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Sensitivity Studies on Cross-section Generation and Modeling for BWR Core Simulation Using SAPHYR Code System

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The work presented in this report is a part of cooperative project between Pennsylvania State University and CEA-Saclay. The objective of the project is to establish an accurate and efficient scheme for BWR core calculation with coupled codes of the SAPHYR system and validate this methodology against the available experimental data. The project is divided into three stages and uses as reference design the Peach Bottom 2 plant. The Peach Bottom 2 plant was selected as a reference design because of the available measured data at different conditions, which allows us to validate both cycle and transient calculation capabilities of SAPHYR. In the first stage of the project, the main focus is on performing studies to implement and validate cross-section generation and modeling methodology for boiling water reactor in order to identify and address the major sources of modeling assumptions in this process. The second stage involves studies on core-calculations with coupled 3D neutronics/thermal-hydraulic models and the relevant issues to obtain an optimal representation in terms of accuracy and efficiency. The third stage will focus on the validation of the coupled calculation scheme against the available experimental data.

This paper presents the methodology for BWR assembly calculation with SAPHYR code system and shows results from performed sensitivity studies on cross-section modeling.

KEYWORDS: BWR, Cross-section modeling, SAPHYR code system, Core calculation, Validation

1. Introduction

The reactor core simulations are important part of the reactor analysis and require advanced coupled three-dimensional (3D) models to achieve high accuracy. In the past, application of such coupled 3D neutronics/thermal-hydraulics models in a consistent manner to both cycle and transient calculations was limited because of the limitations in the computer capabilities. Nowadays, in order to provide more advanced analysis tools the code development is aimed at coupling existing codes and applying the same coupled codes to core design and safety analysis. The progress in computer technology and computational methods has made feasible such multi-functional coupled 3D core calculations for power reactors.

In 2003, Reactor Dynamics and Fuel Management Group (RDFMG) at the Pennsylvania State University (PSU) and DM2S at CEA-Saclay started a cooperation project for developing

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an advanced methodology for analysis of boiling water reactor (BWR) core using SAPHYR code system ("SAPHYR" is a French acronym for Advanced System for Reactor Physics). The SAPHYR system includes the lattice physics code APOLLO2 [1], the core calculation code CRONOS2 [2], and the thermal-hydraulic code FLICA4 [3]. The standalone codes have been validated in numerous applications (PWR, VVER, etc.). The modular structure of the codes enables coupling in order to solve complex problems. The advanced and diverse modeling potential of the SAPHYR code system gives opportunity to investigate some important physical aspects of the BWR calculation scheme, including the cross-section generation and modeling in terms of dependencies on history and instantaneous thermal-hydraulic and control variables.

2. Validation Methodology for BWR Core Calculation

2.1. Description of the Project

The project is divided into three stages and uses as reference design the Peach Bottom 2 plant [4] (a General Electric designed BWR/4). The validation against experimental data will give a solid base for further development of the methodology for advanced assembly designs and core configurations.

In the first stage of the project, the cross-section generation and modeling methodology existing at CEA is implemented for BWR application, resembling as much as possible the routine paths for production calculation [5]. The BWR core is of special interest because factors, such as the control rod blade, the internal water rods, the axial variation of the isotopic compositions and the thermal-hydraulic (T-H) conditions create local heterogeneities in the assembly. This research focuses on the physical aspects of the BWR assembly simulations in order to identify and address the major sources of modeling uncertainties, such as the assembly homogenization and the parameterization of cross-sections

The second stage of the project involves studies on core-calculations with and without coupled 3D neutronics/thermal-hydraulic models. On core level, we will examine how the cross-section generation and modeling influences the core calculation in the diffusion approximation. The utilization of some approximations, such as material dilutions, energy discretization, parameterization of libraries, and bypass modeling will be validated in order to improve the core modeling. In addition, the spatial mesh overlays will be studied to obtain an optimal representation in terms of accuracy and efficiency of the coupled core-calculation.

The third stage will focus on validation of the coupled calculation against available experimental data (critical rod positions, flux and temperature distributions, etc.). The goal of the research is to develop a methodology for assessment of uncertainties for a given code system, in our case SAPHYR. We will use a strategy of the Design of Experiment (DOE) method to study the impact of different parameters in the coupling. The sensitivity analysis resulting from the previous stages will be applied to estimate the ranges of variation of the final results and create an acceptance margin. Parameters of main interest are the assembly model and homogenization, the choice of parameters in the neutronic libraries, the spatial discretization in the coupled core calculation, and the different thermal-hydraulic options in terms of numerical and physical models. This is an optimization problem that aims at reducing the difference between the calculation results and the experimental data.

