Validation of coupled neutron physics and thermal-hydraulics analysis for HPLWR

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Abstract – *Within the 5. Framework Program of the European Community a High Performance LWR (HPLWR) is investigated, considering a reference design based on work of Oka et. al. [1] The utilization of supercritical water pressure leads to a strong axial variation of the water density in the coolant channels of the fuel assemblies. The reference design contains in each fuel assembly a number of moderator rods to enhance the over-all mean water density and three radial and three axial zone enrichments for power flattening. This leads to a very complicated neutron physics behavior of the reactor. The validation of applied calculation procedures is mandatory for such new core concepts. In a first exploratory step, before having new relevant experimental information, validation with Monte Carlo simulations seems to be adequate. A specific feature of the actual HPLWR design is the strong feedback between the neutron physics and the thermal-hydraulics calculations. For the coupling with thermal-hydraulic codes deterministic multi-group neutron physics calculations are recommended. In the following in a first step two- and three-dimensional models for Monte Carlo calculations with MCNP are developed. Comparisons of different MCNP models give confidence in the results and show some sensitivities, e.g. with respect to the treatment of the isolation wrappers around the moderator rods. The second step involves the development of a super-cell model of the fuel assembly for deterministic multi-group calculations. Here the comparison with the results of Monte Carlo calculations with MCNP shows the applicability of the super-cell model. Finally, on the basis of this super-cell model a coupling with the thermal-hydraulic code RELAP5 is realized. First results from the coupled calculations are given.*

I. INTRODUCTION

The utilization of supercritical water pressure in the High Performance LWR (HPLWR) under consideration in the 5. Framework Program of the European Community leads to a strong axial variation of the water density in the fuel assemblies. The actual reference design based on work of Oka et. al. [1] contains in each fuel assembly a number of moderator rods to enhance the over-all mean water density and three radial and three axial zone enrichments for power flattening. Together with the strong axial density variation, this leads to a very complicated neutron physics behavior of the reactor. The validation of applied calculation procedures is mandatory for such new reactor concepts. Although experimental validation will be required for a final design, in an intermediate step validation with Monte Carlo simulations seems to be a good approach. Modern Monte Carlo procedures like MCNP are very powerful for the description of complicated nuclear reactor systems. Important drawbacks are still the required large computing times and the lack of continuous temperature variations of the fuel. Moreover, the utilization of the supercritical water pressure leads to a very strong feedback between neutron physics and thermal-hydraulics behavior, making coupled calculations mandatory. For this purpose models with comparable level of discretization for neutron physics and thermal-hydraulics calculations are desirable. In this presentation the thermal-hydraulic calculations are based on a complete reactor system with one core channel with 20 axial nodes. For this model neutron physics calculations for one fuel assembly in an infinite array are adequate. For multi channel thermal-hydraulic core calculations more detailed full core neutron physics calculations would be needed. In section 2 the validation of a simplified fuel assembly model is described. The work starts with a slice model of the fuel assembly as defined for HPLWR benchmark investigations [3]. Complimentary to the 30^0 model of VTT, Finland, at FZK two full two-dimensional MCNP models were developed and compared. After validation, the simplest full 2-D model could be extended to three dimensions. These MCNP models are the basis for the qualification of simplified geometrical models for deterministic multi-group calculations with the code system KAPROS / KARBUS (see reference [4]), described in sections 3 and 4. In section 5 the automatic coupling of the validated simplified deterministic calculation procedures of KAPROS / KARBUS with thermodynamics calculations with the code RELAP5 are described and first results of these coupled calculations are presented.

II. MODELS FOR THE MCNP CALCULATIONS

The geometry of the applied model is based on data supplied in [2]. There are four different materials used in the model - fuel, Ni-based alloy, stainless steel and water. Fuel is uranium dioxide with oxygen-uranium ratio equal to

1.98. According to [1], the fuel enrichment is profiled in radial and axial direction and, therefore, fuel is represented by nine material compositions (three radial and three axial regions), which differ only in the ratio U^{235} to U^{238}. The water within the assembly is divided into three spatial zones on the basis of its density and temperature behavior in axial direction: "moderator", "stagnant water" and "coolant". "Moderator" represents water inside water rods. The water in this region has almost constant axial density, equal to that of the inlet water. "Stagnant water" fills regions, surrounded by flower-shaped walls, i.e. this is a layer between hot "coolant" and cold "moderator". Water referred to as "coolant" is any other water except "stagnant water" and "moderator" within the assembly; mainly, this is water, which surrounds fuel pins. The density of the "coolant" changes very strongly with the height. The space between assemblies has been also taken into account in the model and has been filled with the "coolant".

