# Pin Cell Simulation of the Change in Doppler Broadening and Self-Shielding with the Change in Nuclear Fuel Temperature and Fuel Type by Using OpenMC

**N. Beydoğan, G. Konur, G. Sarici, O.Ş. Çelikten, M. Türkmen, C.N. Sökmen**

*Department of Nuclear Engineering, Hacettepe University, Beytepe, 06800, Ankara, Turkey*

**Abstract.** The main purpose of this study is to determine the uncertainties in modelling due to use of isothermal temperature assumption in the radial direction. For this purpose, unit cells specified in the OECD/NEA Light Water Reactor (LWR) Uncertainty Analysis in Modeling (UAM) benchmark, BWR Peach Bottom-2, the PWR unit cell of Three-Mile Island-1 and the VVER Kozloduy-6, are used. Fuel region of each unit cell is divided into a number of sub-regions, represented as multi-region. Fuel temperature distribution in radial direction is calculated by using the heat equation. Fuel temperature distribution is used in generating the neutron cross-sections for each region. For the simulations, OpenMC code (Monte Carlo particle transport code) coupled with NJOY and ENDF/B-VII.1 neutron cross-section libraries are used. Change of multiplication factor with number of sub-regions and use of temperature gradient in radial direction is investigated.

**Keywords:** Monte Carlo Method, Multiplication Factor, OpenMC, Self-Shielding, UAM

## 1 Introduction

In nuclear fuels, number of neutrons absorbed in the resonance region tend to increase with increasing temperature due to Doppler broadening. This situation leads to decrease the average travel distance of neutrons between the collisions. Some of the neutrons entering into the fuel region from the moderator region are absorbed in the region close to outer surface of the fuel pellet. Therefore, the inner region of the fuel pellet is exposed to a lower neutron flux than the outer region. In other words, the outer region of the fuel pellet shields the inner regions. This phenomenon is known as self-shielding. However, it should be noted that self-shielding depends on the temperature distribution of the fuel due to Doppler broadening. Related with this issue, in the stage of modelling of current reactors, the temperature distribution of the fuel pellet is assumed to be isothermal. In fact, fuel region has a temperature distribution in radial direction. It is clear that use of isothermal temperature assumption would affect the neutronic calculations. Even though uncertainties in modelling due to nuclear data libraries have been studied in OECD/NEA LWR Uncertainty Analysis in Modelling (UAM) benchmark [1], the uncertainties due to effect of temperature distribution on the nuclear cross-sections (e.g., self-shielding, fission) needs to be investigated.

The purpose of this study is to determine the uncertainties in modelling due to use of isothermal temperature assumption in the radial direction. In this manner, multi-region method where the fuel region is represented as volumetrically equal sub-regions in radial direction is utilized in analyses. Change of multiplication factor with the number of sub-regions is investigated.

## 2 Method

This study is performed for three different types of fuel elements reported in the Uncertainty Analysis in Modelling (UAM) benchmark, the square unit cell of Three Mile Island-1 PWR, square unit cell of Peach Bottom-2 BWR and hexagonal unit cell of Kozloduy-6 VVER-1000. Design parameters of the considered reactors are given in Table 1 and unit cell representations are also showed in Figure 1. Geometry, material properties and operating conditions are assumed the same as stated in Exercise I-1 of the UAM benchmark case. Fuel region of each unit cell is divided into a number of sub-regions, up to 16 sub-regions. Fuel temperature distribution in radial direction (without axial distribution) is calculated by using the heat equation (from the conductivity integral).

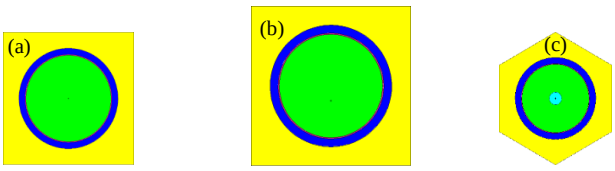


Figure 1. (a) TMI-1 PWR Pin Cell, (b) PB-2 BWR Pin Cell, (c) Kozloduy-6 VVER Pin Cell (in scale).

