Test problem for thermal-hydraulics and neutronic coupled calculation fore ALFREAD reactor core

A Filip¹, G Darie¹, I S Saldikov², A D Smirnov² and G V Tikhomirov²

¹ Department of Nuclear Engineering, Power Engineering Faculty, University Politehnica of Bucharest, Independentei street, 313, Bucuresti, Romania, 060042
² Department of Theoretical and Experimental Physics of Nuclear Reactors, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe highway, 31, Moscow, Russia, 115409

Corresponding author’s e-mail address: ISSaldikov@mephi.ru

Abstract. The beginning of a new era of nuclear reactor requires technological advances and also multiples studies. The European Liquid metal cooled Fast breeder Reactor is one of the designs for the generation IV nuclear reactor, selected by ENEA. A pioneer of its time, ELFR needs a demonstrator in order to prove the feasibility of this project and to acquire more data and experience in operating a LFR. For this reason the ALFRED project was started and it is expected to be under operation by the year 2030. This paper has the objective of analyzing the neutronic and thermohydraulics of the ALFRED core by the means of a coupled scheme. The selected code for neutronic simulation is MCNP and the selected code for thermohydraulics is ANSYS.

1. Introduction

The main goal of the ALFRED project is to play the role of a demonstrator for the European concept of a LFR, thus proving the safety and reliability – in all operating conditions – of the simple engineering solutions adopted (e.g., the extension of the FA up to the cover gas), while reducing uncertainties in design, construction and operation to the largest possible extent. Since ALFRED and ELFR are characterized by different thermal powers, of course not all their core parameters can be maintained equal. Therefore, the issue arose in the choice, for the sake of the demonstration, of the parameters that are necessarily or conveniently to be kept and those which are not. In particular the fuel enrichment and the breeding ratio are different in the two cores and therefore the closure of the fuel cycle does not represent a goal for the ALFRED core. On the other hand, the materials are the same in the two cores, except for the cladding materials: the expected time required for the full qualification of advanced claddings and coatings in lead (foreseen in the ELFR) is not compatible with the foreseen roadmap for ALFRED. [1]

2. ALFRED

ALFRED is a small-size (300 MWth) pool-type LFR and its primary system current configuration is depicted in figure 1 [2].
The 171 FAs are subdivided into two radial zones with different plutonium fractions guaranteeing an effective power flattening, and surrounded by two rows of dummy elements serving as a reflector. Two different and independent control rod systems have been foreseen, namely, Control Rods (CRs) and Safety Rods (SRs), which are assigned regulation/compensation and scram functions assuring the required reliability for cycle reactivity swing control and safe shut-down. [4]

Table 1. ALFRED main parameters [3]

| Parameter                          | Value       |
|------------------------------------|-------------|
| Thermal power                      | 300 MW<sub>th</sub> |
| Coolant mass flow rate             | 25984 kg/s  |
| Total number of FAs                | 171         |
| Pins per FA                        | 127         |
| Coolant inlet temperature          | 400 °C      |
| Coolant outlet temperature         | 480 °C      |
| Mean assembly power                | 1.75 MW     |
| Mean rod power                     | 13.814 kW   |
| Mean wall heat flux                | 0.7 W/m<sup>2</sup> |
| Lead flow average FA               | 144.1 kg/s  |
| Bypass flow average FA             | 2.76 kg/s   |
| Clad maximum temperature           | 550 °C      |

2.1. The Core
The core is made of hexagonal wrapped fuel assemblies. MOX fuel is used in the form of tubular beads. The Active height is large facilitating the natural circulation. The power of the active core is 300 MWt. The reactor consists of 171 fuel assemblies, 12 control rods and 4 shot down rods surrounded by 108 dummy elements (ZrO2-Y2O3), protecting the interior vessel (figure 2) [4]. Each fuel assembly is 8 meters in length and consists of 127 fuel rods, fixed to the base grating. The springs in the upper part prevents the floating of the assemblies caused by rising lead flow and reduces the effects of expansions. The top ends of the assemblies exceed the free surface of molten lead, entering the plenum gas, which facilitates inspection activities and refueling. In this way, the refueling can be done without the intrusion of refueling equipment [3].
2.2. Fuel assembly