II.A. MCNP models for fuel assembly slices

In a first approach a MCNP model for HPLWR fuel assembly slices was developed with the help of a PERL script. This automatized procedure lead to a quite large input data set FZK-S. Subsequently an alternative specification method resulted in a more compact input data set FZK-T. A systematic comparison of the results of K_∞ calculations with these models is summarized in table 1.

Table 1. K_∞ for different geometry models

Description	K_∞
VTT geometry (30^0)	1.1730 ± 0.0006
FZK-S model (360^0)	1.1783 ± 0.0005
FZK-T model (360^0)	1.1790 ± 0.0010
FZK-T-mod, same guide tube modelling as VTT	1.1737 ± 0.0006

We may observe good agreement between the FZK-S and FZK-T model. The comparison of FZK-T, FZK-T-mod and VTT shows that the exact treatment of the guide tubes in the moderator rods leads to ≈ 0.5% difference in K_∞. The agreement between FZK-T-mod and VTT is good.

II.B. MCNP models for the HPLWR fuel assembly

In order to specify accurately the axial water density distribution, all water zones, mentioned before, are divided into several axial planes. To simplify this splitting, some auxiliary code was developed. This code uses a manually created input MCNP "template" file that contains two-dimensional description of the assembly, and an additional file, which contains information about the axial subdivision, and produces a 3-D input model for MCNP. This procedure allows preparing automatically an MCNP input file and enables the specification of different fuel enrichments in the assembly. An initial guess for the "coolant" and "moderator" densities and temperatures was obtained in reference [5] with the RELAP5 code with the assumption of a cosine axial heat distribution and full thermal isolation between "coolant" and "moderator". Properties of "stagnant water" were taken to be the same as "coolant" in the first case, or as "moderator" temperature and densities in the second case. In order to apply the density and temperature data obtained from RELAP5, the fuel assembly is divided into 20 axial sub regions. The temperature for each cell is approximated by the application of data libraries with different temperatures, evaluated by VTT [6] and by appropriate "TMP" input cards for MCNP for thermal scattering. The data library, prepared at 600K was applied for Ni-based alloy, stainless steel and for water. For fuel the 1200K data were used. For more accurate modelling of thermal neutrons transport in water, the S(α,β) treatment for water was included into the calculations. The corresponding S(α,β) table, prepared at 600K also has been taken from the VTT library.

III. AXIAL POWER DISTRIBUTION CALCULATIONS WITH MCNP

On the basis of the 3-D model of the HPLWR fuel assembly, the axial power distribution due to fissions was obtained with MCNP. These calculations were performed for two assumptions for the “stagnant water" density and temperature:

- Equal to properties of "coolant" water,
- Equal to properties of "moderator" water.

The results for both cases are presented in figure1. One can observe a big difference in the axial power distribution depending on the treatment of the stagnant water (despite the fact, that stagnant water only represents 17% of the water in the assembly horizontal cross section). Therefore, for accurate calculations of axial power distributions one should supply the water densities for stagnant water also. On the other hand it has to be noted that the current calculations are based on a thermal-hydraulic model with full isolation between moderator and coolant, which, of course, is not the case for a real system.

IV. HPLWR FUEL ASSEMBLY MODELS FOR DETERMINISTIC CALCULATIONS

Based on the experiences for tight lattice LWR investigations in reference [4], a 1-D super-cell model for the complicated HPLWR fuel assembly was developed. This model consists of a moderator rod and its surroundings. In the radial direction the model has four zones: moderator, rod, wrapper zone with stagnant water and an equivalent fuel zone. The radius of this fuel zone is determined by the volume of the fuel cells per moderator rod and the inter subassembly space. The mean cross sections in the fuel are determined from appropriate cell calculations. Using reflective boundary conditions for bottom and top of this model one can perform 1-D calculations for fuel assembly slices. Extension to a 2-D (R-Z) model easily can be done by the introduction of axial zones and modification of the boundary conditions on bottom and top. In a first step, validation calculations were performed for benchmark specifications for fuel assembly slices from reference [3]. Here good agreement could be observed for the comparison of the deterministic benchmark solutions and of a solution with MCNP, see figure 2. The differences between the

FZK-1 and FZK-2 results are remarkable. Obviously, the observations in section 3 that the treatment of the isolation wrapper has strong influence, are confirmed. After these encouraging results for slice calculations, the deterministic super-cell model was applied for a full height fuel assembly with the same material and geometry specifications as for the Monte Carlo calculations of section 3. The same fuel temperatures and water densities were applied. For the radial fuel enrichments a mean values is used. The comparison of the results of Monte Carlo MCNP and deterministic TWODANT calculations is shown in figure 3. Arbitrary units for the power are used. The mean slice data is normalized to the same maximum value 1. Very good agreement may be observed.

