MCNP5 Core Calculations Coupled with a Simplified Thermal–Hydraulic Model for GTHTR300

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1. Introduction

Temperature-dependent cross sections play an essential role in reactor physics analyses. Temperature changes in reactor core affect the flux and power distributions, and the power distribution in turn results in a new temperature distribution. Therefore, practical neutronic calculations must be coupled with thermal hydraulic feedback to obtain converged results of both temperature and power distributions. In this preliminary study, we present a simplified model that combines the MCNP5 calculation with a simple thermal-hydraulic calculation for GTHTR300 core simulation.

2. Calculation Models and Methods

2.1 Introduction of GTHTR300

GTHTR300 is a gas turbine high temperature reactor design developed at the Japan Atomic Energy Agency. It combines the advantages of the GEN-IV very high temperature gas reactor with simplified plant design, aiming at demonstration of a prototype power plant for future nuclear development in Japan. The core design of GTHTR300 is based on improved HTTR fuel element, which is essentially a hexagonal graphite block inserted with fuel pins made of coated fuel particles. Fig. 1 is a cross-sectional view of the GTHTR300 core, which consists of 90 hexagonal graphite columns: 73 fuel columns, 48 inner and outer replaceable reflector columns, and 18 outer fixed reflector columns. Each fuel column is formed by vertically stacking 8 fuel blocks. Each hexagonal fuel block has a dimension of 100 cm high and 40.5 cm wide, in which 57 fuel pins are inserted and arranged in a hexagonal lattice. [1]

2.2 Coupling of neutronic and thermal hydraulic calculations

The calculation flow of neutronic/thermal-hydraulic coupling is shown in Fig. 2. First, an initial guess for the temperature distribution was given to obtain a power distribution through neutronic calculations. Based on this power distribution, the following thermal-hydraulic calculation can predict a temperature distribution of the reactor including helium, graphite sheath, and fuel elements. The new temperature distribution will be used in the next iteration of neutronic calculation. The process will be repeated until power and temperature distributions converged.



Fig. 1. A cross-sectional view of the GTHTR300 core [2].



Fig. 2. Coupling of neutronic and thermal hydraulic calculation.

The temperature distribution in Table I, which is taken from Ref. [2], was used in this study as the initial guess of the calculation flow. There are only two temperatures, 1 173K and 1423K, for the fuel region in the core. The moderator temperatures range from 900K to 1300K. Uniform helium temperature 1200K is used in our calculations because the temperature variation of helium has little effect on the neutronic properties [3].

2.3 Simulation tools used in neutronic calculations

Continuous-energy Monte Carlo simulations are popular in radiation transport applications because of accurate representations in problem geometry and particle phase space. The Monte Carlo transport code MCNP5 with continuous-energy cross sections based on the ENDF/B-VII.0 library was used in neutronic calculations [4]. The nuclear data libraries in MCNP5 were processed by NJOY99 into the pointwise ACE format cross-section tables evaluated at user-requested temperatures [5]. A high-fidelity GTHTR300 model was built, the core model has great details covering from tiny fuel particles to the entire core structure as shown in Fig. 1 that is corresponding to a fully-loaded core configuration.

Table I.	Initial	Guess	Temperature	Distribution	[2]
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	Inne	er R	R with CR	Fuel	R	R with CR	Fixed R
R	$T_{mod}=1000K$		T _{mod} = 1000K	T _{mod} =900K	$T_{mod} =$	$T_{mod}=1000K$	$T_{mod} = 1000 K$
L1				$T_{f}=1173K$	1000K		
L2				I mod=1000K			
L3	T _{mod}	T_{mod}	T _{mod}	T _f =1423K	$T_{mod} =$	$T_{mod}=$	
L4	= 1000K	= 1100K	= 1100K	1 _{mod} =1150K	1100K	1100K	
L5	T _{mod}	T _{mod}	T _{mod}	$T_{f}=1423K$	$T_{mod} =$	$T_{mod} =$	
L6	= 1100K	= 1200K	= 1200K	I mod=1500K	1200K	1200K	
L7							
L8							
R				T _{mod} =1300K			

R = Reflector, L = Layer, CR = control rods

2.4 A simplified thermal-hydraulic model

Once the power distribution is obtained from the neutronic calculation, simplified thermal hydraulic calculation can be performed to estimate the temperature of the helium coolant channel to the fuel region. A unit cell model containing fuel compact and adjacent coolant channel is shown in Fig. 3. Note that the center region of the fuel compact in GTHTR300 is filled with graphite, while it is filled with helium gas in the HTTR design.



