Neutronics for the GEMINI+ HTGR

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Abstract. Literally at the heart of the Euratom Horizon 2020 project GEMINI+ are the core neutronics (design) calculations. For these calculations on a relatively small (180 MWth) prismatic HTGR with cylindrical core, the 3-D monte-carlo particle transport and depletion code SERPENT version 2 (VTT, Finland) was selected, the main reasons being the flexibility and versatility of this code. This enables the modelling of all relevant details of the reactor without unnecessary approximations. A particularly useful feature of the SERPENT code is the multi-physics input capability. This allows to map a temperature field over the defined geometry, enabling the calculation of converged power and temperature distribution by means of iteration and data exchange between SERPENT and a (steady-state) thermal-hydraulics code. In this particular case the SPECTRA code (NRG, The Netherlands) was used to provide the temperature distribution. 4 to 5 iterations are sufficient to reach simultaneously converged distributions for power and temperature. The paper gives an overview of the performed analyses for the current (June 2020) design of the GEMINI+ HTGR, and results thereof. Neutronics features seem quite promising, but further improvements and therefore further investigations would be desirable.

1. Introduction
The Euratom Horizon 2020 project GEMINI+ [1] is aiming at the (preliminary) design of a reactor system with a net power output of 165 MWth (gross thermal power of 180 MWth including house load), hereby maximising the convergence between European and NGNP Industry Alliance HTGR designs. The GEMINI+ system is currently designed to provide steam (230 t/h at 540 °C and 13.8 MPa) to industrial end users for use in electricity production and/or process heat. The current (June 2020) state of the design is described in [2].

The GEMINI+ reactor is a relatively small (180 MW thermal power) prismatic block type reactor HTGR. The reactor components (fuel blocks, reflector blocks, compacts, coated fuel particles) are very similar to those of existing designs (General Atomics GT-MHR and MHTGR [3,4], Framatome SC- HTGR [5]), although they are fully based on information available in the open literature.

In support of the design and (thermal hydraulic) safety analysis of the GEMINI+ HTGR, reactor (core) physics (neutronics) and depletion calculations have been performed on a limited number of design versions of this reactor [6]. Some of the results will be presented in this paper.

Main characteristics of the reactor (neutronics model) are listed in Table 1. An earlier design featured 10 layers of fuel blocks in the core and slightly different placement of control rod positions in core and (radial) reflector, in the sense that the blocks containing some of the control rod channels may have been rotated, compared to the current (June 2020) 11-layer design. This modification was necessary in view of limitations to the required penetrations of the pressure vessel head [2].
Currently a single batch loading scheme and an operation cycle of 550 full power days is assumed. This may be replaced later by a multi-batch (typically 2 or 3) loading scheme, to improve utilization of the fuel, i.e., to increase the burn-up at final discharge. Furthermore, a single value of the enrichment is assumed. From initial studies, an enrichment of 12% in $^{235}$U seemed to be most practical for now.

**Table 1.** Main configuration characteristics of the SERPENT model of the GEMINI+ prismatic block HTGR.

| Parameter                                            | Value                  | Unit       |
|------------------------------------------------------|------------------------|------------|
| Reactor/core configuration                           |                        |            |
| # Radial rings of fuel blocks (ring around centre column is first ring) | 3                      |            |
| # Fuel block columns                                 | 25                     |            |
| # Control block columns                              | 6                      |            |
| # Axial fuel/control block layers                    | 11                     |            |
| Distance between side faces of adjacent blocks       | 0.2 cm                 |            |
| Core height                                          | 800 / 880 cm           |            |
| # Replaceable reflector rings                        | 2                      |            |
| # Replaceable reflector columns                      | 54                     |            |
| Bottom reflector (with coolant holes)                |                        |            |
| Reflector material                                   | NBG-17 graphite [7]    |            |
| Reflector thickness                                  | 160 cm                 |            |
| Top reflector (with coolant and control rod holes)   |                        |            |
| Reflector material                                   | NBG-17 graphite [7]    |            |
| Reflector thickness                                  | 120 cm                 |            |
| Core barrel                                          |                        |            |
| Core barrel inner radius                             | 199.1 cm               | cm         |
| Core barrel effective outer radius                   | 207.1 cm               | cm         |
| Core barrel material                                 | Alloy 800H             |            |
| Core barrel height (in SERPENT neutronics model)     | 1080 / 1160 cm         | cm         |
| Reactor Pressure Vessel                              |                        |            |
| RPV inner radius                                     | 234.1 cm               | cm         |
| RPV outer radius                                     | 244.05 cm              | cm         |
| RPV material                                         | Alloy SA508             |            |
| RPV height (in SERPENT neutronics model)             | 1080 / 1160 cm (10 / 11 layer core) | cm |
| Fuel block configuration                             |                        |            |
| Block height                                         | 80 cm                  | cm         |
| Hexagon flat-to-flat distance                        | 36 cm                  | cm         |
| Block material                                       | NBG-17 graphite [7]    |            |
| Triangular pitch                                     | 1.9 cm                 | cm         |
| # channels with fuel compacts                        | 216 (w/o BP) / 210 (with BP) |            |
| Compact channel diameter                             | 1.27 cm                | cm         |
| # small coolant channels                             | 6                      |            |
| Small coolant channel diameter                       | 1.27 cm                | cm         |
| # large coolant channels                             | 102                    |            |
| Large coolant channel diameter                       | 1.6 cm                 | cm         |
| Control rod channel diameter                         | 13 cm                  | cm         |

