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Abstract

In the frame of the European contract HTR-N, a work package is devoted to the code validation and method improvements as far as the high temperature gas-cooled reactor (HTGR) core modelling is concerned. Institutions from three countries are involved in this work package: FZJ in Germany, NRG and IRI in the Netherlands, and CEA in France. The present work is based on a benchmark problem proposed by JAERI through the IAEA. It concerns the HTTR’s start-up core physics experiments that were a good opportunity for the European partners to validate their calculational tools and methods. The number of fuel columns necessary to achieve the first criticality and the excess reactivity for 18, 24, and 30 fuel columns in the core had to be evaluated. Pre-test and post-test calculational results, obtained by the partners, are compared with each other and with the experiment. Parts of the discrepancies between experiment and pre-test predictions are analysed and tackled by different treatments. In the case of the Monte Carlo code TRIPOLI4, used by CEA, the discrepancy between measurement and calculation at the first criticality is reduced to Δk/k ∼ 0.85%, when considering the revised data of the HTTR benchmark [Fujimoto, private communication]. In the case of the diffusion codes, this discrepancy is reduced to Δk/k ∼ 0.8% (FZJ) and 2.7 or 1.8% (CEA).

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1. Introduction

The HTGR appears as a promising concept for the next generation of nuclear power reactors. It forms the subject of a renewed interest from the industry on the one hand (Lecomte, 1999) and from countries like Japan and China on the other. In this context, the European nuclear community must have operational tools capable to perform conceptual design studies, industrial calculations (reload calculations and the associated core follow) as well as best-estimate or reference calculations. This implies in a near future, besides the reference Monte Carlo codes, to have methods based on multigroup diffusion and transport codes able to model the HTGR core with its inherent characteristics (neutron streaming phenomenon, coated fuel particles (CFP), control rods inserted in the reflector,...) whatever the concept may be.

Core physics calculation tools are available in Europe both for pebble bed and block-type fuel and are validated for the former HTGR concept conditions and a limited set of fuel types, such as uranium or thorium. Validation and qualification steps are always needed.
Indeed, although code-to-code comparison and critical facilities have been used for validation in the past, only a small amount of validation is available at elevated temperature or from comparisons at operating plants. Moreover, on one hand the codes and their associated methods may have progressed and on the other hand, the HTGR design evolutions and changes lead today to some new core configurations (geometry, fuel, ultra high-burn-up, actinide burning...) for which references do not exist and which impose additional requirements.

For all these reasons described before, the first work package of the HTR-N European contract has two objectives: first to contribute to the code validation and secondly to qualify and improve the methods for modelling the HTGR. The work package related effort was based on the HTTR and HTR-10 reactors recently started-up and for which benchmarks have been proposed by the IAEA (Co-ordinated Research Project 5). Both reactors provide experimental data for the validation of the codes in an extended spectrum of fuel cycles and core geometries. For example, the HTTR represents the first opportunity to model an annular core and to be able to compare with the experiment.

Institutions from three European countries, the FZJ in Germany, NRG and IRI in the Netherlands, and CEA in France, have joined this work package with the aim to validate their calculational methods. Pre-test and post-test calculational results are compared with each other and with the experiment. Parts of the discrepancies between experiment and pre-test predictions are analysed and tackled by different treatments (Raepsaet et al., 2002). In the case of the Monte Carlo code TRIPOLI4, used by CEA, the discrepancy between measurement and calculation at the first criticality has been reduced to $\Delta k/k \sim 0.85\%$, when considering the revised data of the HTTR benchmark. In the case of the diffusion codes, this discrepancy amounts to $\Delta k/k \sim 0.8\%$ (FZJ) and 2.7 or 1.8% (CEA).

2. Nuclear data and the Monte Carlo calculations

2.1. Nuclear data

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

2.2. The Monte Carlo calculations

In order to model the HTTR, the European partners have used two Monte Carlo codes. First, the KENO code used at IRI applies a multigroup data library (172-group) processed by the SCALE4 code system. The KENO calculations should then be considered as transport calculations and as an alternative to the core diffusion calculations. The second code named TRIPOLI4 used at 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 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 by TRIPOLI4 consists of generating multigroup cross-sections (172-group) with the transport code APOLLO2 (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.

3. Cross-section generation for the diffusion calculation

3.1. Cell calculations and the coated fuel particles

The 1D or 2D transport/3D diffusion code systems: WIMS/PANTHER, SCALE4/BOLD VENTURE, APOLLO/CRONOS, and TOTMOS-DORT/CPITATION are used at NRG, IRI, CEA, and FZJ, respectively. The different stages needed to generate the cross-section for the core calculations are presented in Tables 1 and 2 for the four code systems.

