RICERCA DI SISTEMA ELETTRICO

Sviluppo di un codice di cinetica spaziale di nocciolo per sistemi LFR


Report RdS/2012/035
SVILUPPO DI UN CODICE DI CINETICA SPAZIALE DI NOCCIOLA PER SISTEMI LFR


Settembre 2012

Report Ricerca di Sistema Elettrico
Accordo di Programma Ministero dello Sviluppo Economico - ENEA
Area: Governo, gestione e sviluppo del sistema elettrico nazionale
Progetto: Nuovo nucleare da fissione: collaborazioni internazionali e sviluppo competenze in materia nucleare

Responsabile del Progetto: Mariano Tarantino, ENEA
Sviluppo di un codice di cinetica spaziale di nocciole per sistemi LFR

Descrittori
Tipologia del documento: Rapporto tecnico
Collocazione contrattuale: Accordo di programma ENEA-MSE: tema di ricerca "Nuovo nucleare da fissione"
Argomenti trattati: Termoidraulica del nocciole, Neutronica, Generation IV Reactors, Analisi di sicurezza

Sommario
The development of a new multi-physics simulation tool is presented for the quasi-3D analysis of a lead-cooled fast reactor core with the hexagonal fuel element configuration, as currently proposed within the framework of the European project LEADER. The tool implements coupled neutronic (NE) and thermal-hydraulic (TH) models. In the NE module a 2D + 1D full-core multi-group diffusion solver has been developed, while in the TH module the 3D problem is split in 1D (axial) problems along each hexagonal assembly thermally coupled to each other in the transverse directions. The two modules are coupled by exchanging the power distribution (from NE to TH) and the temperature map (from TH to NE). The code is benchmarked against pure TH and pure NE analytical solutions and the results of a coupled NE/TH simulation are also presented.

Note

Deliverable congiunto ENEA – CIRTEN
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INDEX

1. INTRODUCTION AND MOTIVATIONS................................................................. 3

1.1 GENERAL FRAME (POLITO)............................................................................. 3

1.2 REACTOR DESIGN UNDER INVESTIGATION (POLITO - ENEA)..................... 7

2. MODEL DESCRIPTION ....................................................................................... 8

2.1 RELEVANT TIME SCALES ............................................................................. 9

2.2 THERMAL-HYDRAULIC MODEL................................................................... 10

2.3 NEUTRONIC MODEL ................................................................................... 14

2.4 NEUTRONIC/THERMAL-HYDRAULIC COUPLING STRATEGY......................... 16

3. RESULTS ........................................................................................................... 17

3.1 A PURE-TH MODEL PROBLEM................................................................. 18

3.2 A PURE-NE MODEL PROBLEM .................................................................. 20

3.3 A COUPLED TH/NE MODEL PROBLEM: CRITICALITY SEARCH .................. 21

4. CONCLUSIONS AND PERSPECTIVE ............................................................ 25

ACKNOWLEDGMENTS ....................................................................................... 31

CODE ABSTRACT .............................................................................................. 26

PUBLICATIONS AND THESIS RELATED TO THE WORK PERFORMED IN THE
PRESENT RESEARCH .......................................................................................... 31

REFERENCES .................................................................................................... 32
1. INTRODUCTION AND MOTIVATIONS

The work carried out in 2012 constitutes a development of the computational tool for the dynamic analysis of lead-cooled reactors. The work started over one year ago and in this deliverable it reaches the full development of implementation of the coupling between neutronic (NE) and thermal-hydraulic (TH) computational modules. The resulting code has been named FRENETIC (Fast REactor NEutronics/Thermal-hydraulICs), which is part of the present deliverable.

1.1 GENERAL FRAME (POLITO)

Fast reactors present some very advantageous aspects to attain the objectives established within the Generation IV program. In particular, the fast neutron system is the only one that allows a more efficient use of the nuclear fuel with respect to thermal systems, hence significantly extending the time perspectives connected to the natural Uranium energy resource. Furthermore, the use of a fast neutron spectrum permits to transmute by means of nuclear fission very dangerous radioactive products, characterized by a long decay life and potentially proliferating, into short-life nuclides, as fission products, absolutely no-use for military applications.

The European Union (EU) sees at present the Sodium-cooled Fast Reactor as the reference choice among Generation IV reactor designs [1], while the Lead-cooled Fast Reactor (LFR) and the Gas-cooled Fast Reactor are being considered as alternative technologies [2].

In the LFR line, on which we shall focus here, a first design, ELSY (European Lead-cooled System) [3], was proposed within the 6th European Framework Program (FP6); that design is now being further developed within FP7 under the Lead-cooled European Advanced DEmonstration Reactor (LEADER) project [4], with the aim of contributing to the design of the Advanced Lead Fast Reactor European Demonstrator (ALFRED) [5], towards the full-scale first-of-a-kind European Lead Fast
Reactors (ELFR) [6]. Several Italian groups are involved in the project, universities (CIRTEN), as well as ENEA and industry (Ansaldo). Many interactions and synergies have been developed between the activities on the subcritical system and those on the study of the lead-cooled critical reactor. In the future, the knowledge achieved in one field may be of significant interest in the other.