2.2. APOLLO2 Calculation scheme for BWR assemblies

The first process under investigation is the generation of cross-sections for BWR core analysis and involves evaluation of several important approximations such as

- assembly models without rod;
- assembly models with control rod;
- reflector representation;

Another important process, evaluated in this research is the cross-section parameterization, i.e. modeling of cross-section dependencies on thermal-hydraulics and control parameters. The set of instantaneous parameters (fuel temperature and void fraction) covers the whole range of operating conditions of BWR. We take into account a history variable representing the impact of the void fraction on fuel depletion [5].

Figure 1 shows a schematic representation of a BWR assembly for APOLLO2 calculation. The cells outside the assembly box are defined as homogeneous mixtures of the box material, the outside coolant, and the absorber material (if present) based on their volume fractions. This approximation allows simplifying the assembly geometry and reduces the number of calculation meshes. However, the effect of this approximation must be estimated in the framework of the assembly homogenization.

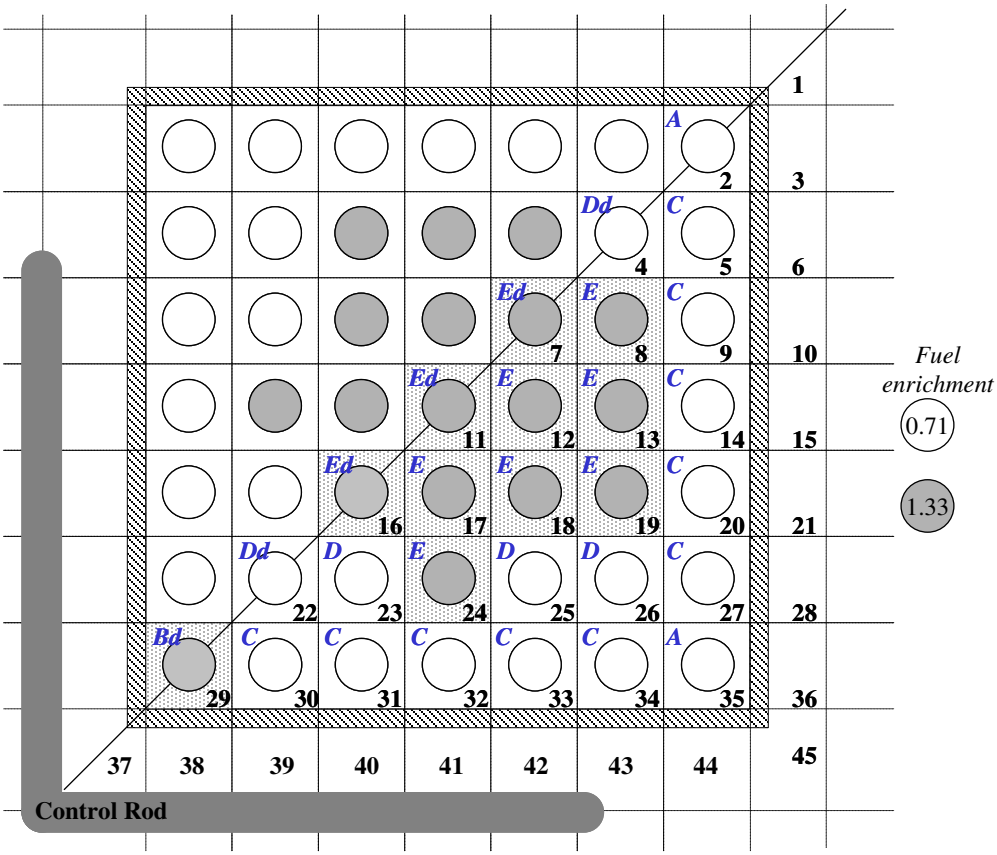

Fig. 1 Assembly model for APOLLO2, 7x7 configuration

2.2.1 Unrodded assembly

In the assembly cross-section calculation with APOLLO2, we utilize a scheme analogous to a scheme applied for PWR cross-section generation [6]. Figure 2 shows a schematic representation of the calculation.