The double heterogeneity of the CFP and the self-shielding in the resonance region are taken into account in all cases either directly in the 1D fuel pin
Table 1
Core cross-sections generated by SCALE and TOTMOS

<table>
<thead>
<tr>
<th>SCALE/4</th>
<th>NITAWL/TOTMOS</th>
</tr>
</thead>
<tbody>
<tr>
<td>172 groups</td>
<td>123 groups</td>
</tr>
<tr>
<td>1D spherical cell</td>
<td>1D spherical cell</td>
</tr>
<tr>
<td>Self-shielding + Dancoff</td>
<td>Self-shielding + Dancoff</td>
</tr>
<tr>
<td>172 groups–$P_{ij}$</td>
<td>123 groups–$P_{ij}$</td>
</tr>
<tr>
<td>1D cylindrical fuel cell</td>
<td>1D cylindrical fuel cell</td>
</tr>
<tr>
<td>$B^2_{crit}$</td>
<td>$B^2_{crit}$</td>
</tr>
<tr>
<td>172-group cell-averaged $\sigma_{172gr}$ (isotopic)</td>
<td>123-group cell-averaged $\sigma_{123gr}$ (10 B) adjusted from $S_n R^2$ BP cell</td>
</tr>
<tr>
<td>172 groups–$P_{ij}$ 1D cylindrical core</td>
<td>123 groups–$P_{ij}$ 1D cylindrical BP cell</td>
</tr>
<tr>
<td>172-group fuel-averaged $\sigma_{172gr}$ (isotopic) for KENO ($P_3$)</td>
<td>4-group cell-averaged $\sigma_{4gr}$ (isotopic) for CITATION</td>
</tr>
</tbody>
</table>

Table 2
Core cross-sections generated by WIMS and APOLLO

<table>
<thead>
<tr>
<th>WIMS-7</th>
<th>APOLLO2</th>
</tr>
</thead>
<tbody>
<tr>
<td>69 groups–$P_{ij}$</td>
<td>172 groups–$P_{ij}$</td>
</tr>
<tr>
<td>1D cylindrical fuel cell</td>
<td>1D cylindrical fuel cell</td>
</tr>
<tr>
<td>Double heterogeneous</td>
<td>Double heterogeneous</td>
</tr>
<tr>
<td>Self-shielding</td>
<td>Self-shielding</td>
</tr>
<tr>
<td>$B^2_{crit}$</td>
<td>$B^2_{crit}$</td>
</tr>
<tr>
<td>16 groups–$P_{ij}$</td>
<td>172 groups–$P_{ij}$</td>
</tr>
<tr>
<td>2D ‘multi-pin’</td>
<td>2D</td>
</tr>
<tr>
<td>$B^2_{crit}$</td>
<td>$B^2_{crit}$</td>
</tr>
<tr>
<td>Heterogeneous leakage</td>
<td>Homogeneous leakage</td>
</tr>
<tr>
<td>No equivalence*</td>
<td>No equivalence*</td>
</tr>
<tr>
<td>2-group block region-averaged $\sigma_{2gr}$ (isotopic) for PANTHER</td>
<td>8-group block-averaged $\sigma_{8gr}$ (isotopic) for CRONOS</td>
</tr>
<tr>
<td></td>
<td>172-group fuel-averaged $\sigma_{172gr}$ (isotopic) for TRIPOLI</td>
</tr>
</tbody>
</table>

* No equivalence factor has been applied between the transport (16 groups) → diffusion (2 groups) calculations (WIMS-PANTHER) and the transport (172 groups) → diffusion (8 groups) calculations (APOLLO-CRONOS).

cylindrical calculations or using a 1D spherical model associated with the use of Dancoff factor. The double heterogeneity model of APOLLO2 is also available in 2D geometry (Fig. 1) but was not used because of the need to generate cross-sections for the annular fuel pin region in the TRIPOLI4 calculations. Therefore, these cross-sections have also been used in the 2D calculations.

The 2D $P_{ij}$ transport calculations performed with WIMS on the fuel element correspond to a multicell approximation whilst those carried out with APOLLO2 are an actual $P_{ij}$ transport calculation in a general geometry. Finally, it has to be mentioned...
that in the FZJ cell calculations no extra leakage term is used ($B_2 = 0$) whereas in all other cell (or element) calculations a critical $B_2$-crit search has been performed.

3.2. Burnable poison

The burnable poisons (BPs) in the fuel blocks present an axial heterogeneity. The $\text{B}_4\text{C}$ pellets are stacked with graphite disks put between them and can be modelled explicitly or not, throughout the cross-section generation process. The effect of the inhomogeneous distribution of the BPs in the axial direction is evaluated at NRG and FZJ, afterwards also in the post-test diffusion calculations of CEA.

3.3. Neutron streaming modelling

In the preliminary calculations the increased neutron streaming in the coolant channels and in the large holes of the core and the reflector is considered in the FZJ and NRG calculations. Later on, this enhanced neutron streaming is also taken into account in the post-test core calculations of CEA.