N.B. The (effective) inner and outer diameter of the core barrel and the pressure vessel as stated here may slightly deviate from what is stated in [2]. This, however, does not influence the neutronic characteristics of the core.
| Parameter | Value | Unit |
|-----------|-------|------|
| Control rod configuration (model - simplified) | - | - |
| # core rods | 6 | - |
| # reflector rods | 18 | - |
| Rod geometry | Annular | - |
| Rod length | 800 / 880 cm | (10 layer core / 11 layer core) |
| Inner radius | 3.75 cm | |
| Outer radius | 5.25 cm | |
| Absorber material | B,C | - |
| Absorber material density | 2.52 g/cm³ | |
| Fuel compact configuration | - | - |
| Matrix material | C | - |
| Matrix material density | 1.75 g/cm³ | |
| # coated particles per compact | 2500 *) | - |
| Compact cylinder height | 5.0 cm | |
| Compact cylinder radius | 0.625 cm | |
| Coated particle configuration | - | - |
| Kernel diameter | 500 micron | |
| Kernel material | UO₂ | - |
| Kernel density | 10.4 g/cm³ | |
| Buffer layer thickness | 95 micron | |
| Buffer layer material | C | - |
| Buffer layer density | 1.05 g/cm³ | |
| Inner PyC layer thickness | 40 micron | |
| Inner PyC material | C | - |
| Inner PyC density | 1.90 g/cm³ | |
| SiC layer thickness | 35 micron | |
| SiC material | SiC | - |
| SiC density | 3.18 g/cm³ | |
| Outer PyC layer thickness | 40 micron | |
| Outer PyC material | C | - |
| Outer PyC density | 1.90 g/cm³ | |
| Burnable poison (BP) configuration (see Figs. 3 and 4 for locations of the burnable poison cylinders in the fuel blocks). | - | - |
| Height | 75.0 cm | |
| Outer radius of annular graphite cylinder | 0.625 cm | |
| Material of annular cylinder | C | - |
| Density of annular cylinder | 1.75 g/cm³ | |
| Burnable poison (BP) material mixture | B₄C in graphite | - |
| Fraction fBP of B₄C in graphite | 0.0 - 1.0 *) | - |
| Density of B₄C in mixture | 2.52 g/cm³ | |
| Density of C in mixture | 1.75 | |
| Outer radius RBP of BP material mixture | 0.2 - 0.525 *) cm | |
| Subdivision of BP material for accurate depletion calculation - # concentric rings of equal volume | 10 | - |

*) The number of coated particles per compact, as well as the fuel enrichment and the parameters of the burnable poison cylinders have been/are being varied in the neutronics studies, in order to arrive at an acceptable / optimised configuration (ongoing in December 2020/January 2021).
Figure 1. Horizontal cross section (z = 1000 cm plane; near the top of the core) of the SERPENT neutronics model for the current (June 2020) version of the GEMINI+ reactor. Control rod identifiers are given. The outer (light grey) section is the pressure vessel. Dimensions are given in Table 1. Also indicated (in green) are 5 representative (due to symmetry; for C4 this is not exact, but in rather good approximation) core columns (C1 - C5).

Figure 2. Vertical cross section (x = 0 cm plane) of the SERPENT neutronics model for the current (June 2020) version of the GEMINI+ reactor (11 layers of fuel blocks in the core). Note that the visible reflector control rods (RR8 and RR17, in green) have been fully inserted in this case. Further note that the aspect ratio shown in the drawing is not entirely realistic. Actual dimensions are given in Table 1.
2. The SERPENT Code

The main code employed for the core neutronics calculations is SERPENT version 2.1.31 in combination with JEFF 3.1.1 nuclear data [8]. SERPENT is a continuous energy monte carlo neutron (and photon) transport code, capable of modelling arbitrary geometry. The later includes the modelling of explicit coated particles in compacts. Integrated into the code is a detailed burn-up/depletion calculation method, featuring a semi-automatic subdivision to distinguish between cells that may initially contain the same material, but deviate during depletion due to differences in local flux (and spectrum). Further features used in the GEMINI+ neutronics calculations are the following:

- Generation and use of explicit random particle distributions.
- Multiphysics input option.

2.1. Explicit coated particle modelling

SERPENT (versions 2.1.x) has the capability to generate random spatial distributions of spheres, e.g., in a cylinder. This was used to generate the random particle positions in a stack of 15 compacts in a fuel block, e.g., 15 x 2500 = 37500 coated particles per 15 compacts. Strictly speaking, a random distribution should be generated for a single (5 cm high) compact (no coated particles crossing the outer boundary of the compact), of which 15 should be put in a stack subsequently. However, the difference in $k_{\text{eff}}$ between these two approaches is only a few pcm, so it was decided to use the simpler approach in further analyses, as described above. All compact channels of all fuel blocks are subsequently filled with the same distribution of coated particles in matrix material.