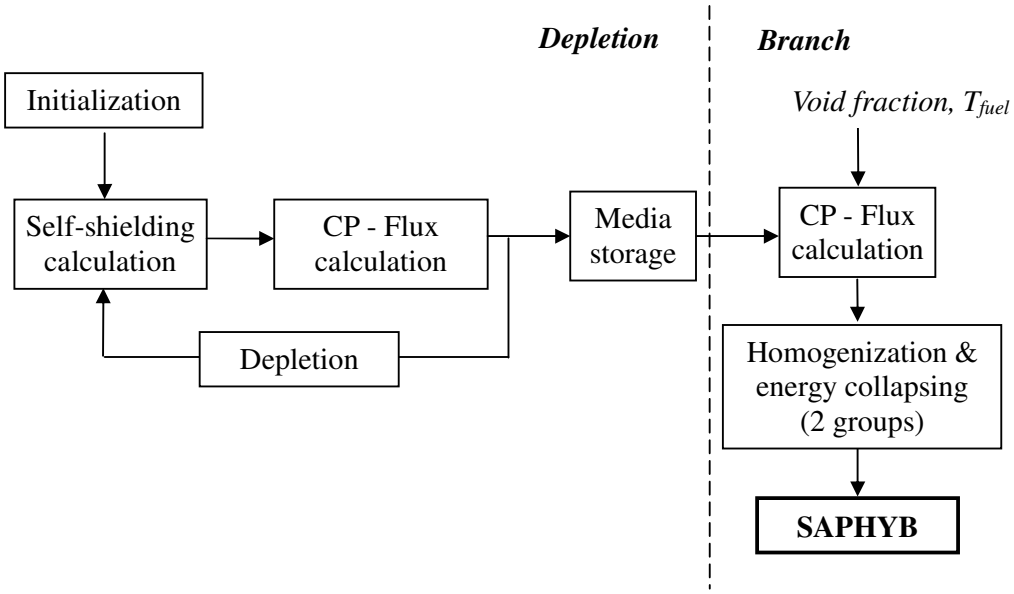

Fig.2 Schematic representation of APOLLO2 calculation for unrodded assembly

2.2.1.1 Depletion

During depletion calculation, APOLLO2 performs a self-shielding calculation (similar to that for PWR assembly) on pin-cell level, where the moderator, the cladding, and the fuel rings are identified in each cells. The gap and the clad are homogenized based on volume fractions. Only one calculation is performed for analogous cells of a given assembly. To take into account the peculiarity of a BWR assembly, the flat-flux collision probability formalism is applied with linear angular flux (UP1) option for U238, and isotropic (UP0HETE) flux option for the remaining isotopes (Gd155, Gd157, Gd156, Gd158, and U235). To take into account the heterogeneities of the flux inside the assembly, the calculation cell is divided into sectors (figure 3). The rings are necessary to be able to calculate well the self-shielding of U238 and the depletion of the different isotopes of Gadolinium.

Next, the code performs a flux calculation on a multi-cell sectored (two sectors per quadrant) geometry by the collision probabilities (CP) method. The CP method uses a flat-flux hypothesis in each calculation region; the calculation cell of the BWR assembly is divided into eight sectors and six rings in the fuel region (Fig 3). The flux calculation is performed with 99-group energy structure, which is well adapted for UO_2 fuel and which gives faster results than 172 groups. The assembly is considered in infinite medium and a critical Buckling search is performed to adjust the reactivity of the assembly at 1.0.

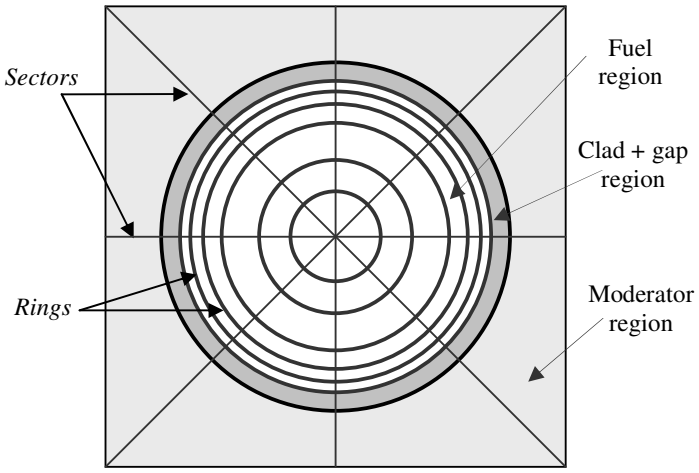

Fig. 3 Calculation cell for BWR in APOLLO2

The output of the depletion is stored in a file containing the media for the base case and is further used in the branch calculation. The base cross sections are calculated at 560 K moderator temperature (saturated conditions at 7.03 MPa), 889 K fuel temperature, and for the three void fractions 0%, 40%, and 70% (depletion axes) [7]. The three void fractions accounts for the different axial spectral history in the core during depletion. In the core calculation, the value of the nodal history variable, HV_{i+1}, at given burnup, BU_{i+1}, is computed from the previous value, HV_i, and the instantaneous value, IV_{i+1}, of the variable by equation 1:

