Comparative Study on Fuel Assembly of Modular Gas-cooled Fast Reactor using MCNP and OpenMC Code

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Abstract. The design study of GFR concepts comprises neutronic analysis of fuel pin and fuel assembly. The Monte Carlo method has advantages in three-dimensional (3D) geometry modeling but requires a high computation time. In this research, the comparative study of Gas-cooled Fast Reactor (GFR) using the Monte Carlo code. The GFR feasibility design study will be carried out with natural uranium with plutonium as fuel cycle inputs. The Monte Carlo method simulates GFR model at full-scale and heterogeneous three-dimensional (3D) using Evaluated Nuclear Data File (ENDF/B-VIII.b5) nuclear data. The code of Monte Carlo methods will be used in this research are the Monte Carlo N-Particle (MCNP) and OpenMC. The comparison of the GFR fuel assembly calculation simulation results is made between the MCNP and OpenMC code. The equilibrium cycle configuration is used as the basis model for the comparisons. The comparison of MCNP and OpenMC code gives a good agreement in criticality calculation of GFR that achieves delta k\textsubscript{eff} less than 1%. The (U-Pu)\textsubscript{N} fuel is a good candidate to be chosen in GFR research that gives k\textsubscript{eff} more than 1.1 in fissile contain 10%Pu and has the highest thermal conductivity. The Zircaloy-4 is the best candidate for material cladding in GFR design that provides the highest k\textsubscript{eff}.

1. Introduction
Modular long life reactors are very prospective for remote areas with small to medium power consumption levels. This reactor is also good when combined with large turbines so that competitive nuclear energy can be obtained. In Indonesia, many remote areas that require electricity are only a few hundred MWe so that sometimes large conventional nuclear reactors are not suitable and the need for small and medium electricity availability is needed (Zaki Su’ud, 2017; Zaki Su'ud, 2013).

GFR is one of the advanced reactors concept selected by the Generation IV International Forum (GIF). Modular GFR was chosen due to having use potential recycle of all actinides and closed fuel cycle also from using fast reactor can utilize the natural uranium during operation as the fuel (M. Ilham, 2017). Another side, the main advantages of modular GFR compare another advanced reactor concept is using helium gas as main coolant (Poette, 2015; R. Stainsby, 2011) because of that we need to understand of GFR fuel design through simulation and modeling.

Development of GFR concept includes neutronic analysis of fuel design i.e. fuel pin and assembly. The study of neutron behavior in nuclear reactor means to understand the interaction of a subatomic particle with the matter. Power distribution and others reaction rate of every point in the nuclear reactor is an interesting investigation for the researcher and nuclear designer. To determine quantitatively of the particle behavior is needed the understanding about particle interaction through simulation of moving particle and mathematical description of particle distribution time dependent. Theory of particle interaction that correlated with particle
scattering is known theory of particle transport. The approach to determine particle distribution in the system generally has two methods such as Monte Carlo and deterministic. Monte Carlo method has prominent in realistic 3D geometry modeling but needs high time computing (Romano, 2013).

In this study, we want to investigate several crucial aspects of modular such types of material fuel, cladding and percentage of fissile contain. The design goal is to combine various features of GFR. The design study used the MCNP and OpenMC code to simulate the full-scale and 3D modeling of fuel pin and assembly of modular that proposed and investigated. The research goal is to determine the characteristic of plutonium fuel in the gas-cooled fast reactor and reasonable multiplication factor, fissile contain, fuel rod and assembly dimensions also the feasibility of fuel and cladding material type for advanced research.

