Test case specifications for coupled neutronics-thermal hydraulics calculation of Gas-cooled Fast Reactor

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Abstract. The paper is focused on development of the coupled neutronics-thermal hydraulics model for the Gas-cooled Fast Reactor. It is necessary to carefully investigate coupled calculations of new concepts to avoid recriticality scenarios, as it is not possible to ensure sub-critical state for a fast reactor core under core disruptive accident conditions. Above mentioned calculations are also very suitable for development of new passive or inherent safety systems that can mitigate the occurrence of the recriticality scenarios. In the paper, the most promising fuel material compositions together with a geometry model are described for the Gas-cooled fast reactor. Seven fuel pin and fuel assembly geometry is proposed as a test case for coupled calculation with three different enrichments of fissile material in the form of Pu-UC. The reflective boundary condition is used in radial directions of the test case and vacuum boundary condition is used in axial directions. During these condition, the nuclear system is in super-critical state and to achieve a stable state (which is numerical representation of operational conditions) it is necessary to decrease the reactivity of the system. The iteration scheme is proposed, where SCALE code system is used for collapsing of a macroscopic cross-section into few group representation as input for coupled code NESTLE.

1. Introduction

The future prognosis of depletion of fossil fuel and limitation of CO₂ release into the atmosphere cause a new interest in nuclear energy as the only energy source with high capacity without CO₂ production. Together with increasing pressure from public to reduce the amount of long-lived radionuclides and enhance safety of nuclear power plants, the new concepts of Generation IV reactors have been proposed. The proposed designs should enter to the operation within the first half of the 21st century. One of these concepts refers as Gas-cooled Fast Reactor (hereinafter GFR) and objectives of the design are to improve all aspect on nuclear power generation such as: 1) safety and reliability, 2) economics, 3) sustainability, 4) availability, 5) proliferation and physical protection. There is a large amount of reactor-grade plutonium available, and thus breeding of fissile material is no longer the primary target for the fast reactors in the short term. This enables a shift from high power density fast reactors to designs that are self-sustaining and put more emphasis on the safety, especially passive and inherent safety systems [1,2]. The purpose of the paper is to provide the test case model of GFR assembly for the comprehensive analysis and for the cross verification of the coupled codes.
2. GFR2400 design

Research of the GFR2400 is directed towards fulfilling the ambitious long term goals of Generation IV concepts. This reactor is the newest on the evolutionary path of fully ceramic GFRs featuring ceramic fuel. Structural materials in the form of silicon carbide fiber are allowing high temperatures and good mechanical stability across a wide range of temperature gradient. An important innovation of the current design is the application of refractory metallic liners in the form of W14Re layer to enhance the fission product retention of the cladding, resulting in a significant neutronic penalty during normal operation. However, this concept is advantageous under transient conditions and involves spectrum softening. Helium is used as an efficient primary coolant. Since it introduces practically no moderation the GFR's neutron spectrum is one of the hardest among the fast reactors, making it ideal for recycling all actinides, including minor actinides (MAs). Helium is inert and transparent, eliminating most problems related to coolant interaction with structural materials and making online visual inspection of the core possible. Also void reactivity effect is low due to neutronic transparency of coolant. The core outlet temperature is not limited by the coolant characteristics, making it attractive for potential heat applications [3,4].

As mentioned in [5] the European experience in gas cooled reactor technology was unparalleled with more than a thousand reactor years of gas thermal reactor operating experience and a number of in-depth design studies has been developed for the gas cooled fast reactors. The evolution of fuel designs includes designs of coated particle fuel with or without a binding matrix, silicon carbide blocks with dispersed microparticle fuel inside, the idea of silicon carbide plates with fuel pellets arranged in a honeycomb structure, finally arriving to the current design of a hexagonal lattice of cylindrical fuel rods consisting of a column of fuel pellets inside the composite silicon carbide cladding (Figure 1) [3].

