element with 24 triangles that have the same area.

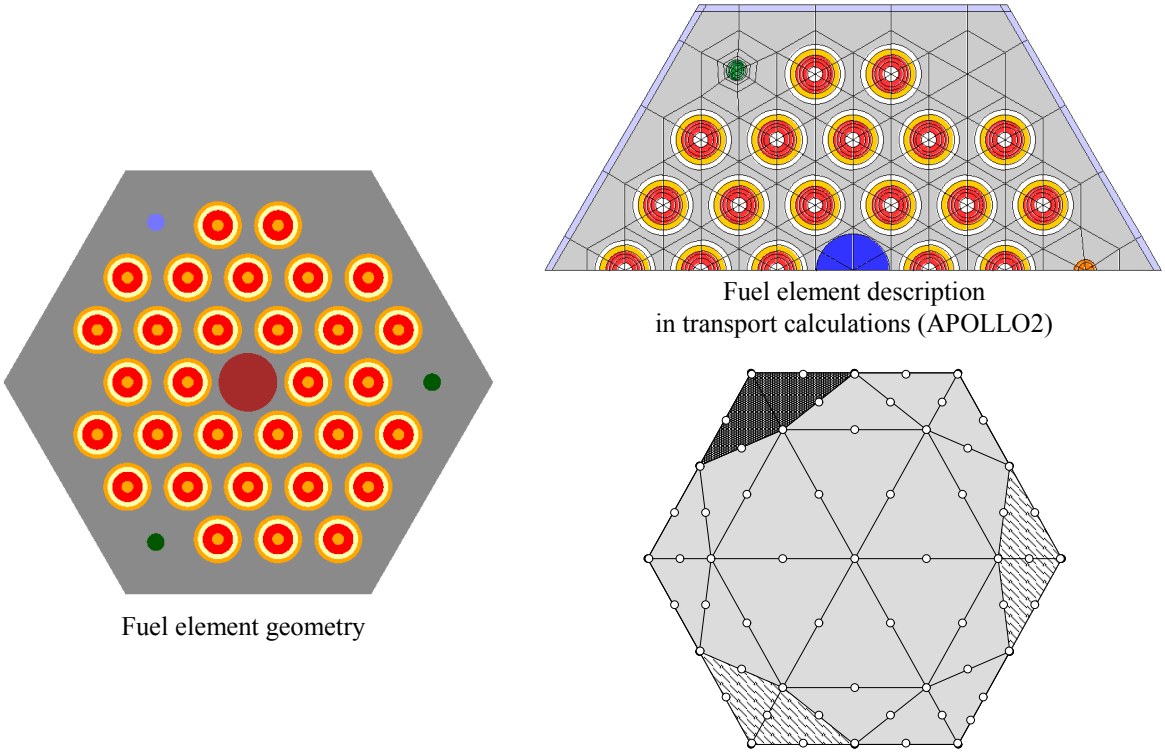


Figure 5: Fuel element modelling in the improved Transport – Diffusion calculation scheme

4.2. STREAMING MODELLING

For the improved Transport – Diffusion calculation scheme, the streaming effect is taken into account by using anisotropic diffusion coefficients in the core calculations. These diffusion coefficients are evaluated in the fuel element transport calculation performed by APOLLO2.

However, the Benoist method [8] (also called *TIBERE* model) used for treatment of the neutron streaming might not be applicable in the large channels of the control rod graphite blocks (three large channels per block). Therefore, an analytical model (Benoist [9]) has been tested on a control rod block alone. With this formulation, the corrected diffusion coefficient is given by:

$$\frac{D_k}{\frac{1}{3}\lambda_m} = 1+\frac{V_c}{V_t}\left(1+\frac{c}{\lambda_m}Q_k\right) \qquad (1)$$

$$k = r\,(radial)\ or\ z\,(axial)$$

where:

- $Q_r = 1-1/\Delta$
- $Q_Z = 2-\frac{3\pi}{4}B_Z c$
- c is the channel radius
- λ_m is the mean free path of the moderator (graphite)
- $V_c = \pi c^2$ is the channel volume
- V_t is the cell volume
- B_Z is the axial buckling

and: $\Delta = \dfrac{\gamma}{\gamma+1-\dfrac{2b'}{1-b'\dfrac{V_c}{V_t}}}$, $b' = \dfrac{\gamma+\frac{1}{2}}{\gamma+1}$, $\gamma = \dfrac{c}{\lambda_m}$

In order to validate these models (*TIBERE* and analytical model), Monte-Carlo and diffusion calculations have been performed on the simplified geometry presented on Figure 6.