2. Design and Calculation Method

Modular GFR reactor system is a nuclear reactor with a fast neutron spectrum used high-temperature helium gas as the coolant and the capability of the core to work in closed cycles (Figure 1). GFR system combined the advantages of fast spectrum system with long-term availability of uranium and waste minimize through fuel reprocessing and fission products of long live actinide. Table 1. Presented fuel assembly characteristics of GFR reactor system that analyzed in this paper. We used the code MCNP6 (Monte Carlo N-Particle) and OpenMC (Open Monte Carlo). Both codes are based on the Monte Carlo method for criticality calculation and capable of simulating complex physical phenomenon in the detailed 3D model and continuous energy cross section representation. Description of the fuel pin and assembly shown in figure 2 and table 2 respectively, such as the fuel is a cylindrical rod region, the gap is an annular region cylindrical region that is empty and surround the fuel, the cladding is an annular cylindrical region that is a barrier for the dispersion of fission product and coolant is the outermost region that surrounds the cylindrical rod and has a hexagonal outer surface. In table 3 shown related fuel candidates that investigated in GFR concept comprised the fuel material with carbide (U-Pu)C, nitride (U-Pu)N, oxide(U-Pu)O₂, and metallic (U-Pu)Zr to attain the good candidate. In table 4 shown the cladding candidates that used material composition type such as SS HT9, SS 316, SiC and zircaloy-4 with density value are 7.874 gr/cm³, 8.0 gr/cm³, 3.210 gr/cm³, and 6.56 gr/cm³, respectively.

| Parameter                      | Value     | Units   |
|-------------------------------|-----------|---------|
| Geometry                      | Hexagonal |         |
| Apothem                       | 11.16     | cm      |
| Side                          | 12.88645801 | cm      |
| Height                        | 71        | cm      |
| Perimeter                     | 77.31874805 | cm      |
| Heavy Metal (HM) Composition  | U/PU(90-97/3-10) | % weight |
Table 2. Fuel Basic Cell Characteristic

| Parameter | Fuel | Gap | Cladding | Coolant | Cell |
|-----------|------|-----|----------|---------|------|
| Geometry  | Cylindrical rod | Cylindrical tube | Cylindrical tube | Hexagonal prism | Hexagonal prism |
| External radius (cm) | 0.4256 | 0.4285 | 0.4785 | | |
| Apothem (cm) | | 0.64 | 0.64 | | |
| Side (cm) | 0.74 | 0.74 | | | |
| Height (cm) | 71 | 71 | 71 | 71 | 71 |
| Perimeter (cm) | 2.6741237 | 2.6923449 | 3.0065042 | 4.44 | 4.44 |
| Area (cm²) | 0.5690535 | 0.0077814 | 0.1424712 | 0.7014939 | 1.4208 |
| Volume (cm³) | 40.4028 | 0.5524779 | 10.115457 | 49.806065 | 100.8768 |
| Volume fraction | 0.4005163 | 0.0054768 | 0.1002754 | 0.4937316 | 1 |
| Density (gr/cc) | 7.55 | 0.037 | 3.21 | 0.037 | |
| Mass (g) | 305.04114 | 0.0204417 | 32.470617 | 1.8428244 | |
| Heavy metal mass (g) | 244.03291 | 0 | 0 | 0 | 244.03291 |

Table 3. Fuel Candidates

| Material Composition | Carbide (U-Pu)C | Nitride (U-Pu)N | Oxide (U-Pu)O₂ | Metallic (U-Pu)Zr |
|----------------------|-----------------|-----------------|----------------|------------------|
| Theoretical density (gr/cc) | 13.6 | 14.3 | 11 | 15.6 |
| Heavy atom density (gr/cc) | 12.95 | 13.53 | 9.75 | 14 |
| Melting Point (°C) | 2420 | 2780 | 2430 | 1080 |
| Thermal conductivity (W/m/K) | 16.5 | 14.3 | 2.9 | 14 |

Table 4. Cladding Candidates

| Material Composition | SS HT9 | SS 316 | SiC | Zircaloy-4 |
|----------------------|--------|--------|-----|------------|
| Theoretical density (gr/cm³) | 7.874 | 8.0 | 3.210 | 6.56 |
| Melting Point (°C) | 1325-1530 | 1375-1400 | 2730 | 1850 |
| C | 0.20% | C | 0.04% | C | 29.95% | O | 0.12% |
| Si | 0.40% | Si | 0.51% | Si | 70.05% | Cr | 0.10% |
| P | 0.03% | P | 0.02% | | | Fe | 0.10% |
| S | 0.02% | S | 0.02% | | | Ni | 0.05% |
| V | 0.30% | Cr | 17.00% | | Zr | 98.23% |
| Cr | 11.50% | Mn | 1.01% | | Sn | 1.40% |
| Mn | 0.60% | Fe | 66.90% | | | | |
Fe 84.95%  Ni 12.00%  
Ni 0.50%  Mo 2.50%  
Mo 1.00%  
W 0.50%

In this research, we analyzed neutron population on two-generation differently in GFR system based on fuel pin and assembly. Then known that multiplication factor (k) and an infinite multiplication factor (k_{inf}) on reaction chain (Duderstadt, 1976; Faw, 2002; Stacey, 2001).