The typical configuration of an LFR core is shown in Figure 1.

![Figure 1. Scheme of ELFR reactor vessel, containing the active core surrounded by the barrel, the hot leg, the pump, the heat exchanger (HX) and the decay heat removal heat exchanger (DHR), all immersed in the lead pool [7].](image)

The computational tools for the description of the global behavior are of particular importance. In order to obtain these objectives it is necessary to develop models that can account simultaneously for the various phenomena and processes that characterize the system. This feature requires the integration of reactor physics, thermal-hydraulics and mechanics in a multi-physics computational tool that should be characterized by flexibility, suitable to carry out parametric evaluations and comparative assessments among the different configurations being proposed. The methods for the dynamic analysis are particularly relevant because of the role they play in the safety evaluations. The study of the transient response is also essential for all the stability and reliability analyses.
The study of the dynamics of fast lead-cooled systems requires the development of suitable coupled neutronic-thermal-hydraulic computational tools. As far as neutronics is concerned, to perform accurate evaluations of the transient regime and stability behavior of these systems, highly-simplified techniques, such as point kinetics, may turn out to be completely inadequate. The full space and spectral behavior has to be described in its whole detail. The overall behavior may be strongly influenced by the thermal-hydraulic features. The thermal fluid-dynamics of lead-cooled fast-neutron systems demands for a specific modelization to account for the typical characteristics of fluid-flow and heat-exchange of liquid metals [8]. These aspects and the geometric characteristics call for specific physical and numerical techniques [9].

A new multi-physics simulation tool, FRENETIC (Fast REactor NEutronics/Thermal-hydraulicCs), is presented for the quasi-3D analysis of a lead-cooled fast reactor core with the hexagonal fuel element configuration, as currently proposed within the framework of the European project LEADER. The tool implements coupled neutronic (NE) and thermal-hydraulic (TH) models.

The model assumes a uniform distribution of the different (TH and NE) relevant parameters at the hexagon level (see Figure 2), i.e., it cannot treat transients at the so-called sub-assembly level (e.g., severe transients leading to loss of structural integrity of single pins or groups of pins, etc); this assumption is well justified for several operational and accidental transients of interest.
As the name says, the code has the ambition to provide (approximate) solutions for core design and/or safety analysis in a computationally effective (i.e. relatively fast) way, thanks to the fact that the 3D problem is solved with a simplified approach.

In a first step of this development, we recently coupled a TH model for a single hexagonal element to a point kinetics NE model [10]. The objective of the present work is the extension of that analysis to the full core configuration.

In the NE module, a 2D + 1D full-core multi-group diffusion solver has been developed based on a coarse-mesh nodal scheme and adapted to cope with the hexagonal geometry. In the TH module, the hexagonal elements, described by 1D (axial) transient advection and conduction in the coolant coupled to conduction in the fuel pins, are thermally coupled to each other in the transverse directions to obtain the full-core evolution of the distribution of the TH variables. The two modules are coupled by transferring to the TH module the distribution of the power source computed by the NE module, which is the driver of the TH evolution; alternately, the temperature distribution computed by the TH module is input at each time step to the NE module in order to update the cross sections.

Figure 2. Hexagonal fuel element with identification of the cross-section homogenization region (shaded in light blue).
The coupling between the TH and the NE modules is performed explicitly using the commercial TISC\textsuperscript{®} platform [11]. Although, for the time being, the NE model is steady state, this solution will allow high flexibility in terms of using different internal time steps for the two modules, according to the different NE and TH timescales; furthermore, it is very fast if compared with I/O on data files, and it allows to keep two separate main codes (NE and TH) that can be, as such, also independently run to separately test and validate them.

The code is benchmarked against pure TH and pure NE analytical solutions and the results of a coupled NE/TH pseudo-transient (criticality search) are also presented. The convergence of the numerical solution is demonstrated both in space and time by computational experiments.

1.2 REACTOR DESIGN UNDER INVESTIGATION (POLITO – ENEA)

In the first steps of the research activity, the definition of a reference LFR design to be adopted for the development of the computational modules has been carried out. ELFR project is characterized by hexagonal fuel elements surrounded by a wrapper, as it can be seen in the sketch reported in Figure 3. Several modifications have been introduced, with the intent to scale down the system power and obtain a demonstrator reactor ALFRED (Advanced Lead Fast Reactor European Demonstrator), whose deployment is the main objective of the LEADER project. As a consequence, in the frame of this research activity here described, the reactor design with hexagonal fuel elements has been selected.
The system characteristics have been retrieved from the available ELFR data. The reactor is characterized by an almost full-scale power (thermal power = 1500 MW) and corresponding core dimension and thermal characterization. However, the modelling tool developed can be easily adopted for the analysis of different systems based on the same core geometry and fluid flow pattern, and can be fruitfully used for the dynamic analyses of the design of the ALFRED reactor.

