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Iteration-Free Coupled Monte Carlo with Thermal Hydraulic Method

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Abstract - *Monte-Carlo (MC) neutron transport codes are widely used for the analysis of existing and future reactor systems due to their capability of simulating complex fuel assembly and core geometries without any significant approximations. Therefore, many institutions developed their own MC-based coupled codes. The coupling is usually referred to the integration between the neutron transport and depletion solutions. Typically, however, such coupled MC analysis is performed without including the thermal-hydraulic (TH) feedback, or in other words, assuming fixed TH conditions. However, providing MC codes with such a feedback is particularly essential because it will allow for more realistic and accurate modeling of the system behavior. In order to couple the transport solution with TH feedback, iterative scheme is generally applied. The most common coupling scheme is the fixed point iterative method, in which power and temperature distributions are iteratively and sequentially exchanged between the transport MC and TH solvers, respectively. Such an approach requires many iterations and hence many MC solutions, per a single time-point, which results in considerably higher CPU requirements. Recently, Generalized Perturbation Theory (GPT) equivalent method that relies on collision history approach was implemented in Serpent MC code. This method allows computing the sensitivity of any parameter due to the perturbation of any input parameter. Here, this feature was used to obtain the sensitivity of relative power change in region j to the relative change in the thermal-hydraulic properties in any region i in the system. This work uses these sensitivity coefficients to compute accurate temperature-dependent power distribution. The main advantage of this method is that it requires only a single transport calculation, in which these sensitivity coefficients are computed. Thereafter, the iterations to converge the TH conditions are performed with no additional MC simulations. The method was tested on a 3D BWR assembly and the results indicate that the proposed method achieves the same accuracy compared to the typical fixed-point iterative approach.*

I. INTRODUCTION

Monte-Carlo (MC) neutron transport codes are widely used for the analysis of existing and future reactor systems due to their capability of simulating complex fuel assembly and core geometries. Typically, MC analysis is performed assuming fixed thermal-hydraulic (TH) conditions. However, providing MC codes with such a feedback is very important and allows realistic and accurate modeling of the system behavior.

Such coupling was accomplished and reported in various publications. For example, in (Joo et al., 2004 [1]), a reduced height mini Pressurized Water Reactor (PWR) core was simulated using MC code McCARD with a simplified thermal feedback module. Continuous energy MC transport code MCNP (Briesmeister, 2000) coupled with the sub-channel TH code STAFAS [2] was applied for the analysis of High Performance Light Water Reactor (HPLWR) fuel assembly. A new coupled system MCNP5/SUBCHANFLOW for the pin- and fuel assembly-wise simulation of LWR and innovative reactors was developed in (Ivanov et al., 2011 [3]). Analysis of a fully coupled core was presented by Kotlyar et al., 2011 [4].

All of the above and many other coupling methodologies rely on an iterative procedure to perform coupled MC-TH analysis. More specifically, the solution usually starts with an initial guess of temperature and density distributions in the core. Power distribution data obtained by the neutron transport calculations using the MC solver. The spatial power distribution is transferred to the thermal-hydraulic module to obtain the updated temperatures and densities. This procedure is repeated until a convergence criterion is achieved, e.g. power residuals are below certain value.

Such an iterative approach is typically implemented in many diffusion codes (e.g. DYN3D [5]) and was also adopted for coupled MC codes. In the deterministic approach, the diffusion solution is relatively inexpensive (i.e. depends on the problem and/or number of energy groups), whereas this is certainly not the case for the transport solution obtained with MC. Achieving a converged solution may require tens of iterations, which will slowdown the solution by the same factor. Moreover, this iterative approach has to be done sequentially; no parallelism is possible. This problem is considerably amplified when the procedure also includes the depletion feedback that is essential for fuel cycle analysis. Moreover, recent studies [6] presented the effect of various iterative coupling schemes on numerical stability and accuracy of the results and suggested that iterative methods are required to stabilize the solution.

Recently, a collision history-based approach to sensitivity calculations was implemented [7] in an extended version of Serpent. The equivalence of this approach to the Generalized Perturbation Theory (GPT) was shown in [7]. This method allows computing the sensitivity of virtually any quantity (to any input parameter) that can be estimated with standard direct Monte Carlo criticality source simulations.

In the current study, this feature was used to obtain the sensitivity of relative power change in a burnable region j to the relative change in the thermal-hydraulic properties (e.g. fuel and coolant temperature and coolant density) in any region i in the system. Here, this ratio will be referred to as the sensitivity coefficient. The GPT-enabled Serpent version allows computing all the sensitivity coefficients in a single run.

This work uses these sensitivity coefficients to compute accurate temperature-dependent power distribution. The advantage of this method is that it requires no iterations and, thus, no additional transport calculations. Further studies would be needed to demonstrate the practicality and the computational efficiency of this method.