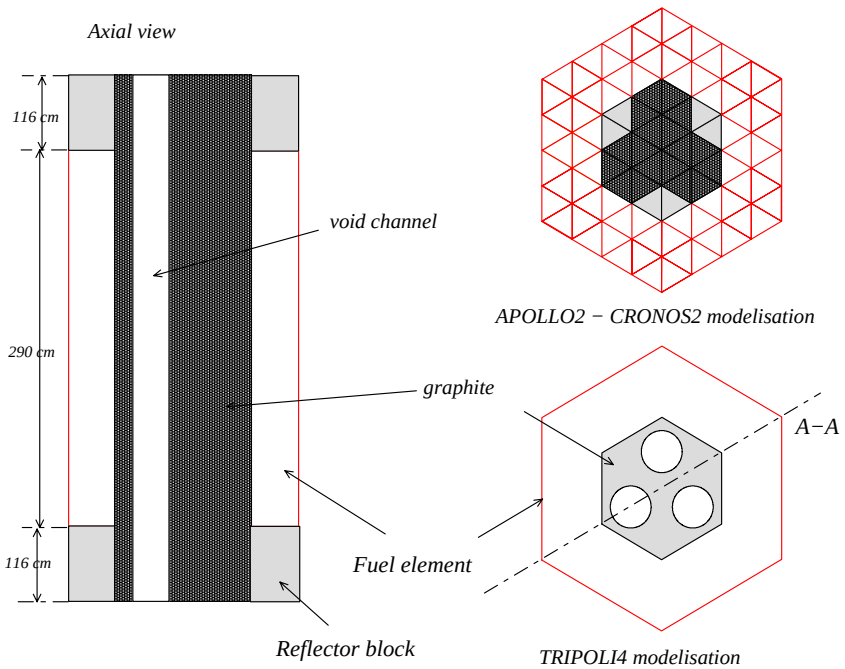


Figure 6: Geometry used for the evaluation of the streaming effect

In the analysed configuration, the control rod block is surrounded by fuel elements and the axial structure of the geometry is the same as HTTR's core. The results are gathered in Table II. The streaming effect calculated by CRONOS2 is underestimated when the anisotropic diffusion coefficients are evaluated by the *TIBERE* model. The underestimation of the streaming effect is the consequence of a non-adequate calculation of the axial diffusion coefficient (underestimation of – 20 to – 25 % on D_z calculation). On the other hand, the use of an analytical model for the axial diffusion coefficient allows obtaining results in good agreement with the reference (Monte-Carlo method).

Table II: Streaming effect calculated on the simplified geometry

	TRIPOLI4	**CRONOS2 -** Diffusion 8 gr	
		TIBERE model	Analytical formulation
Streaming effect	560 ± 135	267	570

5. ANALYSES OF THE RESULTS OBTAINED WITH AN IMPROVED TRANSPORT – DIFFUSION MODELLING

5.1. DIFFUSION CALCULATIONS RESULTS

As far as the diffusion calculations are concerned, new developments carried out in APOLLO2 and CRONOS2 take into account:

- ➲ The exact position of the BP in the fuel block by using new finite elements mesh in the core model,
- ➲ The streaming effect by generating anisotropic diffusion coefficients from both 2D-Pij calculations and analytical formulation.

The use of the HTTR-FC2 data associated with a complete description of the axial heterogeneity of the BP poison led to the new core diffusion calculation results. This was done for six different energy structures (2, 4, 6, 8, 13 and 20 groups) in CRONOS2 without observing a main trend.

The final results are partially gathered in the Figures below. Figure 7 illustrates, with 8 energy groups, the impact of the different model assumptions on the reactivity as a function of the number of fuel columns loaded into the core. Figure 8 shows a streaming effect ranging from 2.25 % in the 18 columns core configuration to 1.8 % in the full core configuration. These results highlight also the importance of the used leakage model for evaluating the neutron streaming in the control rods graphite blocks. Indeed, the first model (*TIBERE* model) gave some values varying from 1.8 to 1.5 %.

It is noticeable that the number of fuel columns needed to achieve criticality increases by about 7 or 8 in comparison with the results obtained with a simplified Transport – Diffusion calculation scheme (Table I). However, at first criticality, a discrepancy remains between the diffusion and the Monte-Carlo calculations ($0.9\ \% < \Delta k/k < 1.7\ \%$). This underscores the limits of a method based on a cross section homogenisation from a fundamental mode calculation (infinite medium) that 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 APOLLO2 transport calculations, before homogenising and collapsing locally the cross sections inside the fuel element.