Indeed, as far as the core diffusion models are concerned, the streaming effect is treated by the use of anisotropic diffusion coefficients ($D_z \neq D_r$). These diffusion coefficients can be estimated by a heterogeneous neutron leakage model included in the transport code, as it is the case for WIMS-7 (NRG) and APOLLO2 (not available in the first set of calculations). The homogenised fuel block regions contain, therefore, anisotropic or modified isotropic diffusion coefficients taking into account the presence of large coolant channels or control rod guides which increases neutron streaming in the axial direction.

The MARCOPOLO (FIZ) 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. As the heterogeneous neutron leakage model was not available in the SCALE4 (IRI) and APOLLO2 code, the group constants provided to CRONOS-2 (CEA) and BOLD VENTURE (IRI) have consequently only homogeneous diffusion coefficients.

4. The experiment and the preliminary calculational results

In the benchmark problem proposed by JAERI (IAEA, 2002–2003) the first part concerned the number of fuel columns necessary to achieve the first criticality. The fuel columns were gradually loaded one after another from the outer region of the core (Fig. 2). In these conditions, a thin annular core configuration was obtained in the course of loading (18 columns), the rest of the core being loaded with some dummy fuel blocks. This specific geometry is very close to the one that can be encountered in current HTGR designs proposed today, i.e. GT-MHR and PBMR-SA (IAEA, 2001). It represents one of the first opportunities to model such core geometry and to be able to compare with the experiment. Finally, the excess reactivity for 18, 24, and 30 fuel columns in the core had to be evaluated and form also the subject of the present study.

Calculations performed with the different code systems are presented in Table 3 together with the experimental results (IAEA, 2002–2003; de Haas and Wallerbos, 1998; de Haas and Turkcan, 2000; Fujimoto et al., 1999; Raepsaet and Damian, 1999). The HTTR got critical with 19 fuel columns in the core with an excess reactivity of 1.5%. The experiments lead also to the following values for both core configurations available in Table 3: $\Delta k_{eff} = 12 \pm 3.3\%$ for the first one and a “barely subcritical” state for

Fig. 2. HTTR core loading. Fuel columns order.
Table 3

<table>
<thead>
<tr>
<th>CITATION</th>
<th>PANTHER</th>
<th>BOLD VENTURE</th>
<th>KENO</th>
<th>TRIPOLI</th>
<th>CRONOS</th>
<th>EXPERIMENT</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffusion, 4 groups</td>
<td>Diffusion, 2 groups</td>
<td>Diffusion, 13 groups</td>
<td>Monte Carlo, 172 groups</td>
<td>Monte Carlo, 172 groups and pointwise</td>
<td>Diffusion, 8 groups</td>
<td></td>
</tr>
<tr>
<td>3D triangle</td>
<td>3D hexagonal</td>
<td>R-Z</td>
<td>3D</td>
<td>3D hexagonal</td>
<td>1 region/block</td>
<td></td>
</tr>
<tr>
<td>Finite element</td>
<td>Finite element</td>
<td>Finite difference</td>
<td>Finite element</td>
<td>Finite element</td>
<td>Finite element</td>
<td></td>
</tr>
<tr>
<td>6 meshes/block</td>
<td>7 meshes/block</td>
<td>24 meshes/block</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

| 30 columns | 1.1607\textsuperscript{a} | 1.1595 | 1.1885\textsuperscript{b} | 1.1600 ± 0.0005 | 1.1463 ± 0.0009 | 1.1698\textsuperscript{c} | 1.1363 ± (> 3.6%) |
| 18 columns | 1.0254\textsuperscript{d} | 1.0240 ± 0.0005 | 1.0171 ± 0.0009 | 1.0580\textsuperscript{e} | 1.0580\textsuperscript{e} | 1.0580\textsuperscript{e} | Subcritical |

\textsuperscript{a} CR insertion considered \( \Delta k = 0.004 \).

\textsuperscript{b} Corrected for the BPs effect from the KENO calculations.

The second core arrangement. The first value leads to a multiplication factor of 1.1363 with nevertheless an important uncertainty.

All preliminary calculations underestimate the number of fuel columns needed for the first criticality. The diffusion calculations lead to 10–16 fuel columns according to the modelling hypotheses (see Section 5) and the Monte Carlo calculations lead to 17 fuel columns. The Japanese predictions for the HTTR criticality are: 14 fuel columns determined by diffusion calculation, and 16 fuel columns in the case of Monte Carlo calculation (Fujimoto et al., 1999). As can be seen in Table 3, the corresponding discrepancy between the calculational results and the experiment at least ranges from \( \Delta k = 0.017 \) to 0.058 at 18 fuel columns loading, that means near the first criticality, and from \( \Delta k = 0.01 \) to 0.052 at full core.