![Figure 1. Hexagonal lattice of cylindrical fuel type representation [6].](image)

The starting concept of the fuel assembly in the GoFastR project was the plate-type concept consisting of the carbide fuel with silicon carbide fiber reinforced silicon carbide (SiCf/SiC) cladding. The goal was to achieve a more realistic and feasible, fully ceramic model which would satisfy all the ambitious GFR requirements. The power generation rate of the Gas-cooled Fast Reactor is 2400 MWth thermal power and helium is used as a coolant at a high pressure of 7 MPa to ensure adequate heat transfer. The coolant volume fraction in the core is high in order to have a small pressure drop that allows decay heat removal by natural circulation under pressurized conditions (the large coolant volume fraction of roughly 43 V/Vtot%). To deal with depressurized accidents three dedicated decay heat removal loops (each capable of removing 100% of the decay heat) and six gas reservoirs are available. During normal operation, the power is transferred to the secondary side via three 800 MW power conversion systems equipped with heat exchangers (IHX) and blowers. The secondary coolant is a helium nitrogen mixture and the overall plant efficiency is expected to be around 45% in an indirect Brayton cycle. The design parameters of GFR2400 are specified in Table 1 [3,7].
The core consists of 516 fuel assemblies in a hexagonal geometry. Two different zones are used with different content of Pu: an inner core with lower and an outer core with higher plutonium content (both zones are almost equal size). Reactivity control equipment is represented by 18 control system devices (CSDs) and 13 diverse safety devices (DSDs). The absorber rods in both groups are made up by boron carbide (B₄C, with boron enriched in ¹⁰B to 90%). Wrapper structural material is a special steel alloy (AIM1) and cladding is made from silicon carbide fiber. The axial reflectors and the 480 radial reflectors are from Zr₃Si₂. For these core elements no detailed layout was made, only their expected volumetric composition was determined [3,7]. The core is show in Figure 2.

According to [8] the technical feasibility of Gas-cooled Fast Reactor is critical. The main issues are arising within the reactor safety and operation. This technology requires complex, innovative and expensive security systems to ensure continued pressurisation of the reactor pressure vessel (RPV) and core cooling in accidental situations.

| Table 1. Basic design parameters of GFR2400 [3]. |
|-----------------|-----------------|-----------------|
| Parameter       | Value           | Parameter       | Value           |
| Thermal power [MW] | 2400            | Primary coolant | He              |
| Primary pressure [MPa] | 7              | Pressure drop in core [MPa] | 0.143 |
| Mass flow rate [kgs⁻¹] | 1213          | Bypass flow rate [kgs⁻¹] | 60 |
| Core inlet temp. [°C] | 400            | Core outlet temp. [°C] | 780 |
| Secondary coolant | 20%He, 80%N₂   | Secondary pressure [MPa] | 6.5 |
| IHX inlet temp. [°C] | 346            | IHX outlet temp. [°C] | 750 |

3. Test case

3.1. Geometry and material composition

Hexagonal lattice of the cylindrical fuel rods consisting of the column of the fuel pellets is the proposed design as a test case. The fuel pin with geometric dimensions is shown in Figure 3. As mentioned in section 2, W₁₄Re layer enhances the fission product retention and significantly influences neutronic properties of the system. Outer surface of the fuel pin is covered by silicon carbide fiber which is allowing high temperatures and good mechanical stability. First proposed geometry as the test case is illustrated in Figure 4 which consists of 7 identical fuel pins with height...
165 cm and lattice pitch 11.57 mm. The helium coolant flows between the fuel pins and is pressurized to 7 MPa. Three cases are proposed for investigation in Table 2. Case 1 consists of carbide fuel type and achieves the average value of PuC enrichment within whole core. Case 2 represents inner core fuel assembly material properties with lower enrichment of PuC and case 3 outer fuel assembly with higher enrichment (see Figure 2). Silicon carbide is used for cladding with coating in the form of the W14Re layer and silicon carbide fiber for each case. Flow rate of helium is 273 kgh⁻¹ for 7 pins. Core inlet temperature 400 °C and core outlet temperature should approach to 780 °C according to the power generation equal to 0.15 MWth for 7 pins.