The proposed method was implemented in a script that couples Serpent with a stand-alone thermal-hydraulic solver. The method was then used to perform 3D coupled TH calculations of a typical BWR fuel pin divided into multiple axial layers. The performance of the proposed methods was compared to the traditional beginning-of-step method.

II. CODES AND METHODS

The thermal-hydraulic temperature and density distributions were evaluated by THERMO [4]. This module was verified for single- and two-phase flow regimes. The module calculates the coolant flow distribution in the core channels by requiring the pressure losses in all channels to be uniform.

The solution procedure is based on the assumption that the coolant flows in non-communicating sub-channels (lateral flow is neglected). The drift flux model is used for two-phase (liquid and vapor) flow. Osmachkin correlations for pressure drop for two phase flow and void fraction estimations [8] were adopted. In addition, the W3 [9] correlation for departure from nucleate boiling(DNB) prediction was used here.

The calculation procedure starts by axially dividing each sub-channel into sub volumes (nodes). The thermal conductivity of the cladding and the gap as well as the thermo-physical properties of the coolant (density, viscosity, specific heat etc.) are all assumed to be constant within each node. The fuel pellet is subdivided into a number of radial zones. The fuel thermal conductivity is assumed to be constant in every such zone. Thermal conductivity of the fuel is expressed as a polynomial function of the temperature and burnup. Heat generation in each fuel node is uniform. Heat transfer coefficient between the fuel and coolant is calculated by the use of appropriate heat convection correlations.

In this work a typical fixed-point iterative coupling scheme between the neutronic and TH calculations was implemented:

1. The sequence is initialized with a guess for the temperature and density distributions.
2. Power distribution data obtained by the neutron transport calculations using Serpent.
3. Temperatures and densities for the various materials (e.g. coolant) are calculated for each node by THERMO.
4. The TH parameters are updated.
5. Stages 2–4 are repeated until power distribution is converged.

III. THEORY: DIRECT POWER-TEMPERATURE CORRELATION

The proposed integration approach which relies on the GPT method was implemented in a linkage code. The continuous energy MC neutron transport Serpent [10] code was used here to provide the neutronic solution. In addition, the recent capability implemented in Serpent to obtain sensitivity coefficients was also used here. The practical implementation and description of the GPT method in Serpent is described in [7] and will not be repeated here.

This section presents a straightforward approach to correlate the change in power with the direct change in thermal hydraulic properties (i.e. temperatures and densities). The sensitivity coefficients of interest are:

$$S_i^j \equiv \frac{\partial P_j / P_j}{\partial T_i / T_i} \tag{1}$$

These sensitivity coefficients can be used to predict the temperature/density dependent behavior of the power as shown in eq. 2

$$P_j(T) = P_j(T_0) \cdot \left(1 + \sum_i^N S_i^j(T_0) \cdot \frac{T_i(P) - T(P_0)}{T_i(P_0)}\right) \tag{2}$$

The relation presented in eq. 2 between the power and temperature allows to couple these feedback mechanisms directly without executing MC sequentially and iteratively.

The change in power is simply obtained from solving a set of algebraic equations, which has the following matrix form:

$$\begin{bmatrix} \triangle P_1 \\ \triangle P_2 \\ \vdots \\ \triangle P_i \\ \vdots \\ \triangle P_N \end{bmatrix} = \begin{bmatrix} S_1^1 & S_2^1 & \dots & S_i^1 & \dots & S_N^1 \\ S_1^2 & S_2^2 & \dots & S_i^2 & \dots & S_N^2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ S_1^i & S_2^i & \dots & S_i^i & \dots & S_N^i \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ S_1^N & S_2^N & \dots & S_i^N & \dots & S_N^N \end{bmatrix} \begin{bmatrix} \triangle T_1/T_1 \\ \triangle T_2/T_2 \\ \vdots \\ \triangle T_i/T_i \\ \vdots \\ \triangle T_N/T_N \end{bmatrix}$$

The matrix **S** is the full Jacobian that describes how a change in thermal-hydraulic proprieties in region i will affect the power in region j (cross-terms). The GPT-based Serpent version allows to evaluate this matrix and hence all these cross terms.

Based on the above interpolation scheme, the following method was developed. For simplicity, the superscript j in S_i^j will be omitted in the algorithm description presented below.

However, the practical implementation evaluates the sensitivity coefficients for power in every region j as a function of every perturbed TH property i. Following are the main steps of the algorithm.

