Test case for ALLEGRO MOX pin modeling using SERPENT and ATHLET

K Kaprinayova 1,2, L Zahorszki 1, S P Nikonov 1 and G V Tikhomirov 1

1National Nuclear Research University MEPhI (Moscow Engineering Physics Institute), Department of Theoretical and Experimental Physics of Nuclear Reactors
2Slovak University of Technology, Faculty of Electrical Engineering

katarina.kaprinayova@gmail.com, zahorszki.liliana@gmail.com, niks.ki@mail.ru, GVTikhomirov@mephi.ru

Abstract. This paper is devoted to the test case for ALLEGRO MOX pin modeling using Serpent and ATHLET codes for coupled neutronics - thermal hydraulics coupled calculation. This research can be considered highly actual as ALLEGRO is the demonstrator of the Gen IV reactors and it should show the possibilities of the fast gas cooled reactors. In this paper, coupling scheme and the basic steps of the calculation, Serpent and ATHLET models of the MOX fuel pin divided into ten axial layers, and the calculated axial power distribution for all iterations are introduced. The auxiliary programs responsible for data processing are written in Python and Fortran languages.

1. Introduction
To obtain results usable in the design and operation of nuclear reactors it is needed to consider all physical processes occurring simultaneously in the reactor core, as they have mutual feedbacks on one another. Therefore, to achieve better accuracy, it is necessary to create a multiphysics model. The article provides a test case for the coupled neutronics-thermal hydraulics calculation of the ALLEGRO [1] reactor using the neutron transport code SERPENT [2] and the thermal hydraulics system code ATHLET [3]. A model of one MOX fuel pin has been developed, which includes shielding, reflector and helium cavity in the top and bottom of the heating part, in which the fuel part is divided into 10 layers, has been developed. It is necessary to say that He inside the fuel element is not considered as a simple gas gap, but it is a real thermofluid object according ATHLET terminology.

2. Discussion
Calculations of power distribution, fuel, cladding, reflector, absorber and coolant temperature, coolant density is carried out. The description of SERPENT [2] and ATHLET [3] codes, geometry and material composition of the model and also an iterative calculation scheme is given in the paper. Programs written in Fortran95 and Python are used for processing input and output data. It is assumed that the test case will be used for further modeling of the ALLEGRO reactor (MOX fuel assembly and starting MOX core) and for cross verification of computer codes. The ALLEGRO reactor [1] is presented in the figure 1., the MOX core in figure 2, the MOX fuel assembly in figure 3, the pin models are shown in figure 4, the coupling scheme is depicted in figure 5 and the results are shown in figure 6.
ALLEGRO is the demonstrator reactor of the GFR IV [1] generation reactor type. Estimated power of the reactor will be 75 MWth. ALLEGRO is a needed step for designing prototypes of GFR2400 power plants. The preliminary system design is based on intermediate loops with two primary helium loops. This system includes two intermediate heat exchangers compatible with inlet and outlet temperatures of helium (260/530°C for the start-up and 400/850°C for the demonstration core). The secondary loops are filled with pressurized water.

The reactor shall be operated with two different cores:

- start-up MOX core figure 2, with some experimental GFR subassemblies,
- core using ceramic fuel assemblies.

The start-up MOX core will be used for testing the operation of GFR and the core using ceramic fuel assemblies will be used for testing the new fuel design.

The MOX core will be used for calculations. A fuel assembly figure 3, consists of 169 fuel rods and claddings are made of stainless steel. Most of the geometrical, material and thermophysical characteristics of ALLEGRO are confidential information, so they can be presented only partially.

ATHLET (Analysis of Thermal-hydraulics of Leaks and Transients) [3] was developed by the Gesellschaft für Anlagen- und Reaktorsicherheit (GRS). The original purpose of ATHLET was the analysis of the entire spectrum of leak cases and transients in LWR reactors. Furthermore, the code is also applicable for plants and facilities applying other working fluids like heavy water, helium, sodium, lead or lead-bismuth eutectic.

The structure of ATHLET [3] is highly modular so different physical models can be easily implemented. The code consists of several basic modules: Thermo-fluiddynamics (TFD), Heat Transfer and Heat conduction (HECU), Neutron Kinetics (NEUKIN) and General Control Simulation Module (GCSM). The system of ordinary differential equations is solved fully implicitly with the numerical integration method FEBE.