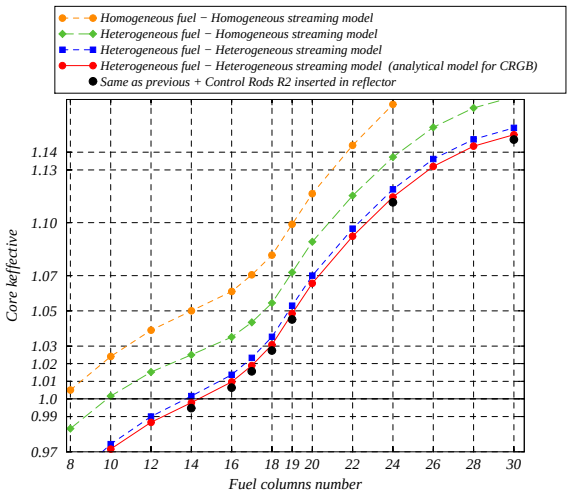


Figure 7: k_{eff} values obtained with different core models

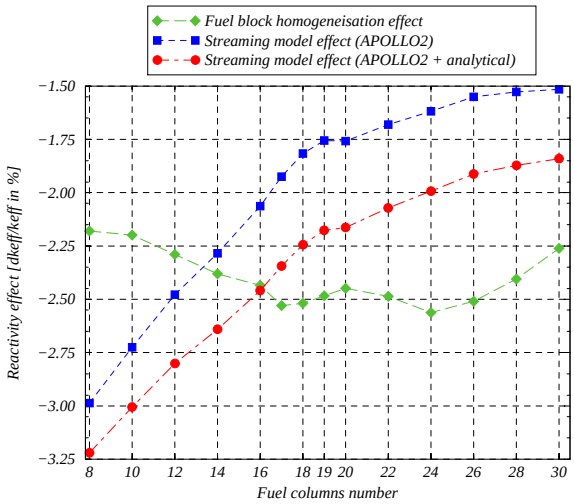


Figure 8: Neutron streaming and fuel block homogenisation effect

5.2. BENCHMARK DATA IMPACT

Table III gathers the benchmark data impact for different core configurations. These values have been calculated with the Monte-Carlo code TRIPOLI4. The impact of the residual air in porosities and the impurities in graphite are much more higher in the thin annular core configuration. Furthermore, it can be stressed that the decrease of the discrepancies between the experiment and the calculation results is correlated to the number of dummy fuel blocks (graphite) discharged during the criticality approach.

Table III: New benchmark data impact for different core configurations

	Number of fuel columns	
	18	**30**
Air in porosity and new impurities in graphite	*0.8 %*	0.3 %
Total impact of revised data (air, impurities, CR inserted in the upper reflector and detector)	*1.27 %*	0.75 %

5.3. FINAL RESULTS

All the final results are gathered in Table IV. In the case of the Monte Carlo code TRIPOLI4, the discrepancy between the measurement and the calculation for the 18 fuel columns configuration is reduced to $\Delta k/k \sim 0.85$ %, when considering the revised data of the HTTR benchmark.

As far as diffusion calculations are concerned, the discrepancy is now reduced to $\Delta k/k \sim 2.75 / 1.78$ % (depending on the number of energy groups), when taking into account the improved models and the revised data. After all, it must be stressed that all the calculation results obtained for the fully loaded core configuration fit the experiment, all the more if one consider the experimental uncertainties.

Altogether it turns out that the following procedures seem to be necessary for a better approach of the experimental results:

⇒ Description of the axial and radial heterogeneities (BP and fuel region) in the whole core calculation,

⇒ Consideration of the environment of the fuel blocks in the transport cell calculations in order to describe the core/reflector coupling accurately,

⇒ Treatment of the enhanced neutron streaming by a leakage model combined with an analytical model

Table IV: Experimental, Monte-Carlo and improved diffusion results

	TRIPOLI4 M. Carlo 172 gr & pointwise 3D	**CRONOS2** **(improved modelling)** • *Diffusion* • *4 groups / 8 groups* • *3D hex - 24 meshes/block* • *3 regions/block*	**EXPERIMENT**
30 col.	1.13833 [1] *± 0.00090*	1.1362 / 1.1451 [1]	1.1363 ± (> *3.6 %)*
24 col.	*	1.1000 / 1.1096 [1]	1.0834 ± (> *2 %)*
19 col.	1.02692 [1] *± 0.00043*	1.0351 / 1.0432 [1]	1.0152 ± ?
18 col.	1.00855 [1] *± 0.00090*	1.0178 / 1.0275 [1]	subcritical

[1] *detector impact included Δk = 0.002*

CONCLUSION

All the problems proposed in the framework of the benchmark have been treated with two different calculation scheme. As far as the Transport – Diffusion calculation scheme (APOLLO2 – CRONOS2) is concerned, an improved modelling that allows taking into account the streaming effect and the fuel element heterogeneity in the core have been used. Moreover, a second calculation scheme based on a Monte-Carlo core calculation with TRIPOLI4 has also been used.

The purpose of the benchmark was to evaluate the number of fuel columns needed to achieve the first criticality. Some discrepancies appear for intermediate core configuration (thin annular core) close to criticality. Parts of these discrepancies were reduced in the Monte-Carlo calculations taking into account the new benchmark data (air in porosity and impurities in graphite). Thus, the discrepancy

between measurement and TRIPOLI4 core calculation is reduced to $\Delta k/k \sim 0.85$ %. As far as the deterministic approach is concerned, some limitations appear in the Transport – Diffusion calculation scheme for thin annular core configuration where fundamental mode approximation seems to be hardly applicable. After all, it can be stressed that all calculation results obtained for the fully loaded core configuration fit well each other and with the experiment, considering the experimental uncertainties.

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