1. Obtain transport solution $P(T_0)$ and $S_i(T_0)$ for a predetermined temperature distribution T_0
2. Solve the heat conduction-convection problem and update the temperature/density distributions T_1
3. Obtain the new TH conditions as weighted average of the current and previous iterations:

$$\bar{T}_1 = (1-\theta)\bar{T}_1 + \theta T_1 \tag{3}$$

4. Update the power by substituting $\bar{T}_1$ into eq. 2
5. Repeat stages 2–4 until convergence is achieved.

Here, an under-relaxation factor $\theta \in [0, 1]$ was used. However, a variable , iteration dependent, relaxation factor could also be considered, e.g. 1/n (n-iteration index). In addition, at the very first iteration $\bar{T}_1 = T_0$.

This approach is similar to the well known fixed-point iterative approach, with an exception that the power distribution is obtained by generating the sensitivity coefficients and solving eq. 2. The direct approach requires sequentially executing the MC transport solver while the proposed approach requires no additional MC executions, which may result in better efficiency. However, each GPT-based MC solution is considerably slower than MC solution without calculation of sensitivity coefficients. The later slow down is proportional to the number of cross-terms in the Jacobian matrix. Therefore, the CPU time may even be longer, more than offsetting the benefits in having no iterations. This trade-off, however, was not studied in the current research but will be addressed in future studies.

IV. RESULTS AND ANALYSIS

In order to demonstrate the performance of the proposed iteration-free approach, a simple BWR cluster model of 7×7 fuel pins is chosen. The fuel lattice pitch is 1.87 cm and axially uniform 3% U-235 enrichment (UO_2 fuel) is considered with reflective radial boundary conditions. The length of the assembly is 366 cm and black boundary conditions are applied at the top and bottom. The assembly power is set to 3.5 MW, inlet water temperature to 287.8 °C and coolant mass flow rate to 29.4 kg/s. This 3D fuel assembly is divided into 36 equidistant layers and hence the dimensions of matrix **S** are 36×36.

The reference solution was obtained by applying a typical fixed-point iterative model described in the methods section. In order to obtain relatively small statistical uncertainties, 500 active fission source iteration cycles with 100,000 histories per cycle were used in the neutron transport calculations with Serpent.

The results are presented in Figs. 1 through 5. The reference solution was obtained by sequentially and iteratively executing the coupled code without relying on sensitivity coefficients. The power distribution was obtained directly by Serpent, which was then used in the thermal-hydraulic module to update the coolant density distribution. In the current study, 20 iterations were used to ensure convergence. The coupled reference solution is represented by the black curve and denoted as the 'reference' in the following figures. The coolant density at the core entry and exit is 730 and 330 kg/m^3 respectively. The coolant density distribution (Fig. 1) determines the power distribution, which in this case is strongly shifted towards the bottom part of the assembly as shown in Fig. 2.

The next stage was to execute the GPT-based Serpent version and obtain the sensitivity coefficients. In order to test the boundaries of this approach, a hypothetical extreme case of uniform coolant density distribution was used to obtain the sensitivity coefficients. Uniform coolant density of 400 kg/m^3 is presented in Fig. 1 (dashed purple curve). As expected, the corresponding power distribution has a cosine shape (Fig. 2). After applying the procedure presented in the previous section, the final solution (represented by the red squares) is much closer to the reference one (Figs. 1–2). It must be pointed out that no additional MC transport solutions are required in the applied iterative procedure. The agreement is relatively poor because the uniform density distribution was used to generate the sensitivity coefficients.

Therefore, it was decided to repeat the calculations with somewhat closer coolant density distribution as is shown in Fig. 3. Generating the sensitivity coefficients with this distribution, which is still relatively far away from the real one, produces power distribution that is in very good agreement with the reference solution (Fig. 4).

Finally, Fig. 5 presents the distribution of sensitivity coefficients in the fuel layer at the mid-plane of the core. As expected, the sensitivity coefficient that were obtained for a uniform coolant density are symmetrically distributed (within statistical uncertainties). For example, the change of 1 kg/m^3 in coolant density at the uppermost layer would have the same effect on the power variation if such change has occurred in the lowest layer. This, of-course, makes sense since the power distribution that corresponds to a uniform coolant density distribution is symmetrical. This figure also shows that the power change in the central layer is most sensitive to the coolant density in that layer and gradually diminishes with distance from this layer. In other words, TH conditions in distant neighbors will only have small effect on power in the mid core fuel layer. The figure also presents the sensitivity coefficient distribution for a non-uniform coolant density. The main difference between the uniform and non-uniform distribution is the asymmetrical effect of neighbors on the power in the central layer.