$$HV_{i+1} = \frac{HV_i BU_i + IV_{i+1}\Delta BU}{BU_{i+1}} \quad (1)$$

2.2.1.2 Branch calculation

In the branch calculations, APOLLO2 performs new CP-flux computations along each depletion axis for the following set of instantaneous parameters: fuel temperatures 553K, 889K, 1973K, and 2000K; and void fractions 0%, 40%, and 70%. The next step is homogenization and collapsing of the effective cross-sections to two energy groups. An equivalence procedure is carried out after the condensation and homogenization in order to guarantee that the effective reaction rates are preserved.

The output of the calculation is a general purpose, parameterized library SAPHYB in which the results (macroscopic and microscopic cross section data resulting from homogenization and collapsing, fluxes, kinetic parameters, equivalence coefficients, etc.) are tabulated for different burnups, instantaneous void fractions, void histories, and fuel temperatures. These multi-dimensional tables account for the cross-term cross-section dependencies on different parameters.

2.2.2 Rodded assembly

For the rodded assembly calculation, we use a specific equivalence technique on two levels involving collision probabilities (for the self-shielding) and discrete ordinates (SN) methods, [7]. Fig. 4 shows a schematic representation of the calculation for rodded assembly in APOLLO2.

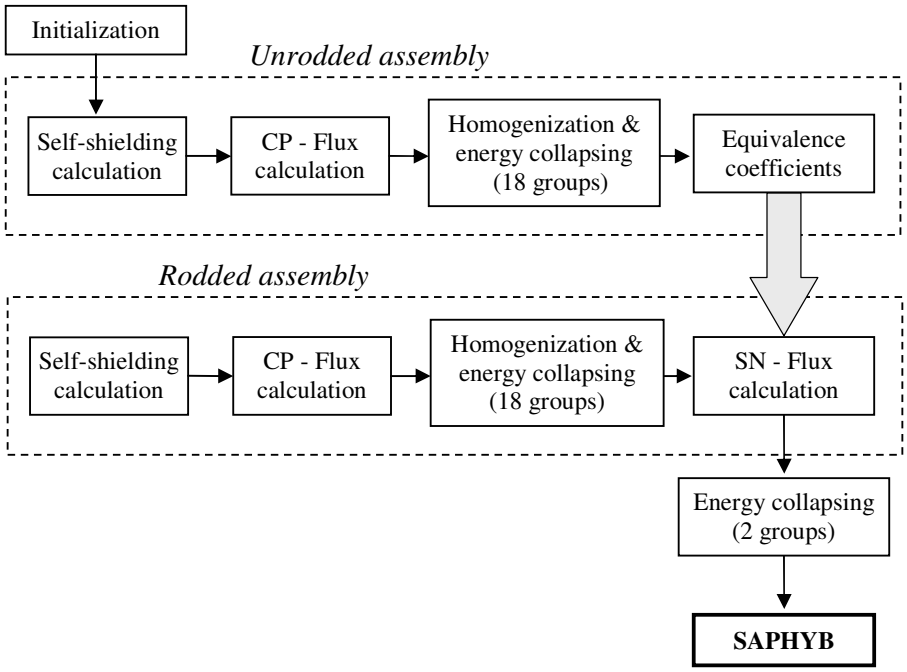

Fig. 4 Simplified schematic representation of APOLLO2 calculation for rodded assembly

The first level of the rodded assembly procedure is a typical self-shielding and CP flux calculation for unrodded assembly with 99 energy groups. Next, the calculation geometry is homogenized and the energy domain is collapsed to 18 groups. After the homogenization, the equivalence coefficients are calculated and stored for later use.

In the second level we apply the same procedure for assembly with control rod. The equivalence coefficients stored in the previous level are applied to correct the leakage and the macroscopic cross sections. This approach is required because the presence of a strong absorber at the periphery (typical for BWR control rod configuration) causes an abrupt drop in the thermal flux. If a typical homogenization is applied directly on a rodded assembly, the equivalence process fails to converge because of the low flux level. Even in the case when convergence is attained, this is only a numerical result and not necessarily the correct physical response.

