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Preliminary neutron kinetic – thermal hydraulic coupled analysis of the ALFRED reactor using PHISICS/RELAP5-3D

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Abstract. The development of a lead-cooled fast reactor (LFR) demonstrator was proposed, mainly in EU, to investigate the feasibility of an industrial size ELFR (European Lead-cooled Fast Reactor). The demonstrator, called ALFRED (Advanced Lead-cooled Fast Reactor European Demonstrator), consists of a pool-type lead-cooled fast reactor, with a nominal thermal power of 300 MWt. This paper aims to verify the capability of the PHISICS/RELAP5-3D coupled approach to simulate transients of such reactor and to evaluate the effects of accidental scenarios relevant for the safety analysis on the system thermal-hydraulics and on the core power spatial evolution. RELAP5-3D®, developed at Idaho National Laboratory (INL), is a thermal-hydraulic system code, validated for a wide range of transient simulations. The code provides the possibility to simulate innovative working fluids (such as lead and lead alloys) and to use a fully integrated multi-dimensional nodalization. In addition, the need to study complex neutronic systems recommended the development of a new kinetic model allowing the calculation with any number of energy groups and also considering the transport for the angular variations. At this purpose, INL developed PHISICS (Parallel and Highly Innovative Simulation for INL Code System) and its coupling methodology with RELAP5-3D. The simulation activity described in this paper has been focused on the safety analysis of ALFRED reactor assuming the occurrence of two unprotected transient scenarios: unprotected loss of flow (ULOF) and unprotected transient overpower (UTOP). At this purpose, a thermal-hydraulic geometrical scheme of the whole reactor has been developed. The models and the outcomes of the calculation are described and discussed in the paper, highlighting the capability of the coupling approach to obtain results consistent with the ones available in the literature.

1. Introduction
In the framework of Generation IV International Forum (GIF) [1], the fast breeder reactors (FBR) were selected as one of the most promising systems to be investigated. They allow a closed fuel cycle, an easier management of radioactive waste by reducing the content of long-lived isotopes and the consume of weapons-grade plutonium (burned as nuclear fuel). Among different FBR design solutions, the lead-cooled fast reactors (LFR) are attractive, mainly for two reasons: lead is chemically inert with respect to air and water and its higher density variation with temperature promotes the instauration of a significant natural flow that provides a considerable reactor grace time during accidental scenarios. As a part of the 7th Framework Program (FP7), the European Commission financed the LEADER (Lead-cooled European Advanced DEMonstration Reactor) project with the final purpose of developing the concept of an industrial size LFR, called ELFR (European Lead-cooled Fast Reactor). To support the reactor design, a small demo reactor (300 MWt), called ALFRED (Advanced Lead-cooled Fast Reactor...
European Demonstrator), was proposed to prove the feasibility of the ELFR and test its safety and reliability in a wide range of operational and accidental conditions [2]. For the purposes of the LFR safety analysis, the presence of such an intense neutron flux leads to the need of a neutron kinetic and thermal hydraulic (NK/TH) coupled simulation of accidental transients which may interest the reactor. Since 2011, INL has been developing the PHISICS reactor analysis toolkit to perform advanced neutron transport calculations coupled with the three-dimensional thermal hydraulic system code RELAP5-3D (R5-3D) [3], [4], [5] and [6]. During a transient simulation, the NK code provides the axial/radial power distribution in input to the TH code that, at its time, returns to the former the thermal hydraulic parameters necessary to compute the neutronic feedbacks and the core reactivity. This approach allows to locally consider the reactivity feedbacks for a better evaluation of the reactor power and the temperature distributions. The PHISICS/RELAP5-3D (P/R) coupled codes have been already used to simulate transients of VVER-440 Russian pressurized water reactors [7], and High Temperature Gas-cooled Reactors (HTGR) [8], [9]. The purpose of this work is to investigate the capability of the P/R coupled codes to simulate LFR transients, in particular, to reproduce ALFRED core power spatial evolution and its effects on the main thermal-hydraulic parameters during two unprotected scenarios: unprotected loss of flow (ULOF) and unprotected transient of over-power (UTOP).

2. Description of ALFRED reactor
ALFRED is a pool type Pb-cooled fast reactor of 300 MWt. The nominal lead temperature field in the core is 673–753 K. Eight steam generators (SGs) remove the reactor power. They are connected with eight secondary cooling systems, which are fed with water at 608 K and 18.8 MPa. Super-heated steam enters the turbine at 723 K and 18 MPa to produce a net electrical power of about 125 MWe [2].