Next proposed geometry is whole fuel assembly (Figure 5 and Figure 6). Inner flow rate of helium for whole assembly is 8462.91 kgh⁻¹ and outer flow within inter-assembly gap is 418.6 kgh⁻¹. Inlet temperature is also 400 °C and power generation rate reaches 4.651 MWth.

3.1.1. $k_{\text{inf}}$ results
The calculation of $k_{\text{inf}}$ was performed for all fuel types. The calculation was performed by SCALE6 KENO VI code [9] system using the multi-group (MG) approach (the used library is ENDF/B-VII.0-238) and the results are shown in Table 3.

### Table 2. Fuel material composition [3].

| Case 1 | Case 2 | Case 3 |
|--------|--------|--------|
| Density [gcm⁻³] | 10.9001984 | 10.9006112 | 10.899764 |
| %V in PuC | 15.84 | 14.12 | 17.65 |
| %V in UC | 84.16 | 85.88 | 82.35 |
| %W Pu | 14.54422677 | 13.32679852 | 16.65979296 |
| %W Am-241 | 0.105392948 | 0.093945206 | 0.117440635 |
| %W U-235 | 80.14544 | 81.7803 | 78.4291 |
| %W C-nat | 4.798422563 | 4.798957869 | 4.797859203 |

### Table 3. Results of $k_{\text{inf}}$ for all fuel types.

| Test case | $k_{\text{inf}}$ | deviation |
|-----------|-----------------|-----------|
| Case 1    | 1.173878        | ± 0.000052|
| Case 2    | 1.103342        | ± 0.000048|
| Case 3    | 1.243441        | ± 0.000051|
For zero incoming current boundary condition, all cases achieve very deep sub-critical state. Therefore, it is necessary to stabilize nuclear system with reflective boundary condition. Obviously, the boron concentration within the helium coolant cannot be used. The first approach is to surround test case with depleted pins to decrease the reactivity of the system (Figure 7). NESTLE code system [10] is used for coupled calculations. NESTLE is able to treat whole assemblies, thus to mitigate the influence of increasing diameter on thermo-hydraulics calculation, it is necessary to surround the test case with the depleted fuel assemblies (Figure 8). All these approaches can be applied also for the test case with whole fuel assembly. Additionally, it is possible to calculate $k_{inf}$ of the whole fuel assembly with included absorber in the form of $B_4C$ in the chosen representative pin position (red pins in Figure 6). The absorber part influences the neutronic properties of the system, but has negligible effect on thermos-hydraulics.

Figure 5. Axial cut of fuel assembly (dimensions in mm).

Figure 6. Cross sectional view of the fuel assembly of GFR2400 [3].

Figure 7. Depleted fuel pins (blue colour) on the edge of system.

Figure 8. Depleted fuel assemblies (red colour) on the edge of system around the test case of 7 fuel pins (blue).

3.2. Iteration scheme

Iteration scheme is presented in Figure 9. NESTLE code system is able to solve either the nodal or Finite Difference Method representation of 4 or 2-group neutron diffusion equation. Therefore, it is necessary to prepare 4 or 2-group macroscopic cross-section library. The sub-module TRITON within the SCALE code system is used for this purpose. TRITON can be used to provide automated,
problem-dependent cross-section processing followed by multigroup transport calculations for one-, two-, and three-dimensional (1D, 2D, and 3D) configurations [9,10].

The convergence of the $k_{\text{eff}}$ is highly dependent from thermo-hydraulic feedback, therefore the criterion for convergence in NESTLE is set to $k_{\text{eff}}$ eigenvalue or to representation of $k_{\text{eff}}$ error criteria. After successful convergence of the coupled calculation, the script checks if stable state is achieved ($k_{\text{eff}} \approx 1.0$). If not, the changes in the peripheral depleted or absorber area have to be made and the calculation is performed again until the stable state is not achieved. It is also possible to add small control rods in the peripheral area to achieve the stable state.