2.2. Multiphysics input

SERPENT has a “multi-physics” input option. This has been used to assign different temperature to different materials in different locations in the model, without the necessity to assign different material names to materials at different temperatures. This feature has been used to import the (steady state) temperature distributions for different materials (fuel kernel, coatings, matrix material of the compacts, block graphite, etc.) as calculated by the thermal hydraulics code SPECTRA for the corresponding thermal hydraulics model [2,8,9,10].

2.3. Statistical uncertainties

As SERPENT uses the (continuous energy) monte carlo method to simulate neutron (and photon) transport, all results come with a statistical uncertainty that is dependent on the number of neutrons per calculation cycles and the number of cycles per calculation for a single point in time. (Most of) the monte carlo calculations were performed using a neutron population of 100000 (“fine” mode) or 400000 (“extra fine” mode), 1000 cycles with 20 or 100 inactive cycles, using around 350 cores, and a hybrid MPI/OpenMP parallelization.

3. The SERPENT Neutronics Model

The current (June 2020) neutronics model with 11 layers of fuel blocks in the core is shown in Fig. 1 (horizontal cross section) and Fig. 2 (vertical cross section). Also indicated are the identifiers of the control rods in the core (“CRx”) and radial reflector (“RR[x]x”), and 5 “representative” fuel columns (“C1” to “C5”). The neutronics model has been restricted to those elements that are of influence on the neutronics behaviour. Therefore, the upper and lower part of the pressure vessel (including the components within those sections) have not been included. Further information on materials and dimensions of the neutronics model is given in Table 1.

Details of the fuel blocks with and without a control rod channel is shown in Figs. 3 and 4. Note that 6 out of 216 and 4 out of 174 compact channels have been replaced by burnable poison cylinders (see below for further explanation).
The initial version of the reactor featured 10 layers of fuel blocks in the core, with 25 full fuel blocks and 6 fuel blocks with a control rod channel per layer. No burnable poison (BP) was used in this version, which, however, exhibited a too high (> 1600 °C) maximum fuel temperature in a Depressurised Loss of Forced Cooling (DLOFC) accident [11]. Therefore, an extra layer of fuel blocks was added in order to lower the (average) power density, increasing the total height of the core, radial reflectors, core barrel and pressure vessel by 80.0 cm [12]. This promises a great improvement (i.e., much lower) in maximum fuel temperature during DLOFC, as was indicated by transient thermal-hydraulic calculations assuming a uniform power distribution [13]. A further assumption in this DLOFC simulation was a “radially flat” power profile.

In addition, burnable poison (B₄C in graphite) was introduced, as indicated in Figs. 3 and 4, for two purposes:

- To tailor the history of the (uncontrolled) $k_{\text{eff}}$ from Beginning-of-Life (BOL; start of operation; $^{135}$Xe-free) to End-of-Life (EOL; 550 full power days; equilibrium $^{135}$Xe and $^{149}$Sm). The main purpose of this is to ensure that the uncontrolled $k_{\text{eff}}$ (i.e., the value for all rods out) is within the range that can actually be compensated by the control/shutdown rods in the reflector and the core, for all operational states of the reactor. See Sections V and VI.
- To improve the (radial) power distribution over the core, as additional measure in response to the too high maximum fuel temperature in the earlier design version with 10 layers of fuel blocks in the core, without BP.

Efforts for the 2nd point are currently (August/September 2020) ongoing and have not yet been fully finalised. The aim is to flatten the (radial) power distribution (as this was the assumption in the DLOFC calculations that showed favourable characteristics with respect to peak fuel temperature [13]), or even to shift the maximum power density to the outer fuel blocks close to the radial reflector, mainly by optimising the (radial) distribution of burnable poison (and possibly the enrichment). See Section VI.

The temperature distribution over the 11-layer geometry in Hot Full Power (HFP) conditions originates from a steady state thermal hydraulics calculation by SPECTRA, assuming a “flat” radial power profile (i.e., the same axial power profile for all fuel columns) and a re-scaled 10-layer axial profile (i.e., from 10 to 11 layers) [2]. The latter originates from the iterative procedure between neutronics (SERPENT) and thermal hydraulics (SPECTRA) that was applied for the initial 10-layer configuration [10]. Only a few iterations already resulted in a converged solution for the temperature and power distribution, as is demonstrated in Fig. 5.
Figure 5. Successive iterations of the axial distribution of the power in the representative fuel columns C1 to C5 at BOL (10-layer core; no burnable poison). Starting with a cosine-shaped axial power distribution (not shown in the graphs) a corresponding temperature distribution was calculated by SPECTRA [10], based on which the power distribution for the next iteration was calculated. This was repeated 4 times, resulting in successive axial power distributions (indicated as “5” up to “8” in the graphs). Note that the power distributions of the 3rd and 4th iterations already nearly coincide, indicating convergence. Relative standard deviation of the power (per half block; half block is the meshing used for the calculation of the neutron flux and derived parameters, e.g., the power) in the results shown is 0.22 % for the peak values.
Note that the axial power profiles for iterations 3 and 4 already almost coincide for the representative fuel columns C1 to C5 (N.B. These representative fuel columns are designated “FA1” to “FA5”, respectively, in [10,11]).