ATHLET [3] provides a modular network approach for the representation of a thermal-hydraulic system. One can simulate a system configuration by connecting basic fluiddynamic elements, these elements are called thermo-fluiddynamic objects (TFO). There are several TFO types and these types are classified mainly into three basic categories: pipe objects, branch objects and special objects.
SERPENT is a multi-purpose three-dimensional continuous-energy Monte Carlo particle [2] transport code, developed at VTT Technical Research Centre of Finland. It can be used in a wide area of applications, such as traditional reactor physics calculations, validation of codes, burn up calculations, multiphysics modeling, neutron and photon transport simulations for radiation dose rate calculations etc.

The accuracy of calculations is determined by the used evaluated nuclear data libraries. SERPENT can perform various calculations with realistic geometry and exact material composition of complex media at various temperatures. SERPENT can utilize MPI parallelization, so the calculations can be divided into several nodes [1].

The neutronics model in SERPENT [2] is one pin, consisting of the MOX fuel, helium cavity, reflector and shielding surrounded by coolant (helium) figure 4. The model is divided into 16 axial layers (10 layers in the fuel part, top and bottom helium cavity, reflector and shielding). Periodic boundary condition is set on the lateral border, black boundary condition is used at the top and bottom of the fuel pin. The effective neutron multiplication factor $K_{\text{eff}}$ should be equal unity so it is adjusted by varying the position of the boundary, because no absorber is present in the coolant. The temperature dependence of the density of the fuel, cladding, reflector, and shielding is not taken into account on this stage of the investigation. Nominal power is equal to 5,4789 kW (the average power of a fuel pin).

In case of ATHLET [3], the model includes two helium TFOs (thermofluid objects), one, the coolant, is located outside the fuel cladding, the other inside, and it includes the gas gap and the two cavities. The fuel cladding, fuel, top and bottom reflectors and shieldings are considered as thermal structures. The materials, dimensions, and the axial division are the same as in the neutronics model. Figure 4 shows the structure of the ATHLET model, HE L001 is the coolant helium, HE-S001 is the helium, which includes gas gap and the helium cavity. The position of the layers in the heat structures is the same as in the TFO. It is assumed that heat is generated only in the fuel part of the pin. The needed values from ATHLET [3] are the density and temperature distributions of the coolant helium and the helium inside the fuel rod, and also the temperature distribution in the fuel, cladding, bottom and top reflectors and shieldings.

![Figure 4. ALLEGRO MOX pin model; Serpent (left), ATHLET (right)](image)

The aim of this multiphysics model is to reflect the physics of a real facility, that can be used for the determination of characteristics of the ALLEGRO reactor [1]. The external iterative scheme is shown in figure 5.

The axial power distribution needed for ATHLET is calculated by the formula:

$$P_i[\%] = \frac{R_{fi}}{\sum_i R_{fi}}$$  \hspace{1cm} (1)
where $P_i \ [%\]$ is the power of the $i$th layer in $\%$, and $R_f$ is the sum of fission reaction rates in $i$th layer obtained from the SERPENT calculation [4]. The steps of the coupled are the following:

1. SERPENT calculation [4]; $keff = 1$;

2. processing the output file by a program written Fortran $\rightarrow$ power distribution;

3. transferring the power distribution to the ATHLET input file (Fortran90 program);

4. ATHLET calculation [3];

5. processing the output file by a program written in Fortran $\rightarrow$ helium density and temperature distribution from two sides of cladding and also temperature distribution in fuel, cladding, bottom and top reflector and shielding;

6. transferring temperatures and densities to the SERPENT input file (Python program);

7. SERPENT calculation [4] with Doppler broadening; $keff = 1$ (by changing the position of boundary);

8. return to step 1 and iterate until the maximum difference in power distribution is less than 2%:

$$\delta P_{i,j} = \frac{P_{i-1,j} - P_{i,j}}{P_{i-1,j}}$$  \hspace{1cm} (2)

where $P_{i-1,j}$ is the power in the $(i-1)_{th}$ iteration, $j_{th}$ layer and $P_{i,j}$ is the power in the $(i-1)_{th}$ iteration, $j_{th}$ layer, according to the formula (2) [4]. Figure 6 shows the power distribution along the length of the fuel part of the pin after each iteration. The power of each layer is given in percentage of the total pin power.

![Figure 5. Iterative scheme](image)

![Figure 6. Power distribution](image)

3. Conclusion

The changes in power distribution were monitored and after seven iterations the calculation was finished. The difference between the sixth and seventh iteration is not significant, the biggest difference is 1.1% and for the other layers, it is 0%. This model is used for further calculation of ALLEGRO MOX fuel assembly and full core model.
References

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