![Figure 9. Iteration scheme.](image)

### 3.2.1. SCALE characteristic equations

The multigroup Monte Carlo procedures are used in SCALE. Typical integro-differential form of the Boltzmann transport equation is solved [9]:

$$
\frac{1}{v} \frac{\partial}{\partial t} \phi(\vec{r}, E, \vec{\Omega}, t) + \vec{\Omega} \cdot \nabla \phi(\vec{r}, E, \vec{\Omega}, t) + \Sigma_t(\vec{r}, E) \phi(\vec{r}, E, \vec{\Omega}, t) = S(\vec{r}, E, \vec{\Omega}, t) + \int dE' d\vec{\Omega}' \Sigma_s(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) \phi(\vec{r}, E', \vec{\Omega}', t)
$$

(3)

where $(\vec{r}, E, \vec{\Omega}, t)$ denotes the general seven-dimensional phase space, $\vec{r}$ position variable, $E$ the particle’s kinetic energy, $v$ the particle’s speed corresponding to its kinetic energy $E$, $\vec{\Omega}$ represents unit vector which describes the particle’s direction of motion, $t$ time variable, $\phi(\vec{r}, E, \vec{\Omega}, t)$ stands for the time-dependent angular flux, $\Sigma_t(\vec{r}, E)$ represents the total cross-section at the space point $\vec{r}$ for particles of energy $E$, $\Sigma_s(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega})$ is the differential scattering cross-section and $S(\vec{r}, E, \vec{\Omega}, t)$ stands for source particles emitted per unit volume and time.

### 3.2.2. NESTLE characteristic equations

As mentioned above, the NESTLE code originates from the multi-problem solution capability, abbreviating Nodal Eigenvalue, Steady-state, Transient, Le core Evaluator. The eigenvalue problem allows criticality searches to be completed, and the external fixed-source steady-state problem can search a specified power level. Transient problems model delayed neutrons via precursor groups. Several core properties can be input as time dependent. The non-linear iterative strategy associated with the Nodal Expansion Method (NEM) is employed. An advantage of the non-linear iterative strategy is that NESTLE can be utilized to solve either the nodal or Finite Difference Method (FDM) representation of the few-group neutron diffusion equation. NESTLE solves the standard NEM formulation for the solution of the three-dimensional, Cartesian geometry, multi-group, eigenvalue neutron diffusion equation [10]:
\[-\nabla \cdot D_g \nabla \phi_g + \Sigma_{bg} \phi_g = \sum_{g'=-1}^{G} \Sigma_{g'g} \phi_{g'} + \frac{\chi_g}{k} \sum_{g'=-1}^{G} v_{g'} \Sigma_{fg} \phi_{g'}, \tag{4}\]

where $D_g$ is diffusion coefficient [cm], $\phi_g$ represents neutron flux [cm$^{-2}$sec$^{-1}$], $\Sigma_{bg}$ stands for total macroscopic cross section [cm$^{-1}$], $\Sigma_{g'g}$ for group-to-group scattering cross section [cm$^{-1}$], $\chi_g$ represents fission neutrons yield, $k$ is so called multiplication factor (or critical eigenvalue), $v_{g'}$ stands for average number of neutrons created per fission and $\Sigma_{fg}$ represents macroscopic fission cross section [cm$^{-1}$].

Macroscopic cross section is written in form:

$$\hat{\Sigma}_{sg} = a_{sg} + \sum_{n=1}^{3} a_{(n+1)sg} \left( \Delta \rho_c \right)^n + a_{sg} \Delta T_c + a_{sg} \Delta \left( T_{ef} \right)^{1/2} + \sum_{n=1}^{3} a_{(n+1)sg} \left( \Delta N_{sp} \right)^n, \tag{5}$$

where $\hat{\Sigma}_{sg}$ represents a macroscopic cross-section for reaction type $x$ and energy group $g$ without transient fission products corrected to local conditions, $a_{sg}$ is an expansion coefficients, $\Delta \rho_c = \rho_c - \rho_c^{(0)}$ is a change in coolant density [g/cm$^3$] from reference condition, $\Delta T_c = T_c - T_c^{(0)}$ stands for change in coolant temperature [$^\circ F$] from the reference condition, $\Delta \left( T_{ef} \right)^{1/2} = \left( T_{ef} \right)^{1/2} - \left( T_{ef}^{(0)} \right)^{1/2}$ is a change in square root of effective fuel temperature [$^\circ F$] from the reference condition and $\Delta N_{sp} = N_{sp} - N_{sp}^{(0)}$ represents a change in soluble poison number density [cm$^{-3} \times 10^{24}$] from the reference condition.