Fig. 3. A unit cell model of the fuel element.

Temperature distribution in coolant channel

The axial temperature distribution of helium in a typical coolant channel was first evaluated from the heat source in the core, which can be derived from the total thermal power of 600 MW and the power distribution obtained from neutronic calculations. Given inlet coolant

temperature 587° C, by using the energy balance equation Eq. (1), the axial coolant temperature distribution can be calculated [6].

$$\frac{\dot{Q}}{\dot{m}} = \left(h_z + \frac{v_z^2}{2} + gz\right) - \left(h_{in} + \frac{v_{in}^2}{2} + gz_{in}\right) , \quad (1)$$

where

- \dot{Q} = total heat source from inlet to location z,
- h_z = enthalpy of helium at location z,
- v_z = flow rate of helium at location z, and
- \dot{m} = mass flow rate of helium.

Assuming no bypass flow and negligible kinetic and potential energy differences, Eq. (1) can be reduced to

$$\frac{Q}{\dot{m}} = h_z - h_{in}.$$
(2)

Temperature of graphite sheath

Fig. 4 shows the geometry detail of the fuel compact. T_c represents temperature of graphite sheath and T_s represents temperature of fuel surface. To estimate the fuel surface temperature from helium temperature, heat convection equation is used.

$$\frac{\dot{Q}}{A_c} = h(T_c - T_b) \quad , \tag{3}$$

where

 A_c = surface area of channel,

h = heat transfer coefficient of helium, and

 T_h = temperature of helium.

The heat transfer coefficient of helium can be calculated by Dittus-Boelter equation [6].

$$h = C \frac{\kappa_{He}}{D_e} R_e^{\ m} P_r^{\ n} , \qquad (4)$$

where

C = 0.023, m = 0.8, n = 0.4, and

 K_{He} = conductivity of helium, which can be easily found in Ref. [6].



Fig. 4. Geometry detail of the fuel compact [7].

Temperature of fuel compact

Starting from the surface temperature of graphite sheath layer T_c , one can easily calculate the surface temperature of the fuel compact T_s by using heat conduction equation.

It is a bit more complicated to calculate the temperature distribution in the fuel compact because it consists of more than ten thousands of tiny TRISO particles embedded in graphite matrix. For simplification, we homogenized the TRISO particles with the graphite matrix in a fuel compact for temperature estimation. Eq. (5) is used to calculate the equivalent thermal conductivity of the graphite matrix and TRISO particles by Maxwell's equation [8].

$$\frac{K_e}{K_g} = \left[1 + 2\frac{\kappa - 1}{\kappa + 2}\varphi\right] \left[1 - \frac{\kappa - 1}{\kappa + 2}\varphi\right]^{-1},\tag{5}$$

where

 K_e = equivalent conductivity of fuel compact,

 K_g = conductivity of graphite matrix [9],

 $\kappa = K_p/K_a$

 K_p = conductivity of TRISO particle, and

 φ = particle volume fraction.

TRISO particle is composed of several layers, as shown in Fig. 5. The conductivity of the homogenized TRISO particle can be estimated by

$$K_{p} = \left[\frac{r_{1}^{2}}{2} + \sum_{n=1}^{5} r_{n}^{3} \left(\frac{1}{r_{n}} - \frac{1}{r_{n+1}}\right)\right] \\ \left[\frac{r_{1}^{2}}{2K_{1}} + \sum_{n=1}^{5} \frac{r_{n}^{3}}{K_{n+1}} \left(\frac{1}{r_{n}} - \frac{1}{r_{n+1}}\right)\right]^{-1}.$$
 (6)

where r_1 to r_6 represents radius of each layer from inner to outer layer, K_1 to K_6 represents thermal conductivity of each layer [10].