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 k = \text{multiplication factor} = \frac{\text{Neutron number in one generation}}{\text{Neutron number in before generation}} \quad (1)
\]

3. Results and Discussion
After modeling and simulation of the fuel assembly of GFR then calculate using MCNP and OpenMC code to get results and data calculation. The results got a good agreement between MCNP and OpenMC calculation. **Figure 3 and 4.** Fuel assembly in XY view-MCNP and OpenMC. We used hexagonal lattice with 7 rings and 127 pins. In **Figure 5 and 6.** Fuel assembly in YZ view-MCNP and OpenMC that shown there are 7 rings of fuel pins and geometry of fuel meats, gaps and claddings.

At initial calculation, we investigated the profile plutonium such as U-PuC, U-PuN, U-PuZr and U-PuO2. **Figure 7, 8, 9 and 10** shown that the multiplication factor higher than 1.00 when the fissile contain higher than 8%. From these calculation obtained delta k_{inf} between MCNP and OpenMC less than 1% with the average value 0.52%.
Table 5. Comparison of fissile contain 10%Pu

| Fissile Contain 10%Pu | MCNP       | OpenMC     | Delta (%) |
|-----------------------|------------|------------|-----------|
| (U-Pu)C               | 1.14005    | 1.14604    | 0.599     |
| (U-Pu)N               | 1.11285    | 1.12363    | 1.078     |
| (U-Pu)O2              | 1.07179    | 1.07309    | 0.13      |
| (U-Pu)Zr              | 1.15167    | 1.15506    | 0.339     |

Table 5. Shown the comparison of fissile contain 10%Pu when calculated with MCNP and OpenMC code. We obtained the infinite multiplication factor for (U-Pu)Zr is the highest value about 1.15 with delta 0.339%. Next, we presented the comparison between OpenMC and MCNP in plutonium fuel with various cladding material types such as SS HT9, SS 316, Zircaloy-4, and SiC in figure 11, 12, 13 and 13. The interesting results that got the highest value of $k_{inf}$ is from zircaloy-4 material type. In figure 11. Shown the comparison between OpenMC and MCNP calculation in (U-Pu)C with cladding zircaloy-4 and containing fissile 10% got the good values are 1.1463 by MCNP and 1.15968 by OpenMC that produced delta difference 1.34%. Figure 12. Shown the comparison between OpenMC and MCNP calculation in (U-Pu)N with cladding zircaloy-4 and containing fissile 10% got the good values are 1.12363 by MCNP and 1.13666 by OpenMC that produced delta difference 0.10%. Figure 13. Shown the comparison between OpenMC and MCNP calculation in (U-Pu)O2 with cladding zircaloy-4 and containing fissile 10% got the good values are 1.09562 by MCNP and 1.08381 by OpenMC that produced delta difference 1.18%. Figure 14. Shown the comparison between OpenMC and MCNP calculation in (U-Pu)O2 with cladding zircaloy-4 and containing fissile 10% got the good values are 1.18425 by MCNP and 1.17967 by OpenMC that produced delta difference 0.46%.
4. Conclusion

In this research, we got the comparison of MCNP and OpenMC code gives a good agreement in criticality calculation of GFR that achieves delta $k_{inf}$ less than 1%. The (U-Pu)N fuel is a good candidate to be chosen in GFR research that gives $k_{inf}$ more than 1.1 in fissile contain 10%Pu and has the highest thermal conductivity. The Zircaloy-4 is the best candidate for material cladding in GFR design that provides the highest $k_{inf}$. The results should simulate and calculate the full core of GFR with (U-Pu)N fuel and Zircaloy-4 cladding for advanced research.

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