As conductivity integral, the temperature-dependent thermal conductivity derived from the Lyons' integral of $kdT$ [2] (used by Combustion Engineering) as seen below is used;

$$k(T) = \frac{38.24}{129.25 + T} + 6.1256 \times 10^{-13} T^3 \qquad (1)$$

In this equation, $T$ is in unit of Kelvin and $k$ in terms of $\mathrm{Wcm^{-1}K^{-1}}$.

Table 1. The parameters of unit cells at HFP (UAM)

| Parameters | TMI-1 PWR | PB-2 BWR | Kozloduy-6 VVER-1000 |
|---|---|---|---|
| Unit cell pitch, [mm] | 14.427 | 18.75 | 12.75 |
| Fuel pellet diameter, [mm] | 9.391 | 12.1158 | 7.56 |
| Fuel pellet material | $UO_2$ | $UO_2$ | $UO_2$ |
| Fuel density, [g/cm$^3$] | 10.283 | 10.42 | 10.4 |
| Fuel enrichment, [w/o] | 4.85 | 2.93 | 3.3 |
| Central void diameter, [mm] | — | — | 1.4 |
| Central void material | — | — | dry air |
| Cladding outside diameter, [mm] | 10.928 | 14.3002 | 9.1 |
| Cladding thickness, [mm] | 0.673 | 0.9398 | 0.69 |
| Cladding material | Zircaloy-4 | Zircaloy-2 | Zr + 1% Nb |
| Cladding density, [g/cm$^3$] | 6.55 | 6.55 | 6.55 |
| Gap material | He | He | He |
| Moderator material | $H_2O$ | $H_2O$ | $H_2O$ |
| Fuel temperature, [K] | 900 | 900 | 900 |
| Cladding temperature, [K] | 600 | 600 | 600 |
| Moderator (coolant) temperature, [K] | 562 | 557 | 560 |
| Moderator (coolant) density, [kg/m$^3$] | 784.4 | 460.72 | 752.5 |

Radial temperature profile of a solid fuel element is directly related with coolant and cladding condition as much as heat generation rate and material properties. Heat generation depends on neutron reaction rate, especially the fission source. Radial conduction equation is given below in Eq. (2)

$$\frac{1}{r}\frac{\partial}{\partial r}\left(k(\vec{r},T)r\frac{\partial T(\vec{r})}{\partial r}\right)+\not{?}q(\vec{r})=0\,. \qquad (2)$$

In Eq. (2), $r$, $T$, $k$ and $\not{?}q$ represent radius, temperature, thermal conductivity and volumetric heat generation rate, respectively. The thermal conductivity depends on material composition and local temperature of the fuel. Assuming the volumetric heat generation rate is constant, small fuel shells with inner radius of $R_i$ and outer radius of $R_0$ are integrated twice over the radius. Thus, Eq. (3) is obtained

$$\int_{T_0}^{T_i} k(T)dT=\overline{q}(R_0^2-R_i^2)/4\,, \qquad (3)$$

where $T_i$ and $T_0$ are inner and outer temperatures of fuel respectively. $\overline{q}$ is the average heat generation rate over the region bounded by $R_i$ and $R_0$.

For the fuel element which is divided into volumetrically equal $n$-regions, total heat conductivity integral,

$$\sum_{j=1}^{n}\left[\int_{T_0^j}^{T_i^j} k_j(T)dT\right]=\sum_{j=1}^{n}\left[\overline{q}_j(R_{0_j}^2-R_{i_l}^2)/4\right]. \qquad (4)$$

By using Eq. (4), volume-averaged temperature of the fuel is calculated for each individual region. It is important to note that in any case of this study, the volume-averaged temperature over the fuel region is kept constant at 900 K. Furthermore, fuel surface temperature is assumed to be 600 K. In this work, as a first step, no iteration scheme is considered for the convergence of volumetric heat generation. Neutron reaction rates, especially fission rates directly affect the heat generation so, volumetric heat generation assumed the same in all sub-regions without the iteration. Change of multiplication factor due to effect of multi-region and radial temperature distribution is compared to use of isothermal temperature distribution in one region.

The considered unit cells are modelled with the aid of OpenMC [3], a Monte Carlo based code. Surface boundary conditions are defined as reflective. As an illustration, multi-region representation (1, 2, 4, 8 and 16 regions, respectively) of TMI-1 PWR unit cell is shown in Figure 2.