2. MODEL DESCRIPTION

The model to be presented in this Section and implemented in FRENETIC aims at a quasi-3D description of the LFR core. This is achieved by coupling a transient 1D+2D TH model to a steady-state 2D+1D NE model. The TH model thermally couples on the horizontal plane 1D axial/vertical models of each hexagonal fuel assembly. The NE model (for the time being) provides a steady-state 2D description of the neutron flux on the horizontal plane, while a cosine shape is assumed in the axial/vertical direction. In order to justify our approach we have to first consider the different time scales of interest for our problem.

Figure 3. Sketch of the ELFR core cross section. Detail of the hexagonal fuel assembly.
2.1 RELEVANT TIME SCALES

Several different and to some extent separate time scales are relevant for the multi-physics problem of the LFR dynamics. These are summarized in Figure 4, distinguishing between TH and NE phenomena.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure4.png}
\caption{Relevant time scales for LFR dynamics.}
\end{figure}

The time scales in Figure 4 are defined and have been estimated as follows:

- \( \tau_{xy} \approx \frac{\delta}{\delta_2} \), where \( \delta = \delta_{Pb} + 2 \times \delta_w \) is the total thickness separating two neighboring hexagons, including the Pb clearance (see Figure 5) and \( \delta = (\delta_{Pb} \times \delta_{Pb} + 2 \times \delta_w \times \delta_w) / \delta \) is the average (weighted) thermal diffusivity of the three layers;

- \( \tau_{pin} = \frac{r_{pin}^2}{C_{pin}} \), where \( r_{pin} \) is the pin radius and \( C_{pin} \) is the pin thermal diffusivity;

- \( \tau_z \approx \frac{H}{v} \), where \( H \) is the active core height (i.e., the length of the portion of pin containing the fuel) and \( v \) is the coolant speed in the axial direction;
• $\tau_{\text{Pb-pin}} = (V_{\text{Pb}} \times c_v \times \rho)/(h \times A)$, where $V_{\text{Pb}}$ is the Pb volume, $c_v$ is the Pb specific heat at constant volume, $\rho$ is the Pb density, $h$ is the heat transfer coefficient between the coolant and the pins, $A$ is the pin-Pb heat transfer area.

### 2.2 Thermal-Hydraulic Model

The TH model in FRENETIC takes advantage of the separation of time scales $\tau_{xy} >> \tau_z$. Since the thermal coupling between neighboring hexagons is relatively slow/weak compared to the Pb transit time along the fuel assembly the 3D problem can be approximated as a set of weakly (i.e., explicitly) coupled 1D problems, to be solved along each fuel assembly. This approach is very similar to what we previously introduced and successfully used in the context of cryogenic cooling of superconducting magnets for nuclear fusion reactors [12].

The TH module of FRENETIC solves implicitly in time (fully implicit or Crank-Nicolson schemes) the transient 1D mass, momentum and energy balances in each fuel assembly for the speed $v(z, t)$, and for the temperature $T_{\text{Pb}}(z, t)$ and pressure $p(z, t)$ pair:

- **1D mass balance**
  \[
  \frac{\partial v}{\partial t} + v \frac{\partial v}{\partial z} + \frac{1}{\rho} \frac{\partial p}{\partial z} = -Fv - g \cos \gamma 
  \]  
  (1)

- **1D momentum balance**
  \[
  \frac{\partial p}{\partial t} + \rho c_s^2 \frac{\partial v}{\partial z} + v \frac{\partial p}{\partial z} - \Phi \frac{\partial}{\partial z}\left(k \frac{\partial T_{\text{Pb}}}{\partial z}\right) = \Phi \left[ \frac{\Pi_{\text{fuel}} h}{A} (T_{\text{fuel},s} - T_{\text{Pb}}) + \nu pF \right]
  \]  
  (2)

- **1D energy balance**
  \[
  \rho c_v \frac{\partial T_{\text{Pb}}}{\partial t} + \rho c_v \frac{\partial T_{\text{Pb}}}{\partial z} + p c_v \Phi T_{\text{Pb}} \frac{\partial v}{\partial z} \frac{\partial}{\partial z}\left(k \frac{\partial T_{\text{Pb}}}{\partial z} \right) = \\
  = \frac{\Pi_{\text{fuel}} h}{A} (T_{\text{fuel},s} - T_{\text{Pb}}) + \nu pF + \sum_{i=1}^{6} \frac{\Pi_{\text{hex}} h_i}{A} (T_i - T_{\text{Pb}})
  \]  
  (3)
In equation (3), thermal coupling terms appear with neighboring hexagons which are treated explicitly in time since they are weak. This coupling simply includes terms like $I_{hex} \times h_i \times (T_i - T_{Pb})$, where $I_{hex}$ is the contact perimeter between the hexagon considered and the $i$-th neighboring hexagon, $h_i$ is the heat transfer coefficient computed from the series of thermal resistances wrapping-Pb clearance-wrapping between the hexagon considered and the $i$-th neighboring hexagon (as shown in Figure 5), and $T_i$ is $i$-th hexagon lead temperature.