2.1. Primary system
Figure 1 shows the vertical view of the reactor block [2]. All the components are contained inside the Reactor Vessel (RV) that is a cylindrical tank with a torospherical bottom head. It is fastened to the reactor cavity from the top with a support system. Inside the RV, there is the Inner Vessel (IV) that accomplishes two functions: it supports the core and it divides the hot plenum from the cold pool. At the bottom, the lower grid, anchored to the IV, allows the coolant to enter inside the active region, moving upward through the core and exiting the active zone via eight circumferential holes. Then, hot fluid flows inside the primary pumps (PP) inlet pipes, welded to the IV. Eight axial PPs are adopted to promote the circulation of the molten lead. They are installed into the hot legs, inside the PP inlet pipes, and they are surrounded by the steam generator tube bundles, placed inside the SG casings. Each SG consists of 542 bayonet tubes with an active length of six meters. Each primary pump and steam generator are integrated in a single vertical unit, located inside the annular volume between the IV and the RV. The primary coolant flows upward through the PPs and downward through the SG tube bundles up to the cold pool. At the top of the IV, the upper grid is designed to push down the fuel assemblies during the reactor operations. The axial distance between the middle of the core and the SG mid-plane, relevant for the instauration of the natural circulation, is about 1.87 m.

2.2. Core configuration
The reactor core, shown in Figure 2 (a) [2], consists of 57 fuel assemblies (FAs) composing the inner core, 114 FAs the outer core, 12 control rods (CR), 4 safety rods (SR) and 108 dummy elements. Each FA consists of a bundle of 127 pins with an active length of 60 cm and a large fuel rod pitch to improve the natural circulation. MOX fuel is used with two different enrichments for inner and outer core. The pins are arranged in a hexagonal wrapper to provide a more stable core geometry and easier handling. A spike, fixed to the lower grid, allows the coolant entrance through multiple openings and a funnel, above the core active region, permits the fluid exit through several fissures. The multiple inlets/outlets design solution is adopted to avoid an instantaneous total blockage. A long stem extends up to the upper grid to facilitate inspection and handling operations. At the top, a ballast avoids the assembly buoyancy within the liquid lead. Figure 2 (b) shows the FA axial design (total height is 8 m) with cross-sectional geometry at key locations [2]. Two independent systems are conceived to guarantee the reactor control and safety functions: the CR system, used for regulation during reactor operations and for SCRAM in
case of emergency, and the SR system, designed only for the reactor SCRAM. Twelve control rods are positioned in the outer core, the one with the higher enrichment. Each CR consists of a bundle of 19 pins contained inside a cylindrical shroud and cooled by the primary lead. The absorber material is B$_4$C (90% $^{10}$B) and it is characterized by an active length of 68 cm. Control rods enter the core from the bottom and are actuated by motors during reactor operations. When fully extracted, the top of CR absorber region is 4 cm below the bottom of the fuel. The control rods are also provided with an electromagnetic connection whose release in case of emergency causes their rapid insertion within the core by buoyancy. The four SRs have the same absorber material of the CRs, but they are positioned in the inner core. They consist of 12 pins cooled by the primary lead and arranged inside a cylindrical shell. The SRs are inserted downward from the top of the core by a pneumatic system drive. If this system fails, a tungsten ballast, added at the top of the SRs, provides a sufficient weight to oppose the buoyancy and insert the SRs into the core, even if with a lower speed. The absorber length is 84 cm and, when fully extracted, the distance from the top of the fuel is 12 cm. The dummy elements are made up of ZrO$_2$ and Y$_2$O$_3$ and their main function is shielding the inner vessel. A more detailed description of ALFRED core can be found in [10].

Figure 1. ALFRED reactor block: vertical view [2].
3. NK/TH model of ALFRED reactor

A computational model to simulate transients involving ALFRED reactor has been developed using data in [2] and [10]. The thermal hydraulic and neutronic nodalizations are discussed separately in subsections 3.1 and 3.2, respectively.