The former results underscore the fact that the HTTR is a real challenge in the reactor physics point of view. The difficulties are amplified by modelling the thin annular core geometry in order to take accurately into account the core/reflector interfaces. Moreover, associated to important axial and radial heterogeneities in the core (BP, many different enrichments), one of the other characteristics of the HTTR core is the presence of a large number of uncommon big channels offering the possibility for the neutrons to leak from the active zone (streaming effect). All these considerations have, therefore, justified additional works for analysing the discrepancies, for improving the methods and for eventually identifying the weaknesses of the codes.

5. First analyses of the results

As far as the diffusion calculations are concerned, the higher \( k_{\text{eff}} \) values obtained by BOLD VENTURE and CRONOS are explained by the fact that the streaming effect is not considered and that the fuel blocks are homogenised in one region. This will be explained in more detail hereafter. In the CITATION core model the fuel block is also homogenised, however neglecting the core/reflector coupling in a few groups diffusion calculation largely counterbalance the resulting effect.

Furthermore, it turns out that the relatively good agreement in the thin annular core assembly between both Monte Carlo codes disappears in the fully loaded core. One reason could be that the \( P_3 \) and multi-group treatment describing the interaction between neutrons and graphite in KENO, compared to point-wise cross-section used in TRIPOLI4, could have a larger impact on the neutron leakage at a fully loaded core with its harder neutron spectrum than in the thin annular core configuration.

However, it must be pointed out that the observed discrepancies decreased with increasing number of fuel columns in the core. Due to the large experimental error at 30 fuel columns loading (full core),
the differences between the calculations and the experiment are within the error interval, whereas at the thin annular core assembly the discrepancies are significant. Two reasons for the latter circumstance can be proposed. The first would be that the two steps transport-diffusion calculation based on the fundamental mode assumption would be less and less appropriate as one goes toward the annular core configuration. The second would concern the level of the actual boron impurity in the dummy fuel blocks and of the residual air (instead of helium) in the graphite pores. As far as the latter is concerned, the impurities of some dummy fuel blocks have been re-measured by JAERI and the following revised data (Fujimoto, 2000) have been recommended for the recalculation of the first criticality (HTTR-FC2):

- air in the pores of the graphite (presence of $^{14}$N and $^{16}$O);
- a higher boron impurity in some dummy fuel blocks (3.10 ppm versus 2.49 ppm); and
- aluminium in the temporary neutron detector holders (presence of $^{27}$Al, $^{15}$N and $^{16}$O).

Finally, in the course of the studies the following reasons for the above-mentioned discrepancies have been identified:

- the neglect of the detailed structure of the HTTR fuel block together with a non-adequate modelling of the fuel and BP unit cells;
- the use of few group homogenised cross-sections in the whole core diffusion calculation without neutron leakage in the transport calculations;
- an inadequate treatment of the axial self-shielding in the BP rods; and
- an underestimation of the neutron streaming.

These main physical effects and their impacts on the core reactivity are briefly depicted in Fig. 3 for the case of the annular core configuration. Similar tendencies can be observed for the full core configuration. Nevertheless, different absolute values are obtained for the quantified physical effects due to the harder neutron spectrum in the fully loaded core. Indeed, the importance of the boron absorption in the BPs is reduced in this case.

All these aspects have been more or less analysed and quantified by the different code systems. It has, thus, allowed a comparison that is presented hereafter. The observed tendencies between the codes are in good accordance and the values indicated in Fig. 3 give an idea of these trends for the annular core configuration. Starting from a best-estimate calculation, neglecting the fact that the BP was axially a succession

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**Fig. 3. Impact of the model assumptions on the reactivity (18 columns case).**
of boron and graphite pellets leads to a predicted reactivity 1.5% lower than considering the actual heterogeneous composition of these BPs. On the opposite, a core calculation that does not take into account the streaming effect will result in an increase of the reactivity of about 1.8%. At this stage, it is interesting to note that by making two strong physical hypotheses a result not far from the best-estimate calculation can be obtained. Finally, a discrepancy on the order of 4% can be achieved if an insufficient description of the fuel block is used to model the high level of radial heterogeneity. All these physical phenomena have been analysed separately in detail and are presented in the following sections.

6. Detailed physical analyses

6.1. Axial homogenisation of the burnable poison

The BPs in the fuel blocks present an axial heterogeneity. The B$_4$C 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 by CITATION and TRIPOLI4.

In the Monte Carlo calculation only the BP rods have been homogenised (B$_4$C–C) in the 3D detailed geometry and compared to the reference case given previously in Table 3. As far as the CITATION diffusion calculation is concerned, it is in the course of the cross-section generation process that the BP adjustment, based on the $S_n$–$R$ cell calculation, has been considered. The cell-averaged cross-sections with and without BP adjustment have then been used in the core calculation. But in the pre-test calculations, the axial heterogeneity of the BP was taken into account by a reduction of the B$_{10}$ concentration in the 1D cell calculation. This leads also to an overestimation of the BP efficiency. Therefore, in the post-test calculations the axially heterogeneous distribution of the BP was considered by another method: it was provided that the absorption rate in the BP regions of the whole core diffusion calculation was the same as in the detailed 2D DORT cell calculations for these regions. Thus, the axial self-shielding was considered by a more accurate method compared to the method of reducing the B$_{10}$ concentration. The reactivity effects of both methods are also shown in Table 4.