Also note that this procedure was only followed at BOL and the resulting temperature distribution was kept unchanged during the entire operating cycle until EOL, as was envisaged from the start of the project [1]. However, in view of the considerable changes in power distribution during the operating cycle from BOL to EOL (see further sections in this paper), this procedure may need to be revised, e.g., by introducing a simplified thermal-hydraulics feedback module running in conjunction with SERPENT, providing temperature distribution feedback for every time step.

A specific remark concerns the number of coated particles in a compact. In the majority of the neutronics calculation this was assumed to be 2500. In the thermal hydraulics analyses [10,11,12,13], however, it is assumed to be 3760. However, the actual number of coated particles in a compact does not significantly impact the maximum fuel temperature of the reactor in steady-state conditions or even in a (DLOFC - Depressurised Loss of Forced Cooling) transient. The latter was shown by NCBJ by comparing the 2 DLOFC cases [14].

4. $k_{\text{eff}}$ History

The search for an optimised configuration (spatial distribution of burnable poison parameters: fraction $f_{\text{BP}}$ of $\text{B}_4\text{C}$ in graphite; radius $R_{\text{BP}}$ of the cylinder containing $\text{B}_4\text{C}$ in graphite; it is assumed that all burnable poison pins in a single fuel block are identical, initially) is executed in phases. In the first phase, which focusses on the optimisation of the (uncontrolled) $k_{\text{eff}}$ history from BOL (Xe-free) to EOL, it is assumed that all burnable poison cylinders in the core are initially identical.

Several combinations of enrichment (12%, 13% and 15%) and burnable poison parameters (fraction $f_{\text{BP}}$ and cylinder radius $R_{\text{BP}}$; uniform values for all blocks in the core) have been investigated [14] and it was found that a uniform enrichment of 12%, burnable poison cylinder radius $R_{\text{BP}} = 0.242$ cm and burnable poison density ($\text{B}_4\text{C}$ in graphite) $f_{\text{BP}} = 0.038$ provided an acceptable behaviour of the uncontrolled (i.e. all control rods out) $k_{\text{eff}}$ as function of time from Beginning of Life (BOL) to End of Life (EOL = 550 full power days), as is shown in Fig. 6. In this stage of the optimisation the main purpose of introducing burnable poison is to minimise $k_{\text{eff}}$ (but still with $k_{\text{eff}}$ sufficiently above 1 until EOL), so that the control and shutdown rods can be effectively used for start-up and shutdown. Ideally, $k_{\text{eff}}$ is approximately constant after reaching Xe-equilibrium (approx. 3 days) or slowly decreasing.

The $k_{\text{eff}}$ at BOL is 1.078 (Xe-free), and 1.018 (Xe-equilibrium) at EOL. This BOL-to-EOL reactivity swing is well within the reactivity range of the reflector control rods (see Section V). It should be noted that, for 12 % enrichment without burnable poison, the $k_{\text{eff}}$ (Xe-free) at BOL would have been above 1.40! A corresponding BOL-to-EOL reactivity swing of about -40% would be impossible to handle by the reflector rods.

In the 2nd phase of the optimisation, the objective is to improve the radial power distribution (see Section VI), by modifying the radial distribution of the burnable poison parameters, to a lesser or larger extent deviating from the uniform distribution given above, keep the enrichment at 12 %. For simplicity only 2 sets of values (of $R_{\text{BP}}$ and $f_{\text{BP}}$) were used for each of the cases: one set of values for the central fuel columns (C1 - C3) and one set for the peripheral fuel columns (C4, C5). In the search for the optimal performance, the total amount of $\text{B}_4\text{C}$ in the core (at BOL) was kept constant. Difference between central and peripheral columns was either in $f_{\text{BP}}$ or $R_{\text{BP}}$. 
Figure 6. Uncontrolled (i.e. all control rods out) $k_{\text{eff}}$ versus operation time for a uniform enrichment of 12%, burnable poison cylinder radius $R_{\text{BP}} = 0.242$ cm and burnable poison fraction (B$_4$C in graphite) $f_{\text{BP}} = 0.038$. Note the equilibrium reactivity worth of $^{135}\text{Xe}$ is approximately $-2840$ pcm. $k_{\text{eff}}$ varies between 1.078 (BOL, no Xe) and 1.018 (EOL, Xe-eq.). The relative standard deviation in $k_{\text{eff}}$ is 12 to 13 pcm, which is consistent with the neutron population parameters: 100000 neutrons per cycle and 1000 cycles per point in time. In the calculation 26 non-equidistant time steps were used.

Fig. 7 shows the $k_{\text{eff}}$ history for several combinations of BP parameters for central and peripheral fuel columns. Case 202 is the case with uniform BP parameters (the same as in Fig. 6). Case 214 turned out to be the most favourable until now (September 2020) concerning the (radial) power distribution. (see Section VI), while it is also marginally superior to case 202 concerning the $k_{\text{eff}}$ history (i.e. $k_{\text{eff}}$ closer to 1.00). BP parameters for this case are given in Table 2.