With this approximation, we assume that the equivalence coefficients are independent of the presence of control rod. Comparison with the Monte-Carlo code TRIPOLI4 for similar assembly geometry [5] at 0% void fraction has shown difference of 200 pcm in k_{eff} and less than 2% deviations in the reaction rates. The use of this approximation will be further studied in a core calculation and validated against experimental data (cold critical states for PB2).

2.2.3 Axial and Radial Reflectors

The axial reflectors in BWR contain stainless steel (upper and lower tie plates), Zircaloy2 (fuel rod cladding), and moderator (liquid + vapor). APOLLO2 does not have an adequate model to treat the high anisotropy caused by the steel. For that reason, the Beta-method developed at CEA [8] is utilized to generate the cross-sections for the upper and lower reflectors. In the Beta-method, the Monte Carlo code TRIPOLI4 uses the source generated by APOLLO2 to generate albedo matrix; based on this albedo matrix CRONOS2 calculates the

cross sections for the media. Further, the cross-sections for the axial reflectors are defined explicitly in the core calculation.

The radial reflector of a BWR contains primarily water at saturated conditions. Based on our sensitivity study (presented in section 2.3 of this paper), we confirmed that the Beta-method is not mandatory to obtain the radial reflector cross-sections. In this case, the cross-sections are simply calculated by APOLLO2 for 1D geometry with two regions: one containing homogeneous mixture of the assembly and the second containing water at saturated conditions. These cross-sections are obtained by flux-volume homogenization.

2.3. Results from Sensitivity Studies

2.3.1 Reflector Model

To generate the cross-sections for the upper and lower reflectors, where substantial amounts of steel are present, we apply the Beta-method, developed at CEA. For the radial reflector we performed a sensitivity analysis on the presence of steel in the reflector region. We compare the albedo matrices, created with the Beta-method for two energy groups. The comparison is presented in the form of a matrix of the relative differences, where the local relative difference is calculated as

$$\Delta\beta = \left(\frac{\beta}{\beta_R} - 1 \right) \times 100 \qquad (2)$$

The effect of the steel after 30 cm of water is considered negligible if the relative difference is less than 3σ, where the value of σ is calculated by the Monte-Carlo code TRIPOLI4.

The relative differences are calculated as follows

$$\Delta\beta = \begin{pmatrix} 0.30 & -10.73 \\ -0.80 & -0.07 \end{pmatrix} \qquad 3\sigma = \begin{pmatrix} 0.41 & 22.70 \\ 0.55 & 0.14 \end{pmatrix}$$

The relative difference in $\beta_{1\to 2}$ is approximately 5σ, whereas the rest remain below 3σ limit. These results show that the albedo matrices are not very sensitive to the presence of steel after a water region of more than 30 cm width. Based on the above analysis the radial reflector cross-sections are calculated with APOLLO2 in a simplified 1D geometry and by a simple homogenization.

2.3.2 Leakage Model

The model most widely used in the industry for generating equivalent nodal parameters is based on zero-leakage single assembly calculation (i.e. in infinite media). However, the zero-current single-assembly boundary condition approach does not model the "true" environment of the assembly in the core (where the leakage of neutrons from or into the assembly might be quite significant) with sufficient accuracy.

Some lattice physics codes, like APOLLO2 employ a volumetric assembly leakage model. The homogenization technique usually adjusts the volumetric leakage trough an equivalent absorption term until the effective multiplication factor k_{eff} becomes 1. Afterwards, the critical buckling is applied to calculate the diffusion coefficient for the homogeneous assembly. The volumetric leakage approach however, treats the leakage as a global correction and zero-current boundary conditions are still used in the assembly calculations. While the volumetric leakage model may fulfill the neutron balance condition and provide a good

estimate of the asymptotic flux behavior inside the assembly, it does not represent the behavior of the neutron flux near the assembly interfaces.

Another more sophisticated approach utilizes the fundamental mode results to determine a critical albedo boundary condition for the assembly. The main characteristic of this approach is that the global leakage rate is partitioned into radial and axial components and the radial components are computed trough the assembly boundary itself instead of uniformly distributing them trough the whole volume. The partial-current albedo boundary condition is determined from the volumetric leakage rate.

APOLLO2 has an ability to model both the volumetric leakage (homogenization calculation with leakage of type A and B) and the surface leakage (leakage of type C). The critical leakage in the latter case is introduced as a surface source term.