The spatial self-shielding effect of the B$_4$C is clearly highlighted. The homogenisation of the BP rods leads to an overestimation of the boron absorption that 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 emphasised 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 this effect has also been evaluated by the CRONOS-2 model (Table 5) for which the BP was initially homogeneous. The obtained multiplication factor are in this case very close to the one calculated by BOLD VENTURE comparable in term of model (homogeneous, no streaming, ...). Moreover, the impact of the BP heterogeneity is similar with regard to those observed with CITATION and TRIPOLI4.

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 on the fuel block enrichment and is smaller for harder neutron spectrum (higher enrichment). The $\Delta\lambda$ values calculated by DORT for a BP cell (Table 6) can be compared to those obtained by TRIPOLI4 with a 3D/2D fuel block geometry (Table 7).

<table>
<thead>
<tr>
<th>BP homogenisation of the BP</th>
<th>TRIPOLI4</th>
<th>CITATION pre-test</th>
<th>CITATION post-test</th>
</tr>
</thead>
<tbody>
<tr>
<td>30 columns</td>
<td>0.0220 (2224)</td>
<td>0.0226 (2292)</td>
<td>0.0296 (3009)</td>
</tr>
<tr>
<td>18 columns</td>
<td>0.0145 (1460)</td>
<td>0.0198 (2000)</td>
<td>0.0268 (2715)</td>
</tr>
</tbody>
</table>

* $10^5 \times \ln (\lambda_1/\lambda_2)$.

<table>
<thead>
<tr>
<th>Heterogeneous description of the BP</th>
<th>CRONOS-2</th>
<th>BOLD VENTURE</th>
</tr>
</thead>
<tbody>
<tr>
<td>30 columns</td>
<td>1.1956</td>
<td>1.1885</td>
</tr>
<tr>
<td>$\Delta\lambda/\lambda_{base}$ (pcm)</td>
<td>0.0216 (2175)</td>
<td>0.0216 (2175)</td>
</tr>
</tbody>
</table>

* $10^5 \times \ln (\lambda_1/\lambda_2)$.
Table 6
Impact of the BP correction factor on the fuel block reactivity

<table>
<thead>
<tr>
<th>BP cell with DORT</th>
<th>Fuel block no.</th>
<th>Fuel block no.</th>
<th>( \Delta k_{\infty} / k_{\text{hete}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>99120 (enrichment 9.9%)</td>
<td>993120 (enrichment 9.9%)</td>
<td>0.0155</td>
<td></td>
</tr>
<tr>
<td>343320 (enrichment 3.4%)</td>
<td>343320 (enrichment 3.4%)</td>
<td>0.0335</td>
<td></td>
</tr>
</tbody>
</table>

Table 7
Fuel block TRIPOLI calculations

<table>
<thead>
<tr>
<th>Fuel block no.</th>
<th>TRIPOLI4 calculations</th>
<th>TRIPOLI4 heterogeneous BP</th>
<th>TRIPOLI4 homogeneous BP</th>
<th>( \Delta k_{\infty} / k_{\text{hete}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>99120 (enrichment 9.9%)</td>
<td>993120 (enrichment 9.9%)</td>
<td>1.4187 ± 0.0005</td>
<td>1.3994</td>
<td>0.0136</td>
</tr>
</tbody>
</table>

BP homogenisation impact.

The comparison of the reaction rates between both calculations displayed in Table 7 leads 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.

6.2. Fuel element radial homogenisation impact

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

- This homogenisation 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 the BPs and their position, smeared over the entire block in a homogeneous model does not allow a thorough representation of local absorptions. An underestimation of the BP absorption is observed. A solution that consists in considering several regions in the block with different group constants in the core diffusion calculation allows taking into account more accurately the block heterogeneities. However, this solution often requires equivalence factors in order to respect either the flux or the absorption rates between finite multigroup transport calculations of the heterogeneous block and broad group diffusion calculations with several homogenised regions per blocks. This point will be discussed later.

The last point has been evaluated with TRIPOLI-4, CITATION and CRONOS-2 in a 2D radial core simplified configuration (without axial neutron leakage). In this case the streaming effect and the BP axial homogenisation are not considered. Therefore, the results given in Table 8, point only towards the radial homogenisation effect. Once again, the physical effect observed here with two different codes and methods leads to very close results.

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 3. 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 8. In CITATION the finite difference method has been applied on the mesh type 1 given in Fig. 4.