Concerning the fuel temperature, two assumptions are made: 1) a single, suitably averaged temperature is assumed to be representative of the temperature profile inside each pin; 2) all pins inside a hexagon are assumed to be described by the same fuel temperature $T_{fuel}(z, t)$. The latter assumption is justified by the uniform distribution of the fission heat source among the pins of any given fuel assembly and provided boundary effects are negligible at the hexagon level.

$T_{fuel}(z, t)$ evolves according to a 1D transient heat conduction model, which includes the heat transfer term $h \times [T_{fuel,s}(z, t) - T_{Pb}(z, t)]$ between the pin surface at temperature $T_{fuel,s}$ and the Pb, which occurs on a time scale $\tau_{Pb-pin}$ defined by the heat

---

Figure 5. Core schematics adopted for the TH model. SS is Stainless Steel.
transfer coefficient $h$ (taken from the Schad modified correlation for pin bundles, see chapter 10 of [13]). In the model we implement this term as $h' \times [T_{\text{fuel}}(z, t) - T_{\text{Pb}}(z, t)]$, where $h' = h \times [T_{\text{fuel},s}(z, t) - T_{\text{Pb}}(z, t)] / [T_{\text{fuel}}(z, t) - T_{\text{Pb}}(z, t)]$ and use in $h'$ an approximate value for $T_{\text{fuel},s}$, estimated assuming a parabolic radial temperature distribution inside the pin (since this is modified only on the time scale $\tau_{\text{pin}} > \tau_{\text{Pb-pin}}$), see Figure 6. Then $T_{\text{fuel},s}$ can be analytically linked to the heat generation rate $q_v(z, t)$ and to $T_{\text{fuel}}(z, t)$ as follows: $T_{\text{fuel},s}(z, t) = T_{\text{fuel}}(z, t) - q_v(z, t) \times r_{\text{pin}}^2/(8 \times k_{\text{fuel}})$, where $k_{\text{fuel}}$ is the fuel thermal conductivity.

![Figure 6. Parabolic radial temperature distribution assumed inside the fuel pin, allowing the estimation of $\Delta T = T_{\text{fuel},s} - T_{\text{Pb}}$ to be used with the heat transfer coefficient found in literature [13].](image)

The $T_{\text{fuel}}(z, t)$ is then computed solving the 1D transient heat conduction equation for each fuel assembly:

- **1D pure heat conduction**

$$
\rho_{\text{fuel}} C_{\text{fuel}} \frac{\partial T_{\text{fuel}}}{\partial t} - \frac{\partial}{\partial z}\left( k_{\text{fuel}} \frac{\partial T_{\text{fuel}}}{\partial z} \right) = \frac{\Pi_{\text{fuel}} h}{A_{\text{fuel}}} (T_{\text{Pb}} - T_{\text{fuel},s}) + \frac{q_{\text{fuel}}}{A_{\text{fuel}}} \quad (4)
$$

The parameters appearing in equations (1-4) are:

- $A$: Pb cross section
- $C_{\text{fuel}}$: fuel specific heat
- $c_s$: sound speed in liquid Pb
- $F$: coefficients accounting for friction effects, defined as in equation (5)
where $f$ is the friction factor and $D_h$ is the hydraulic diameter

- $g$: gravity acceleration
- $k$: Pb thermal conductivity
- $p$: Pb pressure
- $\Pi_{fuel}$: Pb-pin contact perimeter
- $q_{fuel\text{lin}}$: linear power generation inside the fuel, see equation (7)
- $\varpi$: angle between $z$ and vertical direction to take into account buoyancy
- $\varpi$: Gruneisen parameter, defined as in equation (6)

$$\Phi = \left( \frac{\rho \frac{\partial T}{\partial \rho}}{T \frac{\partial T}{\partial \rho}} \right)$$

where $s$ is the entropy.

The set of 1D differential equations (1-4) is solved at each time step for each fuel assembly.

Space derivatives along $z$ are approximated by 1D linear finite elements, equivalent to central difference approximation.

The coupling of the TH model with the NE model is needed because the main driver in the TH evolution is the fission heat source inside the fuel, reported in equation (7),

$$q_{fuel\text{lin}} = A_{fuel} E_f \sum_{g=1}^{G} \Sigma_{f,g} \Phi_g$$

where $A_{fuel}$ is the (total) pin cross section, $E_f$ is the energy produced per fission, $\Sigma_g$ is the macroscopic fission cross section of group $g$, $\Phi$ is the neutron flux value for group $g$ and $G$ is the number of energy groups.
2.3 Neutronic Model