3.1. RELAP5-3D TH nodalization

The overall TH nodalization adopted for simulation purposes is presented in Figure 3. The core is simulated associating a pipe component to each FA, CR and SR (channel-by-channel approach). Instead, all the dummy elements and the core bypass are collapsed in two equivalent pipe components. Globally, the core model consists of 189 pipes, each one composed of 30 axial hydrodynamic volumes. The axial quotes for nodalization have been chosen to be consistent with the assembly design derived from [10]. The core mass flow distribution suggested in [11] is adopted to obtain in full-power steady state condition a coolant temperature radial distribution at core outlet as flat as possible. Heat structures are connected to each pipe component to simulate the thermal power deposited in any core assembly by gamma and neutron emissions due to the fission process. These components allow the calculation of the heat transferred across solid boundaries to primary lead in hydrodynamic volumes. As suggested in [11], specific correlations have been used to assess pressure drops in FAs spike, funnel, spacer grids and rod bundle. In the first three cases, constant concentrated K-coefficients have been introduced. For what concerns the tube bundle, a Reynolds dependent friction factor expression has been implemented in the input:

\[ f = A + B \cdot Re^{-C} \]  

where A, B and C coefficients have been evaluated by using simplified Cheng and Todreas model, [12], and are equals to 0, 0.203 and 0.2, respectively. The R5-3D heat transfer coefficient (HTC) correlation used by default for liquid metals in bundle geometry is the Westinghouse correlation [13].

\[ Nu = 4.0 + 0.33 \left( \frac{P}{d} \right)^{3.8} \left( \frac{Pe}{100} \right)^{0.86} + 0.16 \left( \frac{P}{d} \right)^{5} \]  

However, for p/d ratio greater than 1.2, as for the fuel bundle (1.32), it shows significant discrepancies with respect to experimental data and the most widely used is the Mikityuk correlation [14].

\[ Nu = 0.25 + 6.2 \frac{P}{d} + \left( -0.007 + 0.032 \frac{P}{d} \right) Pe^{0.8-0.024 \frac{P}{d}} \]  

The procedure to implement such correlation in the input deck is described in [15]. In the operational range of temperature, the two models have a similar gradient of Nusselt versus Peclet. Therefore, a
constant HTC multiplication factor equal to 1.262, calculated as the ratio of Mikityuk and Westinghouse correlations, has been applied in the heat structures simulating the heat transfer in the fuel bundle.

**Figure 3.** ALFRED reactor overall TH nodalization.

All the primary system is simulated with one-dimensional components and for all the reactor the sliced approach is used, recommended when calculations involving natural circulation conditions must be performed. The eight PP-SG vertical units are collapsed into an equivalent one which preserves the hydraulic and heat transfer features (total pressure drops and HTC). This modelling approach reduces the required CPU time without influencing the reactor behavior during transient analysis. Mesh reference length adopted for hydrodynamic volumes is equal to about 0.10 ÷ 0.15 m. Such a value ensures an accurate evaluation of thermodynamic properties variations along the flow path, particularly relevant in those regions where lead heat up and cool down take place and large thermal gradients are expected. The design height difference between the core and the SG mid-planes (1.87 m) is maintained in the model since it determines, together with the total pressure drops of the primary system, the asymptotic natural convection flow rate during ULOF transient. The cold pool is simulated by two annular components linked by cross-junctions. This nodalization method, compared with a 3D model, allows to evaluate with enough detail possible natural convection and mixing phenomena occurring in the pool during some transient conditions (such as ULOF), while reducing the computational time [16].

Cold pool significantly contributes to the thermal inertia of the primary system because of the largest amount of lead contained. The three different free levels are included in the nodalization. Primary pressure is fixed by a time dependent volume at the top of the cover gas volume. The SG secondary sides are collapsed into one that is modeled by a kind of “U” flow path, which reproduces the water descending and water/steam ascending sides of the bayonet configuration. This modelling approach for bayonet tubes has been derived from [17]. Primary and secondary circuits are coupled through the heat structures associated to the equivalent steam generator. Also for the SG rod bundle (p/d equal to 1.42) the Mikityuk correlation has been used to evaluate the heat transfer. It has been implemented in the input deck following the procedure in [15]. The constant HTC multiplication factor used is 1.15. The selected TH time step is 5.0E-03 s.