Each FA is constructed by 127 fuel rods. The main elements are (a) the spike, which fits into the lower diagrid to ensure the correct positioning of the FA and which is provided with a high number of orifices along the entire circumference to allow for the lead inlet, thus minimizing the risk for sudden significant flow reduction due to occlusion; (b) the funnel, which facilitates the lead outlet toward the steam generators through a “nose” able to host neutron and temperature instrumentation and sniffers for failed cladding detection; (c) a long stem allowing the upper head to emerge from the coolant for an easy refueling in full visibility and without moving parts in lead, and for hosting a ballast which counterbalances the buoyancy during refueling (when the upper diagrid is removed). Along the extension of the shrouds, at different heights, the hexcan is bumped to make pads against core compaction in case of an earthquake (figure 3) [3].

The presence of a limited number of control and safety rods (12 control rods and 4 safety rods) and the absence of experimental equipment above the core, make feasible the typical refueling operation, characterized by FAs loading from the above of the core (typical solution adopted in SFRs and LWRs).
During normal operating conditions, when the primary pumps are active, the FAs are held in their position thanks to the core upper plate.

2.3. **ALFRED fuel**
The reactor core is composed of wrapped hexagonal Fuel Assemblies (FAs), each one containing 127 fuel pins arranged in a triangular lattice. The 171 FAs are subdivided into two radial zones (57 inner and 114 outer) with different plutonium enrichments, and surrounded by two rows of dummy elements serving as reflector. In particular, the fuel considered for ALFRED consists of annular U–Pu Mixed Oxide (MOX) pellets. As far as the cladding is concerned, the well known Ti-15-15 steel has been selected because it was already qualified and licensed in fast reactors (Phenix, Superphenix). In Tables 3 and 4, the main specifications of the ALFRED reactor and fuel pin parameters are presented. The fuel is composed of MOX pellets with 95% theoretical density and an Oxygen-to-Metal ratio (O/M) of 1.97. The fuel isotopic composition refers to a typical reactor grade Pu from the reprocessing of Pressurized Water Reactor (PWR) spent fuel (4.5% initial enrichment in 235U, 45 MWd t−1 of burn-up, 15 years of cooling and storage [3]).

**Table 3. ALFRED pin design parameters [3].**

| Fuel type              | MOX          |
|------------------------|--------------|
| Enrichment as Pu/(Pu+U)[wt.%] (inner zone) | 21.7         |
| Enrichment as Pu/(Pu+U)[wt.%] (outer zone)     | 27.80        |
| Fuel density [%] of theoretical density          | 95           |
| O/M                                  | 1.97         |
| Cladding                           | Ti-15-15     |
| Fill gas                             | He           |
| Pre pressurization [MPa]             | 0.1          |
| Upper plenum volume [mm³]            | 30,000       |
| Upper plenum length [mm]             | 120          |
| Active length [mm]                   | 600          |
| Lower plenum length [mm]             | 550          |
| Cladding outer diameter [mm]         | 10.5         |
| Cladding inner diameter [mm]         | 9.3          |
| Fuel pallet outer diameter [mm]      | 9            |
| Fuel pallet inner diameter [mm]      | 2            |
| Pin pitch [mm]                       | 13.86        |

**Table 4. Isotopic specification for U and Pu [3].**

| Plutonium | Uranium |
|-----------|---------|
| Isotope   | Fraction (wt.%) | Isotope | Fraction (wt.%) |
| 238Pu     | 2.332    | 235U    | 0.003             |
| 239Pu     | 56.873   | 236U    | 0.404             |
| 240Pu     | 26.997   | 238U    | 0.010             |
| 241Pu     | 6.105    |         | 99.583            |
| 242Pu     | 7.693    |         |                   |