The description of the neutron flux in FRENETIC is based, for the time being, on the multi-group diffusion approximation of the transport equation, see equation (8),

\[ \nabla \cdot D_g(T_{\text{fuel}}, T_{\text{Pb}}) \nabla \Phi_g - \Sigma_{r,g}(T_{\text{fuel}}, T_{\text{Pb}}) \Phi_g + \sum_{g'=1}^{G-1} \Sigma_{s,g'\rightarrow g}(T_{\text{fuel}}, T_{\text{Pb}}) \Phi_{g'} = 0 \]

where \( D \) is the diffusion coefficient, \( \Sigma \) is the removal cross section, \( \Sigma_{s,g'\rightarrow g} \) is the scattering cross section from group \( g' \) to group \( g \), \( k_{\text{eff}} \) is the effective neutron multiplication factor, \( \chi \) is the fission spectrum, \( \nu \) is the number of neutrons produced by each fission reaction. Therefore, delayed neutrons are not present in the current implementation of the code and a steady state is assumed on the fastest time scale \( \tau_{\text{prompt}} \).

In order to perform coupled calculations on a full-core configuration, the energy description of the neutron population needs to be reduced to a small number of groups. We adopt here a set of three-group cross sections since this choice allows us to properly describe the behavior of the fast neutron spectrum within the system, constituting thus a good compromise between accuracy and computational cost.

Since both the diffusion coefficient and the different cross sections depend on both fuel and Pb temperature, the NE model needs the temperature profiles computed by the TH model. Among these dependences the most significant ones (and the only ones taken into account in the present work) are those of the removal and fission cross sections. The cross section database, including their temperature dependence, was generated for a lead-cooled fast system [14]. In Figure 7 the temperature dependence of the fission and capture cross sections for the third energy group \( (g = 3) \) is reported.
While $\Sigma$ decreases both for increasing $T_{\text{fuel}}$ and for increasing $T_{\text{Pb}}$, giving rise to the so-called negative temperature feedback, the capture cross section $\Sigma_c = \Sigma_i - \Sigma_f$ increases for increasing $T_{\text{fuel}}$, due to the increased resonance captures, and decreases for increasing $T_{\text{Pb}}$. The latter behavior, related to the Pb density reduction for increasing temperature, may in turn be responsible of a positive temperature feedback. Although the variation of the cross sections in Figure 7 is relatively small, for relatively small variation of the temperature, it has to be recalled that this variation is then reflected in a corresponding variation of $k_{\text{eff}}$, which albeit relatively small obviously has important implications.

The NE model is solved in FRENETIC adopting the coarse-mesh approach (2D nodal scheme) [15] for the full-core evaluation in hexagonal geometry. Each fuel element constitutes a computational node in the x-y plane, while the axial variable needs to be discretized, to generate a three-dimensional grid for the solution of the diffusion equation. The cross sections are supposed to be homogeneous on each hexagon, as it is customarily performed in nodal method, and a third order expansion of the neutron flux within the hexagon is assumed.

The formulation of the nodal method in hexagonal geometry requires a change of coordinates. A two-dimensional conformal mapping is applied, as sketched in Figure 8. The transverse integration of the balance equations generates a set of equations for the incoming and outgoing currents for the six edges of the hexagon, to be coupled to the neighboring fuel elements [16].

Figure 7. Behavior of fission and capture cross sections for the third energy group as a function of fuel and Pb temperature [14], as assumed in the present work.
For the time being, in the vertical $z$ direction a buckling term is introduced to account for axial neutron losses. This corresponds to imposing a cosine shape of the flux along the axis, with an amplitude such that $\int_0^\pi P(z) \cdot \sin(z) \, dz = P_{\text{hexagon}}$, $P(z)$ is the linear power density distribution along the fuel element and $P_{\text{hexagon}}$ is the total power produced by each hexagonal assembly, according to the neutron flux computed in the 2D hexagonal element.

In perspective, the solution of the time-dependent problem for operational and accidental transient analysis will be performed inverting the full space-energy problem on the time scale of the prompt neutrons. This approach may constitute a reference, and is characterized by a larger computational effort. For this reason, we are envisaging the implementation of a quasi static procedure [17], allowing a good accuracy in the reproduction of spatial and spectral effects with a reduced computational time.

![Hexagonal geometry of the fuel element (left) and its mapping onto a rectangular domain (right).](image)

**Figure 8. Hexagonal geometry of the fuel element (left) and its mapping onto a rectangular domain (right).**

### 2.4 Neutronic/Thermal-Hydraulic Coupling Strategy

The coupling between the TH and the NE models takes advantage of the fact that the neutron dynamics is (much) faster than the thermal-hydraulic dynamics.
We could then separately develop the NE and TH modules of FRENETIC and couple them explicitly on the shortest thermal-hydraulic time-scales ($\sim \tau$), while each module can march forward in time with a time step choice most suitable for the resolution of the respective (minimum) time scales of interest. For the time being, as already observed, only the steady-state neutron distribution is solved for, taking advantage of the fact that the evolution of the prompt neutrons population (the only included in the model for the time being) should occur on the fastest time scale anyway.