Figure 7. Uncontrolled $k_{\text{eff}}$ histories from calculations to improve the radial power distribution (see Section VI), by applying different burnable poison parameters for columns C1 and C2 on the one hand and C3, C4 and C5 on the other. Case 202 (bold “black circles”) is the same as shown in Fig. 6 (uniform BP parameters). Case 214 (bold “purple diamonds”) is the most favourable configuration so far. Neutron population parameters are the same as in Fig. 6, again yielding a relative standard deviation in $k_{\text{eff}}$ of 12 to 13 pcm.
Table 2. Burnable poison parameters for case 214.

| BP parameter | Columns C1, C2 | Columns C3, C4, C5 | Units |
|---------------|---------------|-------------------|-------|
| $f_{BP}$      | 0.038         | 0.038             | [-]   |
| $R_{BP}$      | 0.290         | 0.227             | [cm]  |

5. Control Rods

The reactor configuration features 6 control rods in the core and 18 (6 clusters of 3 each) in the reflector, as shown in Fig. 1. Table 3 shows the $k_{eff}$ for several control rod patterns (each rod is either fully in or fully out) for uniform initial enrichment of 12 % and uniform burnable poison parameters as in case 202, at Cold Zero Power (CZP; “room” temperature conditions: $T = 300$ K), BOL, Xe-free conditions.

Table 3. $k_{eff}$ for characteristic control rod configurations at CZP, BOL, Xe-free for 11 layers core, uniform 12 % initial enrichment and uniform burnable poison parameters (case 202).

| Rod positions | $k_{eff}$                      | Remarks                                      |
|---------------|--------------------------------|----------------------------------------------|
| All CR in; all RR in | 9.14812E-01 (0.012%) | CZP state is subcritical with all rods in: OK |
| All CR in; all RR out | 1.00170E+00 (0.58%) | Core rods in only are not sufficient in this configuration in CZP state: not OK (at BOL) |
| All CR in; RR1/2/3 in; RR10/11/12 in | 9.65733E-01 (0.012%) | Core rods + some reflector rods are sufficient at BOL. This could be OK, as most RR are in anyway during first days of operation (see below). |
| CR1 out; RR1, RR2, RR3 out; other rods in | 9.77099E-01 (0.012%) | Approximately 60 degr. sector free of rods, to accommodate (re-) load: OK |
| CR1 out; RR1, RR2, RR3, RR16, RR17, RR18 out; other rods in | 1.018760E+00 (0.012%) | Slightly over 60 degr. sector free of rods, to accommodate (re-load): not OK |

It is clear that the core rods alone cannot keep the reactor subcritical at BOL, CZP, Xe-free conditions. It is also not possible with only the reflector rods. However, it is possible to maintain subcriticality at BOL, CZP, Xe-free, by all core rods + 6 reflector rods inserted.

Also, it is possible to remove one core rod and the closed set of 3 reflector rods in a 60 degrees sector of the core, while maintaining subcriticality. This is necessary for the (re-) fuelling procedure.

Similar calculations are currently (September 2020) being performed for the “radially optimised” case 214. It is expected that this will yield similar results.

At elevated temperatures (Hot Zero Power - HZP; uniform temperature $T = 600$K) and Hot Full Power (HFP; temperature distribution from the steady-state SPECTRA thermal hydraulics calculation) the reactivity of the core is lower, and it is very well possible to keep the reactor subcritical with reflector rods only. This is desirable as the core rods are envisaged to be fully withdrawn during operation at (full) power.

Fig. 8 shows, for case 202 with uniform initial burnable poison parameters, the $k_{eff}$ at BOL, HZP/HFP, Xe-free, as function of the number of withdrawn control rods from the reflector. The withdrawal pattern of the reflector rods is such that more than 3 (or even more than 1) partially inserted rods are avoided, i.e., reflector rods are, as much as possible, either fully in or fully out. The control rods in the core have been fully withdrawn, as envisaged for full power operation. Note that the total worth of the reflector rods is approximately the same for HZP and HFP, viz. 12.4 %. This is large enough to compensate the full range of uncontrolled $k_{eff}$ values indicated in Fig. 6, even in case of a Xe-free state at any time in the cycle. Similar calculations for case 214 are currently (September 2020) ongoing. Similar results are expected.
Figure 8. $k_{\text{eff}}$ as function of the number of withdrawn control rods in the reflector for case 202 at BOL. All control rods in the core are out. The value for all rods out at HFP corresponds to the initial value in Fig. 6. Relative standard deviation in $k_{\text{eff}}$ is 12 to 13 pcm.

In the current design of the GEMINI+ reactor, also other control rod patterns are being considered, for which, however, no neutronics analyses have been performed (yet) [2].

Also, a reserve shutdown system, in the form of small absorber spheres (approx. 6 mm diameter, containing B$_4$C) is being considered. In the current configuration these spheres are supposed to use the same channels as the core control rods. This may require a re-design of the core control rods, e.g., cruciform shape instead of annular [2]. No neutronics analyses have been performed (yet) on either one of these configurations and it is assumed that the reactivity worth of either a single channel filled with absorber spheres, or an inserted cruciform rod will have a reactivity value very similar to that of the current core control rod design.