Table 8
Fuel block radial description impact on the core reactivity

<table>
<thead>
<tr>
<th>Fuel block no.</th>
<th>TRIPOLI4 heterogeneous BP</th>
<th>TRIPOLI4 homogeneous BP</th>
<th>CRONOS-2 homogeneous BP</th>
<th>( \Delta k_{\infty} / k_{\text{hete}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>30 columns</td>
<td>1.2800 ± 0.0000</td>
<td>1.3195 ± 0.0000</td>
<td>1.3207</td>
<td>0.0244</td>
</tr>
<tr>
<td>18 columns</td>
<td>1.1404 ± 0.0000</td>
<td>1.1854 ± 0.0000</td>
<td>1.1863</td>
<td>0.0396</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Fuel block no.</th>
<th>CITATION heterogeneous BP</th>
<th>CITATION homogeneous BP</th>
<th>( \Delta k_{\infty} / k_{\text{hete}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>18 columns</td>
<td>1.0410</td>
<td>1.0840</td>
<td>0.0388</td>
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</table>
The reduction of the homogenisation effect for the 
fully loaded core is essentially due to the harder spec-
trum observed in this case. This reduces the impact of 
the underestimation of the BP absorption. Moreover, 
the cell calculations are more representative of that 
what exits in the full core. The neutron spectrum seen 
by the BPs in the core calculation becomes closer to 
the one existing in the cell (or 2D) transport calcula-
tions carried out on the blocks with a white boundary 
condition.

On the opposite, in the 18 columns core configura-
tion, the neutron spectrum existing in the cell (or 2D) 
transport calculations, is much more different from the 
one observed in the core. This phenomenon has been 
emphasised by comparing the neutron spectrum in one 
fuel block of one 3D core calculation with the one 
of the same block in infinite medium. This exercise, 
done on the base of Monte Carlo calculations, shows a 
harder neutron spectrum in the last case. Therefore, a 
next step in the calculations to explain the discrep-
ancies with the experiment could be 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 trans-
port calculations and to multiply the number of cases 
to be treated.

To complete this analysis of the impact of the ra-
dial 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 BP in the fuel blocks. Indeed, from the 2D 
transport calculations illustrated in the Fig. 1, the fuel 
element was initially homogenised in one hexagonal 
finite element. Then, with the help of the new avail-
able finite elements, two different meshes were con-
cidered to describe the fuel elements with 24 radial 
meshes: 24 equilateral triangles (type I) or the cutting 
out depicted Fig. 4 (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.

First of all, in the homogenised case, the 2D-diffu-
sion core calculations (CRONOS-2) give results close 
to those obtained by the Monte Carlo where the fuel 
blocks are represented by homogeneous 172-group 
cross-sections (Table 8). When heterogeneous fuel 
block geometry is used, the quantified effects have 
been evaluated for the three core configurations with 
18, 24 and 30 columns, on the basis of a 2D simpli-
fied core with no axial leakage and with an average 
uranium enrichment. The diffusion calculations are 
compared to the Monte Carlo calculation. The results 
obtained for the first configuration are presented in 
Fig. 5. 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 calcu-
lations already cited in Table 8.

Compared to the previous homogeneous hexago-
nal model for which an effect of about 4% can be 
seen, the new heterogeneous model (type II) leads to 
some discrepancies ranging from 1 to 1.5% with the 
reference calculation (TRIPOLI4). This more realistic 
model leads to a higher absorption in the BP in the fuel 
element but nevertheless the resulting gain of ~3% is 
less important than the one expected and mentioned 
in Table 8 for the annular core configuration. As far as 
the full core is concerned, the diffusion–Monte Carlo 
2D-discrepancies become quit acceptable with the use 
of the new finite elements.

Finally, the use of equivalence factors have been 
implemented in order to respect the global absorption 
rate between the APOLLO2 transport calculations 
(172-group) and the CRONOS-2 diffusion calcula-
tions with few groups. This option has not been con-
sidered afterwards because of it small impact (Fig. 5 ) 
on the finite element of type II.

As a conclusion, a detailed description of the fuel 
block improves largely the results by giving a higher 
weight to the BP absorption in the fuel blocks. It allows 
getting quit acceptable values comparing to the refer-
ence TRIPOLI4 2D calculations for the full core but 
a remaining discrepancy of about 1% can be observed 
for the annular core. This could be attributed to the 
cross-section generation stage where the environment
of the BPs would not be representative of the one existing in the annular core configuration. Indeed, in this configuration the BP is surrounded by much more graphite (reflector) that thus increases the absorption flux-weighted cross-section. Besides, it would appear that there is actually no specific trend concerning the energy structure to be retained in the CRONOS-2 calculations. It seems to have no impact on the results when a neutron leakage term is taken into account in the transport calculations (critical buckling search option). This is not the case in the CITATION calculations.