The coupling is performed in practice using the commercial TISC platform [11], which we already successfully used in the modeling of nuclear fusion problems [18].

3. RESULTS

The performance of FRENETIC has been tested in a few selected cases as reported in this Section. We do not aim, for the time being, at providing results especially relevant for any particular LFR design, but rather at convincing the reader (and ourselves) that the new code is doing what it should/what is expected, at least under suitably controlled conditions.

In all cases the cross section of the domain is the same, extending out to (but not including) the reflector region (see Figure 3). The number of hexagons (fuel elements) in the fuel region of the reference configuration is 451, the reactor thermal power is 1500 MW and the axial power form factor is 1.3 [3]. The other main geometrical parameters are listed in Table 1 [3, 6].
Pb flows from below into the core, under the action of an imposed pressure gradient $\nabla p$ (or forced mass flow rate) and gravity force. To obtain the desired flow speed of 1.1 m/s at full power, a $\nabla p$ of 0.235 MPa is imposed. The friction factor correlation for pin bundles is taken from chapter 9 of [13]. The inlet temperature is assumed to be constant and equal to 673 K. In this work the fuel is UO$_2$ [19], while the wrapper material is 18/12 Stainless Steel (similar to AISI 316). Pb properties are taken from [20].

### 3.1 A PURE-TH MODEL PROBLEM

The first computational test aims at comparing the 2D Pb temperature distribution computed at the outlet section of a core of sufficient height to allow a comparison with the fully developed temperature profile which can be analytically computed at the outlet of a straight smooth circular pipe having the same cross section area of the core [21] through equation (9)

$$\frac{T(r) - T_w}{T_{avg} - T_w} = \frac{96}{11} \left[ \frac{3}{16} + \frac{1}{16} \left( \frac{r}{r_{out}} \right)^4 - \frac{1}{4} \left( \frac{r}{r_{out}} \right)^2 \right]$$

(9)

where $T(r)$ is the temperature value at radius $r$, $T_w$ is the wall temperature, $T_{avg}$ is the average temperature, $r_{out}$ is the equivalent cylindrical core radius (2.33 m), in the case of laminar Pb flow and pipe walls subjected to a constant heat flux.

In the computational test, the radial profile of the axial velocity component of a fully developed laminar flow is imposed as boundary condition at the core inlet, and

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<td>Hexagon side length (mm)</td>
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</tr>
<tr>
<td>Number of pins / hexagon</td>
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</tr>
<tr>
<td>Pin diameter (mm)</td>
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</tr>
<tr>
<td>Fuel pin pitch (center-to-center) (mm)</td>
<td>15</td>
</tr>
<tr>
<td>Wrapper thickness (mm)</td>
<td>4</td>
</tr>
<tr>
<td>Pb clearance between assemblies thickness (mm)</td>
<td>5</td>
</tr>
</tbody>
</table>

*Table 1. Main geometrical characteristic of the ELFR core analyzed in this paper.*
the core side boundaries are subjected to the same heat flux of the pipe. The boundaries between hexagons are assumed to be very thin \((\delta = 1 \text{ mm})\), such that they guarantee almost perfect thermal coupling, while still impeding the mixing of the flow.

The computed and analytical outlet temperature profiles are compared in Figure 9. Although the number of fuel elements (hexagons) is fixed in a given reactor design, we treat it in this section simply as the discretization parameter for the 2D problem on the cross section. As expected, the computed results show an increasingly good agreement with the analytical solution, for increasing number of nodes (hexagonal channels) used in the discretization of the fixed domain. This confirms the adequacy of the 2D+1D approach for the treatment of the present 3D problem.

![Figure 9. Comparison between computed and analytical radial profiles of the Pb temperature in a smooth pipe with laminar flow conditions and imposed heat flux on the side walls, for different node numbers (hexagons) used to discretize the fixed core cross section area.](image-url)
3.2 A PURE-NE MODEL PROBLEM

In the second computational test, the 2D distribution of the neutron flux computed by the NE module of FRENETIC is compared with the analytical distribution in the case of a cylindrical bare reactor, for a single energy group and an isothermal reactor [22], as in equation (10),

$$\frac{\Phi(r)}{\Phi_0} = J_0 \left(2.4048 \cdot \frac{r}{r_{out}}\right)$$

(4)

where $\Phi_0$ is the flux at the center of the core and $J_0$ is the Bessel function of order zero.

Also in this case the number of hexagons in the domain has been varied (with a fixed core cross section area). Again, the larger the number of nodes, the better the agreement between computed and analytical profiles (see Figure 10). The small discrepancies at the outer boundary of the domain are related to the somewhat different boundary conditions applied in the two cases: the analytical solution, equation (10), is obtained imposing a zero-flux condition on the boundary, while the computational solution assumes a zero incoming current.

![Figure 10](image.png)

*Figure 10. Comparison between computed and analytical radial profiles of the neutron flux in a cylindrical bare reactor, for different node numbers (hexagons) used to discretize the fixed core cross section area.*
3.3 A COUPLED TH/NE MODEL PROBLEM: CRITICALITY SEARCH

The third computational test aims at assessing the computed solution in the case of a coupled NE/TH model problem, the so-called criticality search (Figure 11).