6. Power and Burn-Up Distribution

As mentioned in Section III, for the DLOFC transient calculations on the current 11-layed design [13] it is assumed that the radial distribution of the power is uniform, i.e., every column of fuel block has the same axial distribution of the power (per coated particle). This leads to an acceptable behaviour (peak fuel temperature < 1600 °C) in case of DLOFC. The calculations also showed that the DLOFC behaviour is less satisfactory when the power in the central fuel columns (C1, C2) is higher than in the peripheral fuel columns (C3, C4, C5). It is expected that the behaviour will even improve further when the power maximum is “pushed” further towards the peripheral fuel columns. As mentioned earlier (Section III), the second task of burnable poison is therefore to improve the radial power distribution. Preferably the (initial) enrichment of the fuel is still uniform (12 % for the current designs).

In Fig. 9 the axial distribution of power per coated particle (average over half block) is shown for all (31) fuel columns in the core for case 202 (uniform BP parameter distribution) at BOL/Xe-free (“A”), 250 days (“B”) and 525 days (“C”). The highest power per coated particle (158 mW) occurs at BOL in column C1 (820 cm). The relative standard deviation of the power in the results shown is 0.22% for the peak values. Note that there is a large spread in peak values at the same elevation (820 cm), indicating a radial power distribution that is peaking in the centre column.
Figure 9. Axial distribution of power per coated particle (average over half block) for all (31) fuel columns in the core for case 202 (uniform BP parameter distribution) at BOL/Xe-free (“A”), 250 days (“B”) and 525 days (“C”). The highest power per coated particle (158 mW) occurs at BOL in column C1 (820 cm). The relative standard deviation of the power in the results shown is 0.22% for the peak values.

Introducing a radial profile in the BP parameters clearly improves this situation, as is shown in Fig. 10, which shows the axial distribution of power per coated particle (average over half block) for all (31) fuel columns in the core for case 214 (radially “optimised” BP parameter distribution; Table 2) at BOL/Xe-free (“A”), 250 days (“B”) and 525 days (“C”). The highest power per coated particle (145 mW) occurs at BOL (“A”) in a peripheral column of type C5 (at 820 cm). Note that the lowest power per coated particle at the same elevation is 138 mW, occurring in a central column of type C2. Clearly the spread in (peak) values at the same elevation has been reduced considerably, compared to case 202, indicating a much more “radially flat” power profile. Also, the highest power does not occur in a central column, but in a peripheral column (C5-type, adjacent to the radial reflector; see Fig. 1), which is considered even more favourable.

Figure 10. Axial distribution of power per coated particle (average over half block) for all (31) fuel columns in the core for case 214 (radially “optimised” BP parameter distribution; Table 2) at BOL/Xe-free (“A”), 250 days (“B”) and 525 days (“C”). The highest power per coated particle (145 mW) occurs at BOL (“A”) in a peripheral column of type C5 (820 cm). Note that the lowest power per coated particle at the same elevation is 138 mW, occurring in a central column of type C2. The relative standard deviation of the power in the results shown is 0.22% for the peak values.
The final distribution of the burn up at EOL (550 full power operation days) is the topic of Figs. 11 and 12. In the SERPENT calculations the burn up has been determined on half block level. Figs. 11 and 12 show the frequency distribution of fuel in a given burn up interval, i.e., the number of blocks containing fuel at a final burn up in the interval indicated, for cases 202 and 214, respectively. Ideally, for a single batch loading scheme all fuel should end with the same final burn up. In the frequency distribution representation this means a single burnup range (at average burn up), containing all (341) blocks. This is clearly not yet achieved in cases 202 and 214, although it can be considered slightly better for case 214 (slightly lower maximum burn up, although still far above average).

**Figure 11.** Frequency distribution of the final burn up (per block) for case 202, i.e., the number of blocks containing fuel in the indicated burn up range. The maximum burn up is 98.5 MWd/kg. The average burn up is 63.8 MWd/kg.

**Figure 12.** Frequency distribution of the final burn up (per block) for case 202, i.e. the number of blocks containing fuel in the indicated burn up range. The maximum burn up is 94.6 MWd/kg. The average burn up is 63.8 MWd/kg.
Further improvement can be expected from flattening the axial power profile.

A point of further discussion/investigation should be the power per coated particle (and per compact). Even for case 214 (“radially optimised” BP parameters) the maximum power per coated particle (averaged over half a block) is 145 mW at BOL. This is higher than achieved/investigated in recent TRISO fuel irradiation tests [15]. The volume of a compact is 6.136 cm$^3$. The power of a single compact filled with 2500 coated particles @ 145 mW would be 362.5 W, or 59.1 W/cm$^3$. This would also be considerably higher than achieved/investigated in those TRISO tests. Further reduction of the maximum power per particle could e.g. be achieved by increasing the number of coated particles per compact (however, see Section IX).

Another, perhaps more feasible, method of reducing the maximum power per coated particle (and per compact) would be again to flatten the axial power profile. In the current configuration, the average power per coated particle is 69.6 mW. The (axial) power peaking factor is therefore 145/69.6 = 2.08 for case 214 at BOL. As can be seen in Figs. 9 and 10, in the early stages of the cycle (“A” and “B”) the power peak occurs in the upper half of the core. Near the end of the cycle (“C”) a similar peak occurs in the lower half of the core, reflecting that the fuel in upper half has been mostly depleted, due to the earlier high power in the upper half.

