Coupled Safety Analysis for Pressurized Water Reactors

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1. Introduction

Simulation of nuclear reactor cores and components relies on detailed physical models with their inherent feedback mechanisms to provide accurate estimates of system behavior. This includes coupling of several solvers into an integrated multi-physics analysis tool. These coupled calculations are capable of describing very complex phenomena in nuclear systems.

The aim of this study is to develop a coupled neutronics and thermal-hydraulics calculation tools to provide realistic simulation of the behavior of a light water reactor (LWR) core. The developed tool is used for a detailed safety analysis of a single fuel rod where density variation in the sub-channel and power distribution in the fuel rod varies strongly.

As a preliminary step, two way coupling between the thermal-hydraulics and neutronics is done. Changes in thermal hydraulic characteristics influence the power profile, however, the feedback mechanisms are not considered. Additionally, only the static effect on the reactivity is analyzed, neglecting the dynamic nature of the feedback.

2. Coupling Method

The developed tool is based on the coupling between well-known and well-validated codes. The tool uses MCNPX 2.7.0 for the neutronics calculation explicitly coupled with a modified version of COBRA IIIC/MIT-2 as a sub-channel thermal-hydraulics code. To speed up the coupled calculation, a parallel processing technique is adopted.

Typically, the iterations proceed until the thermalhydraulics conditions and the power distribution are converging within the required tolerance.

To better understand the developed computational tool; the neutronics model, thermal hydraulics model as well as auxiliary routines coupling them to each other are explained in this section.

2.1 MCNPX Neutronics Model

The Monte Carlo transport code, MCNPX [1], is used to calculate the energy deposited in the fuel rods due to the fission process. This energy corresponds to the power distribution in the fuel rods and is therefore used to generate the axial power distribution.

The heating in MCNPX is calculated directly using F6 tally which is used as a track length estimator of energy deposition in a cell.

The F6 tally is a volume tally, calculated in MeV/g by MCNPX as follows [1]:

$$F_6 = W_t T_l . \sigma_{TOT} \left(E \right) . h\left(E \right) . \frac{\rho_a}{m_c}$$
(2.1)

Where:

 W_i : Particle weight T_l : Track length (cm) $\sigma_{TOT}(E)$: Total microscopic cross section (barn) h(E): Heating number (MeV/collision) ρ_a : The atom density (atoms/barn-cm) m_c : mass of the cell (g)

In this study, a power conversion was necessary to be compatible with the modified COBRA IIIC/MIT-2 input deck format. The heating energy was converted into kW power units by using the following expression:

$$Q_{rod,z} = \frac{Q_{TOT}}{\sum_{z=1}^{Z} e_{rod,z}} e_{rod,z}$$
(2.2)

Where:

 $e_{rod,z}$: The heating energy in Mev/g function of the axial height z, Q_{TOT} : Fuel rod total power in kW, and $Q_{rod,z}$: The fuel rod power in KW for COBRA

input as a function of the axial height.

A critical issue for coupling is to account for the macroscopic cross-sections temperature dependence . To update the cross-sections, there are several techniques [2, 3], of different accuracy, memory requirements and computational costs.

In this study, the Pseudo Material Approach, also known as stochastic mixing, was used because it does not need any modification to the existing MCNPX cross section library. This approach is not an interpolation in the classical sense. This method relies on the stochastic nature of the MCNPX code and there are no nuclear data generated at some intermediate temperature [4].

It can be shown that the Doppler-broadening of the cross sections induces dependence proportional to the square root of the absolute temperature [5].

If for instance the average fuel temperature computed from thermal-hydraulics code T_{fuel} and cross section data are available for fuel temperatures at T_{low} and T_{high} from the ENDF library. Therefore, the pseudo fractions, f_{low} , f_{high} and cross-section are:

$$f_{low} = \frac{\sqrt{T_{high}} - \sqrt{T_{fuel}}}{\sqrt{T_{high}} - \sqrt{T_{low}}}$$
(2.3)

$$f_{high} = 1 - f_{low} \tag{2.4}$$

$$\Sigma_{Pseudo} (T_{fuel}) = f_{low} \Sigma_{low} (T_{low}) + f_{high} \Sigma_{high} (T_{high})$$
(2.5)

2.2 COBRA Thermal-Hydraulics Models

COBRA IIIC/MIT-2, referred to as COBRA, is a well verified code widely used in nuclear industry. It is a member of the COBRA family which is based on the sub-channel analysis method [6, 7] which solves the continuity, momentum, and energy transport equations.

The COBRA code can compute flow and enthalpy distributions in nuclear fuel rod bundles and core for both steady-state and transient conditions. It is used for thermal-hydraulics analysis of the Departure-from-Nucleate-Boiling Ratio (DNBR) in PWR sub-channels, as well as for 3-D whole PWR core simulation with one or more channels per fuel assembly [8].

The COBRA code consists of three main models that almost describe the entire physical phenomena associated to fuel rod and fuel assembly design and safety analysis. These models are flow transport, fuel heating and flow heat transfer models [8].

In this study, several modifications have been adapted to the code to enhance its capabilities and to accelerate the convergence of its numerical scheme.

2.3 Auxiliary FORTRAN Subroutines

Three subroutines were written in FORTRAN language to establish the coupling scheme. These subroutines were used generally in:

- 1. Reading the outputs files for both MCNPX and COBRA to extract the required data.
- 2. Performing some mathematical operations to prepare the data required for both MCNPX and COBRA input decks.
- 3. Adjusting the cross-sections for MCNPX using the extracted temperatures from COBRA to account for Doppler Effect.