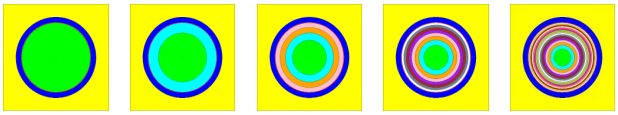

Figure 2. TMI-1 PWR unit cell divided into a number of sub-regions.

OpenMC is a Monte Carlo particle transport simulation code which uses ACE formatted cross-sections. Simulations are performed by using the neutron cross-section libraries generated for the calculated temperature of each sub-region by NJOY99 [4]. The code produces outputs such as multiplication factor and neutron flux. In this study, OpenMC simulations for 2250 batches where the first 250 cycles are inactive, and all simulations are performed for 100000 source particles.

Fuel temperature distribution is used in generating the neutron cross-sections for each region and then neutron crosssection libraries for each region are generated by using the NJOY code. NJOY99 is a nuclear data processing system which is a system of processing modules intended to convert raw nuclear data in the ENDF format into the forms useful for practical applications.

## 3 Results

The results are obtained for 1, 2, 4, 8 and 16 sub-regions. Fuel temperature distribution inside TMI-1 PWR unit cell

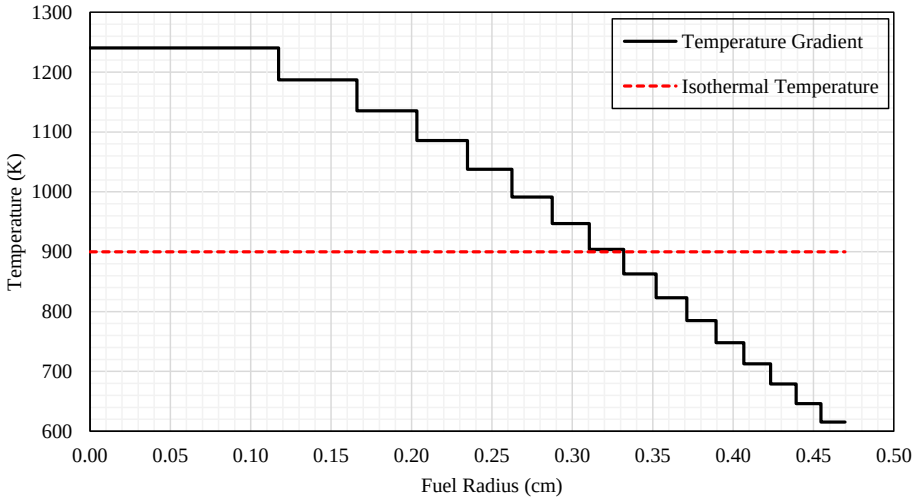


Figure 3. TMI-1 PWR temperature distribution for 16-region case.

for 16 sub-regions is shown in Figure 3. Despite that no iteration on the temperature calculations is carried out, profile of the TMI-1 PWR temperature distribution is in agreement with a different study [5]. As expected, the temperature decreases gradually from fuel centreline to fuel surface. When surface temperature is fixed to 600 K, the maximum temperature was calculated to be about 1240 K at the innermost sub-region. Noting that the volume-averaged fuel temperature is 900 K.

Calculated multiplication factors and standard deviation for various sub-regions are given in Table 2. Results show that the multi-region demonstration of the fuel instead of one-region model affects the multiplication factors because of modelling the temperature gradient. This difference is due to the generation of new nuclear data libraries according to the calculated temperatures. Although the temperature averaged over the fuel region is fixed to 900 K, it is calculated that Doppler calculation for multi-region is different from the one-region approximation.

In order to observe the effect of the use of multi-region approximation and temperature gradient, $k_{\text{eff}}$ values for each reactor type, which are given in Table 2, are subtracted from the one-region multiplication factor value of that reactor ($\delta k = k_i - k_1$, where $i$ represents the region number). The results are given in Figure 4. According to Figure 4, use of multi-region method and temperature gradient leads to 60–80 pcm difference for the VVER, and 80–100 pcm difference for the PWR and BWR from one-region and isothermal temperature distribution approximation.