### 3.2. PHISICS NK nodalization

PHISICS is the toolkit called by RELAP5-3D to solve the NK problem. For this purpose, it is adopted the same internal coupling structure previously developed for NESTLE code [3], [4]. It is shown by Figure 4. PHISICS uses the nodal method to solve the second order formulation of the transport equation in an unlimited number of energy groups. The nodal solver integrated in PHISICS is named INSTANT. The self-shielded macroscopic cross sections needed as input terms in the transport equation are linearly interpolated for all the core materials starting from a N dimensional Cartesian grid. The dimensions of the Cartesian grid are core thermal-hydraulic parameters, such as fuel and coolant temperature, density of the coolant or boron concentration. The number of tabulated dimensions and the points per dimension
are unlimited [4]. For the purposes of ALFRED NK calculations, five fuel temperatures in the range of 603-3373 K and five coolant temperatures in the range of 603-1373 K have been selected to constitute a 25 points-2D interpolation grid. At each time step, the thermal input parameters (fuel and coolant temperatures) for the PHISICS interpolation are provided by the solution of the TH problem performed by RELAP5-3D code. The macroscopic cross sections related to each 2D-grid point are obtained with the cell/lattice calculation module (named ECCO) integrated in ERANOS code [18]. Then, they are tabulated in a .xml file, given in input to the coupled simulation. Cell calculations have been performed adopting a 33 energy groups structure and the P1 approximation for scattering treatment and evaluating thermal expansion and Doppler effect (JEFF 3.1 nuclear data library). The axial distribution of core materials simulated for each assembly type is shown in Figure 5. The NK nodalization foresees 36 axial mesh and, radially, a neutronic node associated to each assembly. Material compositions have been derived from [19]. Non-reentrant current boundary conditions are used to close the neutronic problem. For each time step, the convergence criteria are: 1 pcm for the k-effective value and 1.0E-04 for the neutron flux. The convergence limits are expressed in terms of the ratio between the values of the control parameter in two subsequent iterations. The axial/radial power map resulting from the solution of the transport equation is used from RELAP5-3D as a boundary condition to solve the TH problem and provide the thermal parameters for the next time step iteration. PHISICS/RELAP5-3D coupling structure allows the user to differentiate the time steps of the NK and TH problem, to speed up the simulations. For the current simulation activity, the NK time step has been chosen ten times higher than the TH one (5.0 E-02). This is a good compromise between the instance of maintaining enough result accuracy and the one of reducing the computational time.

Figure 4. PHISICS7RELAP5-3D: coupling structure.

Figure 5. ALFRED core NK nodalization: material axial distribution for each assembly type.
4. Simulation results

4.1. Full-power steady state condition

First, an analysis of the core critical configuration at Beginning of Life (BOL) condition has been performed. The fission power, the lead outlet temperature and the centerline fuel temperature have been computed for each FA and their radial distributions are shown by Figure 6 (a), (c) and (d), respectively. Fission power decreases moving from the center towards the periphery of the core, with a partial increase in the first ring of the outer core (which presents a higher fuel enrichment). The maximum value is in the central FA (2.34 MW). Figure 6 (b) represents, assembly per assembly, the relative error computed in absolute terms between the mass flow rate obtained by simulation and the one derived from [11]. Its maximum value is 0.32%, so the mass flow distribution is reproduced in the model with adequate accuracy. Combining the fission power computed by PHISICS and the assembly flow rate adopted, the resulting distribution of the lead outlet temperature is quite flat. The difference between the maximum and minimum coolant temperatures at the core outlet is ~23 K. The target fuel temperature for ALFRED core design is 2273 K [11]. It is derived from the fuel melting point (~ 3000 K) by applying a safety margin to envelop the temperature excursions during accidents. The deviation of the simulation result (2310 K) from the reference value is acceptably low (~ 40 K). The real design issue is to demonstrate, as discussed in Sections 4.2 and 4.3, that in transient conditions the maximum fuel temperature is below the melting point of an adequate safety margin. Figure 6 (d) represents the centerline fuel temperature radial distribution at the axial level where the maximum value of this parameter occurs (0.35 m from bottom of active fuel). Figure 6 (e) shows the axial/radial distribution of the neutron flux, obtained considering the FAs arranged in the core diameter going from top-right to bottom-left corner and the axial levels from bottom of active fuel (BAF) to top (TAF). The neutron flux has nearly symmetrical profiles in both direction, with a maximum value at the core center (2.56E+15 n/cm²/s).

Figure 6. ALFRED core critical configuration at BOL: (a) fission power, (b) relative error on mass flow, (c) lead outlet temperature, (d) centerline fuel temperature, (e) neutron flux.
4.2. ULOF transient