A convenient way to show this effect is the axial offset $F_{AO}$:

$$F_{AO} = (P_{upper} - P_{lower}) / (P_{upper} + P_{lower})$$

In this equation $P_{upper}$ is the power in the upper half of the core and $P_{lower}$ is the power in the lower half. Fig. 13 shows the axial offset as function of operation time for cases 202 and 214. The curves nearly coincide, going from 0.58 at BOL to -0.43 and -0.45 at EOL. The presence of a power- (flux-) dependent absorber ($^{135}$Xe) just after BOL already reduces the initial power peak ($F_{AO}$ starts at 0.58 and decreases to approx. 0.45 at Xenon equilibrium, $t = 3$ days). This is also an indication that increasing the BP density in the upper half of the core could be effective, perhaps even without axially profiling the enrichment, in decreasing the initial power peak in the upper half at BOL, thereby also decreasing the power peak in the lower half towards EOL.

![Figure 13. Axial offset as function of operation time for cases 202 and 214.](image-url)
7. Temperature Coefficients

An important aspect for safe operation of any nuclear reactor are the temperature coefficients of reactivity $\alpha$. In HTGRs usually the following distinction is made:

- Fuel ("$\alpha_F$"), material in the kernel and the coating layers.
- Moderator ("$\alpha_M$"), matrix material of the compacts and the graphite of the fuel blocks constituting the core.
- Reflector ("$\alpha_R$"), graphite of top-, bottom- and radial reflectors.

The temperature coefficients of reactivity have been calculated as follows:

$$\alpha_x = \left[\frac{1}{k_{\text{eff},x}} - \frac{1}{k_{\text{eff,ref}}}\right] / \Delta T_x$$

In this equation $x = F$ (Fuel), $M$ (Moderator), $R$ (Reflector) or $A$ (all materials), and $k_{\text{eff,ref}}$ is the multiplication factor for the reference state. This concerns the reference temperature distributions at CZP (all materials at 300 K), HZP (all materials at 600 K) and HFP (temperature distribution as calculated by SPECTRA at BOL and used in the HFP calculations presented so far). $\Delta T_x$ is the (spatially uniform) increase in temperature of the materials ($F, M, R, A$) of interest. In the calculations $\Delta T_x = 30$ K was used. To obtain sufficient accuracy in the calculated values, the calculations of $k_{\text{eff,ref}}$ and $k_{\text{eff,x}}$ were performed with 1000 cycles, 400000 neutrons per cycle and 100 inactive cycles. This resulted in a standard deviation of 5 pcm in the calculated values of $k_{\text{eff}}$ and, consequently, an uncertainty of 0.3 pcm/K in the calculated values of $\alpha_x$.

Table 4 shows the temperature coefficients of reactivity as calculated for the BOL, Xe-free state of case 202. For most states/configurations, the coefficients for all ($F, M, R$) materials are negative. However, for the HZP and HFP states, in which core rods and/or reflector rods have been withdrawn, the coefficients for the reflector are (slightly) positive. A positive coefficient of reactivity for the reflector temperature is a well-known phenomenon in HTGRs.

Table 4. Temperature coefficients of reactivity (fuel, moderator, reflector) for case 202, BOL (Xe-free), in pcm/K. The uncertainty in the calculated values of the temperature coefficients is 0.3 pcm/K.

| Configuration/State | $\alpha_F$ (Fuel) | $\alpha_M$ (Moderator) | $\alpha_R$ (Reflector) | Sum | $\alpha_A$ |
|---------------------|-------------------|------------------------|------------------------|-----|----------|
| CZP, all rods in    | -10.0             | -38.1                  | -162.0                 | -210.1 | -48.7    |
| HZP, all rods in    | -6.8              | -4.0                   | -0.8                   | -21.6 | -20.2    |
| HZP, core rods in, reflector rods out | -4.6 | -10.2 | 0.4 | -14.4 | -15.1    |
| HZP, all rods out   | -4.1              | -8.6                   | 1.2                    | -11.5 | -11.3    |
| HFP, core rods out, reflector rods in | -5.3 | -9.7 | 0.3 | -14.7 | -14.4    |
| HFP, all rods out   | -3.1              | -7.4                   | 1.9                    | -8.6  | -9.7     |

Comparing the sum of the ($F, M, R$) coefficients with the coefficient for temperature change in all materials shows that the reactivity effects are reasonably linear at HZP and HFP, but strongly non-linear at CZP.

The current coefficients have been calculated for a uniform increase of 30K in temperature for the material ($F, M, R, A$) under consideration. To take into account the influence of localised changes in temperature on the reactivity in e.g. (transient) thermal hydraulic calculations, e.g., local weight factors can be used. In one-energy group approximation, and under the assumption that absorption is the dominant effect, it can be shown by first-order perturbation theory that the local neutron flux squared can be regarded as the proper weight function/weight factor for reactivity effects, caused by local variations of the effective local macroscopic absorption and fission cross sections [16]. So, in first order approximation (i.e., local variation in effective macroscopic cross section is proportional to local variation in temperature) this is also the case for the reactivity effect of local temperature variations, i.e. the local weight factor.
The results shown so far concern case 202 (uniform initial BP parameter distribution) at BOL. Calculations of temperature coefficients of reactivity are currently (September 2020) ongoing for case 202 beyond BOL and all corresponding states for case 214.