2.4. **Cladding material**
The cladding material proposed for the ALFRED reactor is the austenitic stainless steel Ti-15-15 (Table 5). This class of steels has been adopted as cladding material in fast reactors in the early phase of the development of this technology. After several years of reactor management (Superphenix) and irradiation campaigns (EBRII; Phenix), austenitic chromium-nickel (Cr-Ni) stainless steels have proven the best performance in reactor, showing excellent creep and good swelling resistance. In order to reduce the high swelling propensity caused by irradiation, several titanium-stabilized steels has been proposed, exploiting the capability of TiC precipitates to increase the swelling incubation time.
Moreover, the presence of silicon and boron can change the swelling and the creep features, respectively. Indeed, the concentration of each alloyed element has a paramount effect on the creep, on the swelling behavior and on the ruptures train [5].

Table 5. Ti-15-15 Composition.

| Steel | Cr[wt.%] | Ni[wt.%] | Mo[wt.%] | Mn[wt.%] | Si[wt.%] | Ti[wt.%] | C[wt.%] | B[ppm] |
|-------|----------|----------|----------|----------|----------|----------|---------|--------|
| AIM 1 | 15.0     | 15.0     | 1.50     | 1.50     | 0.90     | 0.40     | 0.09    | 60     |

2.5. Coolant (Lead)
Pure lead is an interesting coolant in fast reactors due to its high mass number and its low absorption cross-section, which are fundamental properties for a fast reactor coolant. It has good thermal characteristics for heat removal. With respect to sodium and lead-bismuth eutectic, it has high melting temperature (327°C, 600 K) and an high boiling point (1749°C, 2022 K) allowing a wide range of operation. [5]

It is steel-aggressive for the core materials both for erosion and corrosion issues (therefore, a flow velocity of less than 2 m s-1 is envisaged, and an oxygen control and/or a coating for cladding are required, respectively) and it is very toxic and polluting, requiring particular attention from production to disposal or recycling. Nevertheless, the stainless steel of which the cladding is made requires further protection, and different coating layers are under development. Among the proposed solutions, the most promising are the FeCrAlY alloy, realized through the so-called GESA (Gepulste ElektronenStrahlAnlage) treatment and the Al2O3 coating realized through Pulse Laser Deposition (PLD). For ALFRED FA, the modeling solution that can be adopted is substitute an external layer of the cladding (40 μm) by a coating which is not affected by corrosion and is featured by a thermal conductivity of 16 W m-1 K-1. Mechanical and irradiation effects on the coating are presently not taken into account.

3. MCNP-ANSYS coupled scheme

3.1. MCNP
MCNP is a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport. Specific areas of application include, but are not limited to, radiation protection and dissymmetry, radiation shielding, radiography, medical physics, nuclear criticality safety, Detector Design and analysis, nuclear oil well logging, Accelerator target design, Fission and fusion reactor design, decontamination and decommissioning. The code treats an arbitrary three-dimensional configuration of materials in geometric cells bounded by first- and second-degree surfaces and fourth-degree elliptical tori.[6]

3.2. ANSYS
ANSYS CFX is an element-based finite-volume method with second-order discretization schemes in space and time. It uses a coupled algebraic multigrid algorithm to solve the linear systems arising from discretization. The discretization schemes and the multigrid solver are scalable parallelized. ANSYS CFX works with unstructured hybrid grids consisting of tetrahedral, hexahedral, prism, and pyramid elements.

3.3. MCNP-ANSYS
In order to perform a neutronic and thermohydraulic analysis of ALFRED reactor core two computational codes are needed to simulate the steady state functioning of the reactor.