The Unprotected Loss of Flow transient is initiated by the loss of power supply to all primary pumps. The reactor scram is supposed to fail and the core power is driven by reactivity feedbacks. During this transient, the secondary system is supposed to remain in normal operation with no control of the feedwater flow rate. Starting from the full-power steady state condition, the loss of all primary pumps takes place after 2 seconds of simulation. After an initial undershoot, with a minimum of 4567 kg/s, the natural circulation flow rate tends to the asymptotic value determined by the primary system pressure drops and the design height difference between the core and the SG mid-planes (Figure 7 (a)). The new value is almost constant, equal to 5905 kg/s (~ 23 % of the nominal flow). Because of the prevalent negative reactivity feedback, the total core fission power follows the same time trend but with enhanced overshoot and undershoot values. However, after these initial oscillations, also this parameter stabilizes to about ~ 205 MW (Figure 7 (b)). At the transient beginning, the unbalance between flow and power in the core causes a sudden increase of the coolant outlet temperature and the clad temperature, followed by stabilization to a new equilibrium value higher than the initial condition (Figure 7 (c) - (d)). ALFRED core design foresees a maximum allowable clad temperature of 1023 K [11]. During the transient simulation, this parameter increases up to 1036 K, so there is a small deviation of 13 K from the reference value. Due to the low amplitude of the clad temperature peak, no clad failures are expected during ULOF transient. Finally, the centerline fuel temperature decreases during this accidental scenario following the fission power behavior (Figure 7 (d)). Other research institutions (ENEA, CEA, PSI, KIT-G, NRG, etc.) have simulated the same ALFRED reactor transient scenarios, but considering the End of Life (EOL) conditions. Many different codes (SIMA-LFR, SPECTRA, TRACE/FRED, CATHARE) have been involved in computational activity. The outcomes of this coordinated work are contained in [20]. The significant neutronic (fuel burn-up, etc.) and thermal-hydraulic (SG tube fouling, core channel plugging, etc.) differences between BOL and EOL reactor conditions, only allow a qualitative comparison between the trends contained in Figure 7 and Figure 8 and the ones reported in [20]. From the qualitative point of view, the outcomes of this simulation activity are comparable with the calculation results in [20].

![Figure 7](image-url)

**Figure 7.** ULOF transient time trends: (a) natural circulation mass flow, (b) total core fission power, (c) average core inlet and outlet coolant temperatures, (d) maximum fuel and clad temperatures.
4.3. UTOP transient

The Unprotected Over-Power transient at full reactor power is initiated by an unexpected positive reactivity insertion. The one simulated is of 250 pcm in 10 s. It represents the possible reactivity perturbation induced in the core as a result of steam generator tube rupture, FA flow blockage or core compaction. The transient is unprotected and the reactor scram is assumed to fail. The secondary circuits are supposed to remain in normal operation with no control of the feed water flow rate. The primary system is maintained in forced circulation. The reactivity insertion is simulated by moving all the control rods out of the core of about 1.3 cm in 10 s with a constant withdrawal rate. Starting from the full-power steady state condition, the reactivity insertion takes place after 2 seconds of simulation. The core power immediately increases (Figure 8 (a)) and consequently also the coolant and structure temperatures rise (Figure 8 (b) - (d)). The power excursion is limited by the prevalent negative reactivity feedback. Among major contributions to it, there are the Doppler Effect and the fuel expansion due to fuel temperature increase. After the initial peak, the system evolves to a new equilibrium state at higher power (~ 350 MW) (Figure 8 (a)). The new coolant core outlet temperature is maintained at about 770 K (Figure 8 (b)). The maximum fuel and clad temperatures occur in the central FA: the former rises up to 2575 K, value sufficiently lower than the MOX melting temperature (~ 2973 K), the latter increases up to 818 K, far lower than the maximum allowable value of 1023 K (Figure 8 (c) - (d)). Even for this transient scenario, the trends reported in Figure 8 are qualitatively comparable with the ones contained in [20].

Figure 8. UTOP transient time trends: (a) total core fission power, (b) average core inlet and outlet coolant temperatures, (c) maximum fuel temperature, (d) maximum clad temperature.

5. Conclusions

Starting from BOL conditions, several unprotected transients defined in the preliminary safety analysis of ALFRED reactor have been simulated by using PHISICS/RELAP5-3D coupled codes. The goal of the activity is to obtain realistic results by calculations performed by means of a thermal-hydraulic and neutronic coupled procedure, considering the codes limitations and physical approximations. First, a complete NK/TH characterization of ALFRED reactor at full-power steady state BOL condition has been performed. From this initial state, ULOF and UTOP accidental scenarios have been investigated. During the transients considered, all the reactor NK/TH parameters are below the limits and the goodness of the ALFRED design under study is demonstrated. Moreover, the calculation outcomes
demonstrate the capability of the P/R coupled codes in simulating LFR transients, giving global results qualitatively comparable with the solutions obtained by other independent codes. Additionally, P/R coupled codes offer the possibility to analyze the local behavior, such as the local temperature peak. Because of the positive feedback obtained by this simulation activity, the coupling methodology discussed in this paper will be used to evaluate the TH performances of the new ALFRED reactor configuration, [21].

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