8. Axial Xe-Oscillations?

In the current design of the GEMINI+ HTGR the core height has been increased to 8.8 m. This has raised the concern of the possibility of occurrence of axial oscillations (axial instability) of the power, related to the changing densities of $^{135}$Xe in the upper and lower half of the core. As a relatively simple first check, the following test was performed for case 202:

- At BOL, HFP, all core rods are out, reflector rods are 50% inserted (all reflector rod tips at 600 cm elevation), followed by full power operation for 3 days until Xe-equilibrium. This was calculated with the normal time steps, also used in the full burn up calculations. At $t = 3$ days, the reactor state is written to a restart file.
- At $t = 3$ days the calculation is continued from the restart file, with the reflector rods fully withdrawn. This calculation was done twice, with different time steps (32 time steps of 0.1 day and 2 time steps of 0.1 day, followed by 15 time steps of 0.2 days, respectively) to detect possible dependence upon the choice of the time steps.

During the entire test, the same HFP temperature profile was used, excluding thermal feedback effects.

Results of this test are shown in Fig. 14. In this figure the axial offset $F_{AX}$ is shown as function of time for the first (“black circles”) and second phase (“red squares” and “green diamonds”) of the test. In the first phase, all reflector rods are 50% inserted. As the total reactor power is being kept constant at 180 MWth, the vast majority of the power is being generated in the lower half of the core, resulting in a strongly negative axial offset: -0.83 at BOL, increasing to -0.80 at Xe-equilibrium. A relatively high concentration of $^{135}$Xe and $^{135}$I has been built up in the lower half, where most of the power is being generated. At $t = 3$ days, the reflector rods are fully withdrawn. This immediately pushes the power peak to the upper half of the core, resulting in a strongly positive axial offset of 0.74. Decaying $^{135}$I into $^{135}$Xe in the lower half suppresses the power in the lower half further for a while, causing the axial offset to increase further to 0.78. Because of the now high power in the upper half, both $^{135}$I and $^{135}$Xe concentrations are increasing in the upper half, while still decreasing in the lower half, until equilibrium is reached again at $t = 4.6$ days, corresponding to the “usual” axial offset of the reactor at HFP near BOL, as shown in Fig. 13. Apart from the little “overshoot”, immediately after withdrawal of the reflector rods, no “oscillatory” behaviour seems to occur.

![Figure 14. Test of axial $^{135}$Xe-related instability.](image)

It should be noted, however, that highly positive or negative values of the axial offset mean that almost the full reactor power is generated in only half the core, resulting in even higher local power densities in coated particles and compacts. This should be avoided anyway. Therefore, it is advisable to
avoid as much as possible partially inserted (reflector) rods during full power operation: rods should, as much as possible, be either fully in or fully out.

In the test presented here, a constant HFP temperature profile has been used, thereby excluding thermal feedback effects. It is desirable to repeat the test with full thermal feedback, also at other points in time in the cycle.

9. Steam Ingress

A final topic is the ability to render the reactor subcritical in case of steam ingress (HZP/HFP state only).

Fig. 15 shows the influence of the steam density in the coolant on the \( k_{\text{eff}} \), for 12\% enrichment and uniform BP parameters as in case 202. In case of 2500 coated particles per compact, the reactor can be kept subcritical with the core rods only with a maximum steam density of 0.09 g/cm\(^3\) steam in the coolant. When both core and reflector rods can be used this is 0.15 g/cm\(^3\). Higher numbers (e.g., 3000) of coated particles per compact result in a lower C/U-ratio (moderator-to-fuel ratio) in the core and a (slightly) higher reactivity increase due to steam ingress. This will not necessarily be detrimental, as some other parameters (e.g., BP parameters, fuel enrichment) may be adapted to lower the uncontrolled (all rods out) BOL \( k_{\text{eff}} \).

Also note that, as can be seen in Fig. 15, the reactivity worth of the control rods decreases with increasing steam density in the core. So, in any case, measures will be necessary to limit the possible amount of steam that can enter the primary circuit.

**Figure 15.** Steam ingress at BOL/HFP and HZP, for 2500 and 3000 coated particles per compact, 12\% enrichment and uniform initial BP parameter distribution as in case 202.

Similar to the calculation of the temperature reactivity coefficients, the analyses of steam ingress will also need to be done for points in time beyond BOL, also for the further optimised configurations of the BP parameter distribution.
10. Conclusions

Extensive neutronics calculations have been performed on the current (June 2020) design of the 180 MWth GEMINI+ HTGR. Neutronics features seem quite promising, but further improvements and therefore further investigations would be desirable, especially concerning:

- Temperature coefficients of reactivity, control rod worths, etc. beyond BOL, also for further optimised configurations of the BP parameter distribution.
- Thermal hydraulic feedback, reflecting the considerable change axial power profile during the operation cycle. In the current calculations, the temperature distribution has been kept constant throughout the operation cycle, as was initially envisaged. Adapting the temperature distribution to the actual power distribution at each point in time would be desirable.
- Further reduction of the axial power peaking, thereby reducing the maximum power per coated particle and also improving the fuel utilisation. Possible methods are axial profiling of BP parameters, axial profiling of enrichment and/or a multi-batch loading scheme.
- Increasing the number of coated particles per compact, possibly in combination with changing the enrichment and/or the BP parameter distribution.

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