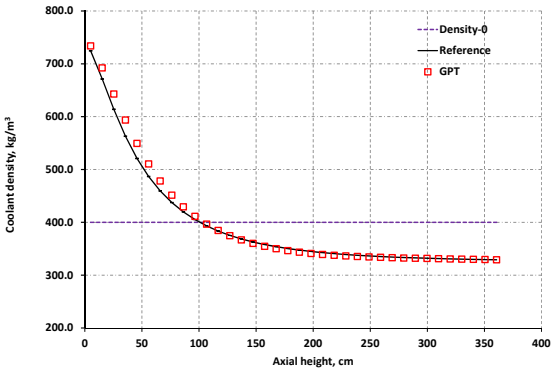

Fig. 1. Coolant density distribution with an initial uniform coolant density distribution guess.

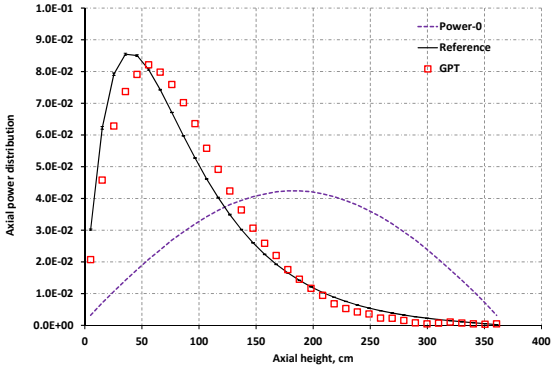

Fig. 2. Power distribution with an initial uniform coolant density distribution guess.

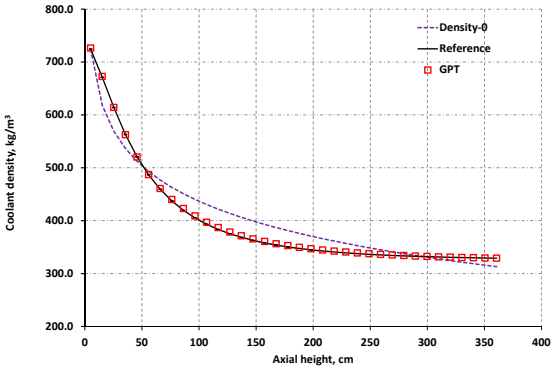

Fig. 3. Coolant density distribution with an initial non-uniform coolant density distribution guess.

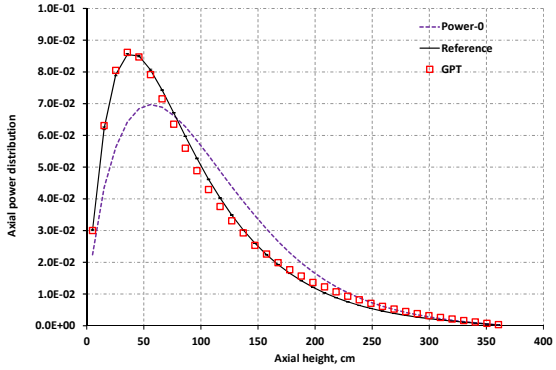

Fig. 4. Power distribution with an initial non-uniform coolant density distribution guess.

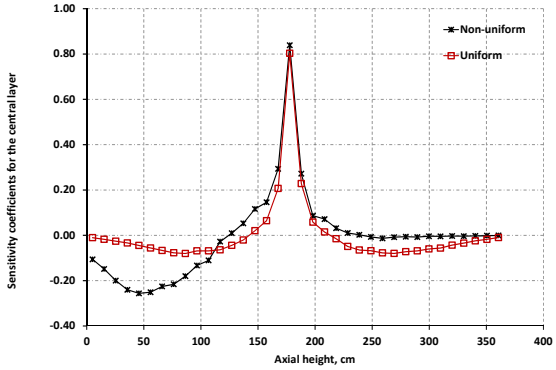

Fig. 5. Distribution of sensitivity coefficients (to coolant density) in the central layer, i.e. $S_1^{18}, ..., S_{36}^{18}$.

V. CONCLUSIONS

The importance of coupling procedure to integrate Monte Carlo neutron transport solution with thermal hydraulic feedback has been recognized and recently became a major topic of research. Coupled MC codes are now routinely used for assessment of new reactor designs.

This study proposes an iteration-free method which takes advantage of the additional information provided in the form of sensitivity coefficients calculated using Generalized Perturbation Theory in Serpent MC transport code. The GPT-enabled Serpent transport solution provides not only the reaction cross sections but also their derivatives with respect to the change in thermal-hydraulic conditions throughout the modeled system.

These derivatives allow obtaining significantly more accurate prediction of the power distribution variation as a function of thermal-hydraulic conditions.

The proposed method offers a potentially iteration-free approach, which could offer a major advantage. However, the

efficiency of the method has not been studied in the current work. The main disadvantage of this method is that calculating the additional sensitivity coefficients slows down the MC transport calculation considerably.

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