For this paper, MCNP and ANSYS code were chosen for creating a coupling scheme (Fig 4) [8]. Although MCNP library does not include materials such as Ti-15-15, it is possible to create it according to weight fraction of isotope composition. In creating the input file necessary for neutronic simulation of the ALFRED core, the precise geometry of a fuel rod is necessary, provided by Table 6 [7]. Data such as density, an estimated temperature of the fuel and material composition is required for a better resolution. According to the used coupled scheme, after the first iteration density of the fuel
and temperature will be replaced with the new data obtained. After the first run of MCNP, power distribution data will be extracted from the output file and used in creating the input file for ANSYS.

The second part of the coupled scheme is represented by the thermohydraulic code ANSYS. It requires the full geometry of the fuel assembly (or a simplified design) considering the same geometrical data used in creating the MCNP input file. Thermo physical properties of the materials are also necessary. Material composition, geometry, viscosity, inlet temperature of coolant are required in ANSYS. The power distribution is resulted from MCNP simulation and is used as an input date for the thermohydraulic code. The resulting data for density and temperature of the coolant are used to recreate the input file for MCNP code. The iteration continues until power distribution and temperature converges.

### Table 6. MCNP and ANSYS Geometry [7].

| Inner diameter | gap | Fuel pallet outer diameter | Gap thickness | Cladding thickness | Cladding outer diameter | Height |
|----------------|-----|---------------------------|---------------|-------------------|------------------------|--------|
| 2 [mm]         | 9 [mm] | 0.15 [mm]                   | 0.6 [mm]      | 10.5 [mm]          | 6000 [mm]              |

### Figure 4. MCNP – ANSYS coupled scheme [8].

3.4. Thermophysical correlation of lead

Density: The density of liquid lead can be related to temperature with a simple linear correlation. Even if purity is not well specified, agreement within data is very strong, with uncertainty under 1%.

$$\rho = 11367 - 1.1944T$$ [kg m$^{-3}$] [5]  \hspace{1cm} (1)

Specific heat capacity at constant pressure: the correlation is suggested as a reasonable choice between available data.

$$c_p = 175.1 - 4.961 \times 10^{-2}T + 1.985 \times 10^{-5}T^2 - 2.099 \times 10^{-8}T^3 - 1.524 \times 10^{-6}T^2$$ [J kg$^{-1}$ K$^{-1}$] [5]  \hspace{1cm} (2)
Thermal Conductivity: The data regarding the thermal conductivity of liquid lead are very dispersed. The proposed correlation is linear and fits well recent data.

\[ \lambda = 9.2 + 0.011T \text{ [Wm}^{-1}\text{K}^{-1}] \] (3)

3.5. Thermo physical properties of Ti-15-15

Density: It is calculated as a function of temperature using the linear expansion correlation.

\[ \rho(T) = \rho_0 \left(1 + \frac{1}{1+\zeta(T)}\right)^3 \text{ [kgm}^{-3}\text{]} \] (4)

Specific heat: Specific heat measurements have been carried out in the range 20÷1000°C (293÷1273 K). The correlation has been selected and implemented.

\[ c_p = 431 + 0.177T + 0.0000872T^{-2} \text{ [Jkg}^{-1}\text{K}^{-1}] \] (5)

Thermal conductivity: The thermal conductivity of the cladding material is a fundamental property because it determines the temperature gradient across the cladding, controlling thermal stress and temperature levels (which determine all the other mechanical properties).

\[ \lambda = 13.95 + 0.01163T \text{ [Wm}^{-1}\text{K}^{-1}] \] (6)

4. Expected results

Through this work it is expected to create a flexible coupled scheme between MCNP code and ANSYS code with the purpose of validation and verification of deterministic calculation. The coupled scheme will provide important data for ALFRED reactor core. Axial power distribution, axial fuel temperature and also fuel temperature can be studied. The iteration process continues until convergence.

Acknowledgment

The authors appreciate the support and effort of National Research Nuclear University MEPhI. This work was accomplished with the financial support of ENEN by the means of ENEN RU II Project number 605149. This work was supported by Competitiveness Program of National Research Nuclear University MEPhI.

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