In the presented sensitivity study, we evaluated the differences introduced by using the above-described three assembly leakage models on both assembly and core level calculations. For the 2D core comparisons we considered a calculation domain (a mini-core) consisting of four assemblies in a checkerboard layout and surrounded by a reflector (Fig. 5) with imposed zero flux conditions at the boundary.

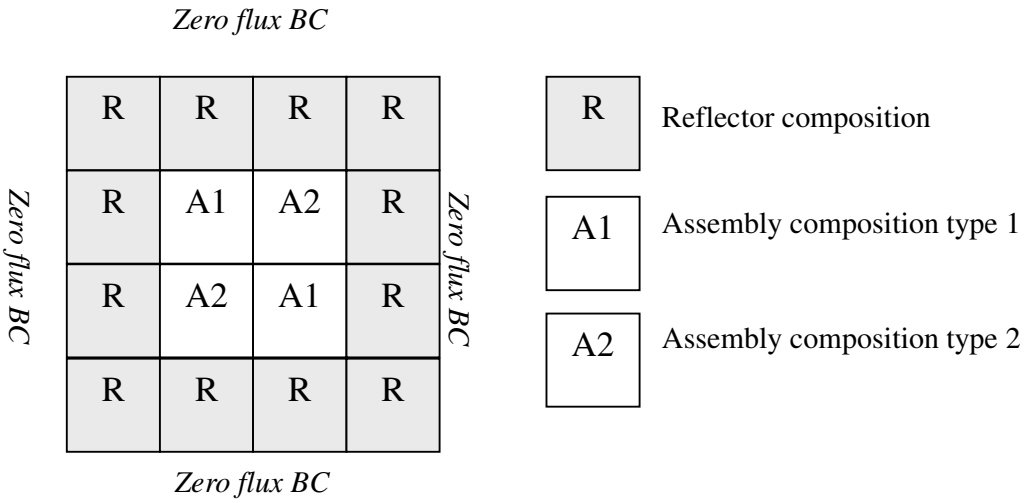

Fig. 5 Calculation domain for CRONOS2

The following three APOLLO2 calculations are performed for unrodded assembly. For each case, the cross-sections calculations are based on the method described previously:

a) assembly without leakage modeling ($B^2 = 0$) ,
b) assembly with volumetric leakage model and critical buckling search,
c) assembly with surface leakage model and critical buckling search.

The results from CRONOS2 in a 2D geometry calculations (at 0 MWd/t exposure, moderator temperature 560K, moderator density 0.739431g/cm^3, fuel temperature 790K) show that the zero current (B^2=0) case yields a deviation in k_{eff} of about 400 pcm compared to the critical leakage case. The difference in the radial power from CRONOS2 calculations differ with about 0.5%. The comparison between volumetric leakage and critical albedo models shows difference of 300 pcm on core level using the above-described mini-core benchmark.

Further comparisons will be performed with "reference" results generated by the APOLLO2 heterogeneous pin-by-pin calculations of the above-described mini-core benchmark The potential of the critical albedo leakage model for approximating the environmental effects into equivalent parameters derived from single-assembly lattice calculations will be investigated in order to improve core simulation results.

2.3.3 Spectral History Modeling

Another important process, which is investigated, is the cross-section parameterization, i.e. modeling of cross-section dependencies on thermal-hydraulics and control parameters. The set of branch parameters (fuel temperature and instantaneous void fraction) covers the whole range of operating conditions of BWR. The cross-sections are tabulated as function of burn-up. We take into account the spectral history by a variable representing the impact of the void fraction on fuel depletion. In the core calculation, the void fraction history is able to establish the differences in assembly cross-sections between axial nodes of an assembly depleted at different void conditions. The formulation of the history of void fraction is given by equation 2:

$$HV = \frac{1}{BU_c} \int_O^{BU_c} \alpha(BU)\, dBU \tag{2}$$

where α(BU) is the instantaneous void fraction and BU_c is the burn-up at the time of the calculation. It defines the correct cross-section to be used from the SAPHYB.

2.3.4 Void Fraction Modeling in APOLLO2

In APOLLO2, the two-phase density ($D_{2\phi}$) is calculated as a function of the void fraction (α) as shown in equation 3:

$$D_{2\phi} = \alpha D_{vapor} + (1-\alpha) D_{liquid} \tag{3}$$

The assumption of saturation allows using the void fraction as a simplified history model for cross-section parameterization. In this case the history of the core sub-cooled region is not modeled. Hence, it is important to have an estimate how these off-nominal parameters affect both assembly and core calculations. The effect is calculated first for the assembly using APOLLO2. Next, we study the impact for a 2D core calculation with CRONOS (mini-core benchmark) in order to show the sensitivity of the neutronic results to the assumption of saturation. Further this effect will be studied in a 3D model, because the sub-cooling usually occurs at the bottom of the assembly. Such study will quantify the neutronic importance of sub-cooled regions of the core/assembly inlet during steady state and transient conditions..