Before the criticality search strictly speaking is started, a preliminary, purely NE simulation is performed, aimed at computing $k_{\text{eff}}$ in the “cold reactor” condition, i.e., with the whole reactor at the same temperature level (assumed here equal to the Pb inlet temperature). The resulting $k_{\text{eff}}$ is $k_{\text{eff,cold}} = 1.09476$. (Note that $k_{\text{eff,cold}} > 1$, as expected, because during the reactor start-up the temperature increases and the negative temperature feedback introduces a negative reactivity, such that $k_{\text{eff}}$ is reduced becoming closer to 1 at full power). The fission terms in the diffusion equations are then divided by $k_{\text{eff,cold}}$.

At this point the procedure reported in Figure 11 is followed: starting again from a uniform temperature in the core (assumed equal to the Pb inlet temperature), the cross sections are evaluated and the neutron fluxes are calculated. The distribution of the power generation from fission reactions is computed from the flux shape, assuming that the power level is the nominal reactor thermal power (1500 MW). The power distribution is then used in the TH module to compute the new temperature distribution. Then, unless the relative temperature variation with respect to previous value is smaller than a given tolerance $tol = 10^{-6}$ in our case, the value of the different cross sections is updated in the NE module, using the new (updated) temperature values, and a new neutron flux shape is computed. In this iterative process the TH module follows the temperature evolution due to the power profile changes, while the NE module performs a steady-state computation at each TH time step using in input the newly computed temperature distribution.

The behavior of $k_{\text{eff}}$ computed at each iteration by the NE module is reported in Figure 12, together with the evolution of the maximum temperature of fuel and Pb. The temperature increase due to the power input is reflected by a progressive reduction of $k_{\text{eff}}$, due to the negative temperature feedback described in Section 2.3. At the end of the criticality search test $k_{\text{eff}} < 1$, as $k_{\text{eff}} = 1$ was imposed in the “cold reactor” condition. The steady-state temperature (Figure 13a) and neutron flux (Figure 13b) distributions, which could be used as initial condition for a real transient
calculation, can finally be obtained by a further (slight) renormalization of the fission terms in the diffusion equations. Figure 13 clearly highlights the different spatial distributions of neutron flux and temperature. In particular, as expected, the highest neutron flux is located in the central part of the reactor (Figure 13b), far away from the boundaries where the leakages strongly reduce the flux. This leads to Pb temperature peaking at the outlet of central assemblies (Figure 13a).

Because of the severe conditions associated to the full power input in a cold configuration, if we use the formula reported in Section 2.2 \( T_{\text{fuel},s}(z, t=0+\Delta t) \) would result to be \( < T_{\text{Pb}}(z, t=0+\Delta t) \), which makes no sense. Whenever this occurs, we force \( T_{\text{fuel},s}(z, t) = T_{\text{Pb}}(z, t) \), and this explains the delayed reaction of the Pb to the pin temperature increase, because the heat transfer is inhibited until the \( T_{\text{fuel},s} \) computed as in Section 2.2 becomes larger than \( T_{\text{Pb}} \) (see Figure 12). These ad-hoc recipes are justified by the fact that we are not following a real transient here, but rather trying to find a sufficiently accurate NE/TH coupled steady-state condition of the reactor core.

Figure 14 shows the numerical convergence analysis where the effect of the two discretization parameters has been considered, namely the (uniform) axial mesh size \( \Delta z \) (Figure 14a) and the (uniform) time step \( \Delta t \) adopted by the TH module (Figure 14b). It is seen that the computed solution can be considered as reasonably independent of \( \Delta z \) and \( \Delta t \).
Figure 11. Procedure for the criticality search.
Figure 12. Behavior of the $k_{\text{eff}}$ (solid symbols, left axis) and of the maximum temperature of fuel (solid line) and Pb (dashed line) during the criticality search test ($t = 0.1 \text{ s}, z = 0.01 \text{ m}$).

Figure 13. 2D maps of the Pb temperature (a) and of the fast ($g = 1$) neutron flux (b) at three different axial locations in the core.
4. CONCLUSIONS AND PERSPECTIVE

The new code FRENETIC has been presented for the coupled neutronic/thermal-hydraulic analysis of lead-cooled fast nuclear reactors, as currently foreseen in the European program within the Generation IV framework.

Both the neutronic and thermal-hydraulic modules of FRENETIC have been benchmarked against analytical solutions. The results of a criticality search have also been discussed, showing the present capabilities of the code to tackle a coupled neutronic/thermal-hydraulic problem. Grid size and time step independence of the numerical solution has been proven by computational experiment.

