High-temperature reactor for hydrogen productions - a step towards future green energy

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Abstract. This article presents review of technology of high-temperature gas reactors and its features. In addition, it contains description of simple computation of neutron-physical characteristics of high-temperature reactor using GETERA and COMSOL Multiphysics programs and comparison of results with results obtained by precision Monte-Carlo program MCU.

1. Introduction

The key words of “small” and “modular” make the small modular reactors (SMRs) different than other reactors. “Small” denotes the reactor’s decreased power size. “Modular” denotes the primary coolant system enveloped by a pressure boundary; and modular construction of components. Modular design requires compact architecture that is built in facility.

Small modular reactors are an important strategic direction for the development of ROSATOM on international markets due to a number of factors:

- The need of emerging markets in Africa, Asia and Latin America for nuclear power generation
- The modularity of SMRs and the possibility of building power under the small need for generation
- Requirements of markets to reduce the cost of generation and reduce the size of investments
- High speed and ease of construction of SMRs due to factory assembly
- Growth in the use of renewable energy sources and the need for uninterrupted sources “in the base”
- Trend for green energy and environmental concerns

HTGR technology is well advanced through the decades of international research, development, and commercialization efforts. Pebble bed and prismatic reactor are the two major design variants. Both are in use today. In either case, the basic fuel construction is the TRISO-coated particle fuel. The unique construction and high burnup potential of the TRISO fuel enhances proliferation resistance. The HTGR safety relies mostly on passive and inherent design features. The choice of low core power density limits the decay heat generation rate to the extent that can be safely removed by thermal conduction only [1].

The HTGR coolant temperature (950 °C) is the highest among the Generation IV reactors. This enables not only for efficient power generation by either steam or gas turbine, but also for high-temperature heat application and attractive cogeneration. The HTGR -based hydrogen production, steelmaking, and
seawater desalination have been found cost competitive. Coupling hydrogen production with nuclear power plants is a promising technology for addressing society’s economically and environmentally unsustainable dependence on fossil fuels. Nuclear energy is a large-scale energy resource that can consistently be provided to the hydrogen production facility. Since hydrogen is an energy carrier as clean as the method used to produce it, coupling the two technologies provides an important pathway for mitigating climate change and depletion of fossil fuel reserves [2].

In this paper the high-temperature reactor based on plutonium-thorium fuel is investigated in terms of the export potential and the use of high-temperature heat for hydrogen productions. It is assumed that for Russia, having significant stocks of reactor-grade plutonium and being able to reprocess the fuel from thermal and fast reactors, the reactor can possess the high breeding factor and, as a consequence, high efficiency and safety.

2. Methodology
The main goal of current investigation is computation of neutron-physical characteristics of high-temperature reactor with thermal power equal to 600 MW (HTGR-600). However, some simple thermal hydraulics and thermal conductivity calculations are involved in this investigation too.

For computations are used these programs:

- GETERA, this is one-dimensional code, which uses first collision probability method (FCP) to solve the neutron transport equation in elementary cell of nuclear reactor fuel load. In the slowing down diapason (2.15 eV - 10.5 MeV) the neutron flux density is calculated in 26-group approximation based on the library BNAB-93. In the thermalization range (0.0 - 2.15 eV) the code uses a special 100-group neutron cross-section library based on the ENDF/B-IV and JENDL-2 evaluated nuclear data files [3].
- COMSOL Multiphysics, this is a general-purpose simulation software for modeling designs, devices, and processes in all fields of engineering, manufacturing, and scientific research, which can solve partial differential equations by finite element method (FEM). Three-dimensional models for calculations can be loaded from any CAD-programs [4].
- T-FLEX CAD, this is Russian CAD-program [5].
- MCU (Monte Carlo Universal), this is a project on development and practical use of a universal computer code for simulation of particle transport (neutrons, photons, electrons, positrons) in three-dimensional systems by means of the Monte Carlo method [6].