V. COUPLING OF KAPROS / KARBUS WITH RELAP5

A specific feature of the actual HPLWR design is the strong feedback between the neutron physics and the thermal-hydraulics calculations, making the coupling of these calculations mandatory. As a first step for coupled neutron physics and thermal-hydraulic investigations, the super-cell model mentioned before is coupled with the thermal-hydraulic system code RELAP5, being improved for HPLWR applications, see reference [5]. The RELAP5 input model describes the whole reactor system, including a one-channel representation for the core. In this case the fuel assembly model for the neutron physics calculations seems to be adequate. The coupled calculations start with a cosine shape estimate for the power distribution in 20 axial zones in the RELAP5 core model. The resulting axial distributions of the densities of the fuel and coolant and of the temperatures of the fuel, the clad and the coolant in these 20 zones of the model are extracted from the RELAP5 output and processed to input for the KAPROS / KARBUS cross section generation. These cross sections are used for the calculation of an axial power distribution in the super-cell fuel assembly model with the TWODANT code. The feedback of this new axial power distribution to the RELAP5 calculation may be repeated as many times as desired by input. The coupling of these codes RELAP5, KARBUS and TWODANT is organised within the KAPROS system in a new procedure R5PROC. Using appropriate mixing of the new axial power distribution with the previous one (relaxation factor), this procedure proves to converge after 8 to 10 iterations. First preliminary results with a RELAP5 model with full isolation between moderator and coolant are shown in the figures 4 to 6. In figure 4 the criticality is given as a function of the number of iterations for 4, 12 and 69 energy groups. The calculations with 69 groups proved to be sensitive to the relaxation factor. In the case of rel=0.667 no convergence for the criticality is observed. For rel=0.5 the criticality converges and satisfactory agreement may be observed with the 12 group solution. The 4 group results show good convergence behavior, but the deviation from 69 groups is not acceptable. In figures 5 and 6 the axial water density and the mean fuel temperature after 8 iterations are shown for the same energy group cases as in figure 4. We may observe good agreement for the water density for the 12 and 69 group, rel=0.5, solutions. The mean fuel temperature behaves quite sensitive. These first results of coupled calculations show the sensitivity of the coupling for the actual HPLWR reference design. Also the modelling of design details like isolation wrappers and stagnant water must be considered carefully.

VI. CONCLUSIONS

Deterministic multi group two- and three- dimensional models for HPLWR fuel assemblies have been validated with corresponding Monte Carlo calculations with the MCNP code. These investigations show a strong sensitivity of important reactor parameters like criticality and power distributions to the treatment of the wrapper around the moderator rods of the reference design. The axial power distribution is very sensitive to the distribution of fuel assembly densities and temperatures. Therefore, the consistent calculation of neutron physics and thermal-hydraulic characteristics of this fuel assembly type is of high importance. For the assessment of these sensitivities an automatized coupling of the thermal-hydraulic code RELAP5 and the modular code system KAPROS for neutron physics calculations has been realized. First results from these coupled calculations have been presented. They show a convergence for the main results after about 10 iterations.