The extension of the neutronic model to include 3D and transient capabilities is under way. In a separate, parallel effort, the thermal-hydraulic model will be validated against experimental data. Once these two steps are achieved, FRENETIC should be relevant and ready to help in the design and analysis of future lead-cooled fast nuclear reactors.
CODE ABSTRACT

1. NAME OR DESIGNATION OF PROGRAM:

FRENETIC (Fast REactor NEutronics/Thermal-hydraulICs).

2. COMPUTERS

The code runs on any PC or workstation.

3. DESCRIPTION OF PROGRAM OR FUNCTION

The code has the ambition to provide (approximate) solutions for lead-cooled fast reactor core design and/or safety analysis in a computationally effective (i.e. relatively fast) way, thanks to the fact that the 3D problem is solved with a simplified approach.

Reference geometry is the closed hexagonal fuel element configuration, as currently proposed within the framework of the European project LEADER. The tool implements coupled neutronic (NE) and thermal-hydraulic (TH) models.

Main outputs of the code are the TH variables and power 3D distributions in the core at selected times, together with their inlet and outlet values during the whole transient.

4. METHODS

In the NE module, a 2D + 1D full-core multi-group diffusion solver has been developed, based on a 2D coarse-mesh nodal scheme and on the assumption of cosine power distribution in the axial direction. Iterations are performed to compute
the effective multiplication factor of the system. The analysis of the system using the point kinetics method with the quasi static method for the time integration is also an available option.

The NE module can be run in standalone mode to compute neutron flux distribution for a given input temperature.

In the TH module, the hexagonal elements, described by 1D (axial) transient advection and conduction in the coolant coupled to conduction in the fuel pins, are thermally coupled (in explicit, thanks to the weak thermal coupling between assemblies) to each other in the transverse directions to obtain the full-core evolution of the distribution of the TH variables.

Space derivatives along the axial direction are approximated by 1D linear finite elements, equivalent to central difference approximation. The set of equations for each assembly is solved implicitly in time (fully implicit or Crank-Nicolson schemes).

Also the TH module can be run in standalone mode to compute TH variables distribution and evolution in the core (or in a single channel) for a given power generation.

The two modules are coupled by transferring to the TH module the distribution of the power source computed by the NE module, which is the driver of the TH evolution; alternately, the temperature distribution computed by the TH module is input at each time step to the NE module in order to update the cross sections.

5. Restrictions on the complexity of the problem

The model assumes a uniform distribution of the different (TH and NE) relevant parameters at the hexagon level, i.e., it cannot treat transients at the so-called sub-assembly level (e.g., severe transients leading to loss of structural integrity of single pins or groups of pins, etc); this assumption is well justified for several operational and accidental transients of interest.

The target domain of the model is the full core (active core length inside the barrel) with closed assemblies configuration.
6. **Typical Running Time**

The running time depends on the type of transient analyzed, but each time step requires ~10 s to be executed, when the coupled code is run.

7. **Unusual Features**

- 

8. **Related or Auxiliary Programs**

The installation of the commercial software TISC® (http://www.tlk-thermo.com) is recommended (but not mandatory) to speed up computations.

9. **Status**

Available.

10. **References**

Progress in multi-physics modeling of innovative lead-cooled fast reactors:

Multi-physics modeling of innovative lead-cooled nuclear fast reactors:
Full-core coupled neutronic/thermal-hydraulic model of innovative lead-cooled fast reactors:

A full-core coupled neutronic/thermal-hydraulic code for the modeling of lead-cooled nuclear fast reactors:

11. **Hardware Requirements**

The code runs on PC and workstation.

12. **Programming Language(s) Used**

The code is written in FORTRAN 90.

13. **Software Requirements**

The program has been tested on WINDOWS workstation.

The installation of the commercial software TISC® (http://www.tlk-thermo.com) is recommended (but not mandatory) to speed up computations.

For the code compilation the use of Microsoft Visual Studio 2005 with Intel Fortran Compiler is recommended.
14. OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS

If the TISC® software is installed, the two files “TISCSlibf.dll” and “TISCSlibf.lib” containing the TISC® connection libraries for the fortran must be in the running folder. Compile the code in 32 or 64 bit depending on the processor and on TISC® libraries available.

If the TISC® software is not installed, the code lines containing the string “&tisc&” in source files “tiscclient.f90” (in both “neutronic” and “coolant” projects) must be commented before compiling, and files “TISCSlibf.dll” and “TISCSlibf.lib” must be removed from both “neutronic” and “coolant” projects. Compile the code in 32 or 64 bit depending on the processor.

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16. MATERIAL AVAILABLE

CD-ROM with source files and test cases.

17. CATEGORIES

• Nuclear fast reactors multi-physics modeling
• Numerical tool for optimization, stability and sensitivity studies

Keywords: Generation IV, Lead-cooled Fast Reactor, Neutronics, Thermal-Hydraulics, Modeling.

ACKNOWLEDGMENTS

We thank M. Canella for helping with the preliminary implementation of the nodal equations in the neutronic module.

PUBLICATIONS AND THESIS RELATED TO THE WORK PERFORMED IN THE PRESENT RESEARCH


REFERENCES


