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# Efficient Geometry and Data Handling for Large-Scale Monte Carlo – Thermal-Hydraulics Coupling

J. Eduard Hoogenboom

[1]*Delft Nuclear Consultancy, IJsselzoom 2, 2902 LB Capelle aan den IJssel, The Netherlands*

[*]E-mail: hoogenboom@delftnuclearconsultancy.nl

Abstract

Detailed coupling of thermal-hydraulics calculations to Monte Carlo reactor criticality calculations requires each axial layer of each fuel pin to be defined separately in the input to the Monte Carlo code in order to assign to each volume the temperature according to the result of the TH calculation, and if the volume contains coolant, also the density of the coolant. This leads to huge input files for even small systems. In this paper a methodology is developed to overcome this problem. The method is implemented in MCNP5.

The method is demonstrated for an infinite lattice with 3x3 BWR-type fuel pins with cladding and moderator/coolant explicitly modeled. For all pins 60 axial zones are considered with different temperatures. The results of the axial power distribution per fuel pin are compared to a standard MCNP5 run in which all 9x60 cells for fuel, cladding and coolant are explicitly defined and their respective temperatures determined from the TH calculation. Full agreement is obtained.

***KEYWORDS: Monte Carlo, MCNP5, Thermal-hydraulics,***

## I. Introduction

To run a Monte Carlo reactor calculation with temperatures in the system derived from a thermal-hydraulics calculation, the temperatures must be addressed in the input to the MC calculation as the neutron cross sections are temperature dependent. For the MCNP5 Monte Carlo code this is done by adding an extension to the nuclide identification name in the input file. The user should take care of providing cross section data at the requested temperature. As there will be many different temperatures in different reactor volumes, it is not practical to generate cross section data at all required temperatures for all nuclides concerned. For large reactor systems this will not only require considerable computing time, but will also give memory problems to store all cross section data. Another approach[(1)], called stochastic mixing, uses a mix of nuclides at two different temperatures. This requires cross sections at a fixed series of temperatures. Then for a medium at temperature *T*, all nuclides in that medium must be specified at the nearest lower and higher temperature for which cross section data are available. With properly chosen atom fractions for the same nuclide at the two temperatures sampling of the nuclides in a collision results on average in representing the correct temperature *T*.
As each axial volume of each fuel rod or coolant channel can have a different temperature, for each small volume the material composition must be given with a double set for each nuclide. For a 17x17 PWR fuel assembly with an axial division of 100 zones this leads to the definition of $17^2$x100x3=86,700 different materials to be defined and entered in the MC input file. This will be impractical and a more efficient method is needed.

## II. Method

A new method was proposed by Ivanov[(2)] and in the current work an independent implementation realised in MCNP5. The basic method for efficient handling of thermal-hydraulic data lies in the assignment of the cross sections with the required temperature when a neutron enters a certain zone. Then the MC code must determine in which fuel rod or coolant channel and at which axial zone as used in the TH calculation the neutron is. From the output table of the TH calculation with temperatures per fuel rod and axial zone, the temperature of the fuel, cladding or coolant volume can be determined. Knowing at which set of temperatures cross section data is available, the MC code can calculate for each nuclide in the medium at which two temperatures the nuclide must be represented in the medium and with which atom fractions. Hence, the composition of fuel, cladding and coolant is not fixed, but changes for each neutron entering a medium.

### 1. Geometry description and material composition

Using a dynamically determined material composition the geometry input can be kept simple. For a fuel assembly consisting of identical pin cells (apart from possibly varying temperatures and coolant densities), one can define a single pin cell and introduce a lattice of these pin cells to form a fuel assembly. If the fuel assembly contains different types of fuel pins, e.g. with different composition, each fuel pin type must be defined separately, but they can still be put together in a fuel assembly in a simple way. An axial lattice must also be defined for the different axial TH zones.
All nuclides need to be listed in the input with two arbitrary

nuclide identification extension, as the actual extensions will be determined dynamically during the Monte Carlo simulation. Likewise, the coolant densities can be entered with arbitrary values.