Fig. 5. Layers of TRISO particle [7].

There is no heat generation in the middle graphite rod. In addition, we assumed no heat transfer in the axial direction. Therefore, the temperature inside the central graphite region will be nearly constant, T_g . In another word, there is no heat transfer on the interface of the central graphite rod and the fuel compact. By using adiabatic boundary condition at the inner surface and T_s at the outer surface, the temperature distribution of fuel compact T_{cp} can be calculated.

$$T_{cp}(r) = T_s + \frac{q'''r_a^2}{4K_e} \left[\left(\frac{r_b}{r_a}\right)^2 - 2\ln\left(\frac{r_b}{r}\right) - \left(\frac{r}{r_a}\right)^2 \right],$$
(7)

where q''' = power density of fuel.

For fission energy deposition, we assumed 186/200 energy deposited in the fuel and 14/200 energy deposited in the graphite moderator in the proximity of the fuel. To simplify the heat transfer calculation, we changed the hexagonal unit-cell geometry to an equivalent circular shape, as shown in Fig. 6. The equivalent radius r_0 of the central fuel region can be obtained by conserving the area during geometry transformation.



Fig. 6. Equivalent circular geometry of hexagonal fuel block.

Temperature of outer graphite region

Heat convection equation was used to calculate the temperature of outer graphite moderator T_i near the fuel compact. Heat conduction equation with an outer insulated surface of graphite was used to calculate the maximum graphite moderator temperature T_0 [11].

$$\frac{q''}{h} = \Delta T = T_i - T_b \quad , \tag{11}$$

$$T_o - T_i = \frac{q''' r_o^2}{4K} \left[2 \ln\left(\frac{r_o}{r_i}\right) + \left(\frac{r_i}{r_o}\right)^2 - 1 \right] , \qquad (12)$$

where

q'' = heat flux of outer graphite region, and q''' = power density of outer graphite region.

3. Results and Discussion

The simplified thermal hydraulic model presented previously was verified by comparing with a CFD calculation (ANSYS12/Fluent 12.0.16) [12]. Table. II shows a comparison result. The differences in fuel temperatures predicted by the simplified model and CFD calculations are all within 10K.

Table II. Differences of Temperatures in Helium, Fuel and Graphite Predicted by the Simplified Model and CED Calculations

CFD Calculations								
	T _b	T _c	Ts	T _{cp,max}	To			
ΔT at exit (K)	-2.6	-5.5	-1.7	-5.3	-9.0			

To get a converged result, the neutronic/thermalhydraulic iterations was performed 6 times in this preliminary study. As shown in Fig. 7, the relative difference gets good converged. Fig. 8 is the converged axial power distribution for the eight layers of fuel blocks. The highest power is located at the 5th layer.

After we got a converged power distribution, the calculation of temperature distribution inside a fuel region was performed. The results are shown in Fig. 9. Fig. 10 shows a comparison of maximum fuel temperature distribution using the maximum and average power of each layer. There are almost 200K difference in the comparison, indicating that using average power of each layer to calculate temperature distribution is not appropriate and conservative, block-by-block power distribution needed to be used to get a more accurate and detailed temperature distribution for neutronic/thermal-hydraulic coupling calculations.



Fig. 7. Relative difference in power and temperature in successive iterations.



Fig. 8. Axial power distribution.



Fig. 9. Temperature distribution of fuel compact calculated by using average power of each layer.



Fig. 10. Comparison of maximum temperature distribution of fuel compact calculated by using maximum and average power of each layer.

4. Summary and Future Work

By using this simple thermal hydraulic model and iterations with neutronic calculation, we can obtain converged power distribution and temperature distribution for GTHTR300.

In the future, we will calculate a detailed block-byblock temperature for the neutronic calculation to get more accurate power distribution. The thermal hydraulic/heat transfer model established in this study for VHTR provides a good starting base for future development of coupling scheme with deterministic nodal diffusion code for more realistic core design calculations.

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