ACKNOWLEDGEMENTS

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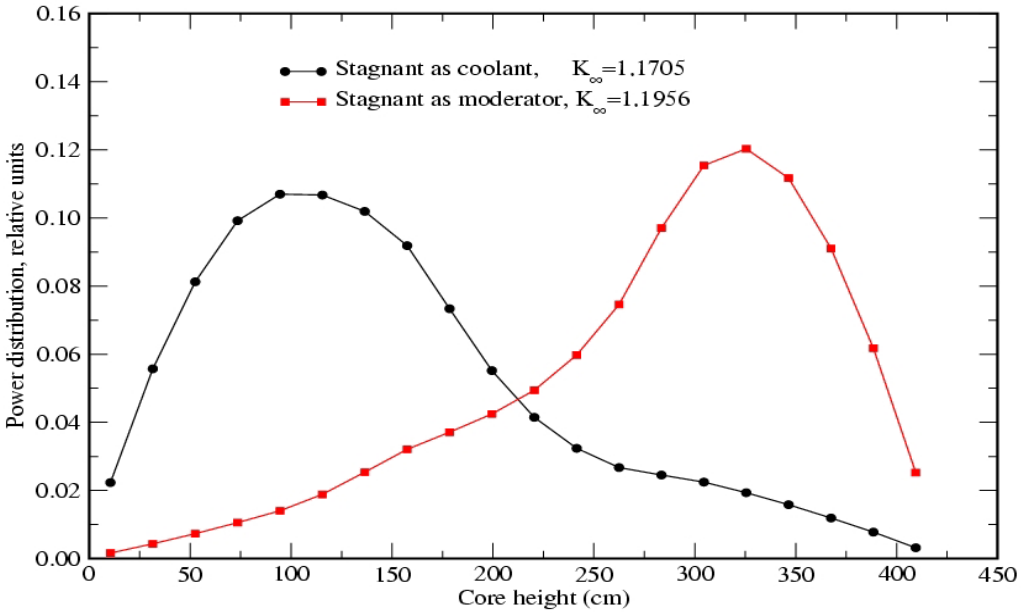

Fig. 1 Comparison of axial power shapes in a HPLWR fuel assembly for different treatments of the stagnant water. The results for K_∞ are also given.

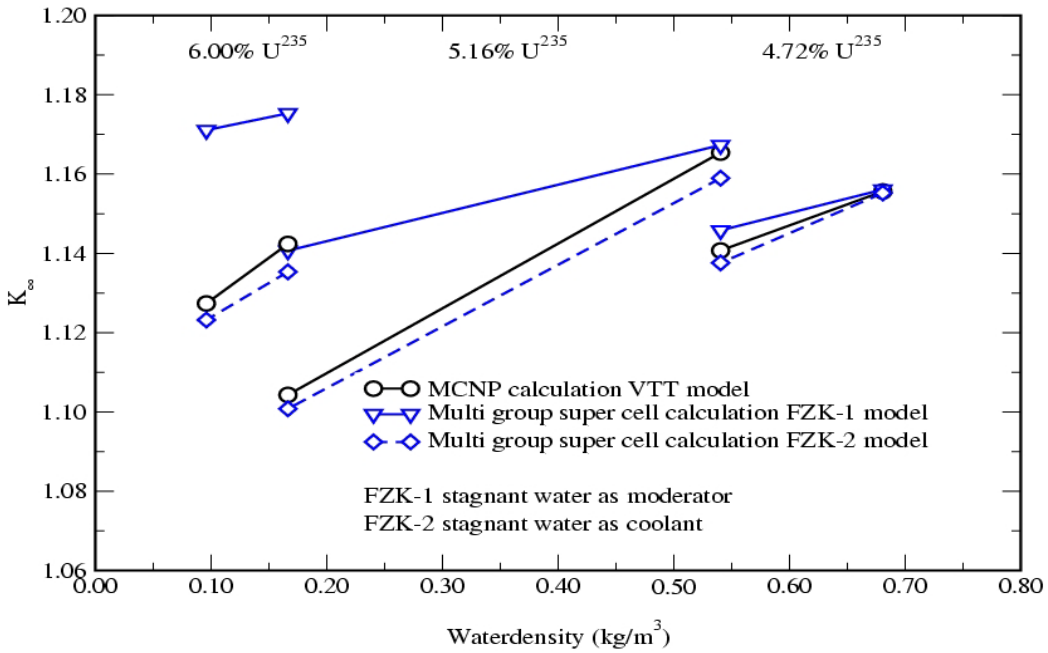

Fig. 2: Comparison of K_∞ values for HPLWR fuel assembly slices from FZK super-cell calculations with Monte Carlo results. The difference between FZK-1 and FZK-2 is only the treatment of the isolation wrapper. Fuel enrichment and water density are varied corresponding to benchmark specifications provided by CEA.