**2. Cross section assignment**

In order to import into computer memory all cross section data that will be needed for a core calculation, given the temperatures from a TH calculation, all nuclides with relevant identification extension must be referenced in the input. All nuclides with identification extensions needed somewhere in the system but not yet referenced, can be referenced as present in a small volume outside the actual system geometry where no neutrons can ever come.

When a neutron enters a certain volume with temperature derived from the TH output, the MC code should determine the pair of actual nuclide identification extensions depending on the actual temperature and the series of temperatures for which cross section data are available.

**3. TH data handling**

It will be efficient if the thermal-hydraulics code lists in an output file for each fuel pin/coolant channel the coolant density, the coolant temperature, the cladding temperature and the average fuel temperature for each axial zone. These data must be read into the Monte Carlo code. For coupled MC-TH iterations, the TH output must be read every time a new MC run starts.

**4. Parallel execution**

In order to maintain the ability of the MCNP5 code for parallel execution, some precautions must be taken. For a serial execution the array with pointers to a specific cross section set per nuclide in a medium can be dynamically redefined for each neutron simulated, but when executing in parallel with different threads, a new array must be defined with separate elements for each thread. This array must be declared threadprivate for proper parallel execution. Likewise, the array for the coolant density must be replaced.

## III. Demonstration

**1. Description of sample case**

The MC-TH coupling scheme is applied to an infinite lattice of a 3x3 pin BWR fuel assemblies. MCNP5 is used as the Monte Carlo code and modified to facilitate the reading of the TH output and dynamically assign nuclide identification extensions and coolant densities. The SubChanFlow[3] code from KIT, Karlsruhe, is used as the thermal-hydraulics code with a small modification to provide a practical output file.

As the aim of this work is to demonstrate the effective use of dynamically assignment of temperatures and coolant densities, no iterations between MC and TH calculations are performed, but a suitable output from a TH run was used in a single MC run.

In the MC run 10,000 neutron histories per cycle were applied and 400 active cycles after 10 inactive cycles, starting from a source distribution that was already available and resembled the converged fission source distribution quite well.

To compare the results a run was performed with the standard MCNP5 code, but with a detailed input, defining each axial zone in each pin cell separately, according to the temperatures and densities from the TH output. The input file for this case contained almost 10,000 lines, while the input for the modified MCMP took only 125 lines.

**2. Results**

Fig. 1 shows the axial power distribution for the central pin of the assembly. The results fully agree, within statistics, with a run of the standard MCNP5 code with separate definition of all cells in the problem. The standard deviation for each power value is in the order of 1 %.

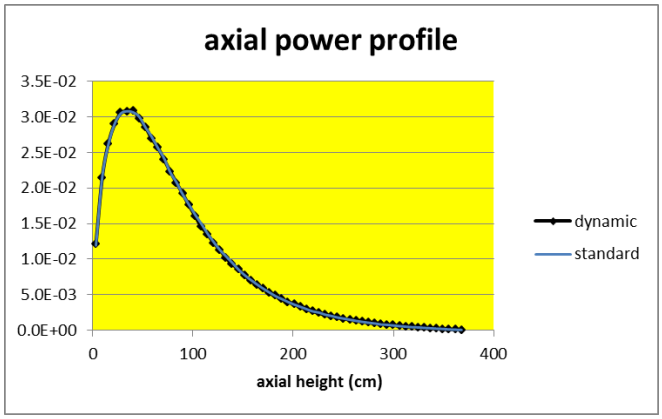


**Figure 1**: A**xial power distribution for central fuel pin for dynamic and standard method**

## IV. Conclusion

The case presented here demonstrates that with limited modification of a general purpose Monte Carlo code, in our case MCNP5, it is possible to execute a coupled MC-TH calculation with detailed assignment of temperatures and coolant densities for all axial zones of each pin cell. This opens the way to MC-TH coupled calculations for large-scale systems with existing Monte Carlo codes with a minimum of cross section data and geometry description.

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**References**

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