To estimate in APOLLO2 the neutronic sensitivity to this hypothesis, we compared two assembly calculations for the following two cases:

1) nominal case (saturated condition) : bypass and in-channel water (fig 6) at saturation temperature (560 K) and corresponding density of 0.739 g/cm^3

2) sub-cooled case : bypass and in-channel water at T=550K and corresponding density of 0.759 g/cm^3

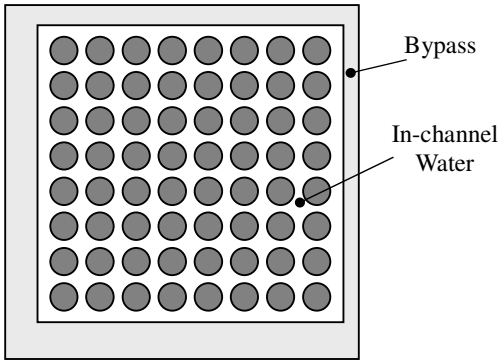

Fig. 6 Bypass and In-channel Water Region in BWR Assembly

These two cases show difference of more than 200 pcm in k_{inf}. At higher burnup the disagreement in k_{inf} is more distinct. Figure 7 shows plot of the k_{inf} deviation between sub-cooled and nominal cases.

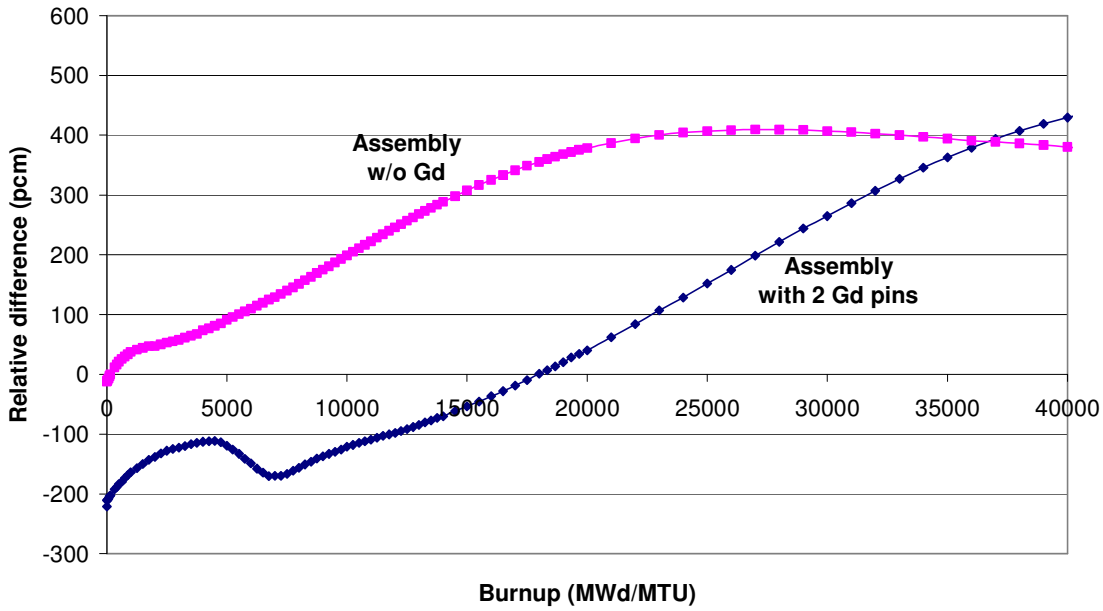

Fig. 7 Deviation of k_{inf} during burnup between sub-cooled and nominal (saturated, zero-void) conditions in assembly calculation

The obtained results on assembly level showed that the sub-cooled spectral history effect is not negligible. Since sub-cooled conditions are present usually in the lower part of the core a full 3D core model will show better the impact of sub-cooled history on axial power distributions. This study will be performed later with CRONOS2 for a 3D geometry to identify if an additional nominal axis for sub-cooled conditions is needed in the depletion calculation.

2.3.5 Bypass Density

The bypass density is not modeled in the geometry of the assembly: we take into account a nominal temperature inside the tube and outside the assembly to define the dilution effects on materials water/box with or without rod.