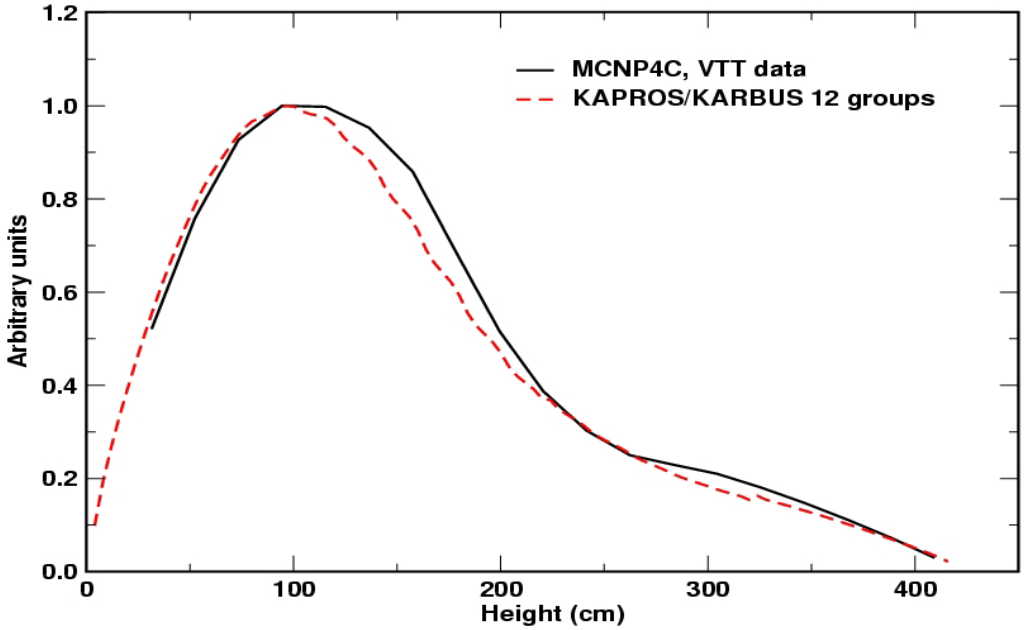

Fig.3: Comparison of axial power distributions in a HPLWR fuel assembly. MCNP4C results are obtained with temperature dependent data libraries from VTT, Finland. KAPROS/KARBUS results are obtained with TWODANT super-cell calculations with 12 energy groups.

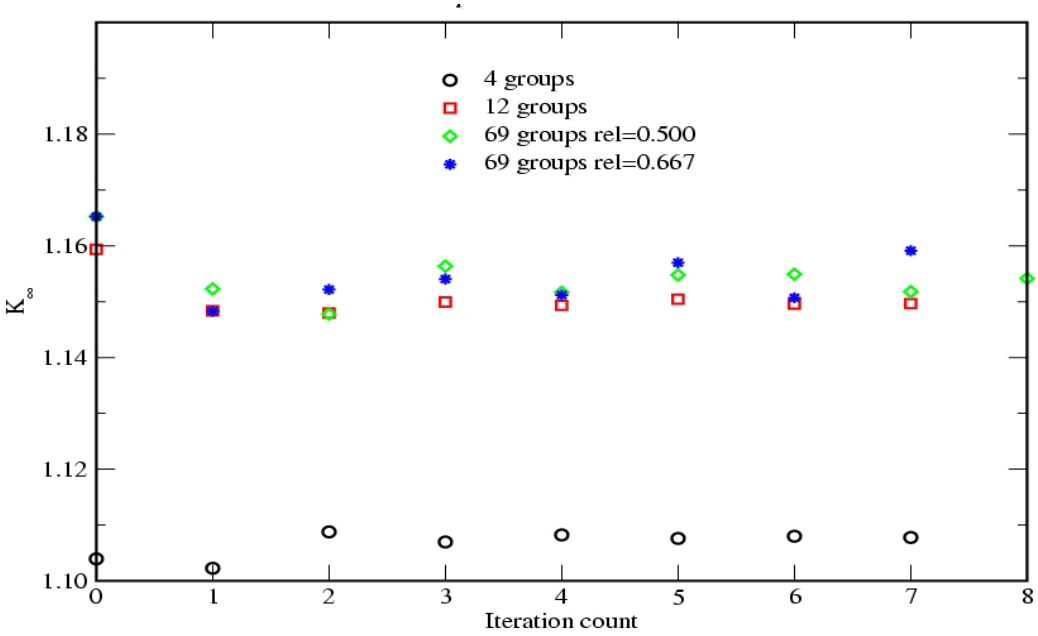

Fig. 4: Reactivity changes during iteration steps for coupled RELAP5/KARBUS calculations with different number of energy groups. The relaxation factors were rel=0.667 for 4, 12 and 69 groups and in addition rel=0.5 for 69 groups