The effective fuel temperature can be evaluated by equation:

$$T_{ef} = T_c + W_c [W_p T_F + (1 - W_p) T_{esf} - T_c] \tag{6}$$

where $W_p$ is a pellet weighting factor, which accounts for resonance flux depression in the interior of the pellet, $W_c$ represents a core statistical weighting factor, that compensates for the lack of detail in the spatial description of the core, $T_F$ stands for a volume average fuel pellet temperature and $T_{esf}$ is a surface average fuel pellet temperature. Thermal-hydraulic feedback is modelled employing a Homogenous Equilibrium Mixture (HEM) model, allowing two-phase flow to be treated. The hydrodynamic model models single and two phase coolant flow up in closed coolant channels. However, only the continuity and energy equations for the coolant are solved, implying a constant pressure treatment. The constant pressure assumption removes the need to consider the momentum equation. The one-dimensional, mass continuity equation along a specified channel for a radial node $ij$ is [10]:

$$A_c^ij(z) \frac{\partial \rho_c^ij(z,t)}{\partial t} = \frac{\partial}{\partial z} \left( G_c^ij(z,t) A_c^ij(z) \right) \tag{7}$$

and the energy conservation equation assuming constant pressure is given by:

$$A_c^ij(z) \frac{\partial}{\partial t} \left( \rho_c^ij(z,t) U_c^ij(z,t) \right) = \frac{\partial}{\partial z} \left( G_c^ij(z,t) A_c^ij(z) U_c^ij(z,t) \right) -$$

$$- \rho_c^ij(z,t) \left( \frac{\partial}{\partial z} \left( \frac{G_c^ij(z,t) A_c^ij(z)}{\rho_c^ij(z,t)} \right) + q_s^ij(z,t) S_c^ij + q_c^ij(z,t) A_c^ij(z) \right) \tag{8}$$

where $\rho_c^ij$ represents coolant density, $G_c^ij$ stands for coolant mass velocity, $U_c^ij$ is coolant internal energy, $q_s^ij$ is volumetric power density from heat deposited directly in the coolant, $A_c^ij$ represents
total cross-sectional area for the coolant flow within the node, $S_{FS}^\omega$ is total fuel rod surface area per unit axial length within the node and $P$ stands for coolant pressure [10].

4. Results

Calculated preliminary results of the test case 1 are shown in Figure 10 and Figure 11. For simplification, the geometry was changed to the square fuel assembly consisting of 9 pins, taking into the account the same volume fractions of materials. 2-group macroscopic cross-section library was prepared by SCALE code system (the used library was ENDF/B-VII.0-238) as the input for NESTE coupled code. The deviance of axial power distribution and fuel temperature from study [11] is caused by the value of $k_{eff} = 1.243582$ together with vacuum boundary condition at the top and the bottom of the fuel assembly. In the study [11], the authors calculated the whole fuel assembly with axial reflectors, that caused increase of the power at the top and the bottom of the assembly. Also the gathering of data from figure in [11] results in the approximate error in power distribution chart. Another results are calculated by FlowVision CFD simulation [12], where the input power distribution is calculated by neutronic code MCU (in this case, the precise geometry was modelled).

![Figure 10. Power density and fuel temperature vs. axial position.](image1)

![Figure 11. Coolant density and coolant temperature vs. axial position.](image2)

5. Conclusion

The overview of the GFR2400 concept is proposed in the paper together with the possible test cases including different enrichment and geometries. Also the procedures how to decrease excessed
reactivity are described by incorporation of the depleted peripheral areas to the system or by replacement of appropriate number of the fuel pins with absorber. The preliminary results are showing good agreement with results of GFR2400 study [11] and FlowVision calculation [12]. However, there is necessary to improve the input data for coupled calculation and to achieve the stable state with $k_{\text{eq}} \approx 1.0$ in the future. The cross checking of the results with other calculation procedures will be performed with other European institutions.

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