In order to reduce the size of the cross-section library and the calculation time it is more efficient to utilize a simplified approach where the bypass is assumed to be at saturated core conditions with 0% void along the core height. The cross-sections for the assembly composition are tabulated using the two-phase density (Eq. 3) of the moderator inside the assembly box (in-channel water).

To estimate the effect coming from the use of different densities for the bypass and the in-channel water we compared two assembly calculations for the following two cases.

1) saturated condition : bypass and in-channel water at saturation temperature (560 K) and corresponding density of 0.739 g/cm^3 with zero void.

2) saturated condition inside and sub-cooled condition for bypass : bypass at T=550K and corresponding density of 0.759 g/cm^3 and in-channel water at saturation with zero void.

These two cases show difference of more than 20 pcm in k_{inf} in the lattice calculation in APOLLO2. The effect on the neutronic calculation in APOLLO2 is very small. This dependence will be further examined in a diffusion calculation with CRONOS2 on a cluster of homogenized assemblies (2D geometry as in fig. 5) in order to identify the main neutronic parameters influenced by the bypass density. Also, the dependence will be further studied in a coupled 3D core calculation where the thermo-hydraulic effects on neutronics could show the necessity of implementing a bypass density correction in the core calculations. Similar problem exists with modeling the internal water rods in a BWR assembly and the effect will be evaluated in a coupled 3D core calculation.

3. Conclusion

The final objective of the cooperative research between CEA-Saclay and Penn State is to implement a refined methodology for a coupled-code calculation of BWR with SAPHYR code system. Qualification of such methodology is a complex task because the calculation is carried out on different levels: cross-section generation and modeling, and consistent coupled 3D core neutronics and thermal-hydraulics representation applicable to both core design and safety analysis. Because of the complexity of the calculation scheme, it is very difficult and time-consuming to identify all the aspects that contribute to the accuracy of final solution. At each step of the qualification process, we evaluate the impact of different factors, e.g. thermal-hydraulics feedback modeling, history effects, energy discretization, and physical approximations.

Our sensitivity studies with APOLLO2 and CRONOS2 show the importance of using appropriate parameters and options in the lattice calculation.

In the next step of the validation process, we will study different energy interval meshing to evaluate the effect of the discretization for a BWR core modeling. Later, we will perform coupled-code calculation using CRONOS2-FLICA4. We take advantage of the techniques developed concurrently at CEA-Saclay to establish an optimal and consistent BWR calculation scheme supplemented by a validation procedure to estimate the predictions of this scheme and establish acceptance criteria for the final results.

References

1) R. Sanchez, A. Hebert, Z. Stankovski, M. Coste, S. Loubiere, C Van Der Gucht and I. Zmijarevic, “APOLLO2 Twelve Years Later “, Mathematics and Computation, Reactor Physics and Environmental Analysis in Nuclear Applications - Madrid - (September 99)
2) J.J. Lautard, S. Loubiere, C. Magnaud, “CRONOS, A Modular Computational System for Neutronic Core Calculations”, IAEA Specialists Meeting, France, September 1990.
3) I. Toumi, A. Bergeron, D. Gallo, E. Royer, D. Caruge, “FLICA-4: A Three-Dimensional Two-Phase Flow Computer Code with Advanced Numerical Methods for Nuclear Applications”, Nuclear Engineering and Design, 200 (2000) 139-155
4) N. H. Larsen, “Core Design and Operating Data for Cycles 1 and 2 of Peach Bottom 2”, EPRI, NP-563, June (1978)
5) F. Bouveret, P. Magat and A. Nicolas, “Two-level Calculation Scheme for Producing Multi-Parameter Libraries using APOLLO-2 for a Dodewaard Fuel Assembly”, Proc. International Conference on Mathematics and Computation, Reactor Physics and Environmental Analysis in Nuclear Applications, 27-30 September 1999, Madrid Spain, pp. 901-908 (1999)
6) A.Santa-Marina et al, “French Calculation Schemes for Light Water Reactor Analysis”, Physor 2004, Chicago 25-29 April 2004
7) C. Poinot, E. Richebois, E. Rigaut, “Les schémas de calcul couple Neutronique-Thermohydraulique pour les réacteurs à eau bouillante : état d’avancement des travaux SERMA en 2000”, SERMA/LCA/RT /01-2896/A
8) E.Richebois et al, “Determination of multi-group and multi-operator Reflector constants application to a power reactor transport calculation”, International Conference on the Physics of Nuclear Science and Technology Long Island, New-York, October 5-8, 1998