Table 2. Calculated multiplication factors for various sub-regions for the interested unit cells

| | 1 Region | 2 Regions | 4 Regions | 8 Regions | 16 Regions |
|---|---|---|---|---|---|
| TMI-1 PWR | 1.41603 | 1.41645 | 1.41693 | 1.41692 | 1.41695 |
| PB-2 BWR | 1.23582 | 1.23648 | 1.23677 | 1.23667 | 1.23679 |
| Kozloduy-6 VVER | 1.33425 | 1.33470 | 1.33496 | 1.33503 | 1.33484 |

*Standard deviations of the OpenMC calculations are about $\pm 0.00006$.

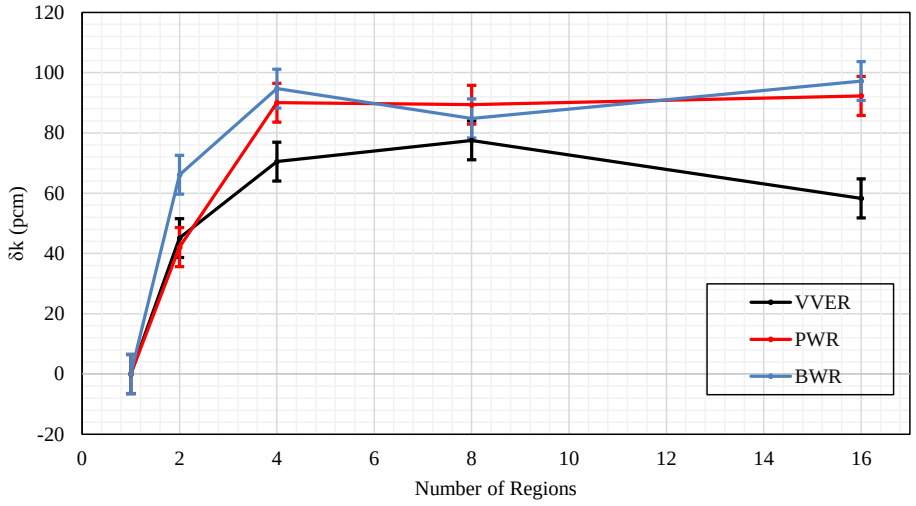


Figure 4. Change of the uncertainty (pcm) of the $k_{\text{eff}}$ due to usage of temperature gradient with the number of regions.

## 4 Conclusion

It is demonstrated in this study that multi-region method allows modelling the temperature distribution effects on the reactor parameters consistently. By increasing the number of sub-regions, the neutronic parameters can be obtained more accurately. Further investigation on how many number of sub-regions is required is needed.

Thermal conductivity is a function of temperature in radial direction and which depends on power generation (fission rate) in the fuel. In this manner, in the future work, a converged volumetric heat generation profile (as fission source distribution from the Monte Carlo calculations) instead of constant volumetric heat generation will be used. In order to perform this modelling, fission rates for each region should be noted and inserted into the model for calculation of the radial fuel temperature distribution again.

### Acknowledgements

This study is supported by The Scientific and Technological Research Council of Turkey (Project Code: 1001-114F375).

### References

[1] Ivanov, K., Avramova, M., Kodeli, I., Sartori E.: Benchmark for Uncertainty Analysis in Modeling (UAM) for Design, Operation and Safety Analysis of LWRs, Volume I: Specification and Support Data for the Neutronics Cases (Phase I), NEA/OECD Nuclear Energy Agency, NEA/NSC/DOC(2007)23, 2007.

[2] Todreas, N.E., Kazimi, M.S.: Nuclear Systems I: Thermal Hydraulic Fundamentals, 2nd Ed., Taylor and Francis, USA, 1993.

[3] Romano P.K., The OpenMC Monte Carlo Code – OpenMC Documentation URL: http://mit-crpg-github.io/openmc, 2013.

[4] MacFarlane R.E., Muir D.W., The NJOY Nuclear Data Processing System, Version 91, Los Alamos National Laboratory report, LA-12740M, 1994.

[5] Türkmen M., Çelikten O.Ş., Sökmen C.N., Uncertainty in modeling due to use of isothermal temperature inside the fuel, Nuclear Engineering and Technology, Submitted Article, 2015.