6.3. Energy group structure

The use of few energetic group collapsed cross-sections in the diffusion calculation and the application of a white boundary condition in the spectrum calculation (fuel block or fuel cell calculations) might be possible reasons for explaining the discrepancies with the experiment.

The non-apparent dependency of the number of group in the CRONOS-2 calculations is likely due to two things. First, the fact that the collapsed cross-sections come from $P_{ij}/2D$ APOLLO2 transport calculations on the whole fuel or control blocks might reduce the impact of the white boundary condition and the number of energy groups used to collapse the cross-sections. Then, the use of a neutron leakage term ($B_{2}\text{crit search}$) in the transport calculation seems to strongly decrease the impact on the reactivity of the energy group structure retained in the diffusion calculation.

However, as it has been mentioned previously, the TOTMOS 1D cell calculations did not consider either an extra neutron leakage term ($B_{2} = 0$) nor any leakage recycling was performed, although a recycling technique is usually applied in the case of (such a small core assembly and) few broad energy groups in the whole core diffusion calculation in order to consider the leakage effects on the neutron spectrum in the cell calculation. Therefore, a scoping study was performed to analyse the influence of different types of leakage feedback: $B_{2}$, $B_{2}$, and albedo recycling, on the multiplication constant of a simplified HTTR reactor model with an annular core (Brockmann and Ohlig, 2000).

The results are available in Table 9. It turns out that considering no leakage iteration in the cell calculations leads to a strong dependence of $k_{eff}$ on the number of groups used in the diffusion calculations and that a 4-group diffusion calculation with neutron
leakage feedback is consistent with a multigroup diffusion calculation. Therefore, the 26 groups energy structure has been retained as an optimum in the final CITATION model between the option of a finer energy structure and a 4 groups structure with leakage feedback slightly difficult to manipulate. However, the main tendency that can be observed here is an increase of the discrepancies (by more than 2%) compared to the experiment.

6.4. Streaming effect

All the obtained values for tentatively quantifying this effect are available in Table 10. First, additional calculations with CITATION have been performed without the streaming correction factors provided by MARCOPOLO. These calculations allow having an estimation of the streaming effect alone.

As far as CRONOS-2 is concerned, the former model does not take into account the streaming effect, the axial heterogeneous composition of the BPs and the heterogeneities of the blocks (case 3 in Fig. 3). Both last cases have been quantified previously (Tables 4, 5 and 8). Table 10 is, therefore, deduced from these last two points.

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 BPs. 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 $\Delta k_{\text{eff}}$ evaluated from KENO and BOLD VENTURE cannot be attributed to the streaming effect only. The homogenisation effect, as described in the previous section, obviously takes place here. A 172 groups 3D transport calculation on the fully detailed core is compared to a 13 groups $R-Z$ diffusion calculation with six homogenised rings. The $R-Z$ and diffusion-related assumptions have a small impact if it is compared to the obtained $\Delta k_{\text{eff}}$ assessments with a KENO hom and BOLD VENTURE on a simplified core. Therefore, the 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 TRIPOLI4, the homogenisation effect would be near 1%. This value is smaller than the one given in Table 5 (2.44%) and should be explained by the absence of BPs in the KENO calculations.

Finally, the Benoist method used for the treatment of the neutron streaming might not be applicable in the large channels of the control rod graph blocks (18 columns) and therefore underestimates this effect that is important in the annular core configuration. Two other analytical models (Benoist) have then been tested in APOLLO2 on a control rod block alone and validated by Monte Carlo calculation. This led to
better results on the whole core. The results are partially gathered in Fig. 6.

It illustrates, with 8 energy groups, the impact of the different model assumptions on the reactivity as a function of the number of fuel columns. It 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 former model gave some values varying from 1.8 to 1.5%.

Another approach has been adopted by CITA TION. In the course of the pre-test calculations it turned out: the streaming effect calculated by the CITATION code using anisotropic diffusion coefficients based on the theory of Benoist was about 33% smaller than the effect calculated by the Monte Carlo code MVP of JAERI (IAEA, 2002–2003), in the case of 18 fuel columns in the core. A possibility of getting more accurate diffusion constants is to adapt these anisotropic diffusion coefficients to the result of the Monte Carlo calculation. Therefore, the neutron streaming coefficients calculated by the MARCOPOLO code were modified by increasing the streaming correction factors of the CR guide and irradiation columns by about 20% (in R- and Z-direction). In this case, the streaming effect calculated by the CITATION code was the same as the reactivity effect resulting from the Monte Carlo calculation with MVP. Now, the increased streaming effects are: 2.54% at 18 fuel columns loading, and 2.03% at full core.

7. New calculational results

Considering the new available data (HTTR-FC2), new Monte Carlo calculations have been performed with TRIPOLI4 for the 18, 19 and 30 columns configurations. The 18 columns case has been treated by taking into account or not the presence of the control rods slightly inserted in the upper part of the reflector ($\Delta k \sim 0.003$).