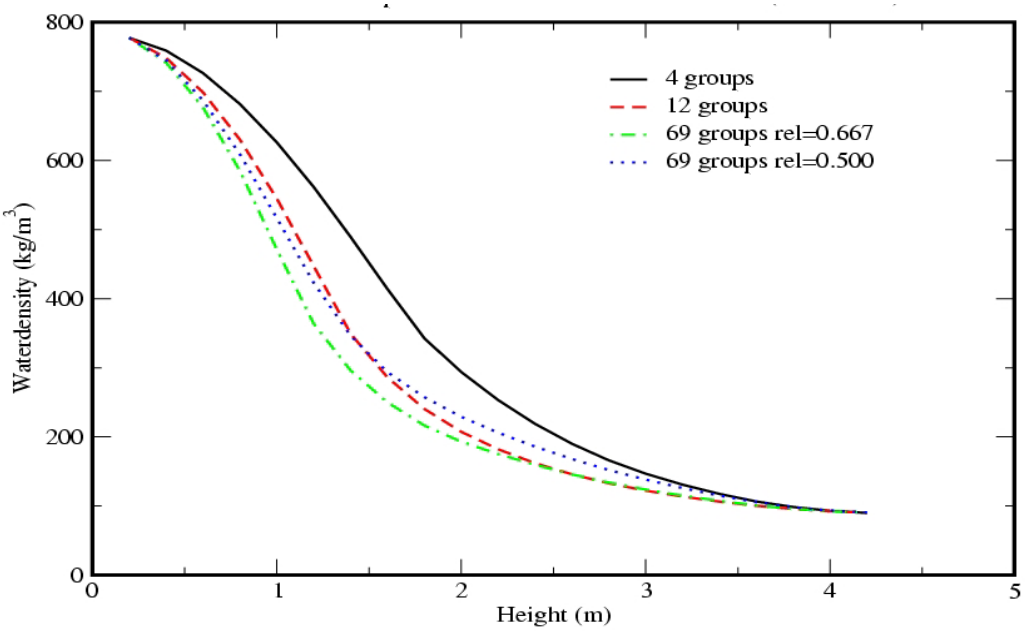

Fig. 5: Axial distributions of the water density after 8 iteration steps of coupled RELAP5/KARBUS calculations. The same cases are plotted as in figure 4.

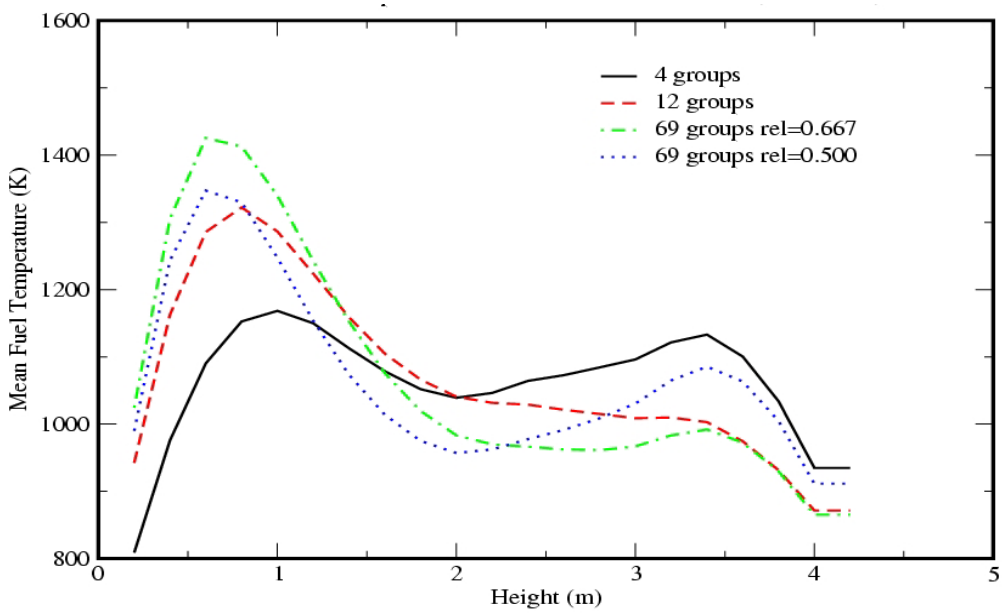

Fig.6: Axial distributions of the mean fuel temperature after 8 iteration steps of coupled RELAP5/KARBUS calculations. The same cases are plotted as in figure 4.