The first step of calculation is preparing of 3D-models. The HTGR-600 vessel and fuel assembly 3D-models are shown on figures 1 and 2. Fuel assembly has 108 coolant holes and central hole for System of Inner-Reactor Control. On figure 2 graphite matrix of assembly is grey and fuel rods are black.

The computational 3D-model of HTGR-600 active core for COMSOL Multiphysics is shown on figure 3. It is huge graphite cylinder of outer and inner reflector with 108 hexagonal prisms of active core inside it. All models are built in T-FLEX CAD.

The second step of calculation is preparing of cross-sections for three-group equation of neutron diffusion (1) with boundary condition (2).

\[ -\nabla \cdot D \nabla \Phi(\vec{r}) + \Sigma(\vec{r}) \Phi(\vec{r}) = \frac{1}{K_{eff}} \left( \chi \left( \frac{\nu_i}{\nu_f} \Sigma_{el} \right) \Phi(\vec{r}) \right) \]

\[ \Phi(\vec{r}_o) = 0 \]

where \( \vec{r}_o \) is radius-vector of any points on outer reflector boundary.

The components of the equation: the vector of neutron fluxes (3), the matrix of diffusion coefficients (4), the matrix of interaction cross-sections (5), the vector of components are fractions of neutrons produced in the corresponding group (6), the matrix of neutron generation cross-sections in groups (7).
Figure 1. 3D-model of HTGR-600 vessel.

Figure 2. 3D-model of fuel assembly.

Figure 3. COMSOL Multiphysics computational model.
\[ \Phi = \begin{pmatrix} \Phi_1(r) \\ \Phi_2(r) \\ \Phi_3(r) \end{pmatrix} \]  \tag{3}

\[ \tilde{D} = \begin{pmatrix} D_1 & 0 & 0 \\ 0 & D_2 & 0 \\ 0 & 0 & D_3 \end{pmatrix} \]  \tag{4}

\[ \tilde{\Sigma} = \begin{pmatrix} \Sigma_{d1} & \Sigma_{d2} & 0 \\ 0 & \Sigma_{d2} & \Sigma_{d3} \\ 0 & 0 & \Sigma_{d3} \end{pmatrix} \]  \tag{5}

\[ \chi = \begin{pmatrix} \chi_1 \\ \chi_2 \\ \chi_3 \end{pmatrix} \]  \tag{6}

\[ v_i \tilde{\Sigma}_f = \begin{pmatrix} v_i \Sigma_{f1} & 0 & 0 \\ 0 & v_i \Sigma_{f2} & 0 \\ 0 & 0 & v_i \Sigma_{f3} \end{pmatrix} \]  \tag{7}

where \( \chi_1 = 0.85; \chi_2 = 0.15; \chi_3 = 0. \)

Constants for this matrix equation obtained from the calculations in GETERA. Computational model for this program is very simple – it is single homogeneous fuel rod with layer of graphite reflector around it. Input data for this calculation is simple too:

- Radius of homogeneous fuel rod (0.625 cm)
- Radius of reflector layer (1.6 cm)
- Average temperature of fuel (850 °C)
- Average temperature of reflector (700 °C)
- Average power density (6.6 MW/m³)
- Nuclear concentrations of \(^{232}\text{Th}, \ ^{238}\text{Pu}, \ ^{239}\text{Pu}, \ ^{240}\text{Pu}, \ ^{241}\text{Pu}, \ ^{242}\text{Pu}, \ ^{16}\text{O}, \ ^{12}\text{C}, \ ^{28}\text{Si}\) in homogeneous fuel rod
- Nuclear concentrations of \(^{12}\text{C}\) in reflector layer

GETERA can solve burnup tasks – and some important values like reactor campaign duration, average burnup of fuel and average coefficient of fuel conversion are calculated by this code.