As far as the diffusion calculations are concerned, new developments carried out in APOLLO2 and CRONOS-2 allow in future to take into account:
the exact position of the BPs in the fuel block by using new finite element mesh in the core model;
the streaming effect by generating anisotropic diffusion coefficients from the previous $P_{ij}$-2D calculations.

The use of the HTTR-FC2 data associated with a complete description of the axial heterogeneity of the BPs has led to new core diffusion calculation results. This has been done for six different energy structures (2, 4, 6, 8, 13 and 20 groups) in CRONOS-2. The final results are partially gathered in Fig. 7. It illustrates, with 8 energy groups, the impact of the different model assumptions on the reactivity as a function of the number of fuel columns.

It is noticeable that the number of fuel columns needed to achieve criticality increases by about seven or eight in comparison with the former results (Table 3). At first criticality, a discrepancy remains between the diffusion and the Monte Carlo calculations ($\Delta k/r < 1.7\%$). 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 elements.

As far as the CITATION calculations are concerned, the conclusions are the followings. The discrepancy between measurement and the pre-test CITATION calculation amounts to $\Delta k/r = 0.0257$ at the first criticality (e.g. 19 fuel columns in the core) for a 4 groups diffusion calculation without leakage feedback. At 30 fuel columns in the core the difference is with $\Delta k/r = 0.0261$ of the same order. Parts of the discrepancies between measurement and former calculations are tackled by improved treatments of the four items, discussed in Section 5.

When applying these improvements and taking the revised data of the HTTR, the first criticality was recalculated for 18 fuel columns, in case of fuel loading from the core periphery. The number of fuel columns, necessary to achieve the first criticality, increased by
about 2 fuel columns compared to the former results, and the discrepancy between measurement and diffusion calculation was reduced from $\Delta k = 0.0287$ to $0.0111$ at 19 fuel columns in the core. The effective multiplication constants obtained in the pre-test and post-test calculations are given in Fig. 8 together with the experimental results.

When summing up all post-test studies, the analysis yields the following effects at 18/19 fuel columns in the core compared to the pre-test results:

- when considering the detailed structure of the HTTR fuel block in the whole core calculation the multiplication factor decreases by about $\Delta k \approx 0.043$;
- the description of the detailed energy dependence of the neutron flux adequately by a fine energy group structure increases the $k_{\text{eff}}$ values by about $\Delta k \approx 0.035$;
- when considering the axial heterogeneity of the BPs by 2D cell calculations, $k_{\text{eff}}$ of the whole core calculation increases by about $\Delta k \approx 0.0068$;
- when treating the neutron streaming effect by modified diffusion constants on the basis of the Japanese Monte Carlo results, $k_{\text{eff}}$ is reduced by about $\Delta k \approx 0.0075$; and
- when taking into account the revised HTTR benchmark data, the multiplication factor is reduced by about $\Delta k \approx 0.009$.

8. Final results and conclusion

All final results are given in Table 11. In the case of the Monte Carlo code TRIPOLI, the discrepancy between measurement and calculation at the first criticality is reduced to $\Delta k/k \sim 0.85\%$, when considering the revised data of the HTTR benchmark. As to the diffusion codes, this discrepancy is now reduced to $\Delta k/k \sim 0.8\%$ (CITATION) and $\sim 2.75\%$ (1.78\%) (CRONOS-2), when taking into account the improved treatments and the revised data.

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...
Table 11
The new core calculations together with the experimental results

<table>
<thead>
<tr>
<th>CITATION</th>
<th>TRIPOLI</th>
<th>CRONOS</th>
<th>EXPERIMENT</th>
</tr>
</thead>
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<tr>
<td>Diffusion, 26 groups</td>
<td>Monte Carlo, 172 group and pointwise</td>
<td>Diffusion, 8 groups (4 groups)</td>
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<td>3D triangular</td>
<td>3D hexagonal</td>
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<td></td>
</tr>
<tr>
<td>3 region/block</td>
<td>3 region/block</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Finite difference</td>
<td>Finite element</td>
<td></td>
<td></td>
</tr>
<tr>
<td>24 meshes/block</td>
<td>24 meshes/block</td>
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<td>30 columns</td>
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<td>1.1363 ± (3.6%)</td>
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<td>1.0834 ± (2%)</td>
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<td>1.0152 ± ?</td>
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<td>18 columns</td>
<td>1.00803 ± 0.00090</td>
<td>1.0275 (1.0178)</td>
<td>Subcritical</td>
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</table>

* CR inserted considered $\Delta d = 0.004$ and detector impact included $\Delta d = 0.002$.

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 BPs 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 BPs by 2D cell calculations (FZJ) or by 3D diffusion calculations (CEA and NRG); and
- 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).

References