3. Numerical Models

3.1 Cell Nodalization

The coupling is performed on a 1-D representation of a fuel rod nodalized in the axial direction with a symmetry condition assumed in the radial boundaries. A node in COBRA represents the boundary of a volume cell. On the other hand, a node in MCNPX represents the center point of the volume cell of a fuel rod or subchannel. The axial nodalization for a single volume cell is shown in Figure 2.1. It is noteworthy, that the nodalization scheme is shifted between COBRA and MCNPX. For data transfer between the two codes, the second node in COBRA at the boundary represents the first node in MCNPX at the cell center as shown in Figure 2.1.



Figure 2.1 Axial representations for data exchange

3.2 Coupling Procedure

The MCNPX and COBRA codes are coupled by exchanging data regarding fuel rod power distribution from the MCNPX simulation with water density, water temperature and fuel rod temperature axial distribution from COBRA simulation. The executable files for MCNPX and COBRA codes with the auxiliary subroutines are run separately and exchange data after each run via one batch file.

At first, MCNPX calculation is performed. Then the power distribution is automatically transferred into COBRA input. Subsequently, the COBRA calculations are performed to obtain the corresponding thermalhydraulics characteristics as a function of the axial height, iteratively until convergence is achieved before running a new MCNPX calculation.

A *converged state* is reached when the difference (relative value) between the coupled quantities at each axial interval of the corresponding iteration and the previous iteration is much smaller than the defined tolerance ε . In this study, a tolerance of 0.001 was used for the convergence criterion.

If the difference between the coupled quantities is larger than the specified tolerance, a new MCNPX/COBRA iteration is required.

To accomplish this, the extracted values form the COBRA code were used to automatically update the MCNPX input deck where the previous values for water density, water temperature and fuel rod temperatures were overwritten. At this step the first coupling iteration was performed.

Then, the coupled iterations were repeated until a converged solution is achieved.

4. Results

To check the coupling procedure a coupled analysis was performed with one typical PWR fuel rod model. The results of the iterations are given for the power distribution over the fuel rod along the rod active length, the water temperature and the water density distributions over the sub-channel including two inactive parts as shown in Figure 2.1.

4.1 Effect of Coupling on Rod Parameters

The need for coupling can be manifested through the effect of density variation on the power distribution. Figure 4.1 shows the fuel rod axial power distribution along the active height for three cases:

- a. An uncoupled case,
- b. Partially Coupled case with water density and temperature effects only 'No Doppler', and
- c. Totally Coupled case as b but with fuel rod temperature feedback (Doppler Effect).



Figure 4.1 Axial Power Distributions

The uncoupled case with constant values produces a power profile following a cosine shape with a maximum at the center.

The converged solution for the partially coupled case with water density and water temperature feedback only produced a power profile with a maximum peak at the lower part of the core due to high moderation.

The totally coupled case with the fuel rod temperature feedback produced a flatter power peak in the lower part of the core. This power peak is flattened because at high power, high fuel temperature, more fission neutrons are captured as the resonance region is widened and hence less power is produced.

4.2 Effect on Axial Power Distribution

The axial power distribution calculated during the iterative procedure is shown in Figure 4.2. The iterations show that the axial power distribution was affected directly by the strong variation in water density and Doppler Effect by the fuel. After seven iterations, the solution converged within the set tolerance.



Figure 4.2 Convergence of the axial Power Distribution

4.3 Effect on Coolant Density Distribution

Figures 4.3 represent the iterative profiles of the coolant density which was strongly affected by the axial power profile. The coolant density decreased faster than the profile of the uncoupled case because the power peak was shifted to the lower part of the core.



Figure 4.3 Convergence of the coolant density distribution

4.4 Effect on CHF and MDNBR

For hot channel safety analysis, the critical heat flux, CHF, and minimum departure of nucleate boiling ratio, MDNBR, are important parameters from the reactor safety point of view.

Figure 4.4 shows the distributions of the local heat flux, critical heat flux and minimum departure of nucleate boiling ratio.

The local heat flux for the uncoupled case follows the cosine power shape while the flux for the totally coupled case follows the coupled power profile since its peak was shifted to the lower part of the core. Similarly, the critical heat flux, CHF, for the totally coupled case exhibits a shifted peak.



Figure 4.4 CHF and MDNBR distribution over the fuel rod

The hot channel minimum departure of nucleate boiling ratio, MDNBR, for a typical PWR is greater than or equal 1.26. As shown in Figure 4.4, the MDNBR value for the totally coupled case is shifted to the left "to the middle of the rod" of the uncoupled case value. The values of MDNBR for both uncoupled and coupled cases are:

> $MDNBR_{Uncoupled} = 1.34997$ $MDNBR_{Coupled} = 1.3859$

5. Conclsions

A new coupled calculation tool with MCNPX 2.7.0 code and a modified version of COBRA IIIC/MIT-2 code has been developed for neutronics/thermal-hydraulics analysis of a fuel rod. The coupling procedure has been realized to iteratively exchange data between MCNPX/COBRA automatically until converged state is achieved.

Comparison of the results with and without coupling showed a significant difference. With this coupled model, the detailed local behavior of various parameters of the fuel rod is more realistic.

The main purpose of this tool is to study the complex behavior of the reactor core. The current work is part of ongoing effort to extend this tool for full core analysis using other physical solvers like fuel performance codes to produce an integrated multi-physics solver that has the capabilities of performing equilibrium core analysis.

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