The third step of calculation is solving three-group equation of neutron diffusion (1) with boundary condition (2) in COMSOL Multiphysics. Three states are calculated – start of the campaign, middle of the campaign and finish of the campaign.

The fourth step of calculation is validation of result of \( K_{\text{eff}} \) calculation in COMSOL Multiphysics by comparison with MCU result for start of campaign state. Computational model for MCU is more complicated and more accurate. Central section of this model is shown on figure 4 and enlarged image of one of the fuel assemblies is shown on figure 5. On those figures graphite of assemblies and reflectors is grey, fuel rods are red and coolant holes are blue. In this configuration fuel rods are heterogeneous. Heterogeneous fuel rod is graphite cylinder with TRISO fuel particles inside it (900 particles in 1 cm³), which are placed randomly in volume of fuel rod.
3. Results
These values are gained from thermal physics calculations:

- Average consumption of helium coolant $G_{He} = 210 \text{ kg/s}$
- Energy conversion efficiency of system with steam turbine $ECF_{st} = 40\%$
- Energy conversion efficiency of system with gas turbine $ECF_{gas} = 58\%$
These values are calculated by GETERA:

- Reactor campaign duration (without refueling) $T = 3996$ days
- Average burnup $B = 167$ MW·days/t
- Average coefficient of fuel conversion $K_{\text{conv}} = 0.98$
- Consumption of reactor-grade plutonium $G_{\text{Pu}} = 280$ kg/year
- $^{233}$U (92% enrichment) production $G_{^{233}\text{U}} = 35$ kg/year

Time dependence of $K_{\text{inf}}$ is shown on figure 6.

![Figure 6. Time dependence of $K_{\text{inf}}$.](image)

**Figure 6.** Time dependence of $K_{\text{inf}}$.

Results of $K_{\text{eff}}$ calculation in COMSOL Multiphysics:

$$K_{\text{eff, start}} = 1.019$$
$$K_{\text{eff, middle}} = 1.017$$
$$K_{\text{eff, finish}} = 1.001$$

For comparison – MCU results of $K_{\text{eff}}$ calculation for start of campaign state:

$$K_{\text{eff, MCU}} = 1.02365 \pm 0.00037$$

In addition, relative error of COMSOL Multiphysics result:

$$\delta K_{\text{eff}} = \left( K_{\text{eff, MCU}} \cdot K_{\text{eff, start}} \right) / K_{\text{eff, MCU}} = 0.45\%$$

Leakage value results are equal for COMSOL Multiphysics and MCU:

$$L = 3.37\%$$

Also from COMSOL Multiphysics are gained some distributions of values. Radial and axial neutron flux distribution in the central section of core are shown on figures 7 and 8. The axial temperature distribution in the central section of core at the termination coolant circulation is shown on figure 9. According to this distribution, there are no reasons to fear of core melting in any accident situation.
Safety of HTGR-600 based on passive systems and the practical impossibility of core melting. Safety approaches, which are usually adopted by the HTGR, are based on three inherent design features:

- A ceramic coated fuel particle that maintains the integrity of the containment shell for fission products at a design temperature limit of 1600 °C;
- The helium coolant is chemically inert and, therefore, does not form explosive gas and has not any phase changes;
- High value of graphite reflector thermal conductivity, low energy density of active zone and negative value of temperature coefficient of reactivity.

Reactor is safety shutdown and cooled by inherent design features without reliance on any equipment or operator action in the event of loss of coolant or station black-out.

Figure 7. The radial neutron flux distribution in the central section of core.
4. Conclusion

The main objective of this paper is to draw attention to HTGR-type reactors, because this technology has a lot of advantages, the world has already introduced development on the HTGR and Russia has its own unique experience in high-temperature reactors. These reactors can work in closed fuel cycle, can use plutonium and thorium as a fuel, according to this paper it is very profitable and safe technology! In addition, verification of calculation scheme using GETERA and COMSOL Multiphysics shows that it is suitable for fast